Dissertation

submitted to the

Combined Faculties for the Natural Sciences and for Mathematics
of the Ruperta-Carola University of Heidelberg

for the degree of

Doctor of Natural Sciences

Put forward by

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born in

Heidelberg

Oral Examination: 15.04.2015

A STATISTICAL FIELD THEORY FOR CLASSICAL PARTICLES

FOUNDATIONS AND APPLICATIONS IN COSMOLOGICAL STRUCTURE FORMATION

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January 2015 – Final Version

Felix Fabis: *A Statistical Field Theory for Classical Particles,* Foundations and Applications in Cosmological Structure Formation, © January 2015

ABSTRACT

We develop a field-theoretical version of kinetic theory based on the pioneering work in [39, 40, 22]. A canonical generating functional for correlators of macroscopic observables is derived using the language of path integrals with the microscopic phase-space coordinates as the fundamental variables determining the dynamics. The findings of the original works are generalised to systems with correlated initial conditions. An exact initial phase-space distribution for a homogeneous and isotropic Gaussian random field is calculated, translated into a diagram language and factorised into connected contributions. The grand canonical generating functional is derived for systems obeying statistical homogeneity and isotropy. Using this, a perturbation theory in terms of coupled integral equations is developed and shown to suffer from inconsistencies due to the presence of initial correlations. We discover hints at a possible cure by using the first order solution for two-point cumulants to reorganise one-loop diagrams. Applied to cosmological structure formation the first order solution for the density power spectrum is found to be the familiar linear growth solution. We argue why our approach should have superior performance in non-linear structure formation compared with the standard approach.

ZUSAMMENFASSUNG

Wir entwickeln eine feldtheoretische Version der kinetischen Gastheorie basierend auf den grundlegenden Arbeiten [39, 40, 22]. Ein kanonisches Erzeugendenfunktional für die Korrelatoren makroskopischer Observablen wird hergeleitet, wobei die Pfadintegralmethode benutzt wird und die mikroskopischen Phasenraum-Koordinaten als fundamentale Variablen die Dynamik beschreiben. Die Ergebnisse der Originalarbeiten werden auf Systeme mit korrelierten Anfangsbedingungen verallgemeinert. Eine exakte anfängliche Phasenraumverteilung für ein statistisch homogenes and isotropes Gaußsches Zufallsfeld wird berechnet, in eine Diagramsprache übersetzt und in verbundene Anteile faktorisiert. Wir geben eine Herleitung des großkanonische Erzeugendenfunktional für statistisch homogene und isotrope Systeme an. Darauf aufbauend wird eine Störungstheorie in Form gekoppelter Integralgleichungen entwickelt und es wird gezeigt, dass diese aufgrund der Anwesenheit von Anfangskorrelationen Inkonsistenzen aufweist. Wir entdecken Hinweise auf eine mögliche Umgehung des Problems indem wir die Lösung erster Ordnung für die Zweipunkt-Kumulanten benutzen um Ein-Schleifen-Diagramme umzusortieren. In der Anwendung auf kosmologische Strukturbildung finden wir das wohlbekannte lineare Wachstum des Dichte-Leistungsspektrums als Lösung erster Ordnung unserer Feldtheorie. Wir argumentieren warum unser Ansatz bei nicht-linearer Strukturbildung der Standardmethode überlegen sein sollte.

Sic parvis magna.

— Motto of Sir Francis Drake

ACKNOWLEDGMENTS

First and foremost I cannot thank my supervisor Prof. Dr. Matthias Bartelmann enough for giving me the opportunity of doing my Ph.D. studies under his guidance. Without his persistent tutoring and unwavering patience many of my misconceptions would have survived until today and would probably have turned this thesis into an unintelligible mess. He was always there to point me in the right direction of research when I was in danger of pursuing irrational avenues and he thus played a large part in the process of me creating this thesis.

I want to thank Daniel Berg, Elena Kozlikin, Robert Lilow, Carsten Littek and Celia Viermann for working on other parts and applications of the field theory presented in this work. Bringing together people all viewing the theory from a different angle has lead to frequent and inspiring discussions which have afforded me a much deeper insight into the inner workings and intricacies of the theory than I would have been able to achieve on my own. I especially like to thank Carsten Littek in particular for helping in proofreading this thesis.

I like to thank Prof. Dr. Jürgen Berges of the Institute of Theoretical Physics at the University of Heidelberg without whose support during the first half of my Ph.D. studies this work would not have been possible. My work was also generously supported by the Transregional Collaborative Research Centre TR 33, 'The Dark Universe', of the German Research Foundation.

The atmosphere provided by my work group at the Institute of Theoretical Astrophysics throughout my studies has never failed to be enjoyable, inspiring and filled with a lot of laughter (thanks to Tim 'Mr. Hilarious' Tugendhat) and of course cake. I especially like to thank my office mates Sven Meyer, Eleonora Sarli, Agnese Fabris and Iva Karovicova for bravely suffering through my occasional antics. Together with Matthias Redlich, Sven Meyer has excelled as my source for sorely needed coding knowledge. I also want to particularly thank Prof. Dr. Björn Malte Schäfer for always providing physical insight when I needed it.

I especially like to thank Anna Zacheus. Her dedicated work always made sure that organisational matters never became an impediment to my studies.

Last but not least, I want to thank my family and friends for always supporting me and providing me with the necessary strength of will to overcome the challenges I faced during my studies.

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$G = 6,67384 \times 10^{-11} \frac{\mathrm{m}^3}{\mathrm{s}^2\mathrm{kg}}$	Gravitational constant
$k_\mathrm{B} = 1.3806488 \times 10^{-23} \frac{\mathrm{J}}{\mathrm{K}}$	Boltzmann constant
$\hbar = \frac{h}{2\pi} = 1.054571726 \times 10^{-34}\,\mathrm{Js}$	Planck constant
$c = 299792458 \frac{\mathrm{m}}{\mathrm{s}}$	Speed of light in vacuum
$H_0 = (74,3 \pm 2,1) \frac{\mathrm{km}}{\mathrm{s} \cdot \mathrm{Mpc}}$	Hubble constant
$1\,\mathrm{pc} = 3.0857 \times 10^{16}\,\mathrm{m}$	One parsec
$1\,\mathrm{Mpc} = 10^6\,\mathrm{pc}$	One Megaparsec
$1\,\mathrm{Gpc} = 10^9\,\mathrm{pc}$	One Gigaparsec

ACRONYMS

d.o.f. degrees of freedom

QM Quantum Mechanics

QFT Quantum Field Theory

MSR Martin-Siggia-Rose formalism

BBGKY Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy

1PI one-particle irreducible

CDM cold dark matter

LSS large scale structure

BAO baryonic acoustic osciallations

SPT Standard Perturbation Theory

SFTCP Statistical Field Theory for Classical Particles

EdS Einstein de-Sitter

TTI time translation invariance

FDT fluctuation-dissipation theorem

FLRW Friedmann-Lemaître-Robertson-Walker

CMB cosmic microwave background

SSA single-stream approximation

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INTRODUCTION

1.1 MOTIVATION AND OUTLINE

The original motivation for this thesis was to find a new approach for the calculation of the time evolution of the statistics of the large scale structure (LSS) in the universe, with the density power spectrum being the main object of interest. Recent observations have provided more and more evidence in favour of the standard ΛCDM-model of cosmology. Especially observations of the cosmic microwave background (CMB), i. e. the remnant radiation released during the epoch of matter-radiation decoupling, have shown that our picture of a nearly flat and statistically homogeneous and isotropic universe, with structures having evolved from small perturbations of the matter density through gravitational interaction in a 'bottom-up' process, seems to fit well with reality. Compared to its predecessor WMAP [12], the latest full sky survey performed by the Planck satellite [50] has lead to sizable improvements in the precision with which the statistics of temperature fluctuations in the CMB can be determined. While at the present time these observations when considered on their own are our most powerful probe for constraining the various parameters of cosmological models, one should always strive to combine information from the observation of different physical effects. Two prominent candidates for this purpose require a good theoretical understanding of structure formation.

- The baryonic acoustic osciallations (BAO) are remnants of waves in the strongly coupled baryon-photon fluid which filled the universe in its radiation dominated epoch. Today, they are observed as a periodic fluctuation in the density of baryonic matter in the universe. More precisely, they lead to a 'bump' in the two-point correlation function ξ of galaxies at around $100\,\mathrm{Mpc}/h$ when calculated from large redshift surveys like the Sloan Digital Sky Survey [24]. If one has a clear theoretical understanding how this feature of the correlation function evolves during the history of the universe it can be used as a 'standard ruler' for measuring distances at different cosmological epochs and thus probe the expansion history of the universe. One especially hopes to constrain different models of dark energy, which governs the accelerated expansion of the universe in the present cosmological epoch.

- Weak gravitational lensing (cf. [5, 3] for reviews of the topic) describes how the signal of light emitted by distant background galaxies is distorted due to the deflection of this light by the LSS between the source and the observer. Since the

matter power spectrum with its time evolution is an input parameter for the theoretical model of weak lensing, observations of this effect allow us to put constraints on the model for the power spectrum. Since this model itself will depend on the cosmological parameters, weak lensing provides yet another way to constrain them.

Using the CMB as a probe for constraining cosmological parameters has the advantage that in order to describe the relevant physics it is sufficient to use theoretical models that are linear in the dynamical variables. In the case of LSS formation this is no longer the case. While linear approximations have been shown to work very well on large enough scales, the dynamics on smaller scales are intrinsically highly non-linear. With many upcoming observations of LSS like Euclid [34] designed to probe scales deeply in the non-linear regime, a more complete theoretical understanding of structure formation is sorely needed when employing effects like the BAO or weak lensing to constrain parameters.

The principal question of structure formation can be summarized as: *How does a distribution of mass evolve under the influence of its own gravity in an expanding spacetime?* Despite the relative simplicity of this question, developing an analytical model that is able to describe this process on a large range of scales has persisted as a very difficult problem over the years. The Standard Perturbation Theory (SPT) that was developed is based upon using the hydrodynamical equations of an ideal and pressureless fluid which is solved perturbatively around the cosmological background. A very extensive and complete review of the developments up to the turn of the millenium can be found in Bernardeau et al. [13].

Until today the most accurate theoretical descriptions of structure formation have been obtained by running numerical N-body simulations. While projects like the Millenium-II simulation (cf. Boylan-Kolchin et al. [16]) and Illustris (cf. Vogelsberger et al. [56]) have reproduced the statistics of the observed LSS to a remarkable degree, they are also very expensive both in terms of time and money. For applications like parameter studies more direct analytical tools would be preferable.

The interest in cosmological structure formation was renewed after the publication of two pioneering papers by Crocce and Scoccimarro [20, 21], where the authors applied methods that originated in Quantum Field Theory (QFT), like Feynman diagrams and their resummation, to the Standard Perturbation Theory that had been developed so far. This sparked a plethora of efforts to transfer other such methods like renormalisation group equations [37, 47] or effective, coarse-grained field theories [48]. These allowed to probe the mildly non-linear scales relevant to the BAO feature but not much further beyond. In addition, they are plagued by the necessity of approximations to the underlying equations of motion like the single-stream approximation (SSA) which a priori limit their validity to length scales above a certain threshold.

The starting point from which this thesis was begun is to combine the description of the dynamics in terms of particles instead of macroscopic observables, which has proven succesful in numeric simulations, with the powerful analytical tools developed in QFT for studying field theories, i. e. in terms of what had been achieved in structure formation we tried to combine 'the best of both worlds'. The theoretical

framework for such an approach had already been developed in a series of papers by Das and Mazenko [22], Mazenko [40, 39]. However, the authors main interest lay in the application of this field theory to the fluctuations of systems in thermal equilibrium and transitions between ergodic and non-ergodic behaviour explored in [42, 23, 41, 52].

Structure formation on the other hand is a process far from thermal equilibrium and starts out from an initially correlated random density field. The main task was thus to find a way how one can implement such initial conditions for a particle based theory and to investigate how this potentially modifies the perturbation equations for macroscopic observables one derives from the microscopic field theory. These problems are adressed in chapters 3 and 4 respectively, which make up the bulk of part i of this thesis. Over the course of working with the theory it became clear that it should not only remove some of the more problematic approximations of SPT, but that it is actually a reformulation of kinetic theory that could also potentially prove to be very powerful in other fields of statistical physics. An example is that one might be able to derive the equations of hydrodynamics from first principles, with the need for heuristic arguments significantly reduced. We therefore provide a thorough introduction into this kind of field theory in chapter 2, where we explain its working principles, the connection to the standard formulations of both equilibrium statistical mechanics as well as non-equilibrium kinetic theory and give reasons why we believe that it posseses some distinct advantages. We also tried to keep the developments throughout part i as general and with as little specialisation to cosmological structure formation as possible.

After that, part ii of this thesis then deals with exactly this specific application of the field theory to the problem of LSS formation. In chapter 6 we briefly explain the physical scenario one is working in by introducing the bare necessities of cosmology and SPT, as well as to argue which of its principal problems are avoided by the particle picture of our approach. Chapter 7 then demonstrates that the implementation of the exact particle dynamics is a rather simple exercise when compared to SPT. In chapter 8 we finally show that the well-known linear growth solution of SPT is exactly reproduced by our field theory with the added benefit of a small-scale cutoff originating in the exact inclusion of initial velocity dispersion. Due to time constraints, we are sadly not able to present calculations of the matter power spectrum beyond the first order of our perturbation expansion. By making a very general comparison between the perturbation expansion of our theory and that of SPT we can however argue that additional contributions will necessarily show up in our theory even at the one-loop order. The investigation of such one-loop effects and their possible resummation present themselves as the logical next step for the author's future work.

At the time of the completion of this thesis, one paper (Fabis et al. [25]) has been submitted for publication which is entirely derived from work found herein. A number of papers (Bartelmann et al. [6, 7, 8], Kozlikin et al. [32], Viermann et al. [55]) have been submitted by other members of our group, which are the result of our cooperative work on this theory and thus contain ideas also found in this thesis. While none of them have been accepted for publication so far, references to the respective electronic preprints can be found in the bibliography.

1.2 NOTATION AND CONVENTIONS

As is usual in field theory we will introduce some notation of our own specifically tailored towards shortening the often extensive length of many expressions we will encounter as well as reducing the amounts of indices.

1.2.1 *Phase-space notation*

We will often deal with properties and quantities that can be attached to the individual particles of an N-particle ensemble moving through a $2dN$-dimensional phase-space, where d is the dimension of real space. In part i of this thesis d is kept arbitrary and in part ii we use $d = 3$. The most basic quantities are the actual phase-space coordinates of the particles, the position $\vec{q}_j(t)$ and the canonical momentum $\vec{p}_j(t)$. We bundle these into the single vector

$$\vec{x}_j(t) = \begin{pmatrix} \vec{q}_j(t) \\ \vec{p}_j(t) \end{pmatrix} . \tag{1.1}$$

Unless explicitly stated otherwise, lower-case latin indices like i, j, k and so on designate quantities as belonging to individual particles. In order to write down expressions that depend on properties of all particles without sums over their labels we introduce the following tensorial notation

$$\mathbf{x}(t) = \sum_{j=1}^{N} \vec{x}_j(t) \otimes \vec{e}_j = \vec{x}_j(t) \otimes \vec{e}_j \, , \tag{1.2}$$

where the second equality introduces the common Einstein summation convention, i. e. repeated indices or labels are summed over their domain space. We also introduced

$$(\vec{e}_j)_i = \delta_{ij} \, , \tag{1.3}$$

which is a N-dimensional column vector, whose j-th entry is unity and all others are zero. Whenever scalar or vectorial quantities that are properties of individual particles appear in bold script they are to be understood in the sense of (1.2). We may for example write for positions or momenta alone

$$\mathbf{q}(t) = \vec{q}_j(t) \otimes \vec{e}_j \, , \qquad \mathbf{p}(t) = \vec{p}_j(t) \otimes \vec{e}_j \, . \tag{1.4}$$

The tensor product has the following general property

$$(A \otimes B) \circ (C \otimes D) = (A \circ C) \otimes (B \circ D) \, , \tag{1.5}$$

where $\circ$ defines some bilinear operation that is well-defined for all quantities involved. In the case of the scalar product we may then define

$$\langle \mathbf{a}, \mathbf{b} \rangle = (\vec{a}_i \otimes \vec{e}_i) \cdot (\vec{b}_j \otimes \vec{e}_j) = (\vec{a}_i \cdot \vec{b}_j) \otimes (\vec{e}_i \cdot \vec{e}_j) = (\vec{a}_i \cdot \vec{b}_j)\delta_{ij} = (\vec{a}_i \cdot \vec{b}_i) \, . \tag{1.6}$$

We will also encounter the phase-space gradient

$$\nabla_j = \begin{pmatrix} \nabla_{q_j} \\ \nabla_{p_j} \end{pmatrix} \quad \rightarrow \quad \boldsymbol{\nabla} = \nabla_j \otimes \vec{e}_j \,, \tag{1.7}$$

where

$$\nabla_{q_j} f(\vec{q}) = \nabla_q f(\vec{q})\big|_{\vec{q}=\vec{q}_j} \tag{1.8}$$

with ∇_q the usual d-dimensional gradient and the same of course holds for ∇_{p_j}. Integration over all of phase-space is written in the shorthand notation

$$\int \mathrm{d}\mathbf{x} = \left(\int \prod_{j=1}^{N} \mathrm{d}^d q_j\right)\left(\int \prod_{j=1}^{N} \mathrm{d}^d p_j\right) = \left(\int \prod_{j=1}^{N} \mathrm{d}\vec{q}_j\right)\left(\int \prod_{j=1}^{N} \mathrm{d}\vec{p}_j\right) \tag{1.9}$$

with obvious restrictions to any kind of subspace. For the rest of this thesis we use the latter vector notation for any integral measures. Another important quantity is the symplectic matrix

$$\mathcal{J} = \begin{pmatrix} 0_d & \mathcal{I}_d \\ -\mathcal{I}_d & 0_d \end{pmatrix} \quad \rightarrow \quad \boldsymbol{\mathcal{J}} = \mathcal{J} \otimes \mathcal{I}_N \,, \tag{1.10}$$

where $\mathcal{I}_N$ is the $N \times N$-dimensional unity matrix and 0_d the $N \times N$-dimensional zero matrix. Whenever matrix valued objects in bold script appear they are to be understood in the above sense. We will also encounter source fields $\mathbf{J}$ and $\mathbf{K}$ which are defined as

$$\mathbf{J}(t) = \begin{pmatrix} \vec{J}_{q_j}(t) \\ \vec{J}_{p_j}(t) \end{pmatrix} \otimes \vec{e}_j \,, \qquad \mathbf{K}(t) = \begin{pmatrix} \vec{K}_{q_j}(t) \\ \vec{K}_{p_j}(t) \end{pmatrix} \otimes \vec{e}_j \tag{1.11}$$

with obvious reduction to the q and p subspaces as in (1.4).

1.2.2 *Field theory notation*

We will encounter expressions which contain a multitude of fields $\Phi(\vec{q}, t)$ and integrations over their arguments or 'labels'. In order to make these expressions manageable we will introduce a few shorthand notations. We abbreviate the combined space and time arguments of fields as simple numbers

$$\Phi(\vec{q}_1, t_1) = \Phi(1) \tag{1.12}$$

and we stress that $\vec{q}_1$ as a field argument never pertains to the position of the particle with index 1 and the same holds true for any such label. We also combine integrations over space and time into

$$\int \mathrm{d}1 \;= \int \mathrm{d}t_1 \int \mathrm{d}\vec{q}_1 \;. \tag{1.13}$$

We will have to deal with vector-valued fields that have multiple components. This is most easily treated with an index notation where greek characters run over these components. We can combine this with the above notation for the field arguments. For example let Φ be a two component vector of fields, then we have

$$\Phi(\vec{q}_1, t_1) = \Phi(1) = \begin{pmatrix} \Phi_A(1) \\ \Phi_B(1) \end{pmatrix} = \Phi_{\mu_1} \quad \Longrightarrow \quad \Phi_{A_1} = \Phi_A(1) = \Phi_A(\vec{q}_1, t_1) \; . \tag{1.14}$$

We will also use an extended Einstein summation convention which for repeated labels μ_1 includes both summing over the components of fields and integration over their spacetime arguments. For two fields this would read as

$$\Phi_{\mu_1} \Psi_{\mu_1} = \sum_{\mu} \int \mathrm{d}1 \, \Phi_\mu(1) \, \Psi_\mu(1) \; , \tag{1.15}$$

which can be understood as a kind of functional scalar product in the component space of the fields. If we write out the components and only have repeated space-time labels left we still understand that integrals are performed as

$$\Phi_{A_1} \Psi_{A_1} = \int \mathrm{d}1 \, \Phi_A(1) \, \Psi_A(1) \; . \tag{1.16}$$

Of course the same notation can easily be extended to tensor-valued fields in the same component space. In some instances, especially when we only have few labels present, we may condense notation even further by understanding the greek indices as encompassing both the field component and the space-time label, i. e. $\mu_1 \to \mu$, and still use the above extended Einstein convention for repeated indices.

1.3 MATHEMATICAL CONCEPTS

There are a few mathematical concepts that are important for this work. We will now introduce the necessary definitions and notational conventions.

1.3.1 *Functional derivatives*

As the name already suggests functional derivatives can be seen as the generalisation of the concept of a derivative from normal functions to functionals. While a basic function $f(x)$ maps an element of some field $\mathbb{K}$ (usually $\mathbb{R}$ or $\mathbb{C}$) into that same field as $f : \mathbb{K} \to \mathbb{K}$, a functional maps functions themselves into a field, usually the one over which the functions are defined. Since this will in most cases include some kind of integration, one could for example write $F : \mathcal{C}^\infty(\mathbb{K}) \to \mathbb{K}$ for some functional $F[f]$, where $\mathcal{C}^\infty(\mathbb{K})$ are the infinitely differentiable functions over the field $\mathbb{K}$. A very simple example for a functional would be for functions $f \in \mathcal{C}^\infty(\mathbb{R})$

$$F[f] = \int_0^1 \mathrm{d}x \, f(x) \; . \tag{1.17}$$

The functional derivative $\frac{\delta F}{\delta f(x)}$ now measures the change in the value of the functional F if the function f is varied. While the actual definition of a functional derivative is more intricate, for the purpose of this work it will be enough to remember that for sufficiently smooth functions the functional derivative obeys the same linearity, product and chain rules as the normal derivative does. The order of mixed functional derivatives can be interchanged arbitrarily and actual computations can be done using that

$$\frac{\delta}{\delta f(y)} f(x) = \delta_{\mathrm{D}}(x - y) \tag{1.18}$$

with obvious extension to functions of multiple variables. We will assume that the reader is familiar with the Dirac delta distribution and its properties. We only mention that for vectorial quantities $\vec{x}, \vec{y}$ we always implicitly understand

$$\delta_{\mathrm{D}}(\vec{x} - \vec{y}) = \prod_a \delta_{\mathrm{D}}(x_a - y_a) \,. \tag{1.19}$$

We will often encounter the case where functional derivatives are applied to the exponential of an integrated product of two functions. For this case we find

$$\begin{aligned}
\frac{\delta}{\delta f(x)} \exp\left\{ \int \mathrm{d}y \, f(y)\, g(y) \right\} &= \frac{\delta}{\delta f(x)} \exp\left\{ F[f,g] \right\} \\
&= \left(\frac{\mathrm{d}}{\mathrm{d}F[f,g]} \exp\left\{ F[f,g] \right\} \right) \frac{\delta F[f,g]}{\delta f(x)} \\
&= \exp\left\{ F[f,g] \right\} \int \mathrm{d}y \, \frac{\delta f(y)}{\delta f(x)} \, g(y) \\
&= \exp\left\{ F[f,g] \right\} \int \mathrm{d}y \, \delta_{\mathrm{D}}(y - x) \, g(y) \\
&= g(x) \exp\left\{ \int \mathrm{d}y \, f(y)\, g(y) \right\}
\end{aligned} \tag{1.20}$$

One may read this in the sense of the exponential function providing an *eigenbasis* of functionals for the functional derivative operator just like it does for the normal derivative. This is important because we will encounter operators which are defined in terms of analytic functions of the functional derivative operator. Let A be such an analytic function with a series representation

$$A(x) = \sum_{n=1}^{\infty} a_n \, x^n \,. \tag{1.21}$$

If this series converges on the entire image of the function $g(x)$, then we may write in general

$$\begin{aligned}
A(g(x)) \exp\left\{ \int \mathrm{d}y \, f(y)\, g(y) \right\} &= \sum_{n=1}^{\infty} a_n \, g(x)^n \exp\left\{ \int \mathrm{d}y \, f(y)\, g(y) \right\} \\
&= \left(\sum_{n=1}^{\infty} a_n \left(\frac{\delta}{\delta f(x)} \right)^n \right) \exp\left\{ \int \mathrm{d}y \, f(y)\, g(y) \right\} \\
&= A\left(\frac{\delta}{\delta f(x)} \right) \exp\left\{ \int \mathrm{d}y \, f(y)\, g(y) \right\} \,.
\end{aligned} \tag{1.22}$$

This relation will see frequent use throughout this thesis. Most of the time we will take functional derivatives w. r. t. vector-valued functions. We understand this in the usual sense of a 'gradient' operator as

$$\frac{\delta}{\delta \vec{f}(\vec{x})} = \begin{pmatrix} \frac{\delta}{\delta f_1(\vec{x})} \\ \vdots \\ \frac{\delta}{\delta f_n(\vec{x})} \end{pmatrix} \tag{1.23}$$

for an n-component function.

1.3.2 *Fourier transform*

We assume that the reader is familiar with the concept of Fourier transforms, so we will only give the conventions used in this work. The Fourier transform of a function $f(\vec{q})$ in real space is defined by

$$\widetilde{f}(\vec{k}) := \int \mathrm{d}\vec{q}\, f(\vec{q})\, \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{k}} \tag{1.24}$$

and the inverse transform is consequently given by

$$f(\vec{q}) = \int \frac{\mathrm{d}\vec{k}}{(2\pi)^d}\, \widetilde{f}(\vec{k})\, \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{k}}\,. \tag{1.25}$$

This implies that the Fourier transform of unity is the Dirac delta distribution

$$\int \mathrm{d}\vec{q}\, \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{k}} = \int \mathrm{d}\vec{q}\, \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{k}} = (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k})\,, \tag{1.26}$$

a relation we will make frequent use of. The above equations formally only hold for integration over all of real and Fourier space. We will however often have to deal with integrations over a finite volume V, so in order to be completely correct we would have to use a discrete Fourier transform. Besides leading to a lot of notational hassle this will not provide any real gain in understanding. Since the Dirac delta distribution is the continuous analogue of the discrete Kronecker delta, all the manipulations we perform using (1.26) can directly be translated into a discrete Fourier language. We thus loose nothing if we still use the above notation of integrations over an infinite space. We only have to keep in mind that

$$(2\pi)^d\, \delta_{\mathrm{D}}(\vec{0}) = \int \mathrm{d}^d q \;= V\,. \tag{1.27}$$

There is also a more physical motivation for using integrations over an infinitely large space. In all our applications we will in principle be free to choose the size of the volume V of the physical system under consideration. As such we will always choose it to be much larger than any of the scales on which we investigate its statistical properties. In this sense the volume can be assumed to be infinite *relative* to the scales of interest.

Throughout this work we will not use the tilde to distinguish between quantities defined in real space and their Fourier counterparts, since we find that the distinction is easily made by the arguments $\vec{q}$ and $\vec{k}$. This is also desirable in the light of our field theory notation introduced in section 1.2.2. We extend the field argument label 1 to mean either $(\vec{q}_1, t_1)$ or $(\vec{k}_1, t_1)$. If we choose expressions to be formulated with quantities in Fourier space we must remember that the extended Einstein convention of (1.15) transforms into

$$\begin{aligned}
\Phi_{\mu_1}\Psi_{\mu_1} &= \sum_{\mu}\int \mathrm{d}1\,\Phi_\mu(1)\Psi_\mu(1) = \int \mathrm{d}t_1 \int \mathrm{d}\vec{q}_1\,\Phi_\mu(\vec{q}_1,t_1)\Psi_\mu(\vec{q}_1,t_1)\\
&= \int \mathrm{d}t_1 \int \mathrm{d}\vec{q}_1 \int \frac{\mathrm{d}\vec{k}_1}{(2\pi)^d}\,\Phi_\mu(\vec{k}_1,t_1)\,\mathrm{e}^{\mathrm{i}\vec{k}_1\cdot\vec{q}_1}\int \frac{\mathrm{d}\vec{k}_2}{(2\pi)^d}\,\Psi_\mu(\vec{k}_2,t_1)\,\mathrm{e}^{\mathrm{i}\vec{k}_2\cdot\vec{q}_1}\\
&= \int \mathrm{d}t_1 \int \frac{\mathrm{d}\vec{k}_1}{(2\pi)^d}\int \frac{\mathrm{d}\vec{k}_2}{(2\pi)^d}\,\Phi_\mu(\vec{k}_1,t_1)\,\Psi_\mu(\vec{k}_2,t_1)\int \mathrm{d}\vec{q}_1\,\mathrm{e}^{\mathrm{i}(\vec{k}_1+\vec{k}_2)\cdot\vec{q}_1}\\
&= \int \mathrm{d}t_1 \int \frac{\mathrm{d}\vec{k}_1}{(2\pi)^d}\int \frac{\mathrm{d}\vec{k}_2}{(2\pi)^d}\,\Phi_\mu(\vec{k}_1,t_1)\,\Psi_\mu(\vec{k}_2,t_1)\,(2\pi)^d\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\\
&= \int \mathrm{d}t_1 \int \frac{\mathrm{d}\vec{k}_1}{(2\pi)^d}\,\Phi_\mu(\vec{k}_1,t_1)\,\Psi_\mu(-\vec{k}_1,t_1)\\
&= \int \mathrm{d}1\,\Phi_\mu(1)\,\Psi_\mu(-1)\,,
\end{aligned} \tag{1.28}$$

where we introduced the notation $-1 = (-\vec{k}_1, t_1)$. If we remember that the 'scalar product' of the field theory Einstein notation involves a factor $1/(2\pi)^d$ and one minus sign in one of the field arguments when evaluated in Fourier space, we can use the same index notation for both real and Fourier space quantities. It will also be useful to keep in mind the following relation between the derivative of a function and its Fourier transform

$$\int \mathrm{d}\vec{q}\;\nabla_q f(\vec{q})\,\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{k}} = \mathrm{i}\vec{k}\,f(\vec{k})\,, \tag{1.29}$$

which can be proven by a straightforward integration by parts and assuming that the function vanishes on the boundaries. The extension of this relation to higher derivatives is trivial.

1.3.3 *Laplace transform*

The Laplace transform is a close relative of the Fourier transform. It is especially useful in treating problems where causality must be observed and as such we will employ it to solve integral equations that involve causal propagators. We use its one-sided definition

$$F(s) := \mathcal{L}_{t\to s}[f(t)] = \int_0^\infty \mathrm{d}t\,f(t)\,\mathrm{e}^{-st} \qquad s\in\mathbb{C}\,, \tag{1.30}$$

where the script $\mathcal{L}$ represents the integral operator defining the Laplace transform. One often calls $f(t)$ the *time-domain* function and $F(s)$ its *frequency domain* counterpart. The inverse transform is usually defined in terms of the so-called *Bromwich integral*

$$f(t) = \mathcal{L}^{-1}_{t\leftarrow s}[F(s)] = \frac{1}{2\pi \mathrm{i}} \lim_{T\to\infty} \int_{\gamma-\mathrm{i}T}^{\gamma+\mathrm{i}T} \mathrm{d}s\, F(s)\, \mathrm{e}^{st} \,, \tag{1.31}$$

where γ is a real number chosen such that it is larger than the real part of all singularities of $F(s)$. This choice makes sure that all these singularities lie on the left hand side of the vertical line in the complex plane along which the integration is performed. While the integral may be performed using for example the Cauchy residue theorem, it is much more common and easier to decompose $F(s)$ into simple functions for which one knows the corresponding time domain functions and thus assemble $f(t)$ by inspection. An easy example for this procedure would be

$$\mathcal{L}_{t\to s}[\mathrm{e}^{bt}] = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{bt}\, \mathrm{e}^{-st} = \frac{\mathrm{e}^{(b-s)t}}{b-s}\Big|_0^\infty = \frac{1}{s-b} \qquad \forall s \text{ with } \Re(s) > b \,. \tag{1.32}$$

Formally we now apply the inverse transform with $\gamma > b$, but the actual logic employed here is

$$\mathcal{L}^{-1}_{t\leftarrow s}\left[\frac{1}{s-b}\right] = \mathcal{L}^{-1}_{t\leftarrow s}\left[\mathcal{L}_{t\to s}[\mathrm{e}^{bt}]\right] = \mathrm{e}^{bt} \,. \tag{1.33}$$

There are some general properties of the Laplace transform that we will need. The effect of a 'time shift' is

$$\begin{aligned}\mathcal{L}_{t\to s}[f(t-a)\,\Theta(t-a)] &= \int_0^\infty \mathrm{d}t\, f(t-a)\,\Theta(t-a)\,\mathrm{e}^{-st} = \int_a^\infty \mathrm{d}t\, f(t-a)\,\mathrm{e}^{-st} \\ &= \int_0^\infty \mathrm{d}t'\, f(t')\,\mathrm{e}^{-s(t'+a)} = \mathrm{e}^{-sa}F(s) \,,\end{aligned} \tag{1.34}$$

where we made the change of variables $t' = t - a$ in the second line and $\Theta(t-a)$ is the Heaviside function. Another very similar relation is

$$\begin{aligned}\mathcal{L}_{t\to s}[f(t+a)] &= \int_0^\infty \mathrm{d}t\, f(t+a)\,\mathrm{e}^{-st} = \int_a^\infty \mathrm{d}t'\, f(t')\,\mathrm{e}^{-s(t'-a)} \\ &= \mathrm{e}^{sa}\int_0^\infty \mathrm{d}t\, f(t)\,\Theta(t-a)\,\mathrm{e}^{-st} = \mathrm{e}^{sa}\mathcal{L}_{t\to s}[f(t)\,\Theta(t-a)] \,,\end{aligned} \tag{1.35}$$

where we again made a substitution $t' = t + a$ in the first line and then renamed $t' \to t$ in the second line. Finally, there is the generalisation of the convolution theorem

$$\begin{aligned}
\mathcal{L}_{t\to s}\left[\int_0^t \mathrm{d}t'\, f(t-t')\, g(t'+a)\right] &= \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-st} \int_0^\infty \mathrm{d}t'\, \Theta(t-t')\, f(t-t')\, g(t'+a) \\
&= \int_0^\infty \mathrm{d}t'\, g(t'+a) \int_0^\infty \mathrm{d}t\, \Theta(t-t')\, f(t-t')\, \mathrm{e}^{-st} \\
&= \int_0^\infty \mathrm{d}t'\, g(t'+a) \int_{-t'}^\infty \mathrm{d}u\, \Theta(u)\, f(u)\, \mathrm{e}^{-s(u+t')} \\
&= \int_0^\infty \mathrm{d}t'\, g(t'+a)\, \mathrm{e}^{-st'} \int_0^\infty \mathrm{d}t\, f(t)\, \mathrm{e}^{-st} \\
&= \mathcal{L}_{t\to s}[f(t)]\, \mathcal{L}_{t'\to s}[g(t'+a)]\,, \qquad (1.36)
\end{aligned}$$

where we substituted $u = t - t'$ in the third line and then renamed $u \to t$ in the fourth line. The standard convolution theorem is obtained by setting $a = 0$.

Part I

NON-EQUILIBRIUM STATISTICAL FIELD THEORY BASED ON PARTICLE DYNAMICS

2

THE CANONICAL GENERATING FUNCTIONAL

In this chapter we will go through the basic ideas of the field-theoretical approach to kinetic theory pioneered by Das and Mazenko in [22, 40, 39]. We will refer to it as Statistical Field Theory for Classical Particles (SFTCP). As shown in Bartelmann et al. [6], the derivation of the generating functional can be done in a more general way with actual fields as the primary variables. However, as the chapter title already suggests we will try to develop a generating functional that has a close connection to the standard canonical partition function of equilibrium statistical physics. In fact, it can be seen as a generalization of this concept to non-equilibrium systems. Because of this we will stick to our more special case where the primary variables are the phase-space coordinates of an N-particle system. This will allow us to mark the difference between the standard equilibrium statistical physics and our approach more clearly as we go along.

2.1 QUICK SUMMARY OF EQUILIBRIUM STATISTICAL PHYSICS

At its very core, equilibrium statistical physics is based only on a few quite simple principles, which we will quickly go through. For a much more thorough discussion we refer the reader to Bartelmann et al. [9]. One usually starts by considering a system of N particles which are subject to some set of equations of motion which can be formulated in the Hamiltonian formalism as

$$\partial_t \mathbf{x} - \boldsymbol{\mathcal{J}} \boldsymbol{\nabla} \mathcal{H} = \boldsymbol{\mathcal{E}}[\mathbf{x}] = 0 \,. \tag{2.1}$$

Given a set of initial conditions $\mathbf{x}^{(\mathrm{i})}$ defining the initial *state* of the system one could then in principle evolve the system to any desired point in time according to the phase-space flow mapping $\mathbf{x}(t) = \Psi_t(\mathbf{x}^{(\mathrm{i})})$ derived from the above equations. However, in practice it is impossible to even measure the initial state due to the large number $\mathcal{F}$ of degrees of freedom (d.o.f.) of the system, let alone solve the equations of motion due to the interactions between them. $\mathcal{F}$ is usually set by the number N of particles, typically of order $N_A \approx 10^{23}$ and larger. We will stick to particles without internal d.o.f. leading to $\mathcal{F} = dN$ for a d-dimensional configuration space and a $2dN$-dimensional phase-space. Equilibrium statistical physics circumvents these problems by looking at the system from a different angle.

- One gives up interest in the precise microscopic description of the system and rather concentrates on characterising the system by a few *macroscopic* observables $\{A\}$. These can be called *collective* in the sense that they are often made

up by contributions from the individual particles and we may consequently write $A(\mathbf{x})$.

- Any real measurement of a macroscopic variable will have to be taken over some period of time T and then averaged afterwards

$$\bar{A}_T = \frac{1}{T} \int_0^T \mathrm{d}t \, A(\Psi_t(\mathbf{x}^{(\mathrm{i})})) \, . \tag{2.2}$$

  Over the course of this measurement the system will travel through states in phase-space with the phase-space flow Ψ_t.

- We can define the average of a macroscopic observable in a different way by introducing the notion of an *ensemble*, a large collection of copies of the same system that have all been prepared in the same macroscopic state but their microscopic states may and usually will differ greatly. Mathematically these can be thought of as a point sampling of the probability density $\mathcal{P}(\mathbf{x})$ in the $2dN$-dimensional phase space Γ, which gives the probability that our actual system is found in the phase-space cell $\mathrm{d}\Gamma = \prod_{i=1}^{N} h_0^{-1} \, \mathrm{d}\vec{q}_i \, \mathrm{d}\vec{p}_i$ [1] around the state $\mathbf{x}$. Then the *ensemble average* is defined as

$$\langle A \rangle = \int \mathrm{d}\Gamma \; \mathcal{P}(\mathbf{x}) \, A(\mathbf{x}) \, . \tag{2.3}$$

  This would correspond to an instantaneous measurement of A on many systems who all have been prepared in the same macroscopic state.

The conceptual leap of statistical physics is now to equate these two different definitions of an average at least approximately. This becomes feasible if the system under consideration meets certain conditions.

- The system must be in equilibrium. This means that the relative fluctuations of the real value of A about its mean $\bar{A}_T$ are small and one can thus use it as a meaningful quantity to characterise the system.

- The system must be ergodic in the sense that on the timescale T of the measurement it travels through such a large amount of states that these cover a sizable fraction of its accessible phase space. Taking the successive time average $\bar{A}_T$ over all these states then becomes comparable to taking the instantaneous average $\langle A \rangle$ over the members of the ensemble occupying these states.

We would thus exchange the task of determining the initial state $\mathbf{x}^{(\mathrm{i})}$ and then solving (2.1) for the problem of finding the ensemble phase-space probability density $\mathcal{P}(\mathbf{x})$. But this is a much easier task if we only constrain the system to have certain values for some macroscopic observables. The very foundation of all further considerations is now the following assumption.

1 h_0 is some discretization constant in order to make phase-space states countable.

Basic postulate of equilibrium statistical physics: *An isolated system conforming to the constraints of consisting of N particles, which occupy the volume V and whose degrees of freedom contain the energy $E = \mathcal{H}$, may be represented by a micro-canonical ensemble of systems under the same constraints. If the phase-space probability density $\mathcal{P}$ of this ensemble is equally distributed initially it is constant in time. This means that averages $\langle A \rangle$ do not change with time and thus the system is in equilibrium. The probability density is given by*

$$\mathcal{P}(\mathbf{x}) = \frac{1}{\Omega(E)} \delta_{\mathrm{D}}(\mathcal{H}(\mathbf{x}) - E) \,, \tag{2.4}$$

where $\Omega(E)$ is the accessible phase space volume defined by

$$\Omega(E) = \int \mathrm{d}\Gamma \, \delta_{\mathrm{D}}(\mathcal{H}(\mathbf{x}) - E) \,. \tag{2.5}$$

For such a system it holds that

$$\langle A \rangle = \frac{1}{\Omega(E)} \int \mathrm{d}\Gamma \, A(\mathbf{x}) \, \delta_{\mathrm{D}}(\mathcal{H}(\mathbf{x}) - E) = \lim_{T \to \infty} \bar{A}_T \,. \tag{2.6}$$

In this language of a phase-space probability density it is easy to make the conceptual step from the micro-canonical to the so-called *canonical* ensemble. Instead of requiring the system to have a set energy we only want to constrain it to have a certain mean energy per degree of freedom, i. e. a certain temperature. This can be achieved by exchanging the Dirac delta distribution in (2.4) for a Boltzmann factor

$$\mathcal{P}(\mathbf{x}) \propto \exp(-\beta \mathcal{H}(\mathbf{x})) \,, \tag{2.7}$$

where $\beta = \frac{1}{k_{\mathrm{B}} T}$. Since the Hamiltonian gives the total energy of the collection of the N particles, the Boltzmann factor compares the exact total energy $\mathcal{H}(\mathbf{x})$ of some phase-space state $\mathbf{x}$ against the mean energy scale $k_{\mathrm{B}} T$ of the system. The larger this ratio gets, the less probable one deems that particular state to be. The *canonical partition function* Z_{C} is then simply the normalisation factor of this probability density.

$$Z_{\mathrm{C}} = \int \mathrm{d}\Gamma \, \exp(-\beta \mathcal{H}(\mathbf{x})) \tag{2.8}$$

It is a very useful quantity because rather than always using the probability density to calculate their averages, values for most macroscopic observables can be obtained by taking appropriate derivatives of the *free energy* $F = -k_{\mathrm{B}} T \ln Z_{\mathrm{C}}$. Our field theoretical approach will rely on a very similar concept for calculating averages of collective quantities.

2.2 GIVING UP EQUILIBRIUM

The big conceptual difference of the new field theory approach is to give up the requirement that the system is in equilibrium. We thus must allow for the macroscopic observables of the system to evolve over time and we consequently introduce two global points in time, the initial time t_{i} and final time t_{f}. This will force us to implement the full time evolution according to (2.1) into our theoretical description. The

initial state $\mathbf{x}^{(\mathrm{i})}$ however is still assumed to be impossible to determine due to the complexity of the system. We can circumvent this problem with the ensemble approach by treating the initial state probabilistically. This is feasible if the evolution of our system up to the initial time has been ergodic in the sense that over its entire lifespan up to t_i it had had the possibility to reach a large enough portion of its phase-space so that it becomes reasonable to attach a continuous probability density $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ to the initial state. In the ensemble sense this again corresponds to an idealized set of copies of the system all prepared to have some set of macroscopic or collective properties that are sufficient to specify $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$.

The time evolution of the ensemble is then contained in the joint probability density $\mathcal{P}(\mathbf{x}^{(\mathrm{f})}, \mathbf{x}^{(\mathrm{i})})$ which gives the probability that the system was in the initial state $\mathbf{x}^{(\mathrm{i})}$ and ends up in the final state $\mathbf{x}^{(\mathrm{f})}$. The ensemble average of any observable A at the final time t_f is consequently given by

$$\langle A \rangle (t_\mathrm{f}) = \int \mathrm{d}\Gamma_\mathrm{f} \int \mathrm{d}\Gamma_\mathrm{i}\, A(\mathbf{x}^{(\mathrm{f})})\, \mathcal{P}(\mathbf{x}^{(\mathrm{f})}, \mathbf{x}^{(\mathrm{i})}) \,. \tag{2.9}$$

Assuming we know $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$, we can use the law of conditional probabilities to write

$$\mathcal{P}(\mathbf{x}^{(\mathrm{f})}, \mathbf{x}^{(\mathrm{i})}) = \mathcal{P}(\mathbf{x}^{(\mathrm{f})} | \mathbf{x}^{(\mathrm{i})})\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \,. \tag{2.10}$$

For a classical deterministic system in a clearly defined initial state $\mathbf{x}^{(\mathrm{i})}$, its state $\mathbf{x}^{(\mathrm{f})}$ at the final time must be the solution $\mathbf{x}_\mathrm{cl}(t_\mathrm{f}; \mathbf{x}^{(\mathrm{i})})$ of the equations of motion (2.1). We have to translate this deterministic relation into a conditional probability density which immediately suggests the use of a Dirac delta distribution leading to

$$\mathcal{P}(\mathbf{x}^{(\mathrm{f})} | \mathbf{x}^{(\mathrm{i})}) = \delta_\mathrm{D}(\mathbf{x}^{(\mathrm{f})} - \mathbf{x}_\mathrm{cl}(t_\mathrm{f}; \mathbf{x}^{(\mathrm{i})})) \,. \tag{2.11}$$

This basic concept is illustrated in Fig. 1. Each point in an equal-time slice represents one possible phase-space configuration of the entire system of N particles. The lower colored area represents the phase-space probability distribution $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ at the initial time t_i. Each point $\mathbf{x}^{(\mathrm{i})}$ within it is transported forward through time to some other phase-space point $\mathbf{x}^{(\mathrm{f})}$ at the final time by means of the classical trajectory $\mathbf{x}_\mathrm{cl}(t; \mathbf{x}^{(\mathrm{i})})$. This transforms the initial distribution into the final distribution $\mathcal{P}(\mathbf{x}^{(\mathrm{f})}) = \int \mathrm{d}\Gamma_\mathrm{i}\, \mathcal{P}(\mathbf{x}^{(\mathrm{f})}, \mathbf{x}^{(\mathrm{i})})$ represented by the upper colored area. The analogue to the canonical partition function of equilibrium statistical physics is again the normalisation of this probability density

$$Z_\mathrm{C} = \int \mathrm{d}\Gamma_\mathrm{i} \int \mathrm{d}\Gamma_\mathrm{f}\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})})\, \delta_\mathrm{D}(\mathbf{x}^{(\mathrm{f})} - \mathbf{x}_\mathrm{cl}(t_\mathrm{f}; \mathbf{x}^{(\mathrm{i})})) \,. \tag{2.12}$$

We still call this a *canonical* partition function since we consider a fixed number of particles N in a fixed volume V. From a conceptual point of view this was all that had to be done in order to include non-equilibrium systems into the description. The big advantage is of course that we may now in principle choose the initial probability density $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ freely. Equilibrium statistics is included as the special case of an initial Boltzmann distribution.

One should also notice that the actual value of Z_C only depends on the normalisation of the initial probability density $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ since the integration over the final state

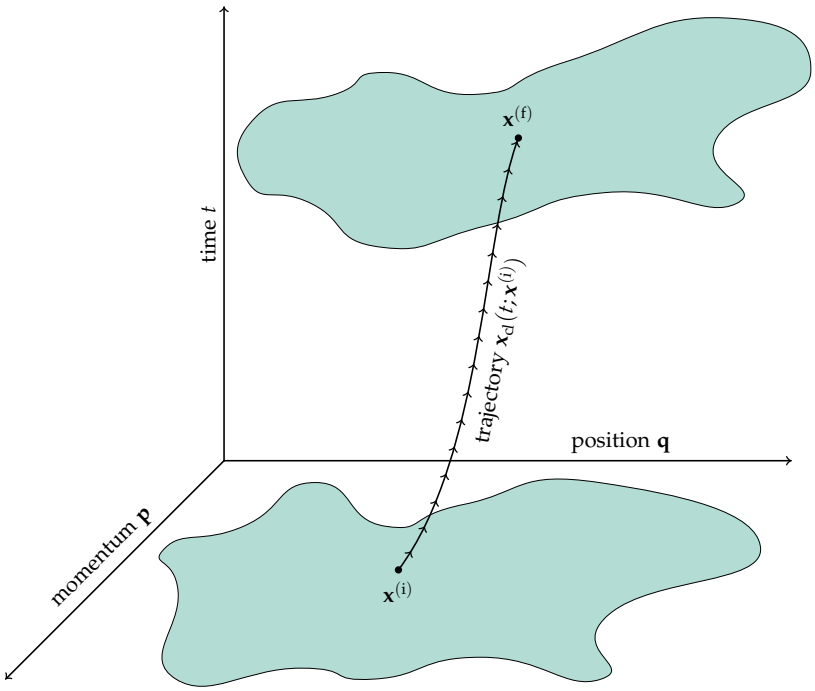


Figure 1: The phase-space evolution of a statistical system made up of N particles.

formally just gives a factor of unity. So if one chooses a properly normalised $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ the partition function will evaluate to unity in contrast to standard equilibrium statistics where the 'physics' is contained in this non-unity normalisation factor. However, due to the way average quantities are calculated in the field theoretical approach it will be preferable to use a properly normalised initial phase-space probability density.

2.3 PATH INTEGRAL FORMULATION

The above expression (2.12) very nicely expresses the concept behind the theory when compared to standard equilibrium statistical physics. In its present form it is however not very helpful for doing actual calculations since one would still need to know the general solution of the equations of motion (2.1). We will thus use what is often called the Martin-Siggia-Rose formalism (MSR) in order to express our generating functional as a path integral. While the principal ideas were originally developed in Martin et al. [36] with applications to statistical systems in mind, it was shown in e. g. Gozzi et al. [26] or Penco and Mauro [45] that path integrals can be used to describe any kind of classical system in this formalism. The great advantage of doing this lies in the fact that it opens up the very formidable toolbox of mathematical techniques developed in QFT to treat interacting systems both in perturbative and non-pertubative ways. Readers unfamiliar with QFT have a wide array of textbooks to choose from. A good introduction focusing directly on the path integral formalism can be found in Srednicki [53] and a more thorough 'classical' introduction in Peskin and Schroeder [46].

2.3.1 *Linking initial and final states*

The idea of the path integral approach in normal quantum mechanics is that as a particle moves through space we move along with it and at every point in time assign a complex-valued weight factor to any possible position and add up these weights. In the standard case, this weight factor is given by $\exp\left\{\frac{\mathrm{i}}{\hbar}S\right\}$, where S is the classical action. Since classical trajectories extremise S, the weight factor will vary by the least amount between points that are close to such a classical trajectory. For points far away it will fluctuate wildly, effectively canceling contributions from neighbouring points. In this way one obtains a transition amplitude $\langle q_\mathrm{f}, t_\mathrm{f} | q_\mathrm{i}, t_\mathrm{i}\rangle$ where most of the weight is centered on classical trajectories. We illustrate this idea in Fig. 2.

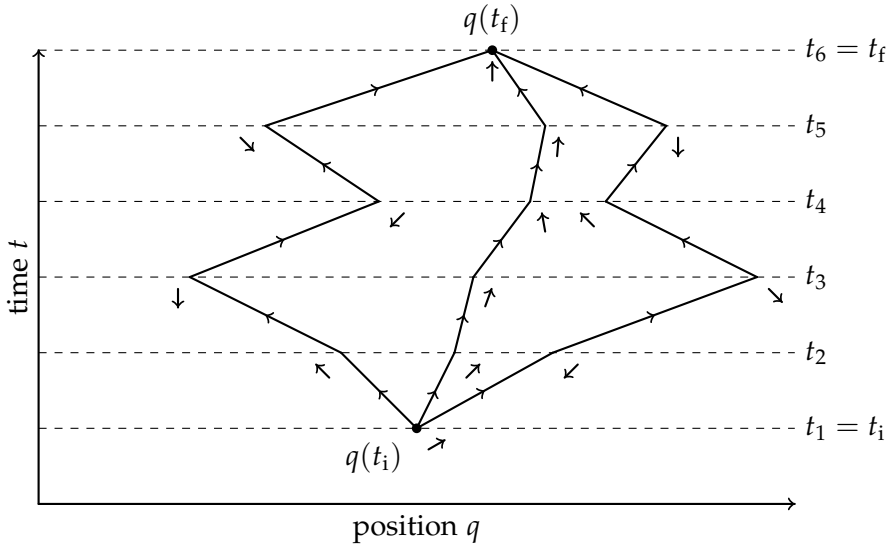


Figure 2: A quantum mechanical particle moving through space from $q(t_\mathrm{i})$ to $q(t_\mathrm{f})$. The arrows next to the particle positions at the instances of time t_j indicate the value of the weight factor $\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S}$ at that position as a unity length vector in the comlex plane. The middle trajectory is the classical one for which most of the vectors point in the same direction and thus add up to a substantial weight. For the other two trajectories the vectors fluctuate a lot more and thus cancel each other out to a large degree when summed up.

We now want to apply the same reasoning to our conditional transition probability $\mathcal{P}(\mathbf{x}^{(\mathrm{f})}|\mathbf{x}^{(\mathrm{i})})$. For our ensemble of particles this of course means that we follow the evolution of the phase-space coordinates of all N particles and at each point in time we assign a weight factor to every possible phase-space configuration $\mathbf{x}(t)$ and add them up. However, we already stated that for a classical deterministic system the only possible phase-space configuration $\mathbf{x}(t)$ at any time is the solution $\mathbf{x}_\mathrm{cl}(t; \mathbf{x}^{(\mathrm{i})})$ of the equations of motion (2.1). So instead of spreading out the weight around the classical trajectory like in quantum mechanics we have to concentrate the entire weight onto it which again leads us to use a Dirac delta distribution[2].

2 One can show that this is actually the limit $\hbar \to 0$ of the Quantum Mechanics (QM) path integral.

In mathematical terms we start by slicing up the time interval $[t_\mathrm{i}, t_\mathrm{f}]$ into $M+1$ intervals of length $\Delta t = (t_\mathrm{f} - t_\mathrm{i})/M$ and define $t_m = t_\mathrm{i} + m\Delta t$ such that $t_0 = t_\mathrm{i}$ and $t_M = t_\mathrm{f}$. At every t_m we insert a factor of

$$\int \mathrm{d}\mathbf{x}(t_m)\, \delta_\mathrm{D}(\mathbf{x}(t_m) - \mathbf{x}_\mathrm{cl}(t_m; \mathbf{x}^{(\mathrm{i})})) = 1 \tag{2.13}$$

into the expression for the conditional transition probability

$$\begin{aligned}\mathcal{P}(\mathbf{x}^{(\mathrm{f})}|\mathbf{x}^{(\mathrm{i})}) &= \delta_\mathrm{D}(\mathbf{x}(t_\mathrm{f}) - \mathbf{x}_\mathrm{cl}(t_\mathrm{f}; \mathbf{x}^{(\mathrm{i})})) \\ &= \delta_\mathrm{D}(\mathbf{x}(t_\mathrm{f}) - \mathbf{x}_\mathrm{cl}(t_\mathrm{f}; \mathbf{x}^{(\mathrm{i})})) \prod_{m=1}^{M-1} \int \mathrm{d}\mathbf{x}(t_m)\, \delta_\mathrm{D}(\mathbf{x}(t_m) - \mathbf{x}_\mathrm{cl}(t_m; \mathbf{x}^{(\mathrm{i})})) \\ &= \left(\prod_{m=1}^{M-1} \int \mathrm{d}\mathbf{x}(t_m) \right) \left(\prod_{m=1}^{M} \delta_\mathrm{D}(\mathbf{x}(t_m) - \mathbf{x}_\mathrm{cl}(t_m; \mathbf{x}^{(\mathrm{i})})) \right) . \end{aligned} \tag{2.14}$$

In the limit $M \to \infty$ of an infinitesimal time grid stepsize, this discretisised expression will go over into a continuous functional integral over all possible phase trajectories that link $\mathbf{x}^{(\mathrm{i})}$ and $\mathbf{x}^{(\mathrm{f})}$, hence the term *path integral*.

$$\lim_{M\to\infty} \prod_{m=1}^{M-1} \int \mathrm{d}\mathbf{x}(t_m) = \int_\mathrm{i}^\mathrm{f} \mathcal{D}\mathbf{x}(t) , \tag{2.15}$$

where the boundaries signal that initial and final states are held fixed and are thus excluded from the functional integration. The Dirac delta distributions go over into

$$\lim_{M\to\infty} \left(\prod_{m=1}^{M} \delta_\mathrm{D}(\mathbf{x}(t_m) - \mathbf{x}_\mathrm{cl}(t_m; \mathbf{x}^{(\mathrm{i})})) \right) = \delta_\mathrm{D}[\mathbf{x}(t) - \mathbf{x}_\mathrm{cl}(t; \mathbf{x}^{(\mathrm{i})})] , \tag{2.16}$$

where the square brackets mark this as a functional Dirac delta distribution, which always has to be understood in the above limit sense, just like the path integral (2.15). We may now rewrite our canonical partition function (2.12) as the path integral expression

$$\begin{aligned} Z_\mathrm{C} &= \int \mathrm{d}\mathbf{x}(t_\mathrm{i})\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \int \mathrm{d}\mathbf{x}(t_\mathrm{f}) \int_\mathrm{i}^\mathrm{f} \mathcal{D}\mathbf{x}(t)\, \delta_\mathrm{D}[\mathbf{x}(t) - \mathbf{x}_\mathrm{cl}(t; \mathbf{x}^{(\mathrm{i})})] \\ &= \int \mathrm{d}\mathbf{x}(t_\mathrm{i})\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \int_\mathrm{i}^\mathrm{f} \mathcal{D}\mathbf{x}(t)\, \delta_\mathrm{D}[\mathbf{x}(t) - \mathbf{x}_\mathrm{cl}(t; \mathbf{x}^{(\mathrm{i})})] \\ &= \int \mathcal{D}\mathbf{x}(t)\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})})\, \delta_\mathrm{D}[\mathbf{x}(t) - \mathbf{x}_\mathrm{cl}(t; \mathbf{x}^{(\mathrm{i})})] . \end{aligned} \tag{2.17}$$

We listed the various notations for the path integral[3] we may use throughout this work. This quantity clearly maps functions into a number, i. e. it is a functional. For reasons that will become apparent soon, we will from now on call it the *canonical generating functional*.

3 Notice that we no longer use the notation $\mathrm{d}\Gamma$ for the integration measure. This is equivalent to setting $h_0 = 1$. The reason is that the field theory approach does not rely on counting states and as such we can take phase-space to be completely continuous.

2.3.2 *The 'other' classical action*

Formulating our generating functional in terms of a path integral has brought us closer to the usual field theory formulation but we still lack a quantity that takes the role of the 'action' of our field theory. As a first step towards such a quantity we now use the following transformation property of the functional Dirac delta distribution which is just the functional analogue of the transformation behaviour of the normal Dirac delta distribution under change of variables. Let φ^a be the components of some vector valued field and F some functional that maps from the space of such vector fields into the real numbers, then it holds that

$$\delta_{\mathrm{D}}[\varphi^a - \varphi_0^a] = \delta_{\mathrm{D}}[F[\varphi^a]] \det\left[\frac{\partial F[\varphi^a]}{\partial \varphi^b}\Big|_{\varphi^a=\varphi_0^a}\right] \quad \text{if} \quad F[\varphi_0^a] = 0\,. \tag{2.18}$$

In our case the role of the vector field is taken by the phase-space coordinates of the particles, i. e. $\varphi^a = x^a(t)$ where the index a runs over all $2dN$ components. The role of the functional is consequently taken by the equations of motion (2.1) which we can reformulate in a component notation as

$$\partial_t x^a - \mathcal{J}^{ab}\partial_b \mathcal{H} = \mathcal{E}[x^a] \quad \text{where} \quad \partial_b = \frac{\partial}{\partial x^b}\,. \tag{2.19}$$

The role of the kernel φ_0^a of the functional is thus taken by the classical solution x_{cl}^a with $\mathcal{E}[x_{\mathrm{cl}}^a] = 0$. The functional Dirac delta distribution in (2.17) may thus be rewritten into

$$\delta_{\mathrm{D}}[\mathbf{x}(t) - \mathbf{x}_{\mathrm{cl}}(t;\mathbf{x}^{(\mathrm{i})})] = \delta_{\mathrm{D}}[\boldsymbol{\mathcal{E}}[\mathbf{x}(t)]] \det\left[\delta_b^a\,\partial_t - \mathcal{J}^{ac}\partial_c\partial_b\mathcal{H}\right]\,. \tag{2.20}$$

The crucial result that the above functional determinant is equal to unity was shown in Gozzi et al. [26]. The proof relies on the causal nature of the Hamiltonian dynamics and the antisymmetry of $\mathcal{J}^{ab}$. We stress here that if one wants to be on the safe side in terms of strict mathematics one should always start from a Hamiltonian formulation of the dynamics, no matter which kind of classical system one wants to describe with this path integral approach. If one wants to use non-canonical equations of motion that cannot be derived from a Hamiltonian one must take care of either showing that the above determinant is a constant or incorporate it into theory.

Expressing the requirement that the phase-space trajectories which receive the entire weight in our path integral are the solutions of the classical equations of motion in terms of these equations themselves has one decisive advantage. In contrast to the actual trajectories they can easily be split into a free and an interacting part. Before we see how to do this, we complete the connection to non-equilibrium QFT by expressing the functional Dirac delta distribution by a functional Fourier transform in analogy to the normal Dirac delta distribution as

$$\delta_{\mathrm{D}}[\boldsymbol{\mathcal{E}}[\mathbf{x}(t)]] = \int \mathcal{D}\boldsymbol{\chi}(t) \exp\left\{\mathrm{i}\int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}} \mathrm{d}t\ \langle \boldsymbol{\chi}(t), \boldsymbol{\mathcal{E}}[\mathbf{x}(t)]\rangle\right\}\,, \tag{2.21}$$

where we had to introduce a new auxiliary field[4] or rather a collection of functions $\vec{\chi}_j(t) = (\vec{\chi}^{\mathrm{T}}_{q_j}(t), \vec{\chi}^{\mathrm{T}}_{p_j}(t))^{\mathrm{T}}$ in the process. In order to make the argument of the exponential dimensionless, these functions must have the inverse dimension of units of their respective phase-space counterparts. In the MSR formalism this auxiliary field is usually associated with a statistical noise contribution to the otherwise deterministic equations of motion. We will soon see that in the approach of Das and Mazenko this field can also be associated with the system's response to interactions between the particles. If we now define our 'action' to be

$$S[\mathbf{x}(t), \boldsymbol{\chi}(t)] := \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \; \langle \boldsymbol{\chi}(t), \boldsymbol{\mathcal{E}}[\mathbf{x}(t)] \rangle = \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \; \langle \boldsymbol{\chi}(t), (\partial_t \mathbf{x}(t) - \boldsymbol{\mathcal{J}} \boldsymbol{\nabla} \mathcal{H}) \rangle \;, \tag{2.22}$$

we can finally write our canonical generating functional in a form that very closely resembles non-equilibrium QFT

$$Z_\mathrm{C} = \int \mathcal{D}\mathbf{x}(t) \int \mathcal{D}\boldsymbol{\chi}(t) \, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \, \mathrm{e}^{\mathrm{i}S[\mathbf{x}(t), \boldsymbol{\chi}(t)]} \;. \tag{2.23}$$

Notice that we can reobtain the classical equations of motion from the action by demanding that its functional derivative w. r. t. the auxiliary field vanishes

$$\frac{\delta S[\mathbf{x}(t), \boldsymbol{\chi}(t)]}{\delta \boldsymbol{\chi}(t)} \overset{!}{=} 0 \quad \Longrightarrow \quad \boldsymbol{\mathcal{E}}[\mathbf{x}(t)] = 0 \,, \tag{2.24}$$

which can be seen as the analogue of the Euler-Lagrange equations for this kind of theory. We now give credibility to the term *generating functional* by following standard QFT procedure and introduce sources for both the phase-space trajectories and the auxiliary field

$$Z_\mathrm{C}[\mathbf{J}, \mathbf{K}] = \int \mathcal{D}\mathbf{x}(t) \int \mathcal{D}\boldsymbol{\chi}(t) \, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \exp\left\{ \mathrm{i} \left(S[\mathbf{x}(t), \boldsymbol{\chi}(t)] + \mathbf{J} \cdot \mathbf{x} + \mathbf{K} \cdot \boldsymbol{\chi} \right) \right\} \;. \tag{2.25}$$

The central dot stands for both the scalar product and integration over time, so explicitly we have

$$\mathbf{J} \cdot \mathbf{x} = \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \; \langle \mathbf{J}(t), \mathbf{x}(t) \rangle \quad \text{and thus} \quad \frac{\delta}{\mathrm{i}\delta \mathbf{J}(t)} \, \mathrm{e}^{\mathrm{i}\mathbf{J}\cdot\mathbf{x}} = \mathbf{x}(t) \, \mathrm{e}^{\mathrm{i}\mathbf{J}\cdot\mathbf{x}} \,, \tag{2.26}$$

where the second relation allows us to exchange instances of $\mathbf{x}$ inside the path integrals for appropriate functional derivatives. These derivatives can then be taken outside the path integrals, a fact that will be very beneficial later on. The same of course holds likewise for $\mathbf{K}$ and $\boldsymbol{\chi}$. At this point the theory is in principle complete and exact since all the information about the time evolution of the microscopic phase-space coordinates is contained in (2.25). Their expectation values at some time $t_\mathrm{i} \leq t \leq t_\mathrm{f}$ are now readily available by taking functional derivatives and turning off the sources

$$\langle \mathbf{x}(t) \rangle = \frac{\delta}{\mathrm{i}\delta \mathbf{J}(t)} \, Z_\mathrm{C}[\mathbf{J}, \mathbf{K}] \big|_{\mathbf{J}=\mathbf{K}=0} \,. \tag{2.27}$$

4 We use the term 'auxiliary field' since its common in most of the literature surrounding the MSR formalism.

One may easily confirm this relation by using (2.26) and then going backwards through the previous calculations until one again arrives at (2.17). Of course the same holds for $\mathbf{K}$ and $\boldsymbol{\chi}$. This then allows us to generalize (2.9) for the expectation value of some observable A, expressible in terms of the microscopic phase-space coordinates as $A(\mathbf{x})$, leading to

$$\langle A(\mathbf{x}(t))\rangle = A\left(\frac{\delta}{\mathrm{i}\delta\mathbf{J}(t)}\right) Z_{\mathrm{C}}[\mathbf{J},\mathbf{K}]\big|_{\mathbf{J}=\mathbf{K}=0} \,. \tag{2.28}$$

The fact that we can now obtain averages at arbitrary times $t_{\mathrm{i}} \leq t \leq t_{\mathrm{f}}$ is another benefit of the path integral approach since it gives us access to the intermediate states of the time evolution of the system.

2.4 INTERACTIONS AND COLLECTIVE FIELDS

The basic obstacle to directly calculating (2.25) is the fact that this is still equivalent to solving the full equations of motion with all interactions included. However, the non-interacting equations of motion can usually be solved analytically, so one would naturally like to set up some kind of perturbation theory around this free solution where the effects of particle interactions are treated in an approximate manner. Fortunately, the path integral approach excels at treating exactly this kind of problem. One of the conceptual achievements accomplished in Mazenko [39] and Das and Mazenko [22] was the scheme how one should treat the 'free' and the 'interacting' part of the theory.

- The free part of the theory is governed by the non-interacting part of the equations of motion. Here the individual particles are decoupled and one can give a general solution for their trajectories. It thus seems natural to treat the free theory on the basis of individual particles.
- In stark contrast, in the interacting part of the theory each particle is connected to all other particles by the interaction. Thus, one cannot treat particle trajectories individually and it seems much more feasible to express the effects of all particle interactions as an interaction between collective quantities which are composed from the individual phase-space coordinates.

2.4.1 *Rewriting the interaction*

We have to demand that we can write this separation in terms of the Hamiltonian as $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_I$. The first part must lead to the 'free and linear'[5] equations of motion while the second part must contain the interactions between the various degrees of freedom. Consequently the equations of motion can be separated as

$$\boldsymbol{\mathcal{E}}[\mathbf{x}] = (\partial_t \mathbf{x} - \boldsymbol{\mathcal{J}}\boldsymbol{\nabla}\mathcal{H}_0) - (\boldsymbol{\mathcal{J}}\boldsymbol{\nabla}\mathcal{H}_I) = \boldsymbol{\mathcal{E}}_0[\mathbf{x}] + \boldsymbol{\mathcal{E}}_I[\mathbf{x}] \,. \tag{2.29}$$

5 More precisely, one must be able to solve the equations of motion obtained from only $\mathcal{H}_0$ analytically. Being linear and not describing any interactions is just the most common case for physical systems composed of classical particles.

Since our action S depends linearly on the equations of motion, we may therefore also separate $S = S_0 + S_I$ where we of course have

$$S_0 = \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \; \langle \boldsymbol{\chi}(t), \boldsymbol{\mathcal{E}}_0[\mathbf{x}(t)] \rangle \; . \tag{2.30}$$

We assume that the interaction Hamiltonian is given by a potential $V(\vec{q}, t)$. This allows us to explicitly write down the interacting part of the action as

$$\begin{aligned} S_I &= \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \; \left\langle \boldsymbol{\chi}(t), -(\mathcal{J} \otimes \mathcal{I}_N)(\nabla_j \otimes \vec{e}_j) V(\vec{q}, t) \right\rangle \\ &= \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \; \left\langle \boldsymbol{\chi}(t), - \begin{pmatrix} \nabla_{p_j} \\ -\nabla_{q_j} \end{pmatrix} V(\vec{q}, t) \otimes \vec{e}_j \right\rangle \end{aligned} \tag{2.31}$$

We can remove the gradient from the potential with the help of the relation

$$\nabla_{q_j} V(\vec{q}, t) = \nabla_q V(\vec{q}, t)\big|_{\vec{q}=\vec{q}_j(t)} = -\int \mathrm{d}\vec{q} \; \left(\nabla_q \, \delta_\mathrm{D}(\vec{q} - \vec{q}_j(t))\right) V(\vec{q}, t) \; , \tag{2.32}$$

where in the second step we first replaced the condition $\vec{q} = \vec{q}_j(t)$ by introducing the integration over the Dirac delta distribution and then integrating by parts to shift the gradient over to it. Since we assume that the particles are confined to some finite volume the boundary terms with a Dirac delta distribution vanish. We may thus continue from (2.31) with

$$\begin{aligned} S_I &= \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \; \left\langle \boldsymbol{\chi}(t), - \int \mathrm{d}\vec{q} \; \left(\nabla_q \, \delta_\mathrm{D}(\vec{q} - \vec{q}_j(t))\right) V(\vec{q}, t) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \vec{e}_j \right\rangle \\ &= -\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \int \mathrm{d}\vec{q} \; \Phi_B(\vec{q}, t) \, V(\vec{q}, t) \; , \end{aligned} \tag{2.33}$$

where we have defined the so called *response field* Φ_B, which in terms of individual particles reads

$$\Phi_B(\vec{q}, t) = \sum_{j=1}^{N} \vec{\chi}_{p_j}^\mathrm{T}(t) \, \nabla_q \, \delta_\mathrm{D}(\vec{q} - \vec{q}_j(t)) \; . \tag{2.34}$$

Furthermore, for a closed system in the absence of external forces[6] the potential $V(\vec{q}, t)$ felt by some particle at position $\vec{q}$ at the time t must be the superposition of the single particle potentials of all particles in the system which can be written as

$$V(\vec{q}, t) = \sum_{j=1}^{N} v_j(\vec{q}, t) \; . \tag{2.35}$$

We now introduce some assumptions about the form of these single particle potentials.

6 External forces with a given potential V are already described by (2.33). They are however not of interest for the purposes of our work.

- All particles are considered identical regarding their interactions which means that the functional form of all v_j is the same.
- The potential only depends on the positions of the source particle at $\vec{q}_j(t)$ and the test particle at $(\vec{q}, t)$.
- This also directly implies that the force acts instantaneously.

The prime example is the Newtonian gravitational potential of a collection of N particles with equal mass m which we will investigate in the second part in the context of cosmology. If these assumptions hold we may rewrite the total potential as

$$\begin{aligned} V(\vec{q}, t) &= \sum_{j=1}^{N} v(\vec{q}, \vec{q}_j(t)) = \int \mathrm{d}\vec{q}\,' \, v(\vec{q}, \vec{q}\,') \sum_{j=1}^{N} \delta_{\mathrm{D}}(\vec{q}\,' - \vec{q}_j(t)) \\ &= \int \mathrm{d}\vec{q}\,' \, v(\vec{q}, \vec{q}\,') \, \Phi_\rho(\vec{q}\,', t) \; , \end{aligned} \tag{2.36}$$

where in the last line we have defined the *particle number density field* as the sum

$$\Phi_\rho(\vec{q}, t) \coloneqq \sum_{j=1}^{N} \delta_{\mathrm{D}}(\vec{q} - \vec{q}_j(t)) \; . \tag{2.37}$$

We use the notation Φ_ρ instead of simply ρ in order to clearly mark this field as a *collective* field which is *distributionally valued*. It only turns into a continuous macroscopic observable due to the integration over the initial phase-space conditions once we calculate its expectation value. The above definition of the total potential implicitly assumes that particles have no self-interaction which means that we demand $v(\vec{q}, \vec{q}\,')\big|_{\vec{q}=\vec{q}\,'} = 0$. The interacting part of the action can thus be formulated purely in terms of collective fields and the single particle potential as

$$S_I = -\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \int \mathrm{d}\vec{q} \int \mathrm{d}\vec{q}\,' \, \Phi_B(\vec{q}, t) \, v(\vec{q}, \vec{q}\,') \, \Phi_\rho(\vec{q}\,', t) \; . \tag{2.38}$$

This expression makes the naming of Φ_B as a 'response field' more transparent since it describes how the particles at $(\vec{q}, t)$ respond to an interaction with the density field at $(\vec{q}\,', t)$ by deviating from their free trajectories. We will see in section 2.5.1 that the auxialiary fields $\vec{\chi}_j$ or rather their conjugate source terms $\mathbf{K}$ can be associated with such deviations. For notational ease we collect these two collective fields into a single two-component vector

$$\Phi(1) = \Phi(\vec{q}_1, t_1) = \begin{pmatrix} \Phi_\rho(\vec{q}_1, t_1) \\ \Phi_B(\vec{q}_1, t_1) \end{pmatrix} \; , \tag{2.39}$$

where we remind the reader that $\vec{q}_1$ as a field argument is *not* the trajectory of an explicit particle but some arbitrary position. If we define the following *interaction matrix*

$$\sigma(1,2) = -v(\vec{q}_1, \vec{q}_2) \, \delta_{\mathrm{D}}(t_1 - t_2) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \; , \tag{2.40}$$

we can then rewrite (2.38) in the very compact and symmetric form

$$\begin{aligned} S_I &= \frac{1}{2}\int \mathrm{d}1 \int \mathrm{d}2\, \Phi^{\mathrm{T}}(1)\,\sigma(1,2)\,\Phi(2) \\ &= \frac{1}{2}\left(\Phi_{\rho_1}\sigma_{\rho_1 B_2}\Phi_{B_2} + \Phi_{B_1}\sigma_{B_1\rho_2}\Phi_{\rho_2}\right) \\ &= \frac{1}{2}\Phi_{\alpha_1}\sigma_{\alpha_1\alpha_2}\Phi_{\alpha_2} = \frac{1}{2}\Phi_{\mu}\sigma_{\mu\nu}\Phi_{\nu}\ . \end{aligned} \tag{2.41}$$

In the second and third line we used all the different versions of our field theory notation in order to give the unexperienced reader an easy example. Remember that α runs over both field types ρ and B, the subindex stands for the spacetime argument or 'label' of the field and if there is no subindex the space-time argument is implicitly contained in the greek index and integrated over for repeated instances.

2.4.2 *Collective sources and correlators*

In order to easily generate averages of these collective fields we introduce a new source field vector

$$H(1) := \begin{pmatrix} H_\rho(1) \\ H_B(1) \end{pmatrix} \tag{2.42}$$

into our theory and couple it to the collective fields

$$H\cdot\Phi = \int \mathrm{d}1\, H^{\mathrm{T}}(1)\,\Phi(1) = H_{\alpha_1}\Phi_{\alpha_1}\ . \tag{2.43}$$

We can now write our canonical generating functional with a clear separation into a free part formulated in terms of microscopic phase-space coordinates and an interacting part formulated in terms of collective fields.

$$Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}] = \int \mathcal{D}\mathbf{x}\int \mathcal{D}\boldsymbol{\chi}\,\mathcal{P}(\mathbf{x}^{(\mathrm{i})})\exp\left\{\mathrm{i}(S_0[\mathbf{x},\boldsymbol{\chi}] + \mathbf{J}\cdot\mathbf{x} + \mathbf{K}\cdot\boldsymbol{\chi} + S_I[\Phi] + H\cdot\Phi)\right\}\ . \tag{2.44}$$

The n-point correlators of the collective fields are now easily obtained by calculating

$$\langle\Phi_{\alpha_1}\dots\Phi_{\alpha_n}\rangle = \frac{\delta}{\mathrm{i}\delta H_{\alpha_1}}\cdots\frac{\delta}{\mathrm{i}\delta H_{\alpha_n}} Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}]\big|_{H=\mathbf{J}=\mathbf{K}=0}\ . \tag{2.45}$$

Notice that we have left out the usual normalisation factor of Z_{C}^{-1} since we assume our generating functional to be normalized to unity at vanishing sources as we already discussed in section 2.2. Connected correlators, i. e. cumulants, can be calculated with

$$G_{\Phi_{\alpha_1}\dots\Phi_{\alpha_n}} = \frac{\delta}{\mathrm{i}\delta H_{\alpha_1}}\cdots\frac{\delta}{\mathrm{i}\delta H_{\alpha_n}} \ln Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}]\big|_{H=\mathbf{J}=\mathbf{K}=0}\ . \tag{2.46}$$

As is usual in QFT we define

$$W_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}] := \ln Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}] \tag{2.47}$$

as the canonical cumulant generating functional.

2.4.3 *Collective fields as operators*

The form of the generating functional (2.44) is only the first step towards a perturbative treatment. At this point we could just switch off the collective part of the expression and solve the free theory. But then the question would be how to reintroduce the interaction into the theory in a systematic way. In order to solve this problem Das and Mazenko took inspiration from QFT and expressed the collective quantities as functional derivatives. As a first step we define an *interaction operator* in terms of these derivatives as

$$\hat{S}_I := \frac{1}{2}\int \mathrm{d}1 \int \mathrm{d}2 \, \frac{\delta}{\mathrm{i}\delta H_{\alpha_1}} \sigma_{\alpha_1\alpha_2} \frac{\delta}{\mathrm{i}\delta H_{\alpha_2}} \,, \tag{2.48}$$

which because of (2.41) satisfies

$$\hat{S}_I \, \mathrm{e}^{\mathrm{i}H\cdot\Phi} = S_I \, \mathrm{e}^{\mathrm{i}H\cdot\Phi} \quad \text{and thus} \quad \mathrm{e}^{\mathrm{i}\hat{S}_I}\mathrm{e}^{\mathrm{i}H\cdot\Phi} = \mathrm{e}^{\mathrm{i}S_I}\mathrm{e}^{\mathrm{i}H\cdot\Phi} \,. \tag{2.49}$$

This 'eigenvalue' relation has the very desirable effect that it expresses the entire interaction as an operator $\hat{S}_I$ which no longer depends on the microscopic quantities $\mathbf{x}$ and $\boldsymbol{\chi}$ of the individual particles. Consequently, we may take the interaction out in front of the path integrals in (2.44) and write the canonical generating functional as

$$\begin{aligned} Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}] &= \mathrm{e}^{\mathrm{i}\hat{S}_I} \int \mathcal{D}\mathbf{x} \int \mathcal{D}\boldsymbol{\chi}\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \exp\left\{\mathrm{i}(S_0[\mathbf{x},\boldsymbol{\chi}] + \mathbf{J}\cdot\mathbf{x} + \mathbf{K}\cdot\boldsymbol{\chi}) + \mathrm{i}H\cdot\Phi\right\} \\ &= \mathrm{e}^{\mathrm{i}\hat{S}_I} Z_{\mathrm{C},0}[H,\mathbf{J},\mathbf{K}] \,, \end{aligned} \tag{2.50}$$

where in the second line we have implicitly defined the free generating functional *with* collective sources H as $Z_{\mathrm{C},0}[H,\mathbf{J},\mathbf{K}]$. Before we try to carry out the path integrals, we also want to move the collective source term out in front of the path integrals. We draw inspiration from (2.28) and make the dependence of the collective fields on the microscopic phase-space coordinates explicit by writing $\Phi(1) = \Phi(\vec{q}_1, \mathbf{x}(t_1), \boldsymbol{\chi}(t_1))$. Since the Dirac delta distribution showing up in the definitions (2.34), (2.37) may be represented in terms of analytic functions, for example by using its Fourier transform as we will do later on, we may employ the relation (2.26) and rewrite

$$\Phi(\vec{q}_1, \mathbf{x}(t_1), \boldsymbol{\chi}(t_1)) \, \mathrm{e}^{\mathrm{i}(\mathbf{J}\cdot\mathbf{x}+\mathbf{K}\cdot\boldsymbol{\chi})} = \Phi\left(\vec{q}_1, \frac{\delta}{\mathrm{i}\delta\mathbf{J}(t_1)}, \frac{\delta}{\mathrm{i}\delta\mathbf{K}(t_1)}\right) \mathrm{e}^{\mathrm{i}(\mathbf{J}\cdot\mathbf{x}+\mathbf{K}\cdot\boldsymbol{\chi})} \,. \tag{2.51}$$

If we now define the *collective field operator* in exactly this way by

$$\begin{aligned} \hat{\Phi}(1) &:= \Phi\left(\vec{q}_1, \frac{\delta}{\mathrm{i}\delta\mathbf{J}(t_1)}, \frac{\delta}{\mathrm{i}\delta\mathbf{K}(t_1)}\right) \\ &= \begin{pmatrix} \hat{\Phi}_\rho(1) \\ \hat{\Phi}_B(1) \end{pmatrix} = \begin{pmatrix} \sum_{j=1}^N \delta_{\mathrm{D}}\left(\vec{q}_1 - \frac{\delta}{\mathrm{i}\delta\vec{J}_{q_j}(t_1)}\right) \\ \sum_{j=1}^N \frac{\delta}{\mathrm{i}\delta\vec{K}_{p_j}(t_1)} \nabla_{q_1}\delta_{\mathrm{D}}\left(\vec{q}_1 - \frac{\delta}{\mathrm{i}\delta\vec{J}_{q_j}(t_1)}\right) \end{pmatrix} \end{aligned} \tag{2.52}$$

we again have a very nice 'eigenvalue relation'

$$\hat{\Phi}(1) \, \mathrm{e}^{\mathrm{i}(\mathbf{J}\cdot\mathbf{x}+\mathbf{K}\cdot\boldsymbol{\chi})} = \Phi(1) \, \mathrm{e}^{\mathrm{i}(\mathbf{J}\cdot\mathbf{x}+\mathbf{K}\cdot\boldsymbol{\chi})} \quad \rightarrow \quad \mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}} \, \mathrm{e}^{\mathrm{i}(\mathbf{J}\cdot\mathbf{x}+\mathbf{K}\cdot\boldsymbol{\chi})} = \mathrm{e}^{\mathrm{i}H\cdot\Phi} \, \mathrm{e}^{\mathrm{i}(\mathbf{J}\cdot\mathbf{x}+\mathbf{K}\cdot\boldsymbol{\chi})} \,. \tag{2.53}$$

We rewrite (2.50) once more to arrive at the final form for the canonical generating functional

$$\begin{aligned} Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}] &= \mathrm{e}^{\mathrm{i}\hat{S}_I}\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}}\int\mathcal{D}\mathbf{x}\int\mathcal{D}\boldsymbol{\chi}\,\mathcal{P}(\mathbf{x}^{(\mathrm{i})})\exp\left\{\mathrm{i}(S_0[\mathbf{x},\boldsymbol{\chi}]+\mathbf{J}\cdot\mathbf{x}+\mathbf{K}\cdot\boldsymbol{\chi})\right\} \\ &= \mathrm{e}^{\mathrm{i}\hat{S}_I}\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}}Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}]\,. \end{aligned} \tag{2.54}$$

We have defined the free generating functional $Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}]$ *without* collective sources H and all microscopic quantities completely decoupled, making its computation a relatively easy task.

2.4.4 *The general form of canonical perturbation theory*

The above relation (2.54) is indeed quite powerful. It tells us that any n-point correlator of the collective field Φ can in principle be calculated to arbitrary order in the single particle interaction potential $\sigma \propto v$ once the free generating functional $Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}]$ is known. To see this we first define the free correlators in accordance with (2.45) as

$$\begin{aligned} \langle\Phi_{\alpha_1}\dots\Phi_{\alpha_n}\rangle_0 &= \frac{\delta}{\mathrm{i}\delta H_{\alpha_1}}\cdots\frac{\delta}{\mathrm{i}\delta H_{\alpha_n}}\left(\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}}Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}]\right)\big|_{H=\mathbf{J}=\mathbf{K}=0} \\ &= \hat{\Phi}_{\alpha_1}\dots\hat{\Phi}_{\alpha_n}\,Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}]\big|_{\mathbf{J}=\mathbf{K}=0}\,. \end{aligned} \tag{2.55}$$

The full correlator with all interactions included is in our operator notation defined by

$$\begin{aligned} \langle\Phi_{\alpha_1}\dots\Phi_{\alpha_n}\rangle &= \frac{\delta}{\mathrm{i}\delta H_{\alpha_1}}\cdots\frac{\delta}{\mathrm{i}\delta H_{\alpha_n}}\mathrm{e}^{\mathrm{i}\hat{S}_I}\left(\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}}Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}]\right)\big|_{H=\mathbf{J}=\mathbf{K}=0} \\ &= \hat{\Phi}_{\alpha_1}\dots\hat{\Phi}_{\alpha_n}\mathrm{e}^{\mathrm{i}\hat{S}_I}\left(\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}}Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}]\right)\big|_{H=\mathbf{J}=\mathbf{K}=0} \\ &= \hat{\Phi}_{\alpha_1}\dots\hat{\Phi}_{\alpha_n}\mathrm{e}^{\mathrm{i}\hat{S}_I[\hat{\Phi}]}Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}]\big|_{\mathbf{J}=\mathbf{K}=0}\,, \end{aligned} \tag{2.56}$$

where we have used that derivatives w. r. t. H commute and defined a different form of the interaction operator

$$\hat{S}_I[\hat{\Phi}] := \frac{1}{2}\int\mathrm{d}1\int\mathrm{d}2\,\hat{\Phi}_{\alpha_1}\sigma_{\alpha_1\alpha_2}\hat{\Phi}_{\alpha_2}\,, \tag{2.57}$$

which follows in a straightforward way from (2.49) if we replace the collective field with its corresponding operator. One can now express (2.56) in terms of the free correlators by expanding the exponential function. Each order of the expansion generates two more collective field operators $\hat{\Phi}$ which are then contracted with the interaction matrix σ.

$$\begin{aligned} \langle\Phi_{\alpha_1}\dots\Phi_{\alpha_n}\rangle &= \hat{\Phi}_{\alpha_1}\dots\hat{\Phi}_{\alpha_n}\left(\sum_{m=0}^{\infty}\frac{\mathrm{i}^m}{2^m m!}\left(\hat{\Phi}_\mu\sigma_{\mu\nu}\hat{\Phi}_\nu\right)^m\right)Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}]\big|_{\mathbf{J}=\mathbf{K}=0} \\ &= \sum_{m=0}^{\infty}\frac{\mathrm{i}^m}{m!}\hat{\Phi}_{\alpha_1}\dots\hat{\Phi}_{\alpha_n}\hat{\Phi}_{\rho_1}\sigma_{\rho_1 B_1}\hat{\Phi}_{B_1}\dots\hat{\Phi}_{\rho_m}\sigma_{\rho_m B_m}\hat{\Phi}_{B_m}\,Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}]\big|_{\mathbf{J}=\mathbf{K}=0} \\ &= \sum_{m=0}^{\infty}\frac{\mathrm{i}^m}{m!}\left\langle\Phi_{\alpha_1}\dots\Phi_{\alpha_n}\Phi_{\rho_1}\Phi_{B_1}\dots\Phi_{\rho_m}\Phi_{B_m}\right\rangle_0\sigma_{\rho_1 B_1}\dots\sigma_{\rho_m B_m}\,, \end{aligned} \tag{2.58}$$

where we have used the symmetry of the interaction matrix (2.40) in the second line. From this one can see that there are in principle only two ingredients in this perturbation theory. First there are the free correlators which are determined by the free equations of motion $\boldsymbol{\mathcal{E}}_0[\mathbf{x}]$ and the initial phase-space probability density $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$. Whether one can give exact or approximate expressions for these correlators will naturally depend on the complexity of the initial conditions. The free equations of motion in contrast should always be chosen such that they describe that particular part of the physical problem one can solve analytically. The second ingredient is the two-particle interaction potential σ which will usually be rather simple.

Finding the general analogue of (2.58) for cumulants is a somewhat more complicated problem. In Appendix B we will show how to derive the perturbative expressions for one-point and two-point cumulants up to second order in σ and already in this case the combinatorial effort will be considerable. It will be one big advantage of the grand canonical approach that it automatically generates the cumulant perturbation series with much less effort than the canonical approach.

2.5 SOLUTION FOR THE FREE THEORY

With the structure of perturbation theory clarified, the only missing piece is the free generating functional $Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}]$ which one needs in order to calculate the free correlators. We first give its general solution in terms of the Green's function or propagator of the free equations of motion and then show how to calculate this propagator for equations of motion of the Hamiltonian type.

2.5.1 *The explicit free generating functional*

We can read off the definition of the free generating functional by combining (2.30) and (2.54) into

$$Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}] = \int \mathcal{D}\mathbf{x} \int \mathcal{D}\boldsymbol{\chi}\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \exp\left\{ \mathrm{i} \left(\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t\ \langle \boldsymbol{\chi}(t), \boldsymbol{\mathcal{E}}_0[\mathbf{x}(t)] \rangle + \mathbf{J}\cdot\mathbf{x} + \mathbf{K}\cdot\boldsymbol{\chi} \right) \right\} . \tag{2.59}$$

We now execute the path integral over $\boldsymbol{\chi}$ and obtain

$$Z_{\mathrm{C},0}[\mathbf{J},\mathbf{K}] = \int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \int_{\mathrm{i}} \mathcal{D}\mathbf{x}\ \delta_{\mathrm{D}}\left[\boldsymbol{\mathcal{E}}_0[\mathbf{x}(t)] + \mathbf{K}\right] \mathrm{e}^{\mathrm{i}\,\mathbf{J}\cdot\mathbf{x}} , \tag{2.60}$$

where we have separated the integration over the initial state from the remaining path integral. Since we are dealing with a Hamiltonian equation of motion, it must be possible to write it as a linear differential operator

$$\hat{\boldsymbol{\mathcal{E}}}_0\, \mathbf{x} = 0 \quad \text{with} \quad \hat{\boldsymbol{\mathcal{E}}}_0 = (\hat{\mathcal{E}}_0 \otimes \mathcal{I}_N) \quad \text{and} \quad \hat{\mathcal{E}}_0\, \vec{x}_j = 0 , \tag{2.61}$$

where $\hat{\mathcal{E}}_0$ has the form of a $2d \times 2d$ matrix. The Dirac delta now tells us that we have to evaluate the system on trajectories which are the solutions to the free equations of motion enhanced by the inhomogeneous source term $\mathbf{K}$ as

$$\hat{\boldsymbol{\mathcal{E}}}_0 \, \mathbf{x} = -\mathbf{K} \, . \tag{2.62}$$

Let us assume that we know the solution and call it $\bar{\mathbf{x}}(t)$. The Dirac delta can be rewritten using (2.18) as

$$\delta_{\mathrm{D}} \left[\hat{\boldsymbol{\mathcal{E}}}_0 \, \mathbf{x} + \mathbf{K} \right] = \frac{1}{\det[\hat{\boldsymbol{\mathcal{E}}}_0]} \delta_{\mathrm{D}}[\mathbf{x} - \bar{\mathbf{x}}] \, . \tag{2.63}$$

Due to the linearity of the equation the functional determinant is a constant of no further consequence and can be absorbed into the normalisation of the path integral. The free generating functional is now trivial to calculate and we find

$$Z_{\mathrm{C},0}[\mathbf{J}, \mathbf{K}] = \int \mathrm{d}\mathbf{x}^{(\mathrm{i})} \, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \int_{\mathrm{i}} \mathcal{D}\mathbf{x} \; \delta_{\mathrm{D}}[\mathbf{x} - \bar{\mathbf{x}}] \, \mathrm{e}^{\mathrm{i}\mathbf{J}\cdot\mathbf{x}} = \int \mathrm{d}\Gamma_{\mathrm{i}} \, \mathrm{e}^{\mathrm{i}\mathbf{J}\cdot\bar{\mathbf{x}}} \, , \tag{2.64}$$

where we have introduced the shorthand notation

$$\int \mathrm{d}\Gamma_{\mathrm{i}} \coloneqq \int \mathrm{d}\mathbf{x}^{(\mathrm{i})} \, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \tag{2.65}$$

for the weighted integration over the initial state. Let us furthermore assume that we know the Green's function $\boldsymbol{\mathcal{G}}$ for the linear differential operator $\hat{\boldsymbol{\mathcal{E}}}_0$. We can then write down the solution to (2.62) for the initial state $\mathbf{x}^{(\mathrm{i})}$ as

$$\bar{\mathbf{x}}(t) = \boldsymbol{\mathcal{G}}(t, t_{\mathrm{i}}) \, \mathbf{x}^{(\mathrm{i})} - \int_{t_{\mathrm{i}}}^{t} \mathrm{d}t' \, \boldsymbol{\mathcal{G}}(t, t') \, \mathbf{K}(t') \, . \tag{2.66}$$

With the help of this result we can write down our final expression for the free generating functional as

$$Z_{\mathrm{C},0}[\mathbf{J}, \mathbf{K}] = \mathrm{e}^{-\mathrm{i}S_K[\mathbf{J},\mathbf{K}]} \int \mathrm{d}\Gamma_i \exp\left\{ \mathrm{i} \int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}} \mathrm{d}t \, \left\langle \mathbf{J}(t), \boldsymbol{\mathcal{G}}(t, t_{\mathrm{i}}) \, \mathbf{x}^{(\mathrm{i})} \right\rangle \right\} \, , \tag{2.67}$$

where we have defined

$$S_K[\mathbf{J}, \mathbf{K}] = \int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}} \mathrm{d}t \int_{t_{\mathrm{i}}}^{t} \mathrm{d}t' \, \left\langle \mathbf{J}(t), \boldsymbol{\mathcal{G}}(t, t') \mathbf{K}(t') \right\rangle \, . \tag{2.68}$$

While the second exponential in (2.67) describes how particles move freely starting out from their initial state $\mathbf{x}^{(\mathrm{i})}$, the S_K term allows us to generate deviations from these free trajectories by acting with operators that contain functional derivatives w. r. t. the source $\mathbf{K}$. We have already shown in (2.52) that these derivatives show up in interactions through the response field Φ_B. We will soon see that we can also express the effects of momentum correlations in the initial phase space probability distribution in terms of these derivatives.

2.5.2 *Green's function for the free Hamiltonian equations*

Given a linear differential operator $L(\vec{r})$ with $\vec{r} \in \mathbb{R}^n$, the general definition for its Green's function is given by

$$L(\vec{r})\, G(\vec{r},\vec{s}) = \delta_{\mathrm{D}}(\vec{r}-\vec{s})\ . \tag{2.69}$$

While this definition allows a general approach to finding G with the help of integral transforms, it does not define G in a unique way since one has to impose initial or boundary conditions by hand. In our case of a non-interacting Hamiltonian system it is more advantageous to directly solve the equations of motion and then identify the Green's function by comparison with (2.66). The Lagrange function of such a non-interacting system will typically only depend on position and velocity up to quadratic order[7] and for a collection of N particles the Hamiltonian equations of motion of individual particles decouple from one another. Thus, for a single particle j we can cast them into the following form augmented by a source term

$$\hat{\mathcal{E}}_0\, \vec{x}_j = (\partial_t \mathcal{I}_{2d} + \mathcal{K}(t))\, \vec{x}_j = -\vec{K}_j\ . \tag{2.70}$$

The $2d \times 2d$-matrix $\mathcal{K}$ is called the *force matrix* which originates from the phase-space gradient acting on the non-interacting Hamiltonian in (2.29). The above equation constitutes a linear system of ordinary differential equations. There are different ways to solve these kinds of systems, but the most convenient approach for our purposes uses matrix exponentials. It is understood most easily if we first consider the one-dimensional case

$$(\partial_t x + a(t)\, x) = g(t)\ , \tag{2.71}$$

where we have the inhomogeneity $g(t)$ on the RHS since we want to solve (2.62) in the end. Obtaining the retarded solution to the homogeneous equation is straightforward and gives

$$\begin{aligned}
&(\partial_t x + a(t)x) = 0 \quad \Rightarrow \quad \partial_t \ln x = -a(t) \\
\Rightarrow &\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\, \partial_{t'} \ln x(t') = \ln x(t')\big|_{t_\mathrm{i}}^{t} = -\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\, a(t') \\
\Rightarrow &\, x(t) = \exp\left\{-\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\, a(t')\right\} x(t_\mathrm{i})\ .
\end{aligned} \tag{2.72}$$

We will denote the initial condition as $x_\mathrm{i} = x(t_\mathrm{i})$. A particular solution to the inhomogeneous problem can be found using the variation of constants. We modify the solution to the homogeneous problem by allowing the parameter x_i to be time-dependent as $x_\mathrm{i} \to x_\mathrm{i}(t)$. The time derivative of this solution then reads

$$\partial_t x(t) = \left(\partial_t \exp\left\{-\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\, a(t')\right\}\right) x_\mathrm{i}(t) + \exp\left\{-\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\, a(t')\right\} \partial_t x_\mathrm{i}(t)$$

7 The most typical examples are free particles as in our case or the harmonic oscillator.

$$= -a(t)\,x(t) + \exp\left\{-\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\,a(t')\right\}\partial_t x_\mathrm{i}(t)\,. \tag{2.73}$$

We insert this back into the inhomogeneous equation (2.71) and find

$$\begin{aligned}
&\exp\left\{-\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\,a(t')\right\}\partial_t x_\mathrm{i}(t) = g(t) \quad \Rightarrow \quad \partial_t x_\mathrm{i}(t) = g(t)\exp\left\{\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\,a(t')\right\} \\
&\Rightarrow x_\mathrm{i}(t'')\big|_{t_\mathrm{i}}^{t} = \int_{t_\mathrm{i}}^{t} \mathrm{d}t''\,g(t'')\exp\left\{\int_{t_\mathrm{i}}^{t''} \mathrm{d}t'\,a(t')\right\} \\
&\to x_\mathrm{i}(t) = x_\mathrm{i}(t_\mathrm{i}) + \int_{t_\mathrm{i}}^{t} \mathrm{d}t''\,g(t'')\exp\left\{-\int_{t''}^{t_\mathrm{i}} \mathrm{d}t'\,a(t')\right\}\,.
\end{aligned} \tag{2.74}$$

We insert this solution back into (2.72) to obtain the general solution to the inhomogeneous problem with initial condition $x_\mathrm{i}(t_i) = x_\mathrm{i}$ as

$$\begin{aligned}
x(t) &= \exp\left\{-\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\,a(t')\right\} x(t_\mathrm{i}) \\
&\quad + \exp\left\{-\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\,a(t')\right\}\int_{t_\mathrm{i}}^{t} \mathrm{d}t''\,g(t'')\exp\left\{-\int_{t''}^{t_\mathrm{i}} \mathrm{d}t'\,a(t')\right\} \\
&= \exp\left\{-\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\,a(t')\right\} x(t_\mathrm{i}) + \int_{t_\mathrm{i}}^{t} \mathrm{d}t''\exp\left\{-\int_{t''}^{t} \mathrm{d}t'\,a(t')\right\} g(t'')\,,
\end{aligned} \tag{2.75}$$

where we have combined the two integrals inside the exponential functions in the last line. One can easily check by inserting the solution back into (2.71) that its validity relies only on two facts:

- The fundamental theorem of calculus
- $\partial_t\,\mathrm{e}^{f(t)} = \mathrm{e}^{f(t)}\partial_t f(t)$

We now replace $x \to \vec{x}_j$, $g \to -\vec{K}_j$ and $a(t) \to \mathcal{K}(t)$. The fundamental theorem of calculus is of course unaffected. The exponential of the matrix A is defined by the series expansion of the exponential function as

$$\mathrm{e}^{A} = \sum_{n=0}^{\infty} \frac{A^n}{n!}\,. \tag{2.76}$$

Let us now assume that the force matrix commutes as $\mathcal{K}(t_1)\mathcal{K}(t_2) = \mathcal{K}(t_2)\mathcal{K}(t_1)$ for arbitrary instances t_1, t_2 in time. Two important special cases of this are constant and nilpotent matrices. We can then show that

$$\begin{aligned}
\partial_t \exp\left\{\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\, \mathcal{K}(t')\right\} &= \sum_{n=1}^{\infty} \frac{1}{n!} \partial_t \left(\int_{t_\mathrm{i}}^{t} \mathrm{d}t_1\, \mathcal{K}(t_1)\right) \dots \left(\int_{t_\mathrm{i}}^{t} \mathrm{d}t_n\, \mathcal{K}(t_n)\right) \\
&= \sum_{n=1}^{\infty} \frac{n}{n!} \mathcal{K}(t) \left(\int_{t_\mathrm{i}}^{t} \mathrm{d}t_1\, \mathcal{K}(t_1)\right) \dots \left(\int_{t_\mathrm{i}}^{t} \mathrm{d}t_{n-1}\, \mathcal{K}(t_{n-1})\right) \\
&= \mathcal{K}(t) \sum_{n=0}^{\infty} \frac{1}{n!} \left(\int_{t_\mathrm{i}}^{t} \mathrm{d}t_1\, \mathcal{K}(t_1)\right) \dots \left(\int_{t_\mathrm{i}}^{t} \mathrm{d}t_n\, \mathcal{K}(t_n)\right) \\
&= \mathcal{K}(t) \exp\left\{\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\, \mathcal{K}(t')\right\} . \qquad (2.77)
\end{aligned}$$

In the second line we have used the commutation property of $\mathcal{K}(t)$ to take the matrix on whose integral the derivative has acted out in front. In cases where $\mathcal{K}(t)$ does not commute with itself at different times one needs to employ a so called Magnus series, but this will not concern us in this work. With the above equation we now see that the solution to (2.70) is given by

$$\vec{\bar{x}}_j(t) = \exp\left\{-\int_{t_\mathrm{i}}^{t} \mathrm{d}t'\, \mathcal{K}(t')\right\} \vec{x}_j^{\,(\mathrm{i})} - \int_{t_\mathrm{i}}^{t} \mathrm{d}t'' \exp\left\{-\int_{t''}^{t} \mathrm{d}t'\, \mathcal{K}(t')\right\} \vec{K}_j(t'') \,. \qquad (2.78)$$

Comparing this equation with (2.66) we can directly read off the Green's function or, in more physical terms, the single-particle phase-space propagator as

$$\mathcal{G}(t,t') = \exp\left\{-\int_{t'}^{t} \mathrm{d}t''\, \mathcal{K}(t'')\right\} \quad \text{and thus} \quad \boldsymbol{\mathcal{G}}(t,t') = \mathcal{G}(t,t') \otimes \mathcal{I}_N \,. \qquad (2.79)$$

Since $\mathcal{K}$ is a $2d \times 2d$-matrix so will be $\mathcal{G}$. For all our applications it will be possible to divide it into four $d \times d$ submatrices as

$$\mathcal{G}(t,t') = \begin{pmatrix} \mathrm{g}_{qq}(t,t')\,\mathcal{I}_d & \mathrm{g}_{qp}(t,t')\,\mathcal{I}_d \\ \mathrm{g}_{pq}(t,t')\,\mathcal{I}_d & \mathrm{g}_{pp}(t,t')\,\mathcal{I}_d \end{pmatrix} , \qquad (2.80)$$

where the g_{qq} and so on are scalar functions.

2.6 COMPARISON WITH STANDARD KINETIC THEORY

So far we have focused on pointing out how SFTCP relates to the quantities familiar from standard equilibrium statistical mechanics. We now argue that it can also be understood as a different formulation of kinetic theory, which is the standard tool for

the investigation of non-equilibrium statistical systems. Its central quantity is the N-particle phase-space distribution function or phase-space density $f^{(N)}(\vec{x}_1, \ldots, \vec{x}_N, t)$ which gives the probability to find a system with $2dN$ generalised coordinates and momenta $\vec{x}_j = (\vec{q}_j^{\,\mathrm{T}}, \vec{p}_j^{\,\mathrm{T}})^{\mathrm{T}}$ somewhere in the phase space cell $\mathrm{d}\vec{x}_1 \ldots \mathrm{d}\vec{x}_N$ around the phase-space point $(\vec{x}_1, \ldots, \vec{x}_N)$ at the time t. The time evolution of $f^{(N)}$ is governed by the Liouville equation

$$\frac{\partial f^{(N)}}{\partial t} + \sum_{j=1}^{N} \left(\dot{\vec{q}}_j \cdot \nabla_{q_j} f^{(N)} + \dot{\vec{p}}_j \cdot \nabla_{p_j} f^{(N)} \right) = 0 \,. \tag{2.81}$$

This states that the phase-space density is constant along the phase-space flow Ψ_t of the system. Let the Hamiltonian be of the form

$$\mathcal{H} = \sum_{j=1}^{N} \left(\frac{\vec{p}_j^{\,2}}{2m} + U^{\mathrm{ext}}(\vec{q}_j) + \sum_{\substack{i=1 \\ i \neq j}}^{N} v_{ij}(\vec{q}_i, \vec{q}_j) \right) \,, \tag{2.82}$$

where U^{ext} is a potential describing an external force and v_{ij} are the pair potentials between the particles which lead to collisions. The Liouville equation then reads

$$\frac{\partial f^{(N)}}{\partial t} + \sum_{j=1}^{N} \left(\frac{\vec{p}_j}{m} \cdot \nabla_{q_j} f^{(N)} - \left(\nabla_{q_j} U^{\mathrm{ext}} + \sum_{\substack{i=1 \\ i \neq j}}^{N} \nabla_{q_j} v_{ij} \right) \cdot \nabla_{p_j} f^{(N)} \right) = 0 \,. \tag{2.83}$$

Due to the typically high dimensionality $2dN$ of phase-space solving this partial differential equation is a very hard task, often impossible for realistic systems. To overcome this obstacle one integrates out the information of most of the phase-space coordinates from the Liouville equation. For $n < N$, one defines the n-particle phase-space distribution functions by

$$f^{(n)}(\vec{x}_1, \ldots, \vec{x}_n, t) \coloneqq \int \mathrm{d}\vec{x}_{n+1} \ldots \int \mathrm{d}\vec{x}_N \, f^{(N)}(\vec{x}_1, \ldots, \vec{x}_N, t) \,. \tag{2.84}$$

and then applies the same kind of integrals to (2.83) itself. This leads to an enormous set of coupled partial differential equations commonly known as the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy (BBGKY) hierarchy (cf. [58, 14, 15, 29, 30]). Its defining feature is that the evolution of $f^{(n)}$ is always coupled to the next higher function $f^{(n+1)}$. The full set of equations still contains the same amount of information as the Liouville equation and is thus equally hard to solve. This forces us to truncate the hierarchy at some level, which means we necessarily have to give up the phase-space information we integrated out. Consider for example the $n = 1$ equation

$$\begin{aligned} &\frac{\partial f^{(1)}(\vec{x}_1, t)}{\partial t} + \frac{\vec{p}_1}{m} \cdot \nabla_{r_1} f^{(1)}(\vec{x}_1, t) - \nabla_{q_1} U^{\mathrm{ext}} \cdot \nabla_{p_1} f^{(1)}(\vec{x}_1, t) \\ &= (N-1) \int \mathrm{d}\vec{x}_2 \, \nabla_{q_1} v_{12} \cdot \nabla_{p_1} f^{(2)}(\vec{x}_1, \vec{x}_2, t) \,. \end{aligned} \tag{2.85}$$

Assuming that the two-particle distribution function factorises as $f^{(2)} \approx f^{(1)} f^{(1)}$ this equation can be decoupled from the hierarchy and then turns into the Boltzmann

equation, which we will encounter later in part ii of this thesis. For a thorough derivation of this result see Lifšic and Pitaevskij [35]. Although we have closed the hierarchy, we have lost all the information about correlations contained in the higher order distribution functions. Together with the assumption that the mean free path of particles is negligibly small against the desired macroscopic resolution, the Boltzmann equation is often used as the starting point for the development of hydrodynamics, which derives equations of motion which directly apply to macroscopic observables like density and momentum.

The link between SFTCP and kinetic theory can be made formal by introducing the single particle phase-space distribution as the collective field

$$\Phi_f(\vec{x},t) = \sum_{j=1}^{N} \delta_{\mathrm{D}}(\vec{x} - \vec{x}_j(t)) = \sum_{j=1}^{N} \delta_{\mathrm{D}}(\vec{q} - \vec{q}_j(t))\, \delta_{\mathrm{D}}(\vec{p} - \vec{p}_j(t)) \,, \tag{2.86}$$

which is just the extension of the collective density field Φ_ρ to all of phase-space. Viermann et al. [55] derived the BBGKY hierarchy for the correlation functions of this collective field, thereby establishing the correspondence $\langle \Phi_{f_1} \dots \Phi_{f_n} \rangle \leftrightarrow f^{(n)}$ with the addition of a self-consistent truncation criterion depending on the order of two-particle interaction one is willing to consider. In the same paper it was also shown that if we define the *momentum density field*

$$\vec{\Phi}_\Pi(\vec{q}_1, t_1) \coloneqq \sum_{j=1}^{N} \vec{p}_j(t)\, \delta_{\mathrm{D}}(\vec{q} - \vec{q}_j(t)) \,, \tag{2.87}$$

then it is straightforward to derive the continuity and Euler's equation for a collisionless gas, expressing conservation of particle number or mass and momentum respectively. In summary, we can now make the following observations.

- The phase-space distribution function $f^{(N)}$ encodes the same information as the quantity

$$\mathcal{P}(\mathbf{x}^{(\mathrm{f})}) = \int_{\mathrm{i}}^{\mathrm{f}} \mathcal{D}\mathbf{x}(t)\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})})\, \delta_{\mathrm{D}}[\mathbf{x}(t) - \mathbf{x}_{\mathrm{cl}}(t_{\mathrm{f}}; \mathbf{x}^{(\mathrm{i})})] \tag{2.88}$$

  of our SFTCP approach and thus we may identify the two. Both distributions are represented by the coloured areas of equal time slices in Fig. 1 and contain the full statistical information about the system and can be used to obtain the expectation values of macroscopic observables.

- Kinetic theory aims at solving the very complex Liouville equation (2.81) in order to describe the time evolution of the system, i. e. $f^{(N)}$ is itself the main dynamic variable in the equation of motion. Looking at Fig. 1, this means that it concentrates on describing how with time the entire coloured area moves through phase-space.

- In contrast, SFTCP concentrates on following only the motion of individual points in Fig. 1 along the classical trajectory. Evolving one of these points from a

clearly defined starting position in phase-space is equivalent to calculating the time evolution of the purely distributional valued $\Phi_f(\vec{x}, t)$ of (2.86), i. e. solving the Klimontovic [31] equation $(\partial_t + \dot{\vec{x}} \cdot \nabla_x)\, \Phi_f(\vec{x}, t) = 0$.

- Only after we have nominally obtained a general solution for this problem do we actually assemble the coloured area in Fig. 1 at the final time by averaging the general solution over its initial conditions with a *continuous* probability density $\mathcal{P}(\mathbf{x}^{(i)})$. So while SFTCP in the end provides the same coarse grained, i. e. smoothed macroscopic information as does the Liouville equation or equivalently the BBGKY hierarchy, its inner dynamical structure is related to the Klimontovic equation.

- This means that we only need to solve the equations of motion (2.1) for the phase-space coordinates of the particles. While this is technically still impossible, these ordinary differential equations are considerably easier to handle than the Liouville equation. As we saw, they can easily be split into a non-interacting and interacting part, with the former leading to simple solutions that can often be obtained analytically, allowing us to set up a perturbation theory around the these 'free' phase-space trajectories in orders of the particle interaction.

- This perturbation theory is formulated directly in terms of the correlation functions of the macroscopic observables, in which we are ultimately interested in, and a response field. The important point we want to stress is that *no phase-space information has been integrated out* in order to write down the perturbative expansion. Summing up all terms of the perturbative expansion is thus equivalent to calculating the expectation values of macroscopic observables with the *full solution* of the Liouville equation (2.81), thereby retaining all the information about the correlations between the *microscopic* degrees of freedom.

We see this as a quite remarkable result. The task of solving a very complex partial differential equation can be reduced to the calculation of normal integrals which then have to be summed up according to (2.58).

3

INITIAL CONDITIONS

In the previous chapter 2 we defined all core elements of SFTCP. Implementing the dynamics by finding the free propagator and the interaction potential is usually a rather straightforward exercise due to the Hamiltonian nature of the equations of motion. This is more complicated in traditional formulations of kinetic theory like hydrodynamics, where the equations of motion are directly formulated in terms of the macroscopic fields and thus take the form of partial differential equations instead of the ordinary type found in Hamiltonian mechanics. In contrast, the problem of initial conditions is easier to handle in these macroscopic approaches since naturally one has only information about these macroscopic observables and not the actual microscopic phase-space coordinates of the constituting particles. As already explained in section 2.2, we will thus need to set up the initial phase-space probability density $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ in such a way that if we reconstruct some macroscopic variable $A(\mathbf{x})$ from the microscopic phase-space information of the theory, their expectation value at the initial time agrees with the known or observed value as

$$\left\langle A|_{t_\mathrm{i}} \right\rangle = \int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})})\, A(\mathbf{x}^{(\mathrm{i})}) \stackrel{!}{=} A^{\mathrm{obs}}\Big|_{t_\mathrm{i}} \,. \tag{3.1}$$

In the language of statistics we would require that the $A(\mathbf{x})$ are unbiased estimators of the initial data. In this chapter we will show how one can construct $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ in the case of point-like particles. Much of our effort will be devoted to treating the case where the only initial information we have are the correlations of a combined density-velocity Gaussian random field.

3.1 POISSON SAMPLING

We will assume that at the initial time we know the macroscopic mass density field $\rho_\mathrm{m}^{(\mathrm{i})}(\vec{q})$ and the momentum field $\vec{\Pi}^{(\mathrm{i})}(\vec{q})$ of some total mass M distributed over the volume V. We want to sample this distribution with N identical particles of equal mass m confined to this volume V. We are free to choose N and m to our liking as long as we fullfill the constraint $Nm = M$. We define the macroscopic *particle number density* field $\rho^{(\mathrm{i})}(\vec{q}) = m^{-1}\rho_\mathrm{m}^{(\mathrm{i})}(\vec{q})$. We can construct an initial phase-space probability density $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ for these particles such that (3.1) holds for $\rho^{(\mathrm{i})}$ and $\vec{\Pi}^{(\mathrm{i})}$. To achieve this we go through all particles and place them randomly somewhere in the volume V and then assign to their momentum the value of the momentum field at that point. The positioning of each particle is considered a statistically independent random

experiment with the probability to place the particle j in the infinitesimal volume $\mathrm{d}\vec{q}_j^{\,(\mathrm{i})}$ around the point $\vec{q}_j^{\,(\mathrm{i})}$ being proportional to the density field at that point and thus

$$\mathcal{P}(\vec{q}_j^{\,(\mathrm{i})})\,\mathrm{d}\vec{q}_j^{\,(\mathrm{i})} = \frac{1}{N}\,\rho^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})})\,\mathrm{d}\vec{q}_j^{\,(\mathrm{i})}\,. \tag{3.2}$$

From this we see that the probability to find a certain particle j inside some subvolume ΔV of V is

$$P(\text{particle } j \text{ in } \Delta V) = \frac{1}{N}\int\limits_{\Delta V}\mathrm{d}\vec{q}^{\,(\mathrm{i})}\,\rho^{(\mathrm{i})}(\vec{q}^{\,(\mathrm{i})}) = p \tag{3.3}$$

and thus the same for all particles. Because of this the probability to find an amount k of the N particles inside ΔV must be given by a binomial distribution

$$P(k \text{ particles in } \Delta V) = \binom{N}{k} p^k (1-p)^{N-k}\,. \tag{3.4}$$

If we make the volume ΔV very small p will tend to zero. If at the same time we make the number of particles N very large such that the expectation value $\langle k\rangle = Np$ stays constant, then the above binomial distribution will turn into a Poisson distribution. This is the reason why this process is often called *Poisson sampling*.

Since we want the particle j at $\vec{q}_j^{\,(\mathrm{i})}$ to have the momentum $\vec{\Pi}^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})})$ we extend (3.2) to the full phase-space coordinates

$$\begin{aligned}\mathcal{P}(\vec{x}_j^{\,(\mathrm{i})})\,\mathrm{d}\vec{x}_j^{\,(\mathrm{i})} &= \mathcal{P}(\vec{q}_j^{\,(\mathrm{i})},\vec{p}_j^{\,(\mathrm{i})})\,\mathrm{d}\vec{q}_j^{\,(\mathrm{i})}\mathrm{d}\vec{p}_j^{\,(\mathrm{i})}\\ &= \frac{1}{N}\,\rho^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})})\,\delta_{\mathrm{D}}(\vec{p}_j^{\,(\mathrm{i})} - \vec{\Pi}^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})}))\,\mathrm{d}\vec{q}_j^{\,(\mathrm{i})}\mathrm{d}\vec{p}_j^{\,(\mathrm{i})}\,.\end{aligned} \tag{3.5}$$

Because we assumed that all particles are placed independently we find for the phase-space probability density of all particles

$$\mathcal{P}(\mathbf{x}^{(\mathrm{i})})\,\mathrm{d}\mathbf{x}^{(\mathrm{i})} = \prod_{j=1}^{N}\mathcal{P}(\vec{q}_j^{\,(\mathrm{i})},\vec{p}_j^{\,(\mathrm{i})})\,\mathrm{d}\vec{q}_j^{\,(\mathrm{i})}\mathrm{d}\vec{p}_j^{\,(\mathrm{i})}\,. \tag{3.6}$$

We now want to confirm (3.1) for the density and momentum fields. We need that

$$\int \mathrm{d}\vec{q}\,\rho^{(\mathrm{i})}(\vec{q}) = N\,. \tag{3.7}$$

This was already used to normalise (3.5) and thus (3.6). The density field was defined in (2.37). We therefore find

$$\begin{aligned}\left\langle\Phi_\rho(\vec{q},t_{\mathrm{i}})\right\rangle &= \int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\,\mathcal{P}(\mathbf{x}^{(\mathrm{i})})\,\Phi_\rho(\vec{q},t_{\mathrm{i}}) = \int \mathrm{d}\mathbf{q}^{(\mathrm{i})}\,\mathcal{P}(\mathbf{q}^{(\mathrm{i})})\sum_{j=1}^{N}\delta_{\mathrm{D}}(\vec{q}-\vec{q}_j^{\,(\mathrm{i})})\\ &= \sum_{j=1}^{N}\int \mathrm{d}\vec{q}^{\,(\mathrm{i})}\,\delta_{\mathrm{D}}(\vec{q}-\vec{q}_j^{\,(\mathrm{i})})\,\frac{1}{N}\,\rho^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})})\\ &= \rho^{(\mathrm{i})}(\vec{q})\sum_{j=1}^{N}\frac{1}{N} = \rho^{(\mathrm{i})}(\vec{q})\,.\end{aligned} \tag{3.8}$$

The expectation value of the macroscopic momentum density field (2.87) at the initial time is found to be

$$\begin{aligned}\left\langle \vec{\Phi}_\Pi(\vec{q},t_\mathrm{i})\right\rangle &= \int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\,\mathcal{P}(\mathbf{x}^{(\mathrm{i})})\,\vec{\Phi}_\Pi(\vec{q},t_\mathrm{i}) = \int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\,\mathcal{P}(\mathbf{x}^{(\mathrm{i})})\sum_{j=1}^{N}\vec{p}_j^{\,(\mathrm{i})}\,\delta_\mathrm{D}(\vec{q}-\vec{q}_j^{\,(\mathrm{i})}) \\ &= \sum_{j=1}^{N}\int \mathrm{d}\vec{q}_j^{\,(\mathrm{i})}\,\delta_\mathrm{D}(\vec{q}-\vec{q}_j^{\,(\mathrm{i})})\,\frac{1}{N}\,\rho^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})}) \\ &\qquad \int \mathrm{d}\vec{p}_j^{\,(\mathrm{i})}\,\delta_\mathrm{D}(\vec{p}_j^{\,(\mathrm{i})}-\vec{\Pi}^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})}))\,\vec{p}_j^{\,(\mathrm{i})} \\ &= \rho^{(\mathrm{i})}(\vec{q})\,\vec{\Pi}^{(\mathrm{i})}(\vec{q})\sum_{j=1}^{N}\frac{1}{N} = \rho^{(\mathrm{i})}(\vec{q})\,\vec{\Pi}^{(\mathrm{i})}(\vec{q})\,. \end{aligned} \tag{3.9}$$

The expected macroscopic momentum field is then defined by

$$\left\langle \vec{\Pi}(\vec{q},t_\mathrm{i})\right\rangle = \frac{\left\langle \vec{\Phi}_\Pi(\vec{q},t_\mathrm{i})\right\rangle}{\left\langle \Phi_\rho(\vec{q},t_\mathrm{i})\right\rangle} = \frac{\rho^{(\mathrm{i})}(\vec{q})\,\vec{\Pi}^{(\mathrm{i})}(\vec{q})}{\rho^{(\mathrm{i})}(\vec{q})} = \vec{\Pi}^{(\mathrm{i})}(\vec{q})\,. \tag{3.10}$$

We thus have shown the relation (3.1) to hold for both the macroscopic density and momentum fields if we use the Poisson sampling method to set up $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$. While the simplicity of the approach is appealing one should be aware of the fact that there are situations which it cannot describe correctly. One such example would be particles which have a 'hard core' which means that each of them has a spherical region of radius r_0 around their position $\vec{q}_j$ that may not be entered by any other particle. A sampling process for this kind of particles would need to make sure that the distance between the positions of two particles is at least $2r_0$ and this is clearly not the case for the independent Poisson sampling.

3.2 POISSON SAMPLING OF CORRELATED RANDOM FIELDS

So far we have assumed that we know the actual initial mass density and momentum fields. There are however many cases where we do not have such information and must consider both these fields as random. We may know the full probability density for these fields or only some of their connected correlation functions, i. e. cumulants. The question is how we can imprint these correlations onto the initial phase-space distribution $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$. A straightforward way can be found in Peebles [44]. Consider a random initial density field with mean

$$\left\langle \rho^{(\mathrm{i})}(\vec{q})\right\rangle = n(\vec{q}) \tag{3.11}$$

and an initial *autocorrelation function* $\xi^{(\mathrm{i})}$ defined by

$$\left\langle \rho^{(\mathrm{i})}(\vec{q}_1)\,\rho^{(\mathrm{i})}(\vec{q}_2)\right\rangle = n(\vec{q}_1)\,n(\vec{q}_2)\,\left(1+\xi^{(\mathrm{i})}(\vec{q}_1,\vec{q}_2)\right)\,. \tag{3.12}$$

It is important to note that the averages in this case are taken over realisations of the random density field $\rho^{(\mathrm{i})}$. We now pick one such realisation and perform a Poisson

sampling of it. For two particles a and b, the joint probability to be at positions $\vec{q}_a^{\,(\mathrm{i})}$ and $\vec{q}_b^{\,(\mathrm{i})}$ is then according to (3.6) proportional to

$$\mathcal{P}(\vec{q}_a^{\,(\mathrm{i})}, \vec{q}_b^{\,(\mathrm{i})}) \propto \rho^{(\mathrm{i})}(\vec{q}_a^{\,(\mathrm{i})})\, \rho^{(\mathrm{i})}(\vec{q}_b^{\,(\mathrm{i})})\, \mathrm{d}\vec{q}_a^{\,(\mathrm{i})} \mathrm{d}\vec{q}_b^{\,(\mathrm{i})} \,. \tag{3.13}$$

We now average this over the realisations of the random field and obtain a mean probability density for the particle positions

$$\bar{\mathcal{P}}(\vec{q}_a^{\,(\mathrm{i})}, \vec{q}_b^{\,(\mathrm{i})}) \propto n(\vec{q}_a^{\,(\mathrm{i})})\, n(\vec{q}_b^{\,(\mathrm{i})}) \left(1 + \xi^{(\mathrm{i})}(\vec{q}_a^{\,(\mathrm{i})}, \vec{q}_b^{\,(\mathrm{i})})\right) \mathrm{d}\vec{q}_a^{\,(\mathrm{i})} \mathrm{d}\vec{q}_b^{\,(\mathrm{i})} \,. \tag{3.14}$$

We see that due to this averaging the correlations of the random density field have been imprinted onto the probability density of the particle ensemble. We now want to make this approach more general. Fig. 3 shows the two-step structure how the canonical ensemble is set up such that it represents systems which are initially described by a combined *random* density-momentum field $(\rho^{(\mathrm{i})}, \vec{\Pi}^{(\mathrm{i})})$.

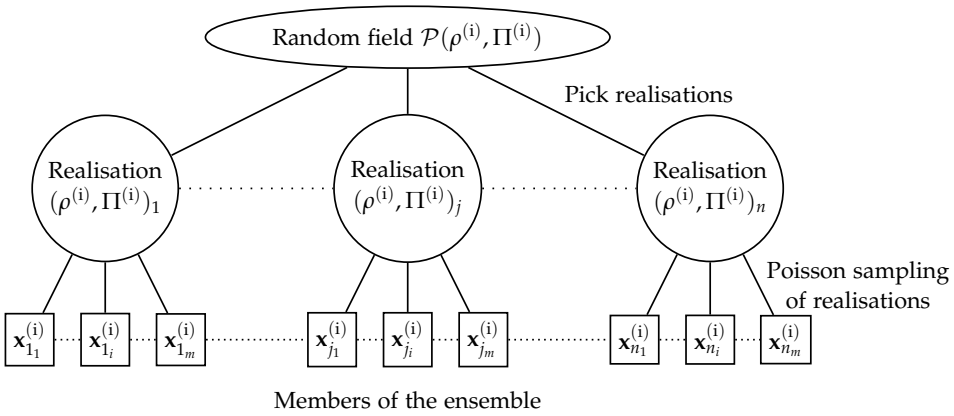


Figure 3: The two-step sampling process defining the canonical ensemble at the initial time. The continuous average $\int \mathrm{d}\mathbf{x}^{(\mathrm{i})} \int \mathrm{d}\mathbf{d}\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}, \mathbf{d}) = \int \mathrm{d}\Gamma_{\mathrm{i}}$ corresponds to the limit $n, m \to \infty$.

We introduce the shorthand notation

$$\rho_j^{(\mathrm{i})} := \rho^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})}) \quad \text{and} \quad \vec{\Pi}_j^{\,(\mathrm{i})} := \vec{\Pi}^{\,(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})}) \,. \tag{3.15}$$

Every particle is now assigned an *initial data vector*

$$\vec{d}_j = \begin{pmatrix} \rho_j^{(\mathrm{i})} \\ \vec{\Pi}_j^{\,(\mathrm{i})} \end{pmatrix} \quad \Rightarrow \quad \mathbf{d} = \vec{d}_j \otimes \vec{e}_j \,, \tag{3.16}$$

which is again collected into an initial data tensor $\mathbf{d}$ with obvious reductions to the $\rho^{(\mathrm{i})}$ and $\vec{\Pi}^{\,(\mathrm{i})}$ subspaces. The probability density for the initial data random field $(\rho^{(\mathrm{i})}, \vec{\Pi}^{\,(\mathrm{i})})$ to be realised with the values of the above data tensor is then assumed to be given as $\mathcal{P}(\mathbf{d})$. Taking an average over the ensemble members then corresponds to taking an average over the combined probability density $\mathcal{P}(\mathbf{x}^{(\mathrm{i})}, \mathbf{d})$. Using conditional probabilities, we can take the average over the second level of Fig. 3 as

$$\mathcal{P}(\mathbf{x}^{(\mathrm{i})}) = \int \mathrm{d}\mathbf{d}\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}, \mathbf{d}) = \int \mathrm{d}\mathbf{d}\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})} | \, \mathbf{d})\, \mathcal{P}\,(\mathbf{d}) \,, \tag{3.17}$$

where we dropped the bar on $\mathcal{P}$ on the LHS since we only used it to signal the averaging in (3.14). Note that this also includes the case where one or both of the fields are known deterministically if we fix them with Dirac delta distributions in $\mathcal{P}(\mathbf{d})$. With regards to normalisation we see that if the sampling probability $\mathcal{P}(\mathbf{x}^{(\mathrm{i})}|\,\mathbf{d})$ conditioned on a single random field realisation is normalised in the sense of

$$\int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\,\mathcal{P}(\mathbf{x}^{(\mathrm{i})}|\,\mathbf{d}) = 1 \tag{3.18}$$

and if $\mathcal{P}(\mathbf{d})$ is also normalised, then $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ in (3.17) is normalised. Note that the conditioned sampling probability does not necessarily need to be chosen as the Poisson sampling in (3.6). However, if we choose Poisson sampling we find

$$\begin{aligned}\mathcal{P}(\mathbf{x}^{(\mathrm{i})}) &= \int \mathrm{d}\boldsymbol{\rho}^{(\mathrm{i})} \int \mathrm{d}\boldsymbol{\Pi}^{(\mathrm{i})} \left(\prod_{j=1}^{N} \frac{1}{N}\,\rho_j^{(\mathrm{i})}\,\delta_{\mathrm{D}}(\vec{p}_j^{\,(\mathrm{i})} - \vec{\Pi}_j^{(\mathrm{i})})\right) \mathcal{P}(\mathbf{d}) \\ &= \int \mathrm{d}\boldsymbol{\rho}^{(\mathrm{i})} \left(\prod_{j=1}^{N} \frac{1}{N}\,\rho_j^{(\mathrm{i})}\right) \int \mathrm{d}\boldsymbol{\Pi}^{(\mathrm{i})}\,\delta_{\mathrm{D}}(\mathbf{p}^{(\mathrm{i})} - \boldsymbol{\Pi}^{(\mathrm{i})})\,\mathcal{P}(\boldsymbol{\rho}^{(\mathrm{i})}, \boldsymbol{\Pi}^{(\mathrm{i})}) \\ &= \left(\prod_{j=1}^{N} \int \mathrm{d}\rho_j^{(\mathrm{i})}\,\frac{1}{N}\,\rho_j^{(\mathrm{i})}\right) \mathcal{P}(\boldsymbol{\rho}^{(\mathrm{i})}, \mathbf{p}^{(\mathrm{i})})\,.\end{aligned} \tag{3.19}$$

This is a properly normalised phase-space probability density if we use a normalised $\mathcal{P}(\mathbf{d})$, since (3.6) obeys (3.18). We now have a very general result. We can for example describe the initial state of our system as an ideal gas if we use a uniform mean particle number density $\bar{\rho}$ in configuration space and a Maxwell-Boltzmann distribution P_{σ_p}, i. e. an uncorrelated centered Gaussian distribution, in momentum space with the momentum dispersion $\sigma_p = \sigma_p(T)$ set by the temperature T. The initial data probability then reads

$$\mathcal{P}(\boldsymbol{\rho}^{(\mathrm{i})}, \mathbf{p}^{(\mathrm{i})}) = \prod_{j=1}^{N} \delta_{\mathrm{D}}(\rho_j^{(\mathrm{i})} - \bar{\rho})\,P_{\sigma_p}(\vec{p}_j^{\,(\mathrm{i})}) \tag{3.20}$$

and the resulting phase-space probability density is

$$\begin{aligned}\mathcal{P}(\mathbf{x}^{(\mathrm{i})}) &= \prod_{j=1}^{N} \int \mathrm{d}\rho_j^{(\mathrm{i})}\,\frac{1}{N}\,\rho_j^{(\mathrm{i})}\,\delta_{\mathrm{D}}(\rho_j^{(\mathrm{i})} - \bar{\rho})\,P_{\sigma_p}(\vec{p}_j^{\,(\mathrm{i})}) \\ &= \left(\frac{\bar{\rho}}{N}\right)^{N} \prod_{j=1}^{N} P_{\sigma_p}(\vec{p}_j^{\,(\mathrm{i})}) = V^{-N} \prod_{j=1}^{N} P_{\sigma_p}(\vec{p}_j^{\,(\mathrm{i})})\,,\end{aligned} \tag{3.21}$$

where we used that $\bar{\rho} = N/V$ in a canonical ensemble. This example obviously does not involve any kind of correlation. We will now move on to similar but more complicated initial conditions which do include correlations and will be used for the remainder of this thesis.

3.2.1 *Phase-space probability density for Gaussian random fields*

An n-component Gaussian random field $\vec{f}(\vec{r})$ is the generalisation of the multivariate Gaussian distribution to fields and is defined as follows. For any number of points

$\vec{r}_1, \ldots, \vec{r}_m$ in the domain space of the field, the joint probability that the field takes on values $\vec{f}(\vec{r}_1), \ldots, \vec{f}(\vec{r}_m)$ is given by

$$\mathcal{P}(\vec{f}(\vec{r}_1), \ldots, \vec{f}(\vec{r}_m)) = \frac{1}{\sqrt{(2\pi)^{n\times m}\det C}} \exp\left\{-\frac{1}{2}(\mathbf{f}-\bar{\mathbf{f}})^{\mathrm{T}} C^{-1}(\mathbf{f}-\bar{\mathbf{f}})\right\} \tag{3.22}$$

with tensors

$$\mathbf{f} = \sum_{i=1}^{m} \vec{f}(\vec{r}_i) \otimes \vec{e}_i \qquad \text{and} \qquad \bar{\mathbf{f}} = \sum_{i=1}^{m} \bar{\vec{f}}(\vec{r}_i) \otimes \vec{e}_i \,, \tag{3.23}$$

where $\vec{e}_j$ in this case has m components. This distribution is fully defined by its mean field

$$\left\langle \vec{f}(\vec{r}) \right\rangle = \bar{\vec{f}}(\vec{r}) \tag{3.24}$$

and its covariance matrix

$$C = \left\langle (\mathbf{f}-\bar{\mathbf{f}}) \otimes (\mathbf{f}-\bar{\mathbf{f}}) \right\rangle \,. \tag{3.25}$$

We will limit ourselves to homogeneous and isotropic Gaussian random fields. For these the mean field is constant in the domain space, i. e. $\bar{\vec{f}}(\vec{q}) = \bar{\vec{f}}$ and any submatrices of C describing the covariance of the field between two points $\vec{q}_1$ and $\vec{q}_2$ may only depend on the distance

$$\left\langle \left(\vec{f}(\vec{r}_1) - \bar{\vec{f}}\right) \otimes \left(\vec{f}(\vec{r}_2) - \bar{\vec{f}}\right) \right\rangle = C_{12}(|\vec{r}_1 - \vec{r}_2|) \,. \tag{3.26}$$

We will take the combined density-momentum field to be a homogeneous and isotropic Gaussian random field with configuration space as the domain space of the field. This might seem a rather arbitrary choice at this point. It is however a natural choice for cosmological structure formation as we will explain in part ii of this thesis. But even aside from this physical motivation the Gaussian distribution is often used as the zeroth order starting point for perturbative approximations to the unknown distribution of some random variable where one only knows a few cumulants, with the Edgeworth series being a prime example. Having an exact solution to the Gaussian problem should thus be of some general value. Due to homogeneity, the mean of the density field is the mean particle number density

$$\left\langle \rho^{(\mathrm{i})}(\vec{q}) \right\rangle = \bar{\rho} = \frac{N}{V} \,. \tag{3.27}$$

This allows us to rewrite the density field in terms of the mean particle number density and a particle number density contrast

$$\rho^{(\mathrm{i})}(\vec{q}) = \bar{\rho}\left(1 + \delta^{(\mathrm{i})}(\vec{q})\right) \qquad \text{with} \qquad \left\langle \delta^{(\mathrm{i})}(\vec{q}) \right\rangle = 0 \,. \tag{3.28}$$

The second property follows directly from (3.27) and the normalisation of the Gaussian distribution. Conservation of mass also directly implies

$$M = \int \mathrm{d}\vec{q}\, \rho_{\mathrm{m}}^{(\mathrm{i})}(\vec{q}) = m\bar{\rho}V \quad \rightarrow \quad \int \mathrm{d}\vec{q}\, \delta^{(\mathrm{i})}(\vec{q}) = 0 \,. \tag{3.29}$$

We can now describe the initial conditions of our system in terms of pairs

$$\vec{d}_j = \begin{pmatrix} \delta_j^{(\mathrm{i})} \\ \vec{p}_j^{\,(\mathrm{i})} \end{pmatrix} \qquad \text{with} \qquad \delta_j^{(\mathrm{i})} = \delta^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})}) \,, \tag{3.30}$$

which get collected into the tensor $\mathbf{d}$ as shown in (3.16). Due to isotropy there may be no preferred direction for the momenta of particles, i. e. no macroscopic overall particle flow, in the system and we thus have a centered Gaussian random field with respective mean and convariance matrix

$$\langle \mathbf{d} \rangle = 0 \,, \qquad C = \langle \mathbf{d} \otimes \mathbf{d} \rangle = C(\mathbf{q}^{(\mathrm{i})}) \,. \tag{3.31}$$

Although the initial data vector (3.30) contains the initial momenta, the covariance matrix will only depend on the initial positions $\mathbf{q}^{(\mathrm{i})}$, since due to (3.15) and (3.19) one must read (3.30) with $\vec{p}_j^{\,(\mathrm{i})} = \vec{\Pi}^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})})$ in mind. The phase-space probability density (3.19) now takes the form

$$\begin{aligned} \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) &= \left(\prod_{j=1}^{N} \int \mathrm{d}\delta_j^{(\mathrm{i})} \, \frac{1}{N} \, \bar{\rho} \, \left(1 + \delta_j^{(\mathrm{i})} \right) \right) \frac{\exp\left\{ -\frac{1}{2} \mathbf{d}^{\mathrm{T}} C^{-1} \mathbf{d} \right\}}{\sqrt{(2\pi)^{(d+1)N} \det C}} \\ &= V^{-N} \left(\prod_{j=1}^{N} \int \mathrm{d}\delta_j^{(\mathrm{i})} \, \left(1 + \delta_j^{(\mathrm{i})} \right) \right) \frac{\exp\left\{ -\frac{1}{2} \mathbf{d}^{\mathrm{T}} C^{-1} \mathbf{d} \right\}}{\sqrt{(2\pi)^{(d+1)N} \det C}} \,. \end{aligned} \tag{3.32}$$

It will prove a lot more convenient to work with the Fourier transform of the Gaussian probability density, which is also called the *characteristic function*

$$\varphi_{\mathbf{d}}(\mathbf{t}) = \int \mathrm{d}\mathbf{d} \, \mathrm{e}^{-\mathrm{i}\langle \mathbf{t}, \mathbf{d} \rangle} \frac{\exp\left\{ -\frac{1}{2} \mathbf{d}^{\mathrm{T}} C^{-1} \mathbf{d} \right\}}{\sqrt{(2\pi)^{(d+1)N} \det C}} = \exp\left\{ -\frac{1}{2} \mathbf{t}^{\mathrm{T}} C \mathbf{t} \right\} \,, \tag{3.33}$$

where the Fourier conjugate $\mathbf{t}$ can naturally also be separated as

$$\mathbf{t} = \vec{t}_j \otimes \vec{e}_j \qquad \text{with} \qquad \vec{t}_j = \begin{pmatrix} t_{\delta_j} \\ \vec{t}_{p_j} \end{pmatrix} \,, \tag{3.34}$$

with obvious restricted quantities $\mathbf{t}_\delta$ and $\mathbf{t}_p$. Using the inverse Fourier transform (1.25) we can rewrite (3.32) as

$$\mathcal{P}(\mathbf{x}^{(\mathrm{i})}) = V^{-N} \int \frac{\mathrm{d}\mathbf{t}}{(2\pi)^{(d+1)N}} \, \mathrm{e}^{\mathrm{i}\langle \mathbf{t}, \mathbf{d} \rangle} \left(\prod_{j=1}^{N} \int \mathrm{d}\delta_j^{(\mathrm{i})} \, \left(1 + \delta_j^{(\mathrm{i})} \right) \right) \exp\left\{ -\frac{1}{2} \mathbf{t}^{\mathrm{T}} C \mathbf{t} \right\} \,. \tag{3.35}$$

With the covariance matrix no longer appearing as its inverse in the exponential function we can now easily split it up into contributions from the $\delta^{(\mathrm{i})}$ and $\vec{p}^{\,(\mathrm{i})}$ subspaces. We start with

$$C = \left\langle \left(\vec{d}_j \otimes \vec{e}_j \right) \otimes \left(\vec{d}_k \otimes \vec{e}_k \right) \right\rangle = \left\langle \begin{pmatrix} \delta_j^{(\mathrm{i})} \\ \vec{p}_j^{\,(\mathrm{i})} \end{pmatrix} \otimes \begin{pmatrix} \delta_k^{(\mathrm{i})} \\ \vec{p}_k^{\,(\mathrm{i})} \end{pmatrix} \right\rangle \otimes (\vec{e}_j \otimes \vec{e}_k)$$

$$= \begin{pmatrix} \left\langle \delta_j^{(\mathrm{i})} \delta_k^{(\mathrm{i})} \right\rangle & \left\langle \delta_j^{(\mathrm{i})} \vec{p}_k^{\,(\mathrm{i})} \right\rangle^{\mathrm{T}} \\ \left\langle \vec{p}_j^{\,(\mathrm{i})} \delta_k^{(\mathrm{i})} \right\rangle & \left\langle \vec{p}_j^{\,(\mathrm{i})} \otimes \vec{p}_k^{\,(\mathrm{i})} \right\rangle \end{pmatrix} \otimes E_{jk}$$
$$= \begin{pmatrix} C_{\delta_j \delta_k} & \vec{C}_{\delta_j p_k}^{\mathrm{T}} \\ \vec{C}_{p_j \delta_k} & C_{p_j p_k} \end{pmatrix} \otimes E_{jk} = C_{jk} \otimes E_{jk} \,. \tag{3.36}$$

Observe that $C_{\delta_j \delta_k}$ is a scalar whereas $C_{p_j p_k}$ is a $d \times d$-matrix. We can give some general statements on the entries of C_{jk} due to the homogeneity and isotropy of the Gaussian random field.

- $\vec{C}_{\delta_j p_k} = 0$ for $j = k$. If the momentum of a particle was correlated with the density at its position, there would be a preferred direction for the momentum field contradicting isotropy.
- $(C_{p_j p_k})_{ab} = 0$ for $a \neq b$, else it would be possible that for example in a $d = 3$ dimensional space, particle j having a certain momentum in x-direction makes it more or less likely for particle k having a certain momentum in y-direction. This again would lead to a preferred direction in the initial momentum field.
- Due to the homogeneity expressed in (3.26) and the previous two arguments, for $j = k$ both $C_{p_j p_k}$ and C_{jk} must be diagonal matrices which are spatially constant. Isotropy then further dictates that $C_{p_j p_j} = \sigma_p^2 \mathcal{I}_d$ with some constant velocity dispersion σ_p.

The next step is to write out the argument of the exponential function in (3.35) as

$$\begin{aligned} \mathbf{t}^{\mathrm{T}} C \mathbf{t} &= \left(\vec{t}_i \otimes \vec{e}_i\right)^{\mathrm{T}} \left(C_{jk} \otimes E_{jk}\right) \left(\vec{t}_l \otimes \vec{e}_l\right) = \left(\vec{t}_i \otimes \vec{e}_i\right)^{\mathrm{T}} \left(\left(C_{jk} \vec{t}_l\right) \otimes \left(E_{jk} \vec{e}_l\right)\right) \\ &= \left(\vec{t}_i^{\,\mathrm{T}} C_{jk} \vec{t}_l\right) \left(\vec{e}_i^{\,\mathrm{T}} E_{jk} \vec{e}_l\right) \,. \end{aligned} \tag{3.37}$$

With the help of (1.3) we find

$$\left(\vec{e}_i^{\,\mathrm{T}} E_{jk} \vec{e}_l\right) = \left(\delta_{ai} (\delta_{aj} \delta_{bk}) \delta_{bl}\right) = \delta_{ij} \delta_{kl} \tag{3.38}$$

and thus

$$\begin{aligned} \mathbf{t}^{\mathrm{T}} C \mathbf{t} &= \left(\vec{t}_i^{\,\mathrm{T}} C_{jk} \vec{t}_l\right) \delta_{ij} \delta_{kl} \\ &= \vec{t}_j^{\,\mathrm{T}} C_{jk} \vec{t}_k = t_{\delta_j} C_{\delta_j \delta_k} t_{\delta_k} + t_{\delta_j} \vec{C}_{\delta_j p_k} \cdot \vec{t}_{p_k} + \vec{t}_{p_j} \cdot \vec{C}_{p_j \delta_k} t_{\delta_k} + \vec{t}_{p_j}^{\,\mathrm{T}} C_{p_j p_k} \vec{t}_{p_k} \\ &= t_{\delta_j} C_{\delta_j \delta_k} t_{\delta_k} + 2\, t_{\delta_j} \vec{C}_{\delta_j p_k} \cdot \vec{t}_{p_k} + \vec{t}_{p_j}^{\,\mathrm{T}} C_{p_j p_k} \vec{t}_{p_k} \,, \end{aligned} \tag{3.39}$$

where we have used $\vec{C}_{p_j \delta_k} = \vec{C}_{\delta_k p_j}$ and exchanged the summation indices in the last line. In analogy to (3.36) we now introduce the matrices

$$C_{\delta\delta} = C_{\delta_j \delta_k} \otimes E_{jk} \qquad C_{\delta p} = \vec{C}_{\delta_j p_k}^{\mathrm{T}} \otimes E_{jk} \qquad C_{pp} = C_{p_j p_k} \otimes E_{jk} \tag{3.40}$$

and can then express (3.39) in our tensor notation as

$$\mathbf{t}^{\mathrm{T}} C \mathbf{t} = \mathbf{t}_\delta^{\mathrm{T}} C_{\delta\delta} \mathbf{t}_\delta + 2 \mathbf{t}_\delta^{\mathrm{T}} C_{\delta p} \mathbf{t}_p + \mathbf{t}_p^{\mathrm{T}} C_{pp} \mathbf{t}_p \,. \tag{3.41}$$

We insert this back into (3.35) and rewrite

$$\mathcal{P}(\mathbf{x}^{(\mathrm{i})}) = V^{-N} \int \frac{\mathrm{d}\mathbf{t}_p}{(2\pi)^{dN}} \mathrm{e}^{\mathrm{i}\left\langle \mathbf{t}_p, \mathbf{p}^{(\mathrm{i})} \right\rangle} \exp\left\{ -\frac{1}{2} \mathbf{t}_p^{\mathrm{T}} C_{pp} \mathbf{t}_p \right\} \times \int \frac{\mathrm{d}\mathbf{t}_\delta}{(2\pi)^N} \exp\left\{ -\frac{1}{2} \mathbf{t}_\delta^{\mathrm{T}} C_{\delta\delta} \mathbf{t}_\delta - \mathbf{t}_\delta^{\mathrm{T}} C_{\delta p} \mathbf{t}_p \right\} \times \left(\prod_{j=1}^{N} \int \mathrm{d}\delta_j^{(\mathrm{i})} \left(1 + \delta_j^{(\mathrm{i})}\right) \right) \mathrm{e}^{\mathrm{i}\left\langle \mathbf{t}_\delta, \boldsymbol{\delta}^{(\mathrm{i})} \right\rangle} . \tag{3.42}$$

We will now solve the integrals in this expression line by line starting with the third one. We find

$$\begin{aligned} &\left(\prod_{j=1}^{N} \int \mathrm{d}\delta_j^{(\mathrm{i})} \left(1 + \delta_j^{(\mathrm{i})}\right) \right) \mathrm{e}^{\mathrm{i}\left\langle \mathbf{t}_\delta, \boldsymbol{\delta}^{(\mathrm{i})} \right\rangle} = \prod_{j=1}^{N} \int \mathrm{d}\delta_j^{(\mathrm{i})} \left(1 + \delta_j^{(\mathrm{i})}\right) \mathrm{e}^{\mathrm{i} t_{\delta_j} \delta_j^{(\mathrm{i})}} \\ &= \prod_{j=1}^{N} \int \mathrm{d}z_j \, z_j \, \mathrm{e}^{\mathrm{i} t_{\delta_j}(z_j - 1)} = \prod_{j=1}^{N} \mathrm{e}^{-\mathrm{i} t_{\delta_j}} \int \mathrm{d}z_j \, (-\mathrm{i}) \frac{\partial}{\partial t_{\delta_j}} \mathrm{e}^{\mathrm{i} t_{\delta_j} z_j} \\ &= (-\mathrm{i}2\pi)^N \mathrm{e}^{-\mathrm{i}\langle \mathbf{t}_\delta, \mathbf{1} \rangle} \prod_{j=1}^{N} \frac{\partial}{\partial t_{\delta_j}} \delta_{\mathrm{D}}(t_{\delta_j}) , \end{aligned} \tag{3.43}$$

where no Einstein convention is applied in this calculation. We substituted $z_j = (1 + \delta_j^{(\mathrm{i})})$ in the second line and introduced the tensor $\mathbf{1} = \sum_{j=1}^{N} 1 \otimes \vec{e}_j$ in the last line. We use this result to write down the integral in the second line of (3.42) as

$$\begin{aligned} &\int \frac{\mathrm{d}\mathbf{t}_\delta}{(2\pi)^N} \exp\left\{ -\frac{1}{2} \mathbf{t}_\delta^{\mathrm{T}} C_{\delta\delta} \mathbf{t}_\delta - \mathbf{t}_\delta^{\mathrm{T}} C_{\delta p} \mathbf{t}_p - \mathrm{i} \left\langle \mathbf{t}_\delta, \mathbf{1} \right\rangle \right\} (-\mathrm{i}2\pi)^N \prod_{j=1}^{N} \frac{\partial}{\partial t_{\delta_j}} \delta_{\mathrm{D}}(t_{\delta_j}) \\ &= (-\mathrm{i})^N (-1)^N \int \mathrm{d}\mathbf{t}_\delta \, \delta_{\mathrm{D}}(\mathbf{t}_\delta) \left(\prod_{j=1}^{N} \frac{\partial}{\partial t_{\delta_j}} \right) \exp\left\{ -\frac{1}{2} \mathbf{t}_\delta^{\mathrm{T}} C_{\delta\delta} \mathbf{t}_\delta - \mathbf{t}_\delta^{\mathrm{T}} C_{\delta p} \mathbf{t}_p - \mathrm{i} \left\langle \mathbf{t}_\delta, \mathbf{1} \right\rangle \right\} \\ &= \mathrm{i}^N \left(\prod_{j=1}^{N} \frac{\partial}{\partial t_{\delta_j}} \right) \exp\left\{ -\frac{1}{2} \mathbf{t}_\delta^{\mathrm{T}} C_{\delta\delta} \mathbf{t}_\delta - \mathbf{t}_\delta^{\mathrm{T}} C_{\delta p} \mathbf{t}_p - \mathrm{i} \left\langle \mathbf{t}_\delta, \mathbf{1} \right\rangle \right\} \Bigg|_{\mathbf{t}_\delta = 0} . \end{aligned} \tag{3.44}$$

In the second line we performed N integrations by parts to move all derivatives from the Dirac delta distributions over to the exponential factor. The boundary terms vanish due to the Dirac delta distributions only picking out contributions at $t_{\delta_j} = 0$. In order to see how we can systematically evaluate the derivatives in (3.44) we abbreviate the argument of the exponential as A and look at the effect of the first three derivatives which we also abbreviate as $\partial_1, \partial_2, \partial_3$. We then have

$$\begin{aligned} \partial_1\partial_2\partial_3 \mathrm{e}^A &= \partial_1\partial_2 \left(\mathrm{e}^A (\partial_3 A) \right) = \partial_1 \left(\mathrm{e}^A (\partial_2 A)(\partial_3 A) + \mathrm{e}^A (\partial_2\partial_3 A) \right) \\ &= \left(\mathrm{e}^A (\partial_1 A)(\partial_2 A)(\partial_3 A) \right) + \left(\mathrm{e}^A (\partial_1\partial_2 A)(\partial_3 A) \right) + \left(\mathrm{e}^A (\partial_2 A)(\partial_1\partial_3 A) \right) \\ &\quad + \left(\mathrm{e}^A (\partial_1 A)(\partial_2\partial_3 A) \right) + \left(\mathrm{e}^A (\partial_1\partial_2\partial_3 A) \right) . \end{aligned} \tag{3.45}$$

However, we know that A depends on the t_{δ_j} only up to quadratic order, so any of its third order derivatives vanish. We will thus only need to consider

$$\frac{\partial}{\partial t_{\delta_j}}\left(-\frac{1}{2}\mathbf{t}_\delta^{\mathrm{T}} C_{\delta\delta}\mathbf{t}_\delta - \mathbf{t}_\delta^{\mathrm{T}} C_{\delta p}\mathbf{t}_p - \mathrm{i}\left\langle \mathbf{t}_\delta, \mathbf{1}\right\rangle\right)\Bigg|_{\mathbf{t}_\delta=0} = -\mathrm{i}(1 - \mathrm{i}\vec{C}_{\delta_j p_n}\cdot\vec{t}_{p_n})\,, \tag{3.46}$$

$$\frac{\partial}{\partial t_{\delta_j}}\frac{\partial}{\partial t_{\delta_k}}\left(-\frac{1}{2}\mathbf{t}_\delta^{\mathrm{T}} C_{\delta\delta}\mathbf{t}_\delta - \mathbf{t}_\delta^{\mathrm{T}} C_{\delta p}\mathbf{t}_p - \mathrm{i}\left\langle \mathbf{t}_\delta, \mathbf{1}\right\rangle\right)\Bigg|_{\mathbf{t}_\delta=0} = -C_{\delta_j\delta_k} = (-\mathrm{i})^2 C_{\delta_j\delta_k}\,. \tag{3.47}$$

From these two equations we see that every derivative leads to a factor of $-\mathrm{i}$ and since every term in (3.44) consists of N derivatives the prefactor i^N is canceled. Starting from (3.45) we find by induction that the entire expression (3.44) takes the form of the polynomial

$$\begin{aligned}\mathcal{C}(\mathbf{t}_p) &= \mathrm{i}^N\left(\prod_{j=1}^{N}\frac{\partial}{\partial t_{\delta_j}}\right)\exp\left\{-\frac{1}{2}\mathbf{t}_\delta^{\mathrm{T}} C_{\delta\delta}\mathbf{t}_\delta - \mathbf{t}_\delta^{\mathrm{T}} C_{\delta p}\mathbf{t}_p - \mathrm{i}\left\langle \mathbf{t}_\delta, \mathbf{1}\right\rangle\right\}\Bigg|_{\mathbf{t}_\delta=0}\\ &= \prod_{n=1}^{N}\left(1 - \mathrm{i}\sum_{\substack{m=1\\ m\neq n}}^{N}\vec{C}_{\delta_n p_m}\cdot\vec{t}_{p_m}\right) + \sum_{\{i,j\}} C_{\delta_i\delta_j}\prod_{\{n\}'}\left(1 - \mathrm{i}\sum_{\substack{m=1\\ m\neq n}}^{N}\vec{C}_{\delta_l p_m}\cdot\vec{t}_{p_m}\right)\\ &\quad + \sum_{\{\{i,j\},\{k,l\}\}'} C_{\delta_i\delta_j}C_{\delta_k\delta_l}\prod_{\{n\}'}\left(1 - \mathrm{i}\sum_{\substack{m=1\\ m\neq n}}^{N}\vec{C}_{\delta_l p_m}\cdot\vec{t}_{p_m}\right) + \dots\end{aligned} \tag{3.48}$$

The fact that in every term of $\mathcal{C}$ each particle index that originates from one of the derivatives may only appear once has numerous consequences. The first is that the sum $\sum_{\{i,j\}}$ runs over all *distinct pairs* of particle indices. For example $\{1,2\}$ and $\{2,1\}$ are not distinct and thus only one of them appears in the sum. Which one is used is arbitrary due to the symmetry of $C_{\delta_i\delta_j}$. On the other hand, $\{1,2\}$ and $\{1,3\}$ are distinct. The second consequence is encoded in the prime on the index $\{n\}'$ of the product in the second term. It means that the indices i,j of the preceding sum are excluded from the product for every term of the sum. The restriction $n \neq m$ on the inner sum is in contrast the consequence of $\vec{C}_{\delta_n p_n} = 0$. In the second line we now have a sum over the distinct 2-tupels of distinct pairs. We call n-tupels $\{\{i_1,j_1\},\dots,\{i_n,j_n\}\}$ of pairs distinct in the sense that for the example of the 2-tupel, $\{\{1,2\},\{3,4\}\}$ and $\{\{4,3\},\{2,1\}\}$ are not distinct, while $\{\{1,2\},\{3,4\}\}$ and $\{\{1,3\},\{2,4\}\}$ are. Since any particle index may appear only once no particle index may be shared between any two pairs of an n-tupel, i. e. $\{\{1,2\},\{2,3\}\}$ does not occur. This is again encoded by the prime on the tupel. The prime on the product index now means that for every term of the sum over tupels of pairs all four indices i,j,k,l in the union of the pairs are excluded. This scheme continues until there are $\lfloor N/2\rfloor$ factors of $C_{\delta_i\delta_j}$.

We stress that $\mathcal{C}(\mathbf{t}_p)$ is a quantity that is purely polynomial in the $\vec{t}_{p_j}$ and consequently also in $\mathbf{t}_p$. If we now insert $\mathcal{C}(\mathbf{t}_p)$ into (3.42) for the last two lines, we can rewrite the initial phase-space probability density as

$$\begin{aligned}
\mathcal{P}(\mathbf{x}^{(\mathrm{i})}) &= V^{-N} \int \frac{\mathrm{d}\mathbf{t}_p}{(2\pi)^{dN}} \, \mathrm{e}^{\mathrm{i}\langle \mathbf{t}_p, \mathbf{p}^{(\mathrm{i})} \rangle} \mathcal{C}(\mathbf{t}_p) \exp\left\{ -\frac{1}{2} \mathbf{t}_p^{\mathrm{T}} C_{pp} \mathbf{t}_p \right\} \\
&= V^{-N} \int \frac{\mathrm{d}\mathbf{t}_p}{(2\pi)^{dN}} \left(\mathcal{C}\left(\frac{\partial}{\mathrm{i}\partial \mathbf{p}^{(\mathrm{i})}} \right) \mathrm{e}^{\mathrm{i}\langle \mathbf{t}_p, \mathbf{p}^{(\mathrm{i})} \rangle} \right) \exp\left\{ -\frac{1}{2} \mathbf{t}_p^{\mathrm{T}} C_{pp} \mathbf{t}_p \right\} \\
&= V^{-N} \, \mathcal{C}\left(\frac{\partial}{\mathrm{i}\partial \mathbf{p}^{(\mathrm{i})}} \right) \int \frac{\mathrm{d}\mathbf{t}_p}{(2\pi)^{dN}} \, \mathrm{e}^{\mathrm{i}\langle \mathbf{t}_p, \mathbf{p}^{(\mathrm{i})} \rangle} \exp\left\{ -\frac{1}{2} \mathbf{t}_p^{\mathrm{T}} C_{pp} \mathbf{t}_p \right\} \\
&= \frac{V^{-N}}{\sqrt{(2\pi)^{dN} \det C_{pp}}} \, \mathcal{C}\left(\frac{\partial}{\mathrm{i}\partial \mathbf{p}^{(\mathrm{i})}} \right) \exp\left\{ -\frac{1}{2} \mathbf{p}^{(\mathrm{i})\mathrm{T}} C_{pp}^{-1} \mathbf{p}^{(\mathrm{i})} \right\} . \qquad (3.49)
\end{aligned}$$

This is our final and exact result for the initial phase-space probability density of a canonical ensemble of N particles in a volume V representing a combined density-momentum field which is a Gaussian random field. If we compare this with our result (3.21) for the ideal gas we can make some interesting observations.

- The uncorrelated Maxwell-Boltzmann distribution P_{σ_p} for individual particles has been replaced by a joint multivariate Gaussian distribution containing correlations between the momenta of all particles. If we turn off the momentum correlations between different particles, i. e. $C_{p_j p_k} = 0$ for $j \neq k$, then according to the arguments following (3.36) we reduce to the Maxwell-Boltzmann case.

- The uniform distribution of the particles in configuration space has been replaced by a statistically homogeneous distribution with correlations between particle positions encoded in the density correlations $C_{\delta_j \delta_k}$, which appear in the polynomial $\mathcal{C}$. This polynomial also contains the cross-correlations between positions and momenta of different particles encoded by the density-momentum correlations $\vec{C}_{\delta_j p_k}$.

- The derivative $\partial / \partial \mathbf{p}^{(\mathrm{i})}$ always appears together with the cross correlations and takes down factors of pure momentum correlations. This allows for density correlations between two particle positions to be mitigated through momentum correlations between intermediate positions. If we turn off all correlations involving density in addition to the momentum cross correlations we fall back to the ideal gas case.

3.3 GENERATING FUNCTIONAL FOR A GAUSSIAN RANDOM FIELD

We now want to insert our result (3.49) for the initial phase-space probability density describing a Gaussian random density-momentum field into the canonical generating functional (2.54). As a first step we will show that the generating functional can be brought into a form where the effects of initial correlations are expressed as operators acting on the generating functional of an ideal gas. In order to organise the various terms in these operators more easily we will introduce a simple yet very effective

diagrammatic language. After that we will combine these diagrams with a technique called the *Mayer cluster expansion* which allows us to treat the combinatorics of the N correlated particles in a systematic way. The result of the cluster expansion will be crucial for calculating the grand canonical generating functional later on.

3.3.1 *Initial correlations as operators*

We first write down the full canonical generating functional

$$Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}] = \mathrm{e}^{\mathrm{i}\hat{S}_I}\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}} \int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\, V^{-N}\mathcal{N}_p\, \mathcal{C}\left(\frac{\partial}{\mathrm{i}\partial\mathbf{p}^{(\mathrm{i})}}\right) \exp\left\{-\frac{1}{2}\mathbf{p}^{(\mathrm{i})\mathrm{T}} C_{pp}^{-1}\mathbf{p}^{(\mathrm{i})}\right\} \\ \times \int_{\mathrm{i}} \mathcal{D}\mathbf{x} \int \mathcal{D}\boldsymbol{\chi} \exp\left\{\mathrm{i}(S_0[\mathbf{x},\boldsymbol{\chi}] + \mathbf{J}\cdot\mathbf{x} + \mathbf{K}\cdot\boldsymbol{\chi})\right\} \ , \tag{3.50}$$

where we defined the normalisation factor for the Gaussian momentum distribution as

$$\mathcal{N}_p := \frac{1}{\sqrt{(2\pi)^{dN}\det C_{pp}}} = \mathcal{N}_p(\mathbf{q}^{(\mathrm{i})}) \ . \tag{3.51}$$

In order to make any progress we need the explicit dependence of the second line in (3.50) on the initial phase-space coordinates. We obtained this solution in (2.67) and we remind the reader that

$$Z_0^{(N)}[\mathbf{J},\mathbf{K}] := \int_{\mathrm{i}} \mathcal{D}\mathbf{x} \int \mathcal{D}\boldsymbol{\chi} \exp\left\{\mathrm{i}(S_0[\mathbf{x},\boldsymbol{\chi}] + \mathbf{J}\cdot\mathbf{x} + \mathbf{K}\cdot\boldsymbol{\chi})\right\} \\ = \exp\left\{\mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t\, \left\langle \mathbf{J}(t), \boldsymbol{\mathcal{G}}(t,t_\mathrm{i})\,\mathbf{x}^{(\mathrm{i})}\right\rangle - \mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \int_{t_\mathrm{i}}^{t} \mathrm{d}t'\, \left\langle \mathbf{J}(t), \boldsymbol{\mathcal{G}}(t,t')\mathbf{K}(t')\right\rangle\right\} \tag{3.52}$$

is an exact equality for the purely dynamical and unaveraged part of the free N-particle generating functional. For the following calculations it will be convenient to define the 'time-averaged' sources

$$\bar{\mathbf{J}}_q = \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t\ \mathbf{J}(t)^{\mathrm{T}}\,\boldsymbol{\mathcal{G}}(t,t_\mathrm{i})\,\boldsymbol{\mathcal{P}}_q \quad \text{and} \quad \bar{\mathbf{J}}_p = \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t\ \mathbf{J}(t)^{\mathrm{T}}\,\boldsymbol{\mathcal{G}}(t,t_\mathrm{i})\,\boldsymbol{\mathcal{P}}_p \ , \tag{3.53}$$

where the projection operators

$$\boldsymbol{\mathcal{P}}_q = \begin{pmatrix} \mathcal{I}_d \\ 0_d \end{pmatrix} \otimes \mathcal{I}_N \quad \text{and} \quad \boldsymbol{\mathcal{P}}_p = \begin{pmatrix} 0_d \\ \mathcal{I}_d \end{pmatrix} \otimes \mathcal{I}_N \tag{3.54}$$

take care of selecting either the position or the momentum subspace. With these we can rewrite

$$\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t\ \left\langle \mathbf{J}(t), \boldsymbol{\mathcal{G}}(t,t_\mathrm{i})\,\mathbf{x}^{(\mathrm{i})}\right\rangle = \left\langle \bar{\mathbf{J}}_q, \mathbf{q}^{(\mathrm{i})}\right\rangle + \left\langle \bar{\mathbf{J}}_p, \mathbf{p}^{(\mathrm{i})}\right\rangle \ . \tag{3.55}$$

The generating functional then takes the form

$$Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}] = \mathrm{e}^{\mathrm{i}\hat{S}_I}\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}}\int \mathrm{d}\mathbf{q}^{(\mathrm{i})}\int \mathrm{d}\mathbf{p}^{(\mathrm{i})}\,\frac{\mathcal{N}_p}{V^N}\,\mathcal{C}\left(\frac{\partial}{\mathrm{i}\partial\mathbf{p}^{(\mathrm{i})}}\right)\exp\left\{-\frac{1}{2}{\mathbf{p}^{(\mathrm{i})}}^{\mathrm{T}}C_{pp}^{-1}\mathbf{p}^{(\mathrm{i})}\right\}$$
$$\times\exp\left\{\mathrm{i}\left\langle\bar{\mathbf{J}}_q,\mathbf{q}^{(\mathrm{i})}\right\rangle+\mathrm{i}\left\langle\bar{\mathbf{J}}_p,\mathbf{p}^{(\mathrm{i})}\right\rangle-\mathrm{i}\,S_K[\mathbf{J},\mathbf{K}]\right\}\,. \tag{3.56}$$

Our first step is to perform the appropriate number of integrations by parts to move all derivatives w. r. t. the initial momenta $\mathbf{p}^{(\mathrm{i})}$ in the polynomial $\mathcal{C}$ from the Gaussian exponential containing C_{pp}^{-1} over to the phase factor containing $\bar{\mathbf{J}}_p$. For each instance of $\mathbf{p}^{(\mathrm{i})}$ we pick up a minus sign in the process. All boundary terms are taken at infinite momenta and vanish becuase C_{pp}^{-1} is positive definite and so must be all of its two-point submatrices, since all of them define Gaussian random fields. On the boundaries, the Gaussian exponential will thus always tend to zero faster than any divergent term in the polynomial $\mathcal{C}$ and the phase factor $\mathrm{e}^{\mathrm{i}\left\langle\bar{\mathbf{J}}_p,\mathbf{p}^{(\mathrm{i})}\right\rangle}$ has an absolute value of unity. Once all derivatives have been transferred we may execute them to find

$$\begin{aligned}
&\int \mathrm{d}\mathbf{p}^{(\mathrm{i})}\exp\left\{\mathrm{i}\left\langle\bar{\mathbf{J}}_p,\mathbf{p}^{(\mathrm{i})}\right\rangle\right\}\mathcal{N}_p\,\mathcal{C}\left(\frac{\partial}{\mathrm{i}\partial\mathbf{p}^{(\mathrm{i})}}\right)\exp\left\{-\frac{1}{2}{\mathbf{p}^{(\mathrm{i})}}^{\mathrm{T}}C_{pp}^{-1}\mathbf{p}^{(\mathrm{i})}\right\}\\
&=\int \mathrm{d}\mathbf{p}^{(\mathrm{i})}\,\mathcal{C}\left(-\bar{\mathbf{J}}_p\right)\exp\left\{\mathrm{i}\left\langle\bar{\mathbf{J}}_p,\mathbf{p}^{(\mathrm{i})}\right\rangle\right\}\mathcal{N}_p\exp\left\{-\frac{1}{2}{\mathbf{p}^{(\mathrm{i})}}^{\mathrm{T}}C_{pp}^{-1}\mathbf{p}^{(\mathrm{i})}\right\}\\
&=\mathcal{C}\left(-\bar{\mathbf{J}}_p\right)\exp\left\{-\frac{1}{2}\,\bar{\mathbf{J}}_p^{\mathrm{T}}\,C_{pp}\,\bar{\mathbf{J}}_p\right\}\,.
\end{aligned} \tag{3.57}$$

In the last line we performed a Fourier transform. This has two convenient consequences. We get rid of the normalisation factor $\mathcal{N}_p$ and the momentum covariance matrix C_{pp} now appears linearly in the exponential. In the N dimensional space of particle indices, we now split this matrix into its diagonal and off-diagonal part as

$$C_{pp} = \left(\sum_{j=k}+\sum_{j\neq k}\right)C_{p_jp_k}\otimes E_{jk} = \left(\sigma_p^2\,\mathcal{I}_d\right)\otimes\mathcal{I}_N+\sum_{j\neq k}C_{p_jp_k}\otimes E_{jk}\,. \tag{3.58}$$

We define the momentum cross-correlation matrix

$$C_{pp}^{\times} = \sum_{j\neq k}C_{p_jp_k}\otimes E_{jk} \tag{3.59}$$

and rewrite the Gaussian exponential

$$\exp\left\{-\frac{1}{2}\,\bar{\mathbf{J}}_p^{\mathrm{T}}\,C_{pp}\,\bar{\mathbf{J}}_p\right\} = \exp\left\{-\frac{1}{2}\,\bar{\mathbf{J}}_p^{\mathrm{T}}\,C_{pp}^{\times}\,\bar{\mathbf{J}}_p\right\}\exp\left\{-\frac{1}{2}\,\bar{\mathbf{J}}_p^{\mathrm{T}}\left(\sigma_p^2\,\mathcal{I}_d\otimes\mathcal{I}_N\right)\bar{\mathbf{J}}_p\right\}\,. \tag{3.60}$$

For the second factor containing the diagonal part, we now reverse the Fourier transform

$$\begin{aligned}
\exp\left\{-\frac{1}{2}\,\bar{\mathbf{J}}_p^{\mathrm{T}}\left(\sigma_p^2\,\mathcal{I}_d\otimes\mathcal{I}_N\right)\bar{\mathbf{J}}_p\right\} &= \int \mathrm{d}\mathbf{p}^{(\mathrm{i})}\,\frac{\exp\left\{\frac{\left\langle\mathbf{p}^{(\mathrm{i})},\mathbf{p}^{(\mathrm{i})}\right\rangle}{2\sigma_p^2}\right\}}{\sqrt{(2\pi\sigma_p^2)^{dN}}}\exp\left\{\mathrm{i}\left\langle\bar{\mathbf{J}}_p,\mathbf{p}^{(\mathrm{i})}\right\rangle\right\}\\
&=\int \mathrm{d}\mathbf{p}^{(\mathrm{i})}\,P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})})\exp\left\{\mathrm{i}\left\langle\bar{\mathbf{J}}_p,\mathbf{p}^{(\mathrm{i})}\right\rangle\right\}\,.
\end{aligned} \tag{3.61}$$

We have identified the Maxwell-Boltzmann distribution P_{σ_p}. This should not be a surprise since we started from a Gaussian random momentum field and just separated off the diagonal part which in the homogeneous and isotropic case is unaffected by correlations and must thus reduce to the special case of a Maxwell-Boltzmann distribution. Reversing the Fourier transform might seem to be a step backwards since it reintroduces an integration we already got rid of. We will see in a moment why this is desirable. Let us first write down the complete generating functional in its present state

$$\begin{aligned} Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}] = \mathrm{e}^{\mathrm{i}\hat{S}_I}\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}}\mathcal{C}\left(-\bar{\mathbf{J}}_p\right)\exp\left\{-\frac{1}{2}\,\bar{\mathbf{J}}_p^{\mathrm{T}}\,C_{pp}^{\times}\,\bar{\mathbf{J}}_p\right\}\int \mathrm{d}\mathbf{q}^{(\mathrm{i})}\int \mathrm{d}\mathbf{p}^{(\mathrm{i})}\,V^{-N}P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})}) \\ \times\exp\left\{\mathrm{i}\left\langle\bar{\mathbf{J}}_q,\mathbf{q}^{(\mathrm{i})}\right\rangle+\mathrm{i}\left\langle\bar{\mathbf{J}}_p,\mathbf{p}^{(\mathrm{i})}\right\rangle-\mathrm{i}\,S_K[\mathbf{J},\mathbf{K}]\right\}\,. \end{aligned} \tag{3.62}$$

For the final step we first need to recognize that

$$\begin{aligned} \frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_{\mathrm{i}})}\exp\left\{-\mathrm{i}\,S_K[\mathbf{J},\mathbf{K}]\right\} &= \frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_{\mathrm{i}})}\exp\left\{-\mathrm{i}\int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}}\mathrm{d}t\int_{t_{\mathrm{i}}}^{t}\mathrm{d}t'\,\left\langle\mathbf{J}(t),\boldsymbol{\mathcal{G}}(t,t')\mathbf{K}(t')\right\rangle\right\} \\ &= \left(-\mathrm{i}\int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}}\mathrm{d}t\int_{t_{\mathrm{i}}}^{t}\mathrm{d}t'\,\mathbf{J}(t)^{\mathrm{T}}\,\boldsymbol{\mathcal{G}}(t,t')\,\boldsymbol{\mathcal{P}}_p\,\delta_{\mathrm{D}}\left(t'-t_{\mathrm{i}}\right)\right) \\ &\quad\times\exp\left\{-\mathrm{i}\int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}}\mathrm{d}t\int_{t_{\mathrm{i}}}^{t}\mathrm{d}t'\,\left\langle\mathbf{J}(t),\boldsymbol{\mathcal{G}}(t,t')\mathbf{K}(t')\right\rangle\right\} \\ &= -\bar{\mathbf{J}}_p\exp\left\{-\mathrm{i}\,S_K[\mathbf{J},\mathbf{K}]\right\}\,, \end{aligned} \tag{3.63}$$

and we can consequently write

$$\begin{aligned} &\mathcal{C}\left(-\bar{\mathbf{J}}_p\right)\exp\left\{-\frac{1}{2}\,\bar{\mathbf{J}}_p^{\mathrm{T}}\,C_{pp}^{\times}\,\bar{\mathbf{J}}_p\right\}\exp\left\{-\mathrm{i}\,S_K[\mathbf{J},\mathbf{K}]\right\} \\ &=\hat{\mathcal{C}}\left(\frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_{\mathrm{i}})}\right)\exp\left\{-\frac{1}{2}\left(\frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_{\mathrm{i}})}\right)^{\mathrm{T}}C_{pp}^{\times}\left(\frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_{\mathrm{i}})}\right)\right\}\exp\left\{-\mathrm{i}\,S_K[\mathbf{J},\mathbf{K}]\right\}\,, \end{aligned} \tag{3.64}$$

where the hat on $\hat{\mathcal{C}}$ signals that we now have an operator expressing correlations. We define a total correlation operator

$$\hat{\mathcal{C}}_{\mathrm{tot}}\left(\frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_{\mathrm{i}})}\right) := \hat{\mathcal{C}}\left(\frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_{\mathrm{i}})}\right)\exp\left\{-\frac{1}{2}\left(\frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_{\mathrm{i}})}\right)^{\mathrm{T}}C_{pp}^{\times}\left(\frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_{\mathrm{i}})}\right)\right\} \tag{3.65}$$

and can now rewrite the generating functional as

$$\begin{aligned} Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}] &= \mathrm{e}^{\mathrm{i}\hat{S}_I}\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}}\int \mathrm{d}\mathbf{q}^{(\mathrm{i})}\int \mathrm{d}\mathbf{p}^{(\mathrm{i})}\,\hat{\mathcal{C}}_{\mathrm{tot}}V^{-N}P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})}) \\ &\quad\times\exp\left\{\mathrm{i}\left\langle\bar{\mathbf{J}}_q,\mathbf{q}^{(\mathrm{i})}\right\rangle+\mathrm{i}\left\langle\bar{\mathbf{J}}_p,\mathbf{p}^{(\mathrm{i})}\right\rangle-\mathrm{i}\,S_K[\mathbf{J},\mathbf{K}]\right\} \\ &= \mathrm{e}^{\mathrm{i}\hat{S}_I}\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}}\hat{\mathcal{C}}_{\mathrm{tot}}\int \mathrm{d}\mathbf{q}^{(\mathrm{i})}\int \mathrm{d}\mathbf{p}^{(\mathrm{i})}\,V^{-N}P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})}) \\ &\quad\times\int_{\mathrm{i}}\mathcal{D}\mathbf{x}\int\mathcal{D}\boldsymbol{\chi}\exp\left\{\mathrm{i}(S_0[\mathbf{x},\boldsymbol{\chi}]+\mathbf{J}\cdot\mathbf{x}+\mathbf{K}\cdot\boldsymbol{\chi})\right\}\,. \end{aligned} \tag{3.66}$$

We have used (3.55) and then (3.52) to reintroduce the path integrals. It is at this point that reversing the Fourier transform in (3.61) pays off. Without it we could not have reobtained the second expression since we would be missing the integral over initial momenta and the corresponding phase factor. The advantage of the second expression is that we may now again freely exchange functional derivatives w. r. t. the sources $\mathbf{J}$,$\mathbf{K}$ with $\mathbf{x}, \boldsymbol{\chi}$. This has been used implicitly to pull the correlation operator out in front of the integrals over initial phase-space coordinates. To do so we have assumed that all three two-point correlation quantities $C_{\delta_i\delta_j}, \vec{C}_{\delta_i p_j}, C^{\times}_{p_i p_j}$ are analytic functions and replaced their dependence on the initial positions by functional derivatives as

$$C_{\delta_i\delta_j}(\vec{q}_i^{\,(\mathrm{i})}, \vec{q}_j^{\,(\mathrm{i})}) \longrightarrow \hat{C}_{\delta_i\delta_j}\left(\frac{\delta}{\mathrm{i}\delta\vec{J}_{q_i}(t_\mathrm{i})}, \frac{\delta}{\mathrm{i}\delta\vec{J}_{q_j}(t_\mathrm{i})}\right) , \tag{3.67}$$

turning all three of them into operators in the process. In contrast, when performing the Mayer cluster expansion later it will be convenient to express everything in terms of $\mathbf{x}, \boldsymbol{\chi}$ and turn off the sources $\mathbf{J}, \mathbf{K}$ temporarily. We now define the canonical generating functional of an ideal gas as

$$Z_\mathrm{C}^\mathrm{id}[H, \mathbf{J}, \mathbf{K}] := \mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}} \int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\, V^{-N} P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})}) \int_\mathrm{i} \mathcal{D}\mathbf{x} \int \mathcal{D}\boldsymbol{\chi} \exp\left\{\mathrm{i}(S_0[\mathbf{x}, \boldsymbol{\chi}] + \mathbf{J}\cdot\mathbf{x} + \mathbf{K}\cdot\boldsymbol{\chi})\right\} \tag{3.68}$$

and can thus write the canonical generating functional of an interacting gas whose initial density and momentum field is a homogeneous and isotropic Gaussian random field in the very concise form

$$Z_\mathrm{C}[H, \mathbf{J}, \mathbf{K}] = \mathrm{e}^{\mathrm{i}\hat{S}_I}\, \hat{\mathcal{C}}_\mathrm{tot}\, Z_\mathrm{C}^\mathrm{id}[H, \mathbf{J}, \mathbf{K}] \,. \tag{3.69}$$

With this very nice result in hand, a few remarks are in order:

- The fact that the covariance matrix (3.36) and all correlations therein do not depend on the momenta of the particles but only on their position was crucial in deriving the above result, especially for the steps in (3.57). As mentioned before this relates to the fact that we assume to know the initial momentum field of the system. If it is not possible to describe the initial state of the system in such a way, finding an analogue of (3.69) is potentially much more difficult.

- In treating the initial correlations we repeated the same logic that we used for the interactions between the particles: Identify the source dependent generating functional of a system that we can treat exactly and obtain the case we are actually interested in by acting with operators which induce the corrections to the exact case. By identifying some ordering parameter we can then also treat the initial correlations in a perturbative manner.

- Note that we could have included the self-correlation of the particle momenta into $\hat{\mathcal{C}}_\mathrm{tot}$. The exact case would then be a collection of particles uniformly distributed in space but without any momentum since we would need to replace

the Maxwell-Boltzmann distribution as $P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})}) \to \delta_{\mathrm{D}}(\mathbf{p}^{(\mathrm{i})})$. We did not do so because the ideal gas is the standard starting point in perturbative approaches to treating the exact dynamics of a collection of particles. Furthermore it eliminates any self-correlations from $\hat{\mathcal{C}}_{\mathrm{tot}}$ which will be convenient for formulating our diagrammatic language for the initial correlations.

- We already mentioned in section 2.5.1 that the source $\mathbf{K}$ allows us to generate deviations from the free trajectories of the particles. It is thus not surprising that $\hat{\mathcal{C}}_{\mathrm{tot}}$ is defined in terms of functional derivatives w. r. t. $\mathbf{K}_p$ since for an isolated system any initial correlations involving the momenta of particles must come from earlier interactions between the particles.

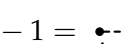
3.3.2 *A diagrammatic language for initial correlations*

When calculating correlators or cumulants of collective fields we still have to treat the initial correlation operator $\hat{\mathcal{C}}_{\mathrm{tot}}$ on the level of all the individual particles for each of its terms. While one can identify certain configurations of the three different correlation quantities defined in (3.36) that will give the same contribution due to the integration over the initial positions of all particles, it quickly becomes so cumbersome to identify and count these configurations by actually writing them down that it just is impractical to do so for higher order correlations. We will thus introduce diagrams representing the three different kinds of correlations $C_{\delta_j\delta_k}, \vec{C}_{\delta_j p_k}, C_{p_j p_k}$ and deduce rules how we may combine them from the form of $\hat{\mathcal{C}}_{\mathrm{tot}}$. The resulting compound diagrams will make it much easier to identify equivalent configurations visually and count them using topological arguments. We start with the Gaussian exponential part in (3.65). We rewrite it in terms of individual particles as

$$\begin{aligned}
&\exp\left\{-\frac{1}{2}\left(\frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_\mathrm{i})}\right)^{\mathrm{T}}\hat{C}^{\times}_{pp}\left(\frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_\mathrm{i})}\right)\right\}\\
&= \exp\left\{-\frac{1}{2}\sum_{j=1}^{N}\sum_{\substack{k=1\\k\neq j}}^{N}\left(\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_j}(t_\mathrm{i})}\right)^{\mathrm{T}}\hat{C}^{\times}_{p_j p_k}\left(\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_k}(t_\mathrm{i})}\right)\right\}\\
&= \exp\left\{-\sum_{\{j,k\}}\left(\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_j}(t_\mathrm{i})}\right)^{\mathrm{T}}\hat{C}^{\times}_{p_j p_k}\left(\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_k}(t_\mathrm{i})}\right)\right\}\\
&= \prod_{\{j,k\}}\left[1+\left(\exp\left\{-\left(\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_j}(t_\mathrm{i})}\right)^{\mathrm{T}}\hat{C}^{\times}_{p_j p_k}\left(\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_k}(t_\mathrm{i})}\right)\right\}-1\right)\right]\,. \qquad (3.70)
\end{aligned}$$

We used (3.59) in the second line and the symmetry $C_{p_j p_k} = C_{p_k p_j}$ in the third line. The pairs $\{j,k\}$ are again those which are *distinct* in the same sense as explained following (3.48). In the last line we inserted a zero into every factor of the product. We now define our first diagram as the operator valued quantity

$$\hat{C}_{p_j p_k} := \exp\left\{-\left(\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_j}(t_\mathrm{i})}\right)^{\mathrm{T}}\hat{C}^{\times}_{p_j p_k}\left(\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_k}(t_\mathrm{i})}\right)\right\}-1 = \quad . \qquad (3.71)$$



The dashed line represents the general form of the operator and the dots represent those particles with their indices for which this general operator form is evaluated. Next we write out the last line of (3.70)

$$\prod_{\{i,j\}} \left(1 + \hat{C}_{p_i p_j}\right) = 1 + \sum_{\{i,j\}} \hat{C}_{p_i p_j} + \sum_{\{\{i,j\},\{k,l\}\}^\star} \hat{C}_{p_i p_j} \hat{C}_{p_k p_l} + \sum_{\{\{i,j\},\{k,l\},\{m,n\}\}^\star} \hat{C}_{p_i p_j} \hat{C}_{p_k p_l} \hat{C}_{p_m p_n} + \dots \,. \tag{3.72}$$

This way of rewriting the Gaussian exponential is actually the first step in performing the Mayer cluster expansion discussed in the next section. Just like for the correlation polynomial defined in (3.48) we again encounter sums over distinct n-tupels of distinct pairs. The only difference is that we have another, less restrictive exclusion rule encoded in the star on the tupel. It means that only *equivalent pairs* are excluded. For example, in (3.72) there are terms like $\hat{C}_{p_1 p_2} \hat{C}_{p_2 p_3}$ but a comparable term $C_{\delta_1 \delta_2} C_{\delta_2 \delta_3}$ does not appear in (3.48). In our diagrammatic language we would write (3.72) as

$$\prod_{\{i,j\}} \left(1 + \; i \;\text{-----}\; j\right) = 1 + \sum_{\{i,j\}} i \;\text{-----}\; j + \sum_{\{\{i,j\},\{k,l\}\}^\star} i \;\text{-----}\; j \;\times\; k \;\text{-----}\; l + \sum_{\{\{i,j\},\{k,l\},\{m,n\}\}^\star} i \;\text{-----}\; j \;\times\; k \;\text{-----}\; l \;\times\; m \;\text{-----}\; n + \dots \tag{3.73}$$

We now want to rewrite the somewhat inconvenient sums over n-tupels of particle pairs into sums over distinct m-tupels $\{i_1, \dots, i_m\}$ of particles. We thus need to make explicit how many particles are actually present in each term of the sums. This can be done by going through all possibilities how indices of the different two-particle lines can be identified with each other. In the diagram language this means that we have to collect all possibilities how we can glue the two-particle lines together. For the double sum in the first line of (3.73) we have to distinguish three principal cases of topology:

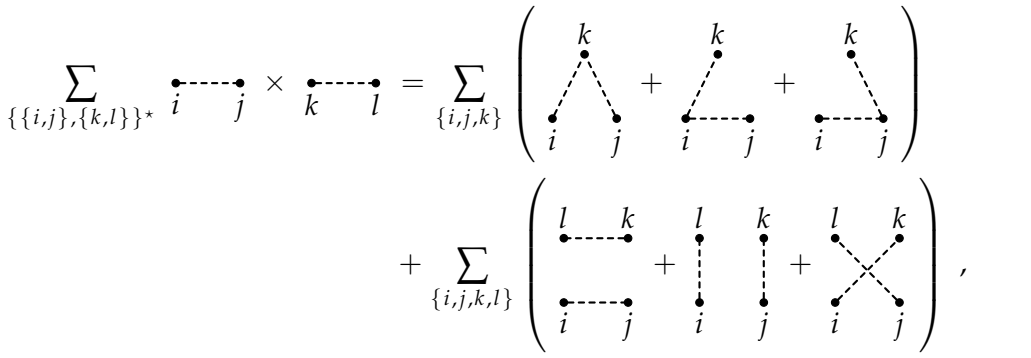
$$i \;\text{-----}\; j \;\times\; i \;\text{-----}\; j \;=\; i \;\text{-----}\!\bigcirc\!\text{-----}\; j \,, \qquad i \;\text{-----}\; k \;\times\; k \;\text{-----}\; j \;=\; \begin{array}{ccc} & k & \\ \diagup & & \diagdown \\ i & & j \end{array} \,,$$

$$i \;\text{-----}\; j \;\times\; k \;\text{-----}\; l \;=\; \begin{array}{c} k \;\text{-----}\; l \\ \\ i \;\text{-----}\; j \end{array} \,. \tag{3.74}$$

Note that for the third case we implicitly understand a product sign to be present between the two disconnected parts of the diagram on the RHS. The rule encoded in the stars in (3.73) excludes equal pairs of particles and thus the corresponding first subdiagram in (3.74) may not appear in any term. We formulate this as a general rule for drawing any kind of diagram involving the line type defined in (3.71).

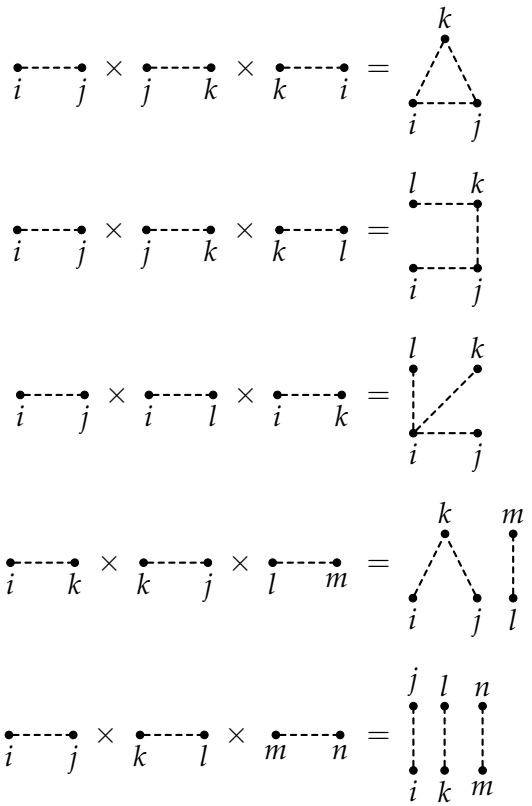
p-LINE RULE : Any pair of distinct particles i and j may at most be connected by one $\hat{C}_{p_i p_j} = i \;\text{-----}\; j$ line. This means that the subdiagram $i \;\text{-----}\!\bigcirc\!\text{-----}\; j$ is *forbidden*.

The complete double sum can then be written as



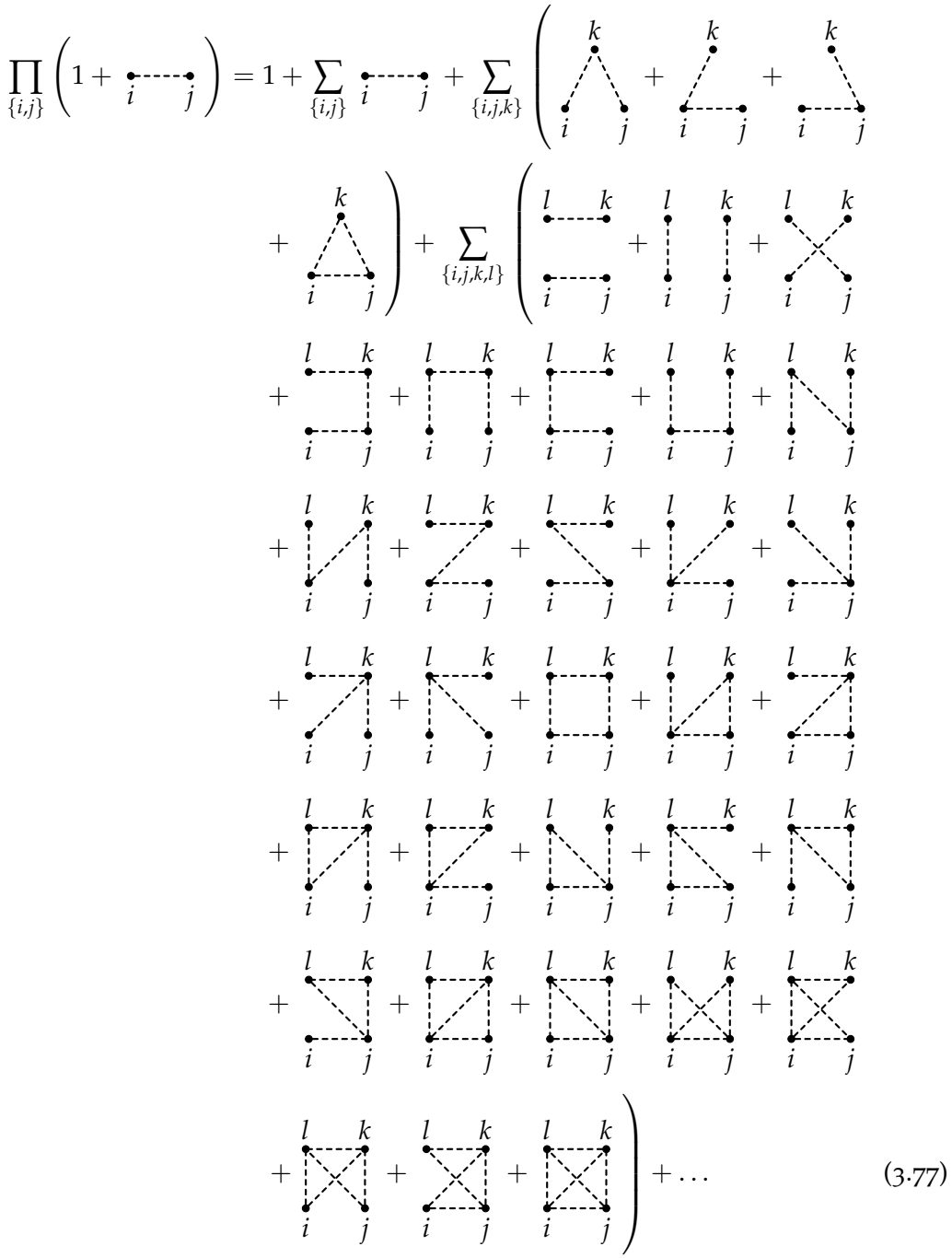
(3.75)

where the sums over three-tupels $\{i,j,k\}$ and four-tupels $\{i,j,k,l\}$ run over all *distinct* tupels in the same sense as for pairs. For example $\{1,2,3\}$ and $\{2,1,3\}$ are not distinct while $\{1,2,3\}$ and $\{1,2,4\}$ are. Taking the sums only over distinct tupels has the effect that we have to draw diagrams that are topolocally equivalent in order to include all possible cases for a certain n-tupel. This might seem cumbersome but it has the advantage of making the combinatorics directly visible. We now also see why we did not include momentum self-correlations since these would result in lines starting and ending at the same particle, i. e.  . This would inflate the number of diagrams we need to draw considerably. For the triple sum in (3.73) we have to distinguish the following topological cases:



(3.76)

Of course there are more possibilities but they are all forbidden by the p-line rule. Just like for the double sum (3.75) we would now draw all possible ways to achieve the above topologies and then sum over the respective distinct n-tupels of particles. This process has to be repeated for any order of correlation lines up to $\lfloor N/2 \rfloor$. By combining the results from all those cascaded sums one finally finds



(3.77)

While this expression is quite extensive we wrote it down explicitly up to 4-tupels since it shows us that we can in principle obtain it by using the following simple recipe: We go through all numbers $1 < n \leq N$ of particles and for each of them draw all diagrams compatible with the above p-line rule and then sum over the respective

distinct n-tupels of particles. Writing down the momentum correlations in this way has the advantage that we immediately see the number of particle momenta that are actually correlated with each other in any term, whereas the double sum in (3.72) and (3.73) for example contains terms with three and four correlated momenta.

In much the same way we can now treat the correlation operator $\hat{C}$ in (3.65) in terms of diagrams. For this we define two more line types

$$\hat{C}_{\delta_j\delta_k} \coloneqq \quad , \tag{3.78}$$

$$\hat{C}_{\delta_j p_k} \coloneqq -\mathrm{i}\hat{\vec{C}}_{\delta_j p_k} \cdot \frac{\delta}{\mathrm{i}\delta\vec{K}_{p_k}(t_\mathrm{i})} = \quad . \tag{3.79}$$

We now want to rewrite (3.48) in the same way as (3.77), i. e. ordered by the number of particles that are correlated. We first look at both types of correlations separately. If we only consider density correlations we have

$$\sum_{\{i,j\}} \hat{C}_{\delta_i\delta_j} = \sum_{\{i,j\}} \quad , \tag{3.80}$$

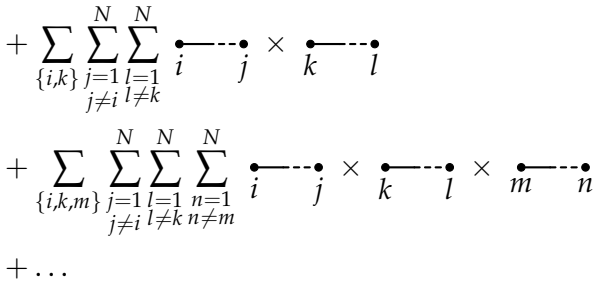
$$\sum_{\{\{i,j\},\{k,l\}\}'} \hat{C}_{\delta_i\delta_j}\hat{C}_{\delta_k\delta_l} = \sum_{\{\{i,j\},\{k,l\}\}'} \quad \times \quad = \sum_{\{i,j,k,l\}} \left(\quad + \quad + \quad \right) \tag{3.81}$$

and so on for higher orders. No topologies with connections between more than two particles are possible due to the exclusion rules encoded in the primes. We can thus formulate our next rule for general diagrams.

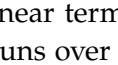
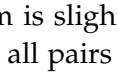
RULE 1 : No $\hat{C}_{\delta_i\delta_j} =$ may be connected to another. All subdiagrams with topology are *forbidden*.

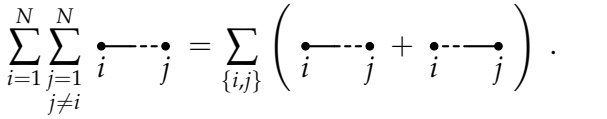
Note that although we never excluded them explicitly, density self-correlations $C_{\delta_j\delta_j}$ for a single particle do not enter into the initial correlations due to the derivative structure in (3.44). As for the momenta there is thus no ○ subdiagram. For the density-momentum correlations we need to consider

$$\prod_{i=1}^{N} \left(1 + \sum_{\substack{j=1 \\ j\neq i}}^{N} \quad \right) = 1 + \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \quad$$



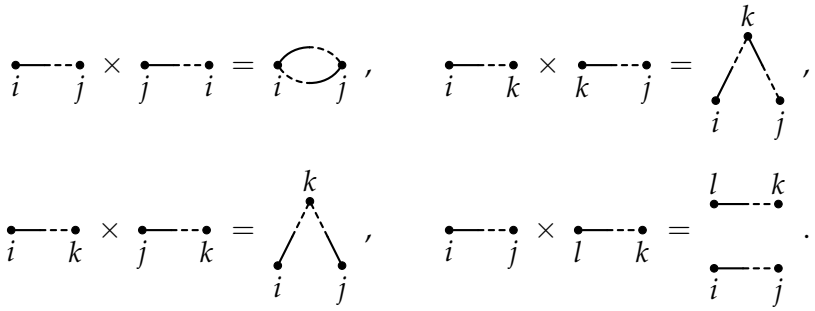
(3.82)

The linear term is slightly different from the linear terms of  and  . The sum runs over all pairs of particles with ordering of the particles taken into account, i. e. both $\{1,2\}$ and $\{2,1\}$ are summed over. The reason is that the diagram is not symmetric like the other two. We can still write it as a sum over *distinct* pairs by adding both possible diagrams



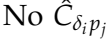
(3.83)

Notice that we again have no self-correlation subdiagrams  , because they actually vanish due to statistical homogeneity and isotropy of the system as explained in section 3.2.1 For the quadratic term we must keep in mind that the indices on the solid δ-line only appear once in the product and thus we again have to sum over distinct pairs $\{i,k\}$. The following topological cases are possible:

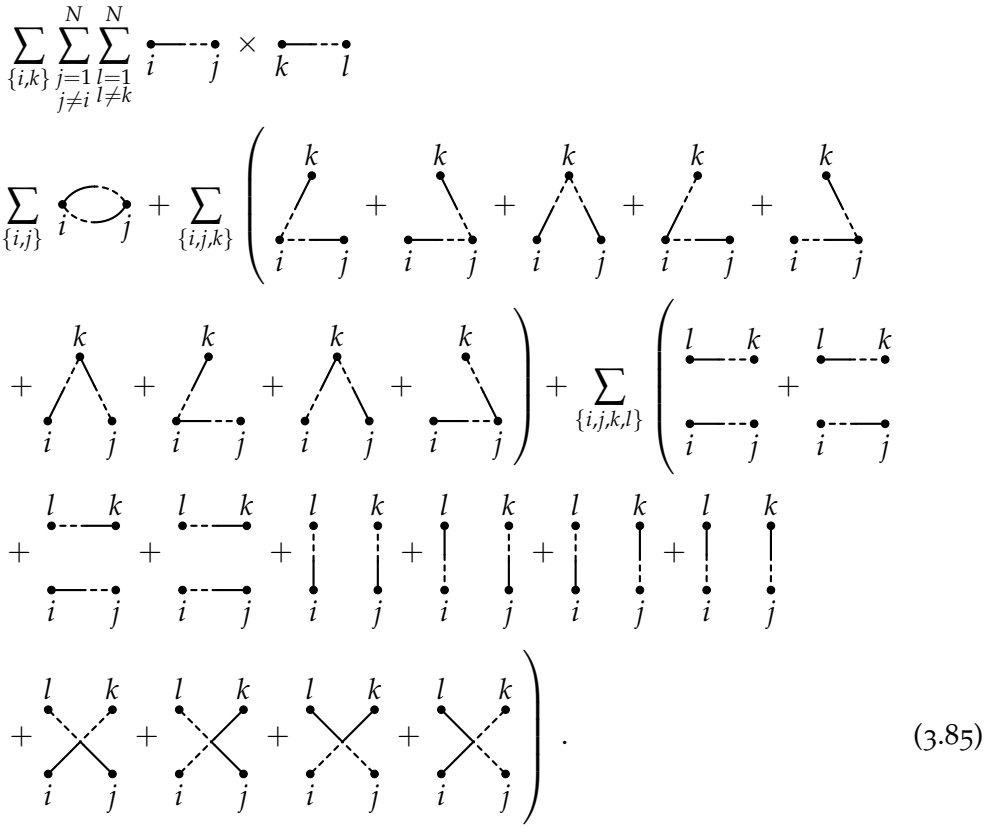


(3.84)

All topologies where two solid δ-lines meet at a point are excluded due to summing over distinct pairs, leading to yet another rule for drawing general diagrams:

RULE 2 : No $\hat{C}_{\delta_i p_j} =$  may be connected to another with the solid δ-end. All subdiagrams with topology  are *forbidden*.

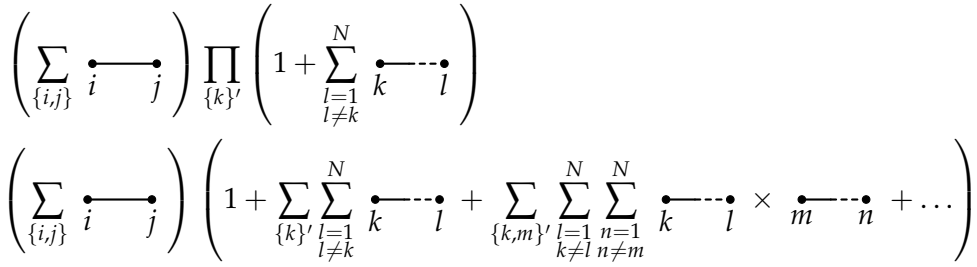
With this rule in mind we write down the quadratic term ordered by the number of particles involved

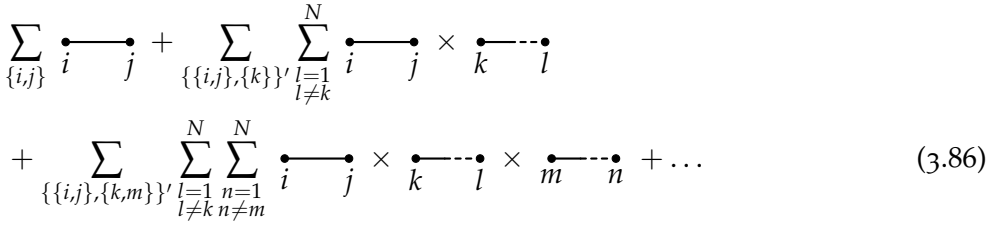


(3.85)

Due to the less restrictive exclusion rules and the non-symmetric nature of the •---• diagram there are quite a few more composed diagrams to consider when compared to the other two line types. Since for the cubic term the number of different topologies is already quite extensive we will abstain from listing them. It should by now be clear that we can find the complete expression for (3.82) in the same way as for (3.73), i. e. go through all particle numbers $1 < n \leq N$, draw all diagrams compatible with Rule 2 and sum over all distinct n-tupels of particles.

Next we have to multiply each term of the sort (3.80),(3.81) and their higher order equivalents with (3.82) with the rule encoded by the prime on the product index in (3.48). For each term in the sums of (3.80),(3.81) it excludes all indices present in that term from the product. For the product with the linear term (3.80) we thus have



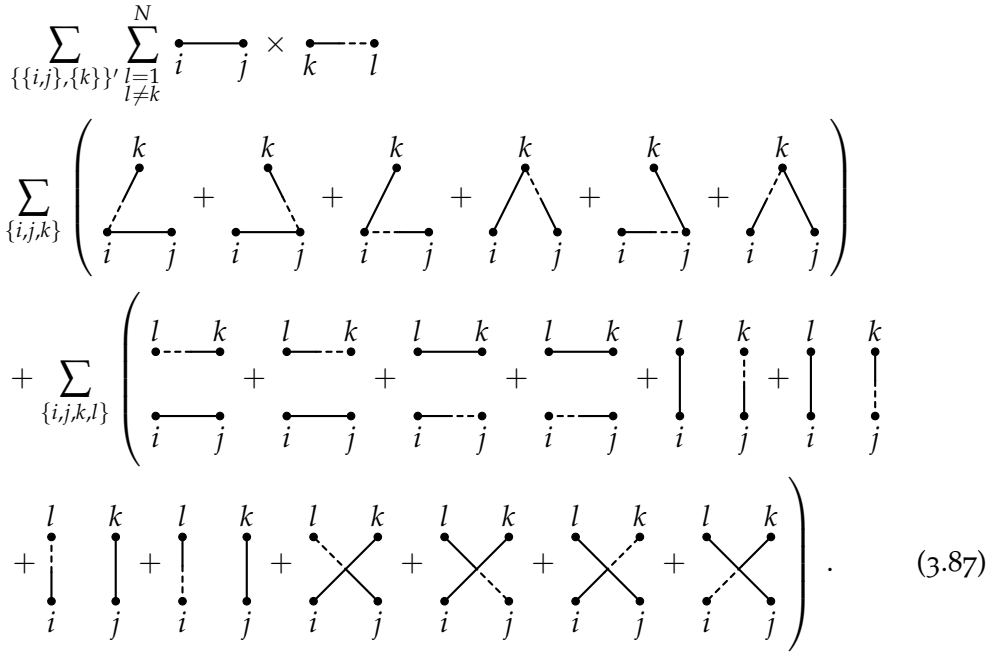


(3.86)

and analogous expressions for the product with (3.81) and all higher order terms. From this we directly see that this last exclusion rule can be transformed into another rule for general diagrams:

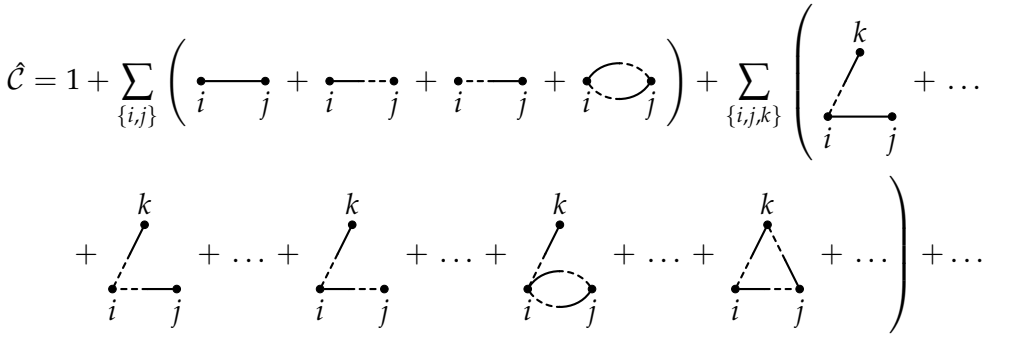
RULE 3 : No $\hat{C}_{\delta_i p_j}$ =  may be connected to a $\hat{C}_{\delta_i \delta_j}$ =  with its solid δ-line. All subdiagrams with topology  are *forbidden*.

We may thus for example write the quadratic term in (3.86) as



(3.87)

We now may write down the correlation operator (3.48) in diagram form as



(3.88)

To arrive at this expression we have written out all terms in (3.86) as in (3.87), done the same for products with higher order terms like (3.81) and added (3.82) with every term written out in the same way as shown (3.85). The dots behind the diagrams stand for all diagrams with the same topology, for example the first dots stand for the diagrams in the second line (3.87). We again see that we can obtain this expression by going through all particle numbers $1 < n \leq N$ and summing all possible diagrams, only this time using both line types and and obeying the Rules 1,2,3 which combine into the

δ-LINE RULE : No particle may have more than one solid δ-line attached to it. All subdiagrams with topology  are *forbidden*.

We now have expressed both factors in the total correlation operator $\hat{\mathcal{C}}_{\text{tot}}$ of (3.65) as sums of diagrams which run over distinct tupels of increasing particle numbers. Both these expansions have the form

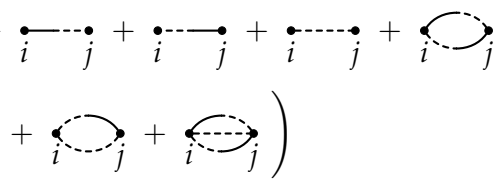
$$\hat{\mathcal{C}} = 1 + \sum_{\delta\text{-RULE}} \left(\text{} \right)$$

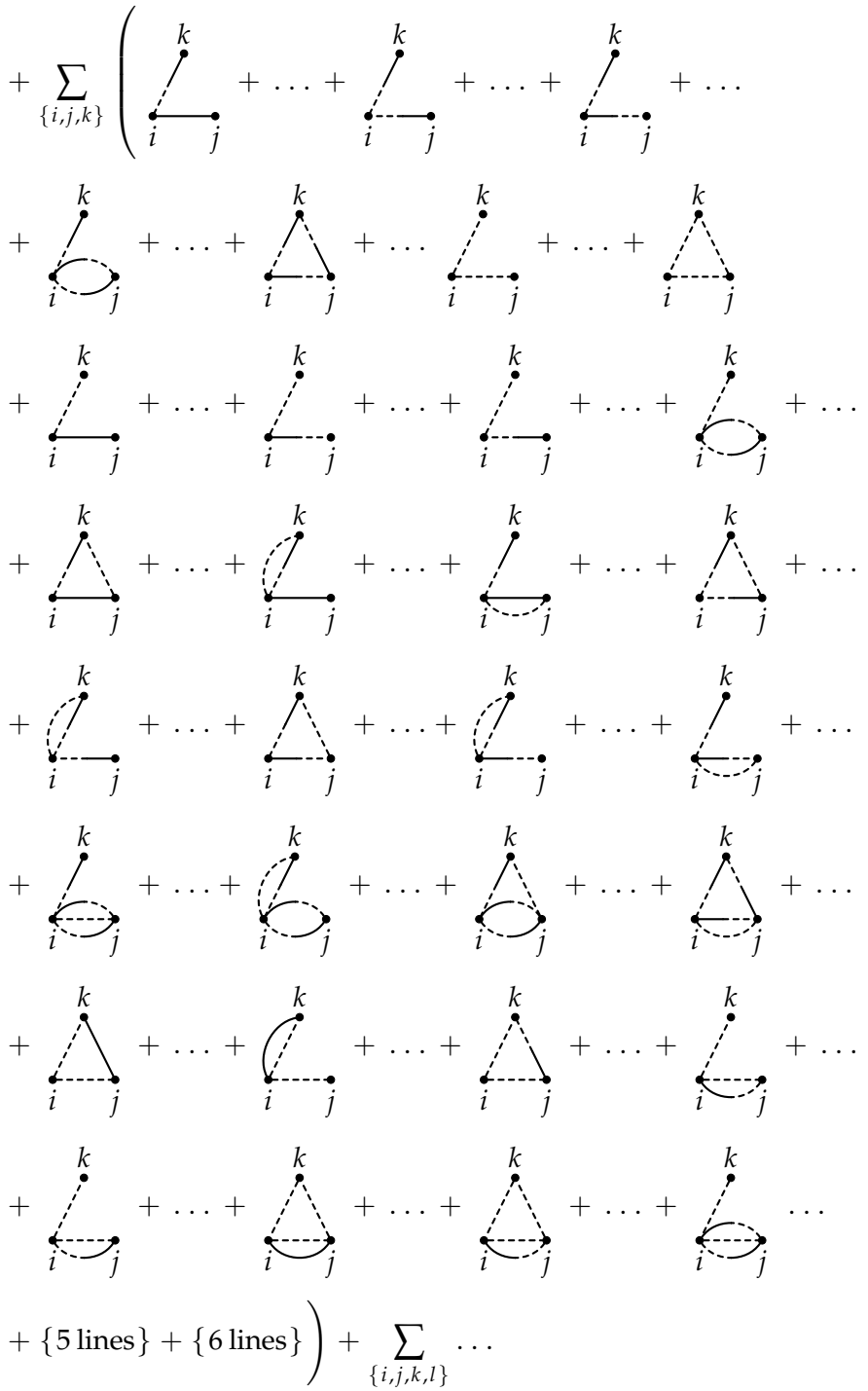
$$\prod_{\{i,j\}} \left(1 + \text{} \right) = 1 + \sum_{p\text{-RULE}} \left(\text{} \right) , \tag{3.89}$$

where the sums run over all possible diagrams for all particle numbers $1 < n \leq N$ that can be constructed with the respective line type subject to their rules. The total correlation operator $\hat{\mathcal{C}}_{\text{tot}}$ is just the product of these two without any additional rules so we find in a schematic sense

$$\begin{aligned}
\hat{\mathcal{C}}_{\text{tot}} &= \hat{\mathcal{C}} \times \prod_{\{i,j\}} \left(1 + \text{  } \right) \\
&= \left(1 + \sum_{\delta\text{-RULE}} \left(\text{} \right) \right) \times \left(1 + \sum_{p\text{-RULE}} \left(\text{} \right) \right) \\
&= 1 + \sum_{\delta\text{-RULE}} \left(\text{} \right) + \sum_{p\text{-RULE}} \left(\text{} \right) \\
&\quad + \sum_{\delta\text{-RULE}, p\text{-RULE}} \left(\text{} \right) \times \left(\text{} \right) \\
&= 1 + \sum_{\delta\text{-RULE}, p\text{-RULE}} \left(\text{} \right) .
\end{aligned} \tag{3.90}$$

The total correlation operator is thus given by summing up all diagrams that can be constructed from all three line types subject to both the δ-line rule and the p-line rule. To illustrate this we write it out for up to three particles:

$$\hat{\mathcal{C}}_{\text{tot}} = 1 + \sum_{\{i,j\}} \left(\text{  } \right)$$



(3.91)

The two-particle sum should be fairly obvious. The three particle sum is already a lot more complicated. In the first two rows we have shown the individual three-particle sums of (3.77) and (3.88). The third row then shows those mixed diagrams which arise by gluing together the respective two-particle sums of (3.77) and (3.88) at one particle dot in every allowed way. The remaining diagrams can then be obtained by adding any number of lines to the diagrams of the first three rows while obeying both rules until at six lines they forbid to add any more lines.

3.3.3 *Mayer cluster expansion of initial correlations*

The Mayer cluster expansion [38] is usually used to reorganize the partition sum of an interacting system in equilibrium statistical physics. Suppose that we have a gas of N interacting particles in thermal equilibrium with canonical partition sum

$$\begin{aligned} Z &= \left(\prod_{j=1}^{N}\int \mathrm{d}\vec{q}_j \int \mathrm{d}\vec{p}_j\right) \exp\left\{-\beta\left(\sum_{j=1}^{N}\frac{\vec{p}_j^{\,2}}{2m} + \sum_{\{j,k\}} v\left(|\vec{q}_j - \vec{q}_k|\right)\right)\right\} \\ &= \left[\prod_{j=1}^{N}\int \mathrm{d}\vec{p}_j \exp\left\{-\beta\frac{\vec{p}_j^{\,2}}{2m}\right\}\right]\left[\left(\prod_{j=1}^{N}\int \mathrm{d}\vec{q}_j\right)\exp\left\{-\beta\sum_{\{j,k\}} v_{jk}\right\}\right] = Z_0 \times I\,. \end{aligned} \tag{3.92}$$

In the above expression Z_0 is the free partition sum of an ideal gas which can be computed exactly, in contrast to the configuration integral I which contains the interaction potentials v_{jk} between the particles. The basic trick of the cluster expansion is now to rewrite this configuration integral in the same way we already did in (3.70) for the momentum correlations. That is one introduces the so-called 'Mayer functions'

$$f_{jk} = \mathrm{e}^{-\beta v_{jk}} - 1 \tag{3.93}$$

and obtains the same expansion for these as we found for $\hat{C}_{p_j p_k}$ in (3.72). One then hopes that with rising number of particles taking part in the interactions the terms are of less and less importance and one thus only needs to calculate some lower particle number terms to get a good approximation for the partition function. One can also obtain the virial expansion of the equation of state of the interacting gas, i. e. an expansion in powers of the mean density, from the Mayer cluster expansion and directly obtain explicit expressions for its coefficients (cf. Landau and Lifschitz [33]).

It is possible to treat the interaction operator $\mathrm{e}^{\mathrm{i}\hat{S}_I}$ in the same way which of course leads to operator valued Mayer functions $\hat{f}_{jk}$. If one then introduces a new line type one can treat both interactions and correlations together in one diagrammatic language. This was done to first order in Kozlikin et al. [32]. While this approach might allow for easier insight into the physical processes on the per particle level one has to give up the interaction being formulated as acting between fields and not individual particles. Since this latter feature is partly responsible for the self-consistent treatment of the interaction in the grand-canonical ensemble we will not pursue this approach any further.

The cluster expansion can be done in a very systematic way by introducing a diagrammatic language for the different terms just like we did in the last chapter for the initial correlations. This is well described in Becker [11] and as such we will follow the argumentation and notation used therein closely. For the purposes of this section it will be more convenient to apply the operators $\hat{\mathcal{C}}_{\mathrm{tot}}$ and $\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}}$ to the generating

functional of the ideal gas and thus again replace all functional derivatives present in these two as

$$\frac{\delta}{\mathrm{i}\delta\vec{J}_{q_j}(t_\mathrm{i})} \longrightarrow \vec{q}_j^{\,(\mathrm{i})} \quad \text{and} \quad \frac{\delta}{\mathrm{i}\delta\vec{K}_{p_j}(t_\mathrm{i})} \longrightarrow \vec{\chi}_{p_j}^{\,(\mathrm{i})} \,. \tag{3.94}$$

We now understand all diagrams to represent their respective non-operator counterparts under the above substitutions. For example $\overset{j}{\bullet}\!\!-\!\!\!-\!\!\bullet\overset{k}{}$ now just means $C_{\delta_j\delta_k}$ instead of its operator version defined in (3.67). Since no more functional derivatives w. r. t. $\mathbf{J}, \mathbf{K}$ are left over we can turn off these sources for now, since they are not needed for the following steps. They will be reintroduced at the end of this section. The free canonical generating functional then reads

$$Z_{\mathrm{C},0}[H] = \int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\, V^{-N} P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})}) \int_{\mathrm{i}} \mathcal{D}\mathbf{x} \int \mathcal{D}\boldsymbol{\chi}\, \mathcal{C}_{\mathrm{tot}}(\mathbf{q}^{(\mathrm{i})}, \boldsymbol{\chi}_p^{(\mathrm{i})})\, \mathrm{e}^{\mathrm{i}(S_0 + H\cdot\Phi)} \,. \tag{3.95}$$

Our aim is now to factorise this expression as much as possible. The motivation behind this is that factors which have the same 'correlation structure', i.e. the same topology when expressed as diagrams, all give the same contribution to the generating functional due to the integration over the entire phase-space evolution. We immediately recognize that with the exception of $\mathcal{C}_{\mathrm{tot}}$ all other quantities can easily be separated into single particle contributions. For the various integral measures this is of course holds by definition

$$\mathrm{d}\mathbf{x}^{(\mathrm{i})} = \prod_{j=1}^{N} \mathrm{d}\vec{q}_j^{\,(\mathrm{i})} \mathrm{d}\vec{p}_j^{\,(\mathrm{i})} \,, \quad \mathcal{D}\mathbf{x} = \prod_{j=1}^{N} \mathcal{D}\vec{x}_j \,, \quad \mathcal{D}\boldsymbol{\chi} = \prod_{j=1}^{N} \mathcal{D}\vec{\chi}_j \,. \tag{3.96}$$

The initial conditions of the ideal gas can also be separated in a straightforward fashion as

$$V^{-N} P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})}) = \frac{\exp\left\{\frac{-\langle \mathbf{p}^{(\mathrm{i})}, \mathbf{p}^{(\mathrm{i})} \rangle}{2\sigma_p^2}\right\}}{V^N \sqrt{(2\pi\sigma_p^2)^{dN}}} = \prod_{j=1}^{N} \frac{\exp\left\{-\frac{\vec{p}_j^{\,(\mathrm{i})\,2}}{2\sigma_p^2}\right\}}{V\sqrt{(2\pi\sigma_p^2)^{d}}} = \prod_{j=1}^{N} V^{-1} P_{\sigma_p}(\vec{p}_j^{\,(\mathrm{i})}) \,. \tag{3.97}$$

Finally we see from the respective definitions of the free action S_0 in (2.30), (2.61) and the collective fields in (2.34), (2.37) that we can also separate them as

$$\exp\left\{\mathrm{i}(S_0 + H\cdot\Phi)\right\} = \exp\left\{\mathrm{i}\sum_{j=1}^{N}\left(S_{0,j} + H\cdot\phi_j\right)\right\} = \prod_{j=1}^{N} \exp\left\{\mathrm{i}\left(S_{0,j} + H\cdot\phi_j\right)\right\} \tag{3.98}$$

where we have the single particle quantities

$$S_{0,j} = \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t\, \vec{\chi}_j^{\,\mathrm{T}}(t)\, \hat{\mathcal{E}}_0 \vec{x}_j \tag{3.99}$$

and

$$\phi_j(1) = \begin{pmatrix} \phi_{\rho_j}(1) \\ \phi_{B_j}(1) \end{pmatrix} = \begin{pmatrix} \delta_{\mathrm{D}}\left(\vec{q}_1 - \vec{q}_j(t_1)\right) \\ \vec{\chi}_{p_j}^{\,\mathrm{T}}(t_1)\, \nabla_q\, \delta_{\mathrm{D}}\left(\vec{q}_1 - \vec{q}_j(t_1)\right) \end{pmatrix} \,. \tag{3.100}$$

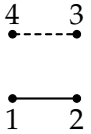
We now define a trace operation

$$\mathrm{Tr}_j = \int \mathrm{d}\vec{q}^{\,(\mathrm{i})} \int \mathrm{d}\vec{p}^{\,(\mathrm{i})}\, V^{-1} P_{\sigma_p}(\vec{p}_j^{\,(\mathrm{i})}) \int_{\mathrm{i}} \mathcal{D}\vec{x}_j \int \mathcal{D}\vec{\chi}_j \exp\left\{\mathrm{i}\left(S_{0,j} + H\cdot\phi_j\right)\right\} \ . \quad (3.101)$$

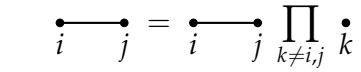
which contains all the ideal gas contributions for a single particle and allows us to write down the free generating functional in the very concise form

$$Z_{\mathrm{C},0}[H] = \left(\prod_{j=1}^{N} \mathrm{Tr}_j\right) \mathcal{C}_{\mathrm{tot}}(\mathbf{q}^{(\mathrm{i})}, \boldsymbol{\chi}_p^{(\mathrm{i})}) \ . \quad (3.102)$$

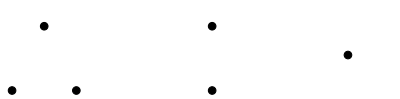
We need to consider how terms in $\mathcal{C}_{\mathrm{tot}}$ factorize once we apply the trace operators. It is obvious that one can factorize parts of a diagram if they are not connected by correlation lines. For the example of some four particles which we label $1, 2, 3, 4$ without loss of generality, there is a term

$\mathrm{Tr}_1\mathrm{Tr}_2\mathrm{Tr}_3\mathrm{Tr}_4$  $= \left(\mathrm{Tr}_1\mathrm{Tr}_2$  $\right) \times \left(\mathrm{Tr}_3\mathrm{Tr}_4$  $\right)$. (3.103)

For this particular term all other particles $5, 6, \ldots, N$ are not correlated. We thus represent them as isolated dots with unity value, i. e. we have to understand all our diagrams in the following sense

 (3.104)

with obvious extension to higher correlation order diagrams. We now adopt the notion that if any number ℓ of particles are connected in any allowed way by the three types of correlation lines they form an *ℓ-cluster*. For now we forget about the actual lines furnishing the clusters and only care about the grouping of particles. We first introduce the notion of a *clustering configuration* which is a set $\{m_\ell\}$ of numbers, where m_ℓ is the number of clusters of size ℓ. This does not specify which particles are in which cluster. In our diagrammatic language we represent such a configuration by visually grouping unlabeled particle dots with a clear spatial separation between clusters. We could for example have

$\{m_1 = N-5, m_2 = 1, m_3 = 1\} =$  , (3.105)

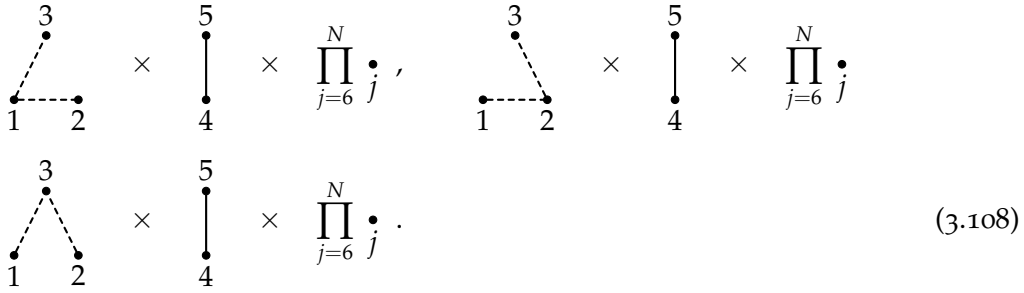
where there are of course $N-5$ isolated 1-particle clusters at the end. Any cluster size not mentioned in $\{m_\ell\}$ is taken to be zero. We call this visual representation of a clustering configuration a *clustering pattern*. Since there are only N particles any clustering configuration must of course obey the constraint

$$\sum_{\ell=1}^{N} \ell \cdot m_\ell = N \ . \quad (3.106)$$

Any clustering configuration $\{m_\ell\}$ has many different *clustering realisations*, where each particle index is clearly assigned to one of the dots of the clustering pattern. We denote these as $[\prod_\ell c_{\ell,1},\ldots,c_{\ell,m_\ell}]$, where $c_{\ell,j}$ is the jth cluster of size ℓ and so on. In order to make this assigment unique we arrange the particle indices in a certain order and this sequence then stands for a particular realisation. We then fix a bijective mapping between this sequence of indices and the clustering pattern. For the clustering configuration in (3.105) we could for example have

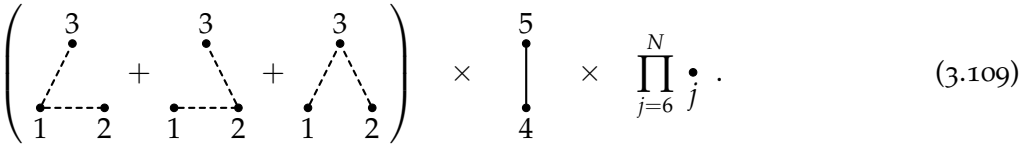
$$[(1,2,3),(4,5),(6),\ldots,(N)] = \quad \begin{matrix} 3 & & 5 & & & & \\ \bullet & & \bullet & & & & \\ & & & & \bullet & \cdots & \bullet \\ \bullet & \bullet & \bullet & & 6 & & N \\ 1 & 2 & 4 & & & & \end{matrix} \,. \tag{3.107}$$

Once all particles are assigned we call the pattern *fixed* because exchanging any two particles would correspond to another sequence of indices and thus to another clustering realisation. For example $[(2,1,3),(4,5),(6),\ldots,(N)]$ is considered to be a different realisation. Each diagrammatic term in (3.91) can now be identified as belonging to a clustering realisation. For example the following three terms all belong to $[(1,2,3),(4,5),(6),\ldots,(N)]$



(3.108)

We may combine these three into



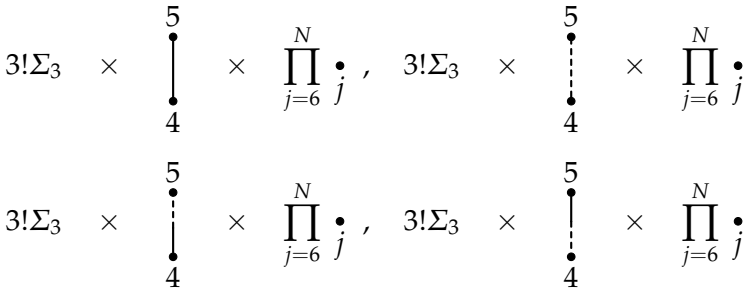
(3.109)

We now take this to its logical conclusion and sum all appropriate terms in (3.91) such that we obtain the sum over all connected diagrams for the particles $1,2,3$ in the $\ell = 3$-cluster. Since there are no disconnected 3-particle diagrams we actually can see this sum directly in (3.91). Then we apply the trace operators for the three particles. For a general ℓ-cluster we now define the *connected ℓ-particle free generating functional*

$$\Sigma_\ell[H] := \frac{1}{\ell!}\left(\prod_{j=1}^{\ell}\mathrm{Tr}_j\right)\mathcal{C}_{\mathrm{con}}^{(\ell)}\,, \tag{3.110}$$

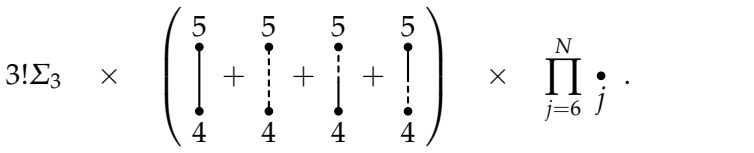
where $\mathcal{C}_{\mathrm{con}}^{(\ell)}$ is the sum of all the connected ℓ-particle diagrams. It is important to note that due to the trace operators this quantity has the *same* value for any ℓ-cluster, no

matter which particles actually form it. Because of this we defined it with a set of *representative* particles $1,\ldots,\ell$. Having summed all diagrams for the three-cluster of the specific realisation $[(1,2,3),(4,5),(6),\ldots,(N)]$, there are now terms like



(3.111)

in the expansion (3.91) of $\mathcal{C}_{\text{tot}}$. We also combine these as



(3.112)

We again complete the process by summing all appropriate remaining diagrams such that we obtain the sum of all connected two particle diagrams for the $\ell = 2$-cluster. If we further recognize that $\Sigma_1[H] = \text{Tr}\bullet$ we can write the entire contribution from the clustering realisation $[(1,2,3),(4,5),(6),\ldots,(N)]$ to (3.102) as

$$3!\Sigma_3 \times 2!\Sigma_2 \times \prod_{j=6}^{N} 1!\Sigma_1 \,. \tag{3.113}$$

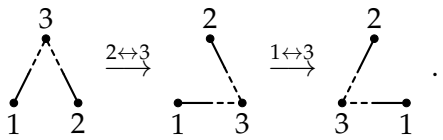
It is now clear that we can write the contribution from any general clustering realisation $[\prod_\ell c_{\ell,1},\ldots,c_{\ell,m_\ell}]$ of a clustering configuration $\{m_\ell\}$ to (3.102) as

$$\prod_{\ell=1}^{N} (\ell!\Sigma_\ell)^{m_\ell} \,. \tag{3.114}$$

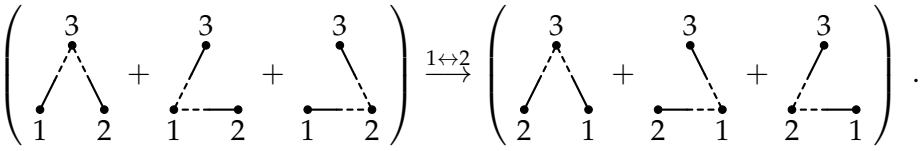
Due to the arguments given following (3.110) this contribution is the same for any clustering realisation. It is thus possible to rewrite the free generating functional as a sum over clustering configurations $\{m_\ell\}$. In order to do so we need to know which clustering realisations are actually present in (3.102) for any given configuration. Once we fixed the bijective mapping between the sequence of numbers in $[\prod_\ell c_{\ell,1},\ldots,c_{\ell,m_\ell}]$ and the clustering pattern it is clear that there are $N!$ different realisations of any configuration. However, once all possible diagrams are summed up for all these realisations some of them lead to identical contributions even prior to the application of the trace operators. There are two classes of transformations of the sequence $[\prod_\ell c_{\ell,1},\ldots,c_{\ell,m_\ell}]$ which leave the corresponding product $\prod_{\ell=1}^{N} \mathcal{C}^{(\ell)}_{\text{con}}(c_{\ell,1}) \times \ldots \times \mathcal{C}^{(\ell)}_{\text{con}}(c_{\ell,m_\ell})$ invariant.

- If we exchange the order of particles inside a cluster, the sum over all connected diagrams for this cluster is invariant. This is most easily seen by first picking

a diagram with a certain topology and then pairwise exchanging the positions of particles in the clustering pattern, which corresponds to a reordering of the sequence of particle indices defining the clustering realisation. This leads to a transformation of the diagram and a simple example for this is



Note that this is the same term which only appears *once* in (3.102), but realised as different diagrams in different clustering realisations. Since we need to make sure that we always describe the same term when transforming diagrams, i. e. the lines must still connect the same *indices* in the same way as before, the topology of diagrams is invariant under such transformations. In consequence, sums of all topological equivalent diagrams are invariant in a diagrammatic sense, i. e. they look the same after applying a transformation as described above. For our simple example we would have

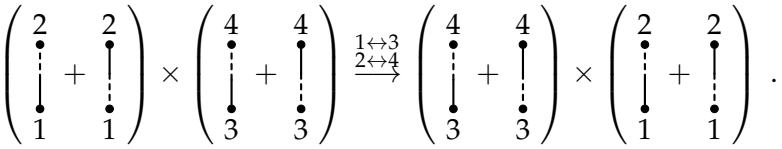


We see that we would get the exact same sum wether we have $(1,2,3)$ or $(2,1,3)$ somewhere in the sequence of the clustering realisation. Since the sum over all connected diagrams of a ℓ-particle cluster can be broken down into sums over all diagrams of all possible topologies we conclude that it must also be invariant in the diagrammatic sense when subjected to transformations as described above. For a certain configuration $\{m_\ell\}$, we thus have to divide out all clustering realisations which can be transformed into one another by a sequence of pairwise exchanges of particle order inside any cluster. There are $\ell!$ permutations of the ordering of particles inside a cluster and m_ℓ clusters of size ℓ which leads to

$$\prod_{\ell=1}^{N} \ell!^{m_\ell}$$

equivalent realisations.

- The second class of transformations is exchanging all particles between two clusters of equal size. Again the same reasoning applies where we first look at specific topologies only. A simple example would be

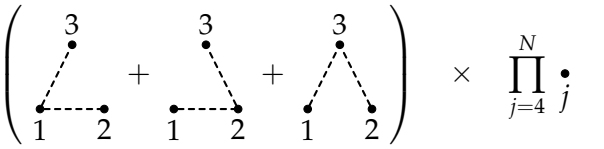


Since this transformation again leaves sums over topologies diagrammatically invariant this also holds for the sum over all possible connected diagrams. Exchanging all particles between two clusters is the same as exchanging the order of the two clusters in the sequence $[\prod_\ell c_{\ell,1},\dots,c_{\ell,m_\ell}]$ of the clustering realisation. Since there are m_ℓ clusters of size ℓ we have $m_\ell!$ permutations of their ordering.

All together we thus find that we can rewrite the free generating functional of (3.102) as a sum over clustering configurations

$$Z_{\mathrm{C},0}[H] = \sum_{\{m_\ell\}^*} \frac{N!}{\prod_{\ell=1}^N (\ell!)^{m_\ell} m_\ell!} \prod_{\ell=1}^N (\ell! \Sigma_\ell[H])^{m_\ell} = N! \sum_{\{m_\ell\}^*} \prod_{\ell=1}^N \frac{\Sigma_\ell[H]^{m_\ell}}{m_\ell!}\,, \tag{3.115}$$

where the asteriks in $\{m_\ell\}^*$ encodes the constraint (3.106). The main advantage of writing the free canonical generating functional in this maximally factorised form is that it will allow us to derive the grand canonical generating functional in an exact way. However, along the way we also discovered the diagrammatic invariance of sums of topological equivalent diagrams. Since the same combinatorial arguments hold for these as for the sum over all connected diagrams this gives us a systematic way to derive the multiplicity of a certain topology of correlations. Take for example the two dashed $\hat{C}_{p_i p_j}$ connecting the three cluster in (3.109). We want to know which contribution this topology alone gives to the generating functional. We can identify



(3.116)

as a member of the clustering configuration $\{m_1 = N-3, m_3 = 1\}$. After applying all trace operators we thus find the contribution from this topology to be

$$\begin{aligned}
&\frac{N!}{(1!^{N-3}(N-3)!)\times(3!^1 1!)}\,\mathrm{Tr}_1\mathrm{Tr}_2\mathrm{Tr}_3 \left(\begin{array}{ccccc} 3 & & 3 & & 3 \\ \diagup\diagdown & + & \diagup\diagdown & + & \diagup\diagdown \\ 1 & 2 & 1 & 2 & 1 \quad 2 \end{array}\right) \\
&\times \prod_{j=4}^N \mathrm{Tr}_j \bullet_j \\
&= \frac{N(N-1)(N-2)}{6}\,\mathrm{Tr}_1\mathrm{Tr}_2\mathrm{Tr}_3 \left(\begin{array}{cc} 3 & \\ \diagup\diagdown & \\ 1 \quad 2 & \end{array}\right) \times \prod_{j=4}^N \mathrm{Tr}_j \bullet_j \\
&\approx \frac{N^3}{2} \left(\begin{array}{cc} 3 & \\ \diagup\diagdown & \\ 1 \quad 2 & \end{array}\right) \times \prod_{j=4}^N \mathrm{Tr}_j \bullet_j\,.
\end{aligned} \tag{3.117}$$

In the second line we used that due to the trace operators all diagrams will give the same result and in the last line we used $N \gg 1$. This scheme of combining

diagrams of equal topology will also be used later when we calculate the cumulants of collective fields in the grand canonical ensemble. It is also interesting to see that in the free theory the scaling of terms with the particle number N and thus with the mean particle number density $\bar{\rho}$ is solely controlled by the correlation structure.

As a last step we need to reintroduce the single-particle sources $\mathbf{J}, \mathbf{K}$ back into the theory. Without them we are unable to rewrite the collective fields as operators and thus cannot execute the path integrals to obtain the free theory solution. We do this by modifying the trace operators as

$$\mathrm{Tr}_j \longrightarrow \mathrm{Tr}_j \exp\left\{ \mathrm{i} \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \, \left(\vec{J}_j(t) \cdot \vec{x}_j(t) + \vec{K}_j(t) \cdot \vec{\chi}_j(t) \right) \right\} . \tag{3.118}$$

Note that in a strict mathematical sense these are different from the sources we turned off at the beginning of this chapter. Each of those pertained to one specific particle of the N particles in the system. The quantities Σ_ℓ however are now defined for a *representative* set of ℓ particles which may stand for any subset of ℓ particles chosen from the overall N particles and the above new sources pertain to the particles of this representative set. We can define such a representative set since all actual ℓ-particle subsets give the same result for Σ_ℓ which was a crucial point in our reasoning for obtaining (3.115). This would no longer be true if we still had had the original sources $\mathbf{J}, \mathbf{K}$ remaining in the theory, since they could in principle lead to different Σ_ℓ for different subsets. By deriving everything without the help of these two sources we circumvented this problem.

With the single particle sources reintroduced as in (3.118) we may then rewrite the connected ℓ-particle generating functional $\Sigma_\ell[H, \mathbf{J}, \mathbf{K}]$ in the familiar way, i. e. we express the collective fields as operators $\hat{\Phi}$, only that they are now defined with the particles of the representative set used to define $\Sigma_\ell[H, \mathbf{J}, \mathbf{K}]$. We can also express the sum of connected ℓ-particle diagrams $\mathcal{C}_{\mathrm{con}}^{(\ell)}$ as an operator by reversing the second replacement in (3.94), only now with the *representative* source $\mathbf{K}$. As such we understand diagrams to represent their respective operators with the quantities $C_{\delta_i \delta_j}, \vec{C}_{\delta_i p_j}, C^{\times}_{p_i p_j}$ appearing as simple functions of the initial positions $\vec{q}_j^{\,(\mathrm{i})}$ of the ℓ representative particles. We thus have

$$\Sigma_\ell[H, \mathbf{J}, \mathbf{K}] = \mathrm{e}^{\mathrm{i}H\hat{\Phi}} \int \mathrm{d}\mathbf{x}^{(\mathrm{i})} \, \frac{P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})})}{V^\ell} \, \hat{\mathcal{C}}_{\mathrm{con}}^{(\ell)} \left(\frac{\delta}{\mathrm{i}\delta \mathbf{K}_p(t_\mathrm{i})} \right) Z_0^{(\ell)}[\mathbf{J}, \mathbf{K}] \tag{3.119}$$

where of course all bold tensorial quantities are now defined w. r. t. the ℓ representative particles and $Z_0^{(\ell)}$ is the ℓ-particle version of (3.52). We also absorbed the factor of $\ell!^{-1}$ in (3.110) into the operator $\hat{\mathcal{C}}_{\mathrm{con}}^{(\ell)}$.

4

THE GRAND CANONICAL ENSEMBLE

So far we have managed to set up all the basic building blocks of the field theory, that is the solution (2.67) to the non-interacting theory, the interaction matrix (2.40) and the corresponding operator (2.48) and the phase-space probability density (3.49) describing the initial state. We then combined both the free theory and a diagrammatic approach to the initial conditions to find a maximally factorised form of the free generating functional in (3.115). One could in principle now proceed and obtain corrections to the correlators or cumulants of the free theory by calculating higher and higher orders in the perturbation scheme of the canonical ensemble. However, at least for systems which obey statistical homogeneity and isotropy the field theoretical description can be translated into the analogue of the grand canonical ensemble of standard equilibrium statistical physics. In the course of this chapter we will see that this has two distinct advantages over the canonical approach:

- Obtaining the free cumulants of the theory is a straightforward process and can be done in a structured scheme. Most of the combinatorial effort has already been taken care of by the Mayer cluster expansion. Furthermore, the free cumulants naturally appear as one of the basic building blocks of perturbation theory.
- Perturbation theory is no longer formulated as a simple series of integrals of the interaction potential and the free correlators but in terms of self-consistent integral equations involving the potential, the free and full cumulants. We will show that this amounts to summing up subclasses of infinitely many terms in the canonical perturbation series even at linear order of the grand canonical perturbation theory.

In this chapter we will first define what we understand to be our grand canonical ensemble and how it is connected to the canonical one. We develop the entire scheme for obtaining explicit expressions for the free cumulants of the collective fields. We then derive the main perturbation equations for the interacting one- and two-point cumulants. We will see which kind of terms in the canonical perturbation series are summed up at the first order of the grand canonical perturbation series and how this can be understood as including a whole class of physical interaction processes with arbitrary numbers of participating particles taken into account. In contrast, for the canonical case (2.58) the number of particles participating in any such process is directly linked to the order of interactions considered.

4.1 THE GRAND CANONICAL GENERATING FUNCTIONAL

We first have to accurately define what we mean by writing down a generating functional for a system described by a grand canonical ensemble. For this we again take a look at standard equilibrium statistical physics. The principle difference w. r. t. to the canonical ensemble is that one no longer fixes the number of particles N in the system, but rather a so-called *chemical potential* μ which gives the necessary energy associated with adding a single particle to the system. The Boltzmann factor is then modified as

$$\mathcal{P}(\mathbf{x}) \propto \exp\left\{-\beta\mathcal{H}(\mathbf{x})\right\} \longrightarrow \mathcal{P}(\mathbf{x}, N) \propto \exp\left\{-\beta\mathcal{H}(\mathbf{x}) - \beta\mu N\right\} \ , \tag{4.1}$$

which means that one compares the energy μN necessary for adding N particles to the system to the mean thermal energy $k_\mathrm{B}T = \beta^{-1}$ in the system. The grand canonical partition sum is then obtained by first integrating over phase space with a fixed general particle number N and then summing over all possible particle numbers leading to

$$Z_\mathrm{GC} = \sum_{N=0}^{\infty} \int \mathrm{d}\Gamma \exp\left\{-\beta\mathcal{H}(\mathbf{x}) - \beta\mu N\right\} \ , \tag{4.2}$$

where Γ is again the appropriate phase-space measure. In a more general sense one introduces some probability distribution $\mathcal{P}(N)$ for the number of particles. In our case we thus have to modify our transition probability from initial to final state

$$\mathcal{P}(\mathbf{x}^{(\mathrm{f})}, \mathbf{x}^{(\mathrm{i})}) \longrightarrow \mathcal{P}(\mathbf{x}^{(\mathrm{f})}, \mathbf{x}^{(\mathrm{i})}, N) = \mathcal{P}(\mathbf{x}^{(\mathrm{f})}, \mathbf{x}^{(\mathrm{i})}|N)\, \mathcal{P}(N) \ . \tag{4.3}$$

Furthermore, we know the transition probability conditioned on a fixed particle number since this is the case described by the canonical ensemble. Using (2.17) we consequently have the following expression for the grand canonical generating functional

$$Z_\mathrm{GC} = \sum_{N=0}^{\infty} \int \mathrm{d}\mathbf{x}\, \mathcal{P}(N)\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})})\, \delta_\mathrm{D}[\mathbf{x}(t) - \mathbf{x}_\mathrm{cl}(t; \mathbf{x}^{(\mathrm{i})})] \ . \tag{4.4}$$

The difficulty now lies in specifying $\mathcal{P}(N)$. Defining a chemical potential seems problematic at best since the energy for adding a particle to the system may in principle depend on the entire instanteneous phase-space state $\mathbf{x}(t)$ and thus on the full interaction of all particles. In contrast to the equilibrium case there is also no easy choice for an energy scale that we could compare the chemical potential with.

However, for our case of a system satisfying statistical homogeneity and isotropy the solution is straightforward. For this we use a well-known textbook approach and imagine our system $\mathcal{S}_\mathrm{GC}$ described by the grand canonical ensemble as being embedded into a much larger system $\mathcal{S}_\mathrm{C}$ which is described by a canonical ensemble. The latter has a fixed particle number N_C and volume V_C while the former only has fixed volume V_GC. Particles can freely be exchanged between $\mathcal{S}_\mathrm{GC}$ and its complement in $\mathcal{S}_\mathrm{C}$. All particles may interact across the boundary defining $\mathcal{S}_\mathrm{GC}$. We illustrate this situation in Fig. 4. Since the system is statistically homogeneous and isotropic any

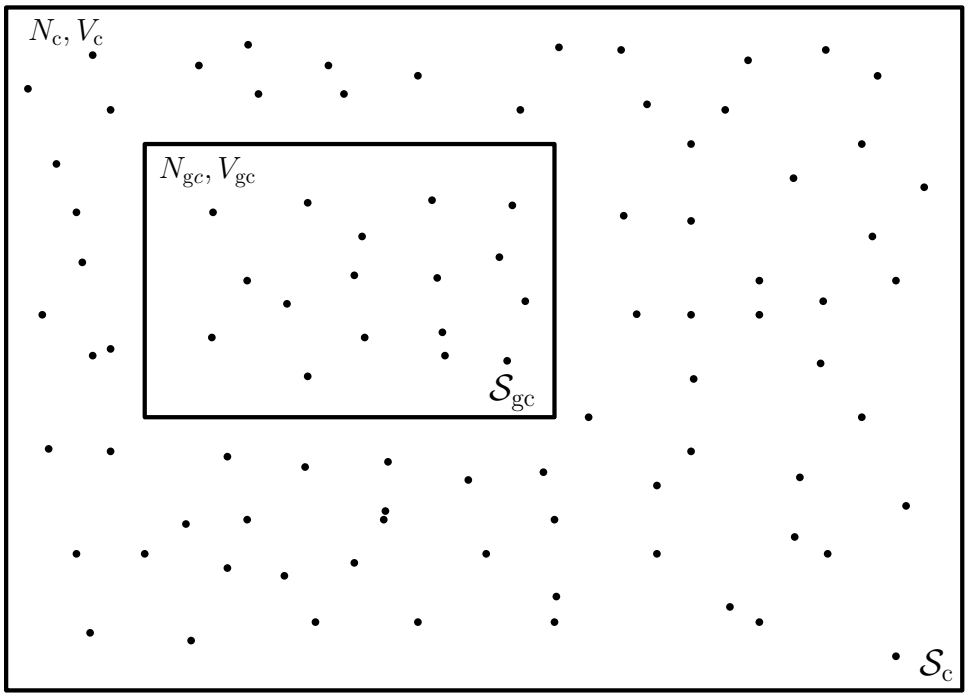


Figure 4: The physical situation of the grand canonical system $\mathcal{S}_{GC}$ embedded into the larger canonical system $\mathcal{S}_C$ used in the derivation of the particle number probability in the grand canonical ensemble.

statistical quantity must be invariant under translation and rotation at all times. Consequently, this must also hold for the probability to find any particle of the system $\mathcal{S}_C$ somewhere in the volume V_C, regardless of any particle interactions or correlations. Since this probability is a scalar quantity and is invariant under translation it must be a constant and proper normalisation tells us that it must be $1/V_C$. It is then straightforward to see that the probability to find this particle in the volume of the grand canonical subsystem is given by

$$p = \frac{V_{GC}}{V_C} \,. \tag{4.5}$$

This constitutes N_C independent Bernoulli experiments each with a random variable X_j which is 1 if the particle is in V_{GC} with probability $P(X_j = 1) = p$. The sum of all N_C random variables X_j is then binomially distributed

$$N_{GC} = \sum_{j=1}^{N_C} X_j \Rightarrow N_{GC} \sim \mathcal{B}\left(N_C, p\right) \,. \tag{4.6}$$

We now assume $\mathcal{S}_C$ to be in the 'thermodynamic' limit of a very large volume $V_C \to \infty$ and particle number $N_C \to \infty$, but we still keep the mean particle number density $\bar{\rho} = N_C/V_C$ constant. The probability p will tend to zero in this limit, i. e. $p \to 0$. Since the expectation value

$$\langle N_{GC} \rangle = N_C \, p = N_C \frac{V_{GC}}{V_C} = \bar{\rho} V_{GC} \tag{4.7}$$

is constant in this limit the binomial distribution will tend towards a Poisson distribution as

$$\mathcal{B}\left(N_{\mathrm{C}}, p\right) \underset{\substack{V_{\mathrm{C}}, N_{\mathrm{C}} \to \infty \\ \bar{\rho} = N_{\mathrm{C}}/V_{\mathrm{C}} = \text{const}}}{\longrightarrow} \mathrm{Pois}\left(\langle N_{\mathrm{GC}} \rangle\right) \,. \tag{4.8}$$

We thus find that the probability density for the number of particles in the grand canonical ensemble is

$$\mathcal{P}(N_{\mathrm{GC}}) = \frac{\langle N_{\mathrm{GC}} \rangle^{N_{\mathrm{GC}}}}{N_{\mathrm{GC}}!} \mathrm{e}^{-\langle N_{\mathrm{GC}} \rangle} = \frac{\bar{\rho}^{N_{\mathrm{GC}}} V_{\mathrm{GC}}^{N_{\mathrm{GC}}}}{N_{\mathrm{GC}}!} \mathrm{e}^{-\langle N_{\mathrm{GC}} \rangle} = \frac{\bar{\rho}^{N} V^{N}}{N!} \mathrm{e}^{-\langle N \rangle} \,, \tag{4.9}$$

if we want to fix the mean particle number density $\bar{\rho}$ at all times. In the last step we dropped the GC-suffix since we now forget about the surrounding canonical system. We insert our result back into (4.4) and find

$$\begin{aligned} Z_{\mathrm{GC}} &= \sum_{N=0}^{\infty} \int \mathrm{d}\mathbf{x} \, \frac{\bar{\rho}^{N} V^{N}}{N!} \mathrm{e}^{-\langle N \rangle} \, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \, \delta_{\mathrm{D}}[\mathbf{x}(t) - \mathbf{x}_{\mathrm{cl}}(t; \mathbf{x}^{(\mathrm{i})})] \\ &= \mathrm{e}^{-\langle N \rangle} \sum_{N=0}^{\infty} \frac{\bar{\rho}^{N} V^{N}}{N!} \int \mathrm{d}\mathbf{x} \, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \, \delta_{\mathrm{D}}[\mathbf{x}(t) - \mathbf{x}_{\mathrm{cl}}(t; \mathbf{x}^{(\mathrm{i})})] \\ &= \mathrm{e}^{-\langle N \rangle} \sum_{N=0}^{\infty} \frac{\bar{\rho}^{N} V^{N}}{N!} Z_{\mathrm{C}}^{(N)} \,. \end{aligned} \tag{4.10}$$

In the last step we identified the N-particle canonical generating functional $Z_{\mathrm{C}}^{(N)}$ pertaining to our grand canonical system with volume V. The normalisation factor $\mathrm{e}^{-\langle N \rangle}$ can be absorbed into one of the path integrals. It is of no consequence since we will only take derivatives of the logarithm of Z_{GC} later on. If we recall the definition (3.49) of the initial phase space probability density $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ we see that it had an overall factor of V^{-N}. This cancels against the above prefactor $\bar{\rho}^{N} V^{N}$ such that we have to exchange $1/V \to \bar{\rho}$ in the definition (3.101) of the trace and thus in the definition (3.119) of the connected free ℓ-particle generating functional. After this there are no explicit instances of the volume V present in the generating functional. We will also never encounter expressions of the form (1.27) when working in the grand canonical ensemble. Considering the statistics of our system to be characterised solely by fixing the mean particle number density $\bar{\rho}$ and the initial phase-space probability distribution $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ with $1/V \to \bar{\rho}$ we can thus safely take the limit where we push the volume $V \to \infty$. We can now insert our final result (3.115) from the previous chapter to obtain

$$\begin{aligned} Z_{\mathrm{GC}}[H] &= \sum_{N=0}^{\infty} \frac{1}{N!} \mathrm{e}^{\mathrm{i}\hat{S}_I} N! \sum_{\{m_\ell\}^*} \prod_{\ell=1}^{N} \frac{\Sigma_\ell[H]^{m_\ell}}{m_\ell!} = \mathrm{e}^{\mathrm{i}\hat{S}_I} \sum_{N=0}^{\infty} \sum_{\{m_\ell\}^*} \prod_{\ell=1}^{N} \frac{\Sigma_\ell[H]^{m_\ell}}{m_\ell!} \\ &= \mathrm{e}^{\mathrm{i}\hat{S}_I} \sum_{\{m_\ell\}} \prod_{\ell'} \frac{\Sigma_\ell[H]^{m_\ell}}{m_\ell!} = \mathrm{e}^{\mathrm{i}\hat{S}_I} \prod_{\ell=0}^{\infty} \sum_{m_\ell=0}^{\infty} \frac{\Sigma_\ell[H]^{m_\ell}}{m_\ell!} \\ &= \mathrm{e}^{\mathrm{i}\hat{S}_I} \prod_{\ell=0}^{\infty} \exp\left\{\Sigma_\ell[H]\right\} = \mathrm{e}^{\mathrm{i}\hat{S}_I} \exp\left\{\sum_{\ell=0}^{\infty} \Sigma_\ell[H]\right\} \,. \end{aligned} \tag{4.11}$$

In the first line we have used the fact that the interaction operator is independent of the particle number to pull it out in front of the sum over N. In the second line we first used that taking the sum over all clustering configurations $\{m_\ell\}$ subject to the constraint (3.106) and then taking the sum over all particle numbers is the same as taking the sum over all clustering configurations without the constraint. The prime on ℓ in the product means that it runs over all cluster sizes present in the clustering configuration of the previous sum. In the next step we reordered the sum in terms of the cluster size ℓ and then used the series definition of the exponential function in the last line. In the non-interacting regime the above result can be schematically summarised as

$$Z_{\mathrm{GC},0} = \sum \text{ diagrams} = \exp\left\{\sum \text{connected diagrams}\right\} \ . \tag{4.12}$$

Readers familiar with QFT will recognize this structure immediately since it appears in the same way for the Feynman diagrams which encode the dynamic correlation function of fields which arise due to the self-interaction of and interactions between fields. In our case, we encoded the instantaneous initial correlations between the phase-space coordinates of classical particles in the diagrams. The topological principle at work behind the Mayer cluster expansion and the so-called *exponentiation of disconnected diagrams* in QFT is however the same, which is why we obtain the same structure of the generating functional. As we already mentioned, we could also have included the interaction into this diagram picture, which would make the analogy complete.

4.2 NON-INTERACTING CUMULANTS

4.2.1 *Definition*

Just like in the canonical ensemble we define the generating functional of connected correlation functions or cumulants by

$$W_{\mathrm{GC}}[H] := \ln Z_{\mathrm{GC}}[H] \tag{4.13}$$

and consequently a general n-point cumulant of the collective fields is obtained by

$$G_{\Phi_{\alpha_1}\dots\Phi_{\alpha_n}} = \frac{\delta}{\mathrm{i}\delta H_{\alpha_1}} \cdots \frac{\delta}{\mathrm{i}\delta H_{\alpha_n}} W_{\mathrm{GC}}[H]\Big|_0 \ , \tag{4.14}$$

where we introduced the shorthand notation $|_0$ to indicate that all source terms should be set to zero once all functional derivatives w. r. t. them have been executed. In the non-interacting regime with $\hat{S}_I = 0$ the cumulant generating functional reads

$$W_{\mathrm{GC},0}[H] = \ln Z_{\mathrm{GC},0} = \ln \exp\left\{\sum_{\ell=0}^{\infty} \Sigma_\ell[H]\right\} = \sum_{\ell=0}^{\infty} \Sigma_\ell[H] \ . \tag{4.15}$$

It is this simple form as a sum that makes calculating the free cumulants much easier when compared to the canonical ensemble. Evaluating the cumulants in the Fourier

space conjugate to position space will be much more convenient. We thus use (1.28) to reinterpret the collective source term as

$$\begin{aligned} \mathrm{e}^{\mathrm{i}H\cdot\Phi} &= \exp\left\{ \mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \int \mathrm{d}\vec{q}\, H(\vec{q},t)^\mathrm{T}\Phi(\vec{q},t) \right\} \\ &= \exp\left\{ \mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \int \frac{\mathrm{d}\vec{k}}{(2\pi)^d}\, H(-\vec{k},t)^\mathrm{T}\Phi(\vec{k},t) \right\} . \end{aligned} \tag{4.16}$$

If we then understand functional derivatives as

$$\frac{\delta}{\mathrm{i}\delta H_{\alpha_1}} = \frac{\delta}{\mathrm{i}\delta\left(\frac{1}{(2\pi)^d} H_\alpha(-\vec{k}_1,t_1)\right)} \tag{4.17}$$

they will take down factors of the Fourier transformed collective fields $\Phi(\vec{k}_1,t_1)$. Hence we will from now on understand all collective fields Φ_{α_1} to be defined in Fourier space with labels $1=(\vec{k}_1,t_1)$. We can write down the free cumulants as

$$\begin{aligned} G^{(0)}_{\Phi_{\alpha_1}\dots\Phi_{\alpha n}} &= \frac{\delta}{\mathrm{i}\delta H_{\alpha_1}}\cdots\frac{\delta}{\mathrm{i}\delta H_{\alpha_n}}\left(\sum_{\ell=0}^{\infty}\Sigma_\ell[H,\mathbf{J},\mathbf{K}]\right)\Big|_0 \\ &= \sum_{\ell=0}^{\infty}\frac{\delta}{\mathrm{i}\delta H_{\alpha_1}}\cdots\frac{\delta}{\mathrm{i}\delta H_{\alpha_n}}\mathrm{e}^{\mathrm{i}H\cdot\hat{\Phi}^{(\ell)}}\int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\,\bar{\rho}^\ell P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})})\,\hat{\mathcal{C}}^{(\ell)}_{\mathrm{con}}\,Z_0^{(\ell)}[\mathbf{J},\mathbf{K}]\Big|_0 \\ &= \sum_{\ell=0}^{\infty}\int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\,\bar{\rho}^\ell P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})})\,\hat{\mathcal{C}}^{(\ell)}_{\mathrm{con}}\left(\frac{\delta}{\mathrm{i}\delta\mathbf{K}_p(t_\mathrm{i})}\right)\hat{\Phi}^{(\ell)}_{\alpha_1}\dots\hat{\Phi}^{(\ell)}_{\alpha_n}\,Z_0^{(\ell)}[\mathbf{J},\mathbf{K}]\Big|_0 \\ &= \sum_{\ell=0}^{\infty} G^{(0,\ell)}_{\Phi_{\alpha_1}\dots\Phi_{\alpha_n}} , \end{aligned} \tag{4.18}$$

where we made it explicit that for every Σ_ℓ the collective field operators $\hat{\Phi}^{(\ell)}$ in Fourier space depend only on the respective ℓ representative particles by using the (ℓ) superscript. One might now think that this is not a very practical expression since it contains an infinite sum over particle numbers. There are however two effects that lead to a truncation of this series. First, if the initial correlations of the system are weak in the sense that higher order diagrams give less and less significant contributions then one may specify a maximum number m of correlation functions to be taken into account. Since this translates into a maximum number of correlation lines one can draw and one needs at least $\ell-1$ lines to connect ℓ particles together, one would then automatically truncate the series in (4.18) at $\ell = m+1$ particles. Furthermore, we will later see that for some specific cumulant which contains r insertions of the density field Φ_ρ the summation is automatically truncated at $\ell = r$.

4.2.2 *Fourier space collective operators*

In order to evaluate the collective field operators acting on $Z_0^{(\ell)}[\mathbf{J},\mathbf{K}]$ we need their explicit form in Fourier space. We start with the full N-particle density field $\Phi_\rho(\vec{q},t)$. Its Fourier transform is easily found to be

$$\Phi_\rho(\vec{k},t) = \int \mathrm{d}\vec{q}\, \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{k}} \sum_{j=1}^{N} \delta_{\mathrm{D}}\left(\vec{q}-\vec{q}_j(t)\right) = \sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{q}_j(t)} = \sum_{j=1}^{N} \phi_{\rho_j}(\vec{k},t)\,, \tag{4.19}$$

where we defined the 1-particle density contributions ϕ_{ρ_j} in Fourier space in the last step. These are of course the Fourier conjugates of (3.100). With the help of (1.29), the transform of the Φ_B-field is also straightforward

$$\begin{aligned}\Phi_B(\vec{k},t) &= \int \mathrm{d}\vec{q}\, \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{k}} \sum_{j=1}^{N} \vec{\chi}_{p_j}^{\mathrm{T}}(t)\, \nabla_q \delta_{\mathrm{D}}\left(\vec{q}-\vec{q}_j(t)\right) = \sum_{j=1}^{N} \mathrm{i}\vec{\chi}_{p_j}^{\mathrm{T}}(t)\, \vec{k}\, \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{q}_j(t)} \\ &= \sum_{j=1}^{N} \phi_{B_j}(\vec{k},t)\,. \end{aligned} \tag{4.20}$$

Their ℓ-particle operator form is obtained by restricting the sum to the representative particle set and performing the same substitution (2.51) as in configuration space. We thus find

$$\hat{\Phi}_\rho^{(\ell)}(\vec{k},t) = \sum_{j=1}^{\ell} \hat{\phi}_{\rho_j}(\vec{k},t) \quad \text{with} \quad \hat{\phi}_{\rho_j}(\vec{k},t) = \exp\left\{-\mathrm{i}\vec{k}\cdot\frac{\delta}{\mathrm{i}\delta\vec{J}_{q_j}(t)}\right\} \tag{4.21}$$

$$\hat{\Phi}_B^{(\ell)}(\vec{k},t) = \sum_{j=1}^{\ell} \hat{\phi}_{B_j}(\vec{k},t) = \sum_{j=1}^{\ell} \hat{b}_j(\vec{k},t)\, \hat{\phi}_{\rho_j}(\vec{k},t) \quad \text{with} \quad \hat{b}_j(\vec{k},t) = \mathrm{i}\vec{k}\cdot\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_j}(t)}\,. \tag{4.22}$$

Consider now a general ℓ-particle cumulant like in (4.18). With the above result for the collective field operators it takes on the form

$$G^{(0,\ell)}_{\Phi_{\alpha_1}\ldots\Phi_{\alpha_n}} = \int \mathrm{d}\mathbf{x}^{(\mathrm{i})}\, \bar{\rho}^{\ell} P_{\sigma_p}(\mathbf{p}^{(\mathrm{i})})\, \hat{\mathcal{C}}^{(\ell)}_{\mathrm{con}} \left(\sum_{j=1}^{\ell} \hat{\phi}^{(\ell)}_{\alpha_1}\right) \ldots \left(\sum_{j=1}^{\ell} \hat{\phi}^{(\ell)}_{\alpha_n}\right) Z_0^{(\ell)}[\mathbf{J},\mathbf{K}]\Big|_0\,. \tag{4.23}$$

Multiplying out the sums of single particle operators we see that we get a sum of ℓ^n terms, each being the product of n single particle operators. Since we can split up the Φ_B-field single particle operators $\hat{\phi}_{B_j}$ into a product of the density operator $\hat{\phi}_{\rho_j}$ and the $\hat{b}_j$ operator and we may rearrange the operators in any order we like, we opt to put all $\hat{\phi}_{\rho_j}$ to the right and execute them first. This means that for any particle number ℓ and any general n-point cumulant we first calculate the density-only cumulant. After that we apply the $\hat{b}_j$ operators in the appropriate way to get mixed cumulants. In each operator product term each *external label* $1,\ldots,n$ coming from the arguments of the fields in the cumulant appears exactly once. We will adopt the notion that such an external label is *carried* by the particle j if the label appears in a density operator $\hat{\phi}_{\rho_j}$ belonging to that particle. In physical terms, for the external

label 1 this means that the particle j contributes the phase $\exp\left\{-\mathrm{i}\vec{k}_1\cdot\vec{q}_j(t_1)\right\}$ to the mode $\vec{k}_1$ of the density field at time t_1. With the help of the ℓ-particle version of (2.66), the effect of the operator on $Z_0^{(\ell)}$ is straightforward to calculate

$$\begin{aligned}
\hat{\phi}_{\rho_j}(1)Z_0^{(\ell)}[\mathbf{J},\mathbf{K}] &= \exp\left\{-\mathrm{i}\vec{k}_1\cdot\frac{\delta}{\mathrm{i}\delta\vec{J}_{q_j}(t_1)}\right\}\exp\left\{\mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\mathrm{d}t\ \langle\mathbf{J}(t),\bar{\mathbf{x}}(t)\rangle\right\}\\
&= \exp\left\{-\mathrm{i}\vec{k}_1\cdot\frac{\delta}{\mathrm{i}\delta\vec{J}_{q_j}(t_1)}\right\}\exp\left\{\mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\mathrm{d}t\ \sum_{i=1}^{\ell}\vec{J}_i(t)\cdot\bar{\vec{x}}_i(t)\right\}\\
&= \exp\left\{-\mathrm{i}\begin{pmatrix}\vec{k}_1\\ \vec{0}\end{pmatrix}^{\mathrm{T}}\bar{\vec{x}}_j(t_1)\right\}\exp\left\{\mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\mathrm{d}t\ \sum_{i=1}^{\ell}\vec{J}_i(t)\cdot\bar{\vec{x}}_i(t)\right\}\\
&= \exp\left\{\mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\mathrm{d}t\ \left\langle\left(-\delta_\mathrm{D}\left(t-t_1\right)\begin{pmatrix}\vec{k}_1\\ \vec{0}\end{pmatrix}\otimes\vec{e}_j\right),\bar{\mathbf{x}}(t)\right\rangle\right\}\times\\
&\quad\exp\left\{\mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\mathrm{d}t\ \langle\mathbf{J}(t),\bar{\mathbf{x}}(t)\rangle\right\}
\end{aligned}\tag{4.24}$$

In the case where the particle j carries not only one but a subset $\{s\}_j$ of all external labels $1,\ldots,n$, i. e. multiple operators $\hat{\phi}_{\rho_j}$ are applied, we get the appropriate product of prefactors of the sort shown in (4.24). If we define the *shift tensor*

$$\mathbf{L}_j(t) := -\sum_{s\in\{s\}_j}\delta_\mathrm{D}\left(t-t_s\right)\begin{pmatrix}\vec{k}_s\\ \vec{0}\end{pmatrix}\otimes\vec{e}_j \tag{4.25}$$

we can write the effect of multiple operators as a shift of the $\mathbf{J}$ source

$$\begin{aligned}
\left(\prod_{s\in\{s\}_j}\hat{\phi}_{\rho_j}(s)\right)Z_0^{(\ell)}[\mathbf{J},\mathbf{K}] &= \exp\left\{\mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\mathrm{d}t\ \left\langle\mathbf{L}_j(t),\bar{\mathbf{x}}(t)\right\rangle\right\}\exp\left\{\mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\mathrm{d}t\,\langle\mathbf{J}(t),\bar{\mathbf{x}}(t)\rangle\right\}\\
&= \exp\left\{\mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\mathrm{d}t\ \left\langle\mathbf{J}(t)+\mathbf{L}_j(t),\bar{\mathbf{x}}(t)\right\rangle\right\}\\
&= Z_0^{(\ell)}[\mathbf{J}+\mathbf{L}_j,\mathbf{K}]\,.
\end{aligned}\tag{4.26}$$

The effect of all density operators in any term of (4.23) is then given by adding the shift tensors for all particles as

$$\left(\prod_{j=1}^{\ell}\left(\prod_{s\in\{s\}_j}\hat{\phi}_{\rho_j}(s)\right)\right)Z_0^{(\ell)}[\mathbf{J},\mathbf{K}] = Z_0^{(\ell)}[\mathbf{J}+\sum_{j=1}^{\ell}\mathbf{L}_j(t),\mathbf{K}] := Z_0^{(\ell)}[\mathbf{J}+\mathbf{L},\mathbf{K}]\,. \tag{4.27}$$

We now know the effect of density operators. The effect of the $\hat{b}$ operators is then very easy to derive. They only contain derivatives w. r. t. to the $\mathbf{K}_p$ source. We thus need the following derivative

$$\begin{aligned}\mathrm{i}\vec{k}_1 \cdot \frac{\delta \bar{\mathbf{x}}(t)}{\mathrm{i}\delta \vec{K}_{p_j}(t_1)} &= \mathrm{i}\vec{k}_1 \cdot \frac{\delta}{\mathrm{i}\delta \vec{K}_{p_j}(t_1)} \left(\mathcal{G}(t,t_\mathrm{i})\, \vec{x}_i^{(\mathrm{i})} - \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t'\, \mathcal{G}(t,t')\, \vec{K}_i(t') \right) \otimes \vec{e}_i \\ &= -\mathcal{G}(t,t_1) \begin{pmatrix} \vec{0} \\ \vec{k}_1 \end{pmatrix} \otimes \vec{e}_j \end{aligned} \tag{4.28}$$

and with this result we find

$$\hat{b}_j(1) Z_0^{(\ell)}[\mathbf{J}+\mathbf{L},\mathbf{K}] = \left(-\mathrm{i} \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \left\langle \mathbf{J}(t) + \mathbf{L}(t), \mathcal{G}(t,t_1) \begin{pmatrix} 0 \\ \vec{k}_1 \end{pmatrix} \otimes \vec{e}_j \right\rangle \right) Z_0^{(\ell)}[\mathbf{J}+\mathbf{L},\mathbf{K}] \,. \tag{4.29}$$

We see that the $\hat{b}$ operators do not lead to any new instances of the source $\mathbf{K}$ or shifts of $\mathbf{J}$ and thus applying multiple operators of this type just takes down factors of the above form. After executing all $\hat{b}$ operators in any term of (4.23) the only functional derivatives left are those w. r. t. $\mathbf{K}_p(t_\mathrm{i})$ in the connected ℓ-particle correlation operator $\hat{\mathcal{C}}_{\mathrm{con}}^{(\ell)}$. Just like the $\hat{b}$ operators they will not lead to an additional shift of the sources in $Z_0^{(\ell)}$ but just take down a factor very similar to that in (4.29). Hence, we can for now assume that we executed these derivatives and set all sources to zero. The unaveraged generating functional will then reduce to

$$\begin{aligned} Z_0^{(\ell)}[\mathbf{J}+\mathbf{L},\mathbf{K}]\Big|_0 = Z_0^{(\ell)}[\mathbf{L},\mathbf{0}] &= \exp\left\{ \mathrm{i} \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \left\langle \mathbf{L}(t), \boldsymbol{\mathcal{G}}(t,t_\mathrm{i})\, \mathbf{x}^{(\mathrm{i})} \right\rangle \right\} \\ &= \exp\left\{ -\mathrm{i} \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \sum_{j=1}^{\ell} \sum_{s\in\{s\}_j} \delta_\mathrm{D}(t-t_s) \begin{pmatrix} \vec{k}_s \\ \vec{0} \end{pmatrix}^\mathrm{T} \mathcal{G}(t,t_\mathrm{i})\, \vec{x}_j^{(\mathrm{i})} \right\} \\ &= \prod_{j=1}^{\ell} \exp\left\{ -\mathrm{i} \sum_{s\in\{s\}_j} \left(\mathrm{g}_{qq}(t_s,t_\mathrm{i})\, \vec{k}_s \cdot \vec{q}_j^{(\mathrm{i})} + \mathrm{g}_{qp}(t_s,t_\mathrm{i})\, \vec{k}_s \cdot \vec{p}_j^{(\mathrm{i})} \right) \right\} . \end{aligned} \tag{4.30}$$

The factors resulting from the application of the $\hat{b}$ operators also simplify significantly into

$$\begin{aligned} b_j(1) &:= \left(-\mathrm{i} \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \left\langle \mathbf{J}(t) + \mathbf{L}(t), \mathcal{G}(t,t_1) \begin{pmatrix} 0 \\ \vec{k}_1 \end{pmatrix} \otimes \vec{e}_j \right\rangle \right) \Big|_0 \\ &= \mathrm{i} \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t \sum_{s\in\{s\}_j} \delta_\mathrm{D}(t-t_s) \begin{pmatrix} \vec{k}_s \\ \vec{0} \end{pmatrix}^\mathrm{T} \mathcal{G}(t,t_1) \begin{pmatrix} \vec{0} \\ \vec{k}_1 \end{pmatrix} \\ &= \mathrm{i}\vec{k}_1 \cdot \sum_{s\in\{s\}_j} \vec{k}_s\, \mathrm{g}_{qp}(t_s,t_1) \,. \end{aligned} \tag{4.31}$$

From this we see that of the four submatrices making up the single particle propagator shown in (2.80) only two actually show up in the cumulants. This fact is unchanged by the correlation operator $\hat{\mathcal{C}}^{(\ell)}_{\text{con}}$ since as already mentioned it will have factors very similar to (4.29). In any physically sensible theory $g_{qq}(t, t_i) = \Theta(t - t_i)$, since this function encodes how the initial position of a freely moving particle influences its momentary position. Furthermore, since we only consider times $t \geq t_i$ we can set $g_{qq}(t, t_i) = 1$. The function $g_{qp}(t, t')$ describes how the position of a freely moving particle changes between times t' and t due to its momentum. For ease of notation we introduce the shorthand notation

$$g_{12} := g_{qp}(t_1, t_2) \quad \text{and} \quad g_1 := g_{qp}(t_1, t_i) \,. \tag{4.32}$$

The fact that also $g_{12} \propto \Theta(t_1 - t_2)$ and $g_{11} = 0$ due to causality allows us to derive a very general theorem for the terms making up (4.23).

Theorem 1. *If in a term contributing to some $G^{(0,\ell)}_{\Phi_{\alpha_1}\dots\Phi_{\alpha_n}}$ a particle 'j' carries only external labels belonging to Φ_B-fields, then the term vanishes.*

Proof. This is best done in an inductive fashion. We begin with a particle j carrying only a single Φ_B-field external label 1. Then the set of external labels is $\{s\}_j = \{1\}$ and with (4.31) we immediately find $b_j(1) = \mathrm{i}\, k_1^2\, g_{11} = 0$. For two Φ_B-fields $\Phi_B(1), \Phi_B(2)$ carried by the particle j the set of external labels is $\{s\}_j = \{1, 2\}$ and we have

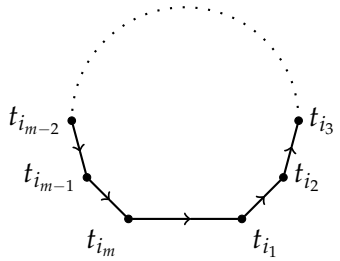
$$\begin{aligned} b_j(1)\, b_j(2) &= \left(\mathrm{i}\vec{k}_1 \cdot \left(\vec{k}_1\, g_{11} + \vec{k}_2\, g_{21}\right)\right) \left(\mathrm{i}\vec{k}_2 \cdot \left(\vec{k}_1\, g_{12} + \vec{k}_2\, g_{22}\right)\right) \\ &= \left(\mathrm{i}\vec{k}_1 \cdot \vec{k}_2\, g_{21}\right) \left(\mathrm{i}\vec{k}_2 \cdot \vec{k}_1\, g_{12}\right) \propto \Theta(t_2 - t_1)\, \Theta(t_1 - t_2) \,. \end{aligned}$$

The only possibility for both Heaviside functions not to vanish would be $t_1 = t_2$. But this leads to factors $g_{11} = g_{22} = 0$.

In the general case of n Φ_B-fields it is advantageous to use a diagrammatic argument. Picture every time coordinate included in the external labels as a point. Due to (4.31) a factor $b_j(1)$ can be seen as a sum of lines between t_1 and all other $n - 1$ time coordinates t_i representing the g_{i1}.

$$b_j(1) \times \ldots \times b_j(n) \to \left(\sum_{m \in \{2,\dots,n\}} \underset{t_1}{\bullet} \!\!\longrightarrow\!\! \underset{t_m}{\bullet} \right) \cdots \left(\sum_{m \in \{1,\dots,n-1\}} \underset{t_n}{\bullet} \!\!\longrightarrow\!\! \underset{t_m}{\bullet} \right)$$

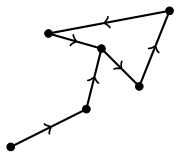
The product $b_j(1)\, b_j(2) \dots b_j(n)$ then results in a sum of $(n-1)^n$ terms each containing n lines connecting all n instances in time. The only restriction on the topology is that there may never be more than one line pointing *away* from any point since these endpoints show up only once in the above product. As in the case $n = 2$, any pair of points connected by two lines, i.e. a closed loop contributes zero. The argument for a two-point loop is easily extended to a general m-point loop as



$$\Theta(t_{i_1} - t_{i_2})\,\Theta(t_{i_2} - t_{i_3}) \ldots \Theta(t_{i_{m-1}} - t_{i_m})\,\Theta(t_{i_m} - t_{i_1}) \Rightarrow t_{i_m} \geq t_{i_1} \geq t_{i_2} \geq \ldots \geq t_{i_m}$$

Again this can only be satisfied if all time coordinates are identical which leads to vanishing propagators. If we connect n dots representing instances of time with $n-1$ lines in any way we always get a tree-like structure. Take for example 6 points and thus 5 lines then we could have:

If we add only one more line in the above example we would always get a closed loop. One possible example for this would be:



It is clear that this also holds for the general case of adding one more line to a tree-like structure of $n-1$ lines connecting n instances in time. Thus, there is no possibility of connecting n instances in time with n lines without creating a closed loop. Since this is the situation for the product $b_j(1)\,b_j(2)\ldots b_j(n)$ all of its terms vanish. □

A straightforward corollary that we can immediately derive from this theorem is the following:

Corollary 2. *Any non-interacting Φ_B-field-only cumulant vanishes:* $G^{(0,\ell)}_{\Phi_{B_1}\ldots\Phi_{B_n}} = 0$.

In a physical sense Theorem 1 is a consequence of the theory respecting the causality of interactions. Consider a term of a general cumulant $G^{(0,\ell)}_{\Phi_{\rho_1}\Phi_{B_2}\Phi_{\alpha_3}\ldots\Phi_{\alpha_n}}$ where both fields $\Phi_\rho(1)$ and $\Phi_B(2)$ are carried by the same particle j. This then leads to a $b_j(2) = i\vec{k}_2 \cdot \vec{k}_1\, g_{12}$ factor which describes how a particle j, which at time t_2 contributes a phase factor as shown in (4.19) to the mode $\vec{k}_2$ of the density field, will deviate from its former free trajectory due to a two-particle interaction it took part in at time t_2 and then again propagate freely forward in time with g_{12} to contribute to the mode $\vec{k}_1$ of the density field at time t_1. If we exchange $\Phi_\rho(1) \to \Phi_B(1)$ we would describe how interactions of the same particle j at times t_1 and t_2 influence the density field at the respective other time. This is represented by the closed loops of arrow lines above. Since we assume our theory to respect causality by using a retarded propagator we

must be able to establish a clear order of how interactions propagate through time and thus terms representing such contradictatory situations must not contribute.

4.2.3 *Effects of correlation operators*

We now assume to have applied all collective field operators present in a general cumulant as shown in (4.23). Since the $\hat{b}$ operators do not generate any new factors of $\mathbf{K}$, the connected correlation operator $\hat{\mathcal{C}}^{(\ell)}_{\text{con}}$, which only contains functional derivatives w. r. t. $\mathbf{K}_p$, will solely act on the shifted $Z^{(\ell)}_0$. We can assemble the effect of any of these operators if we know the effect of the operators represented by the three line types. For the solid density correlation line this is easy since

$$\overset{i}{\bullet}\!\!-\!\!-\!\!\bullet\overset{j}{} \; Z^{(\ell)}_0[\mathbf{J}+\mathbf{L},\mathbf{K}] = C_{\delta_i\delta_j}(\vec{q}^{\,(\mathrm{i})}_i,\vec{q}^{\,(\mathrm{i})}_j)\, Z^{(\ell)}_0[\mathbf{J}+\mathbf{L},\mathbf{K}] \tag{4.33}$$

is just a simple multiplication. Moving on to the density-momentum cross correlation we have

$$\overset{i}{\bullet}\!\!-\!\!-\!\!\bullet\overset{j}{} \; Z^{(\ell)}_0[\mathbf{J}+\mathbf{L},\mathbf{K}] = -\mathrm{i}\vec{C}_{\delta_i p_j}(\vec{q}^{\,(\mathrm{i})}_i,\vec{q}^{\,(\mathrm{i})}_j)\cdot\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_j}(t_\mathrm{i})}\, Z^{(\ell)}_0[\mathbf{J}+\mathbf{L},\mathbf{K}]\,. \tag{4.34}$$

This is basically the same derivative we had to take for the $\hat{b}$ operators and we therefore get the results of (4.28) and (4.29) only with $t_1 \to t_\mathrm{i}$ and $\mathrm{i}\vec{k}_1 \to -\mathrm{i}\vec{C}_{\delta_i p_j}$. This also means that again these derivatives do not generate new factors of $\mathbf{K}_p$ and thus all individual $\bullet\!\!-\!\!-\!\!\bullet$ lines of any diagram only act on the shifted $Z^{(\ell)}_0$ and thus generate factors

$$\begin{aligned}
c_{\delta_i p_j} &:= \left(\mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\mathrm{d}t\,\left\langle \mathbf{J}(t)+\mathbf{L}(t), \mathcal{G}(t,t_\mathrm{i})\begin{pmatrix}0\\ \vec{C}_{\delta_i p_j}\end{pmatrix}\otimes\vec{e}_j\right\rangle\right)\Big|_0 \\
&= -\mathrm{i}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\mathrm{d}t\sum_{s\in\{s\}_j}\delta_\mathrm{D}(t-t_s)\begin{pmatrix}\vec{k}_s\\ \vec{0}\end{pmatrix}^\mathrm{T}\mathcal{G}(t,t_\mathrm{i})\begin{pmatrix}\vec{0}\\ \vec{C}_{\delta_i p_j}\end{pmatrix} \\
&= -\mathrm{i}\vec{C}_{\delta_i p_j}(\vec{q}^{\,(\mathrm{i})}_i,\vec{q}^{\,(\mathrm{i})}_j)\cdot\sum_{s\in\{s\}_j}\vec{k}_s\,\mathrm{g}_{qp}(t_s,t_\mathrm{i}) \\
&= -\mathrm{i}\vec{C}_{\delta_i p_j}(\vec{q}^{\,(\mathrm{i})}_i,\vec{q}^{\,(\mathrm{i})}_j)\cdot\vec{T}_{\{s\}_j}\,.
\end{aligned} \tag{4.35}$$

In the last line we implicitly defined the *transport vector*

$$\vec{T}_{\{s\}_j} := \sum_{s\in\{s\}_j}\vec{k}_s\,\mathrm{g}_{qp}(t_s,t_\mathrm{i}) = \sum_{s\in\{s\}_j}\vec{k}_s\,\mathrm{g}_s\,, \tag{4.36}$$

which encodes how the deviation of the trajectory of particle j due to initial correlations $\vec{C}_{\delta_i p_j}$ travels forward through time to influence the contribution of particle j to the various modes $\vec{k}_s$ of the density field at times t_s. The remaining momentum cor-

relation line i •------• j can be evaluated in a very similar way. With the above reasoning we find

$$\begin{aligned}
&\overset{i}{\bullet}\!\text{------}\!\overset{j}{\bullet}\; Z_0^{(\ell)}[\mathbf{J}+\mathbf{L},\mathbf{K}]\Big|_0 \\
&= \left(\exp\left\{-\left(\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_i}(t_\mathrm{i})}\right)^{\mathrm{T}} C^{\times}_{p_ip_j}\left(\frac{\delta}{\mathrm{i}\delta\vec{K}_{p_j}(t_\mathrm{i})}\right)\right\}-1\right) Z_0^{(\ell)}[\mathbf{J}+\mathbf{L},\mathbf{K}]\Big|_0 \\
&= \left(\exp\left\{-\left(\sum_{s\in\{s\}_i}\vec{k}_s\, \mathrm{g}_{qp}(t_s,t_\mathrm{i})\right)^{\mathrm{T}} C^{\times}_{p_ip_j}\sum_{s\in\{s\}_j}\vec{k}_s\, \mathrm{g}_{qp}(t_s,t_\mathrm{i})\right\}-1\right) Z_0^{(\ell)}[\mathbf{L},\mathbf{0}]\,.
\end{aligned} \tag{4.37}$$

If we again use the transport vector we can define

$$c_{p_ip_j} := \exp\left\{-\vec{T}^{\mathrm{T}}_{\{s\}_i} C^{\times}_{p_ip_j}\vec{T}_{\{s\}_j}\right\}-1\,. \tag{4.38}$$

Once all lines in a $\hat{\mathcal{C}}^{(\ell)}_{\mathrm{con}}$ have been evaluated in this fashion it becomes again a simple function $\mathcal{C}^{(\ell)}_{\mathrm{con}}$ defined individually for each term in (4.23) coming from the product of single-particle operators $\hat{\phi}^{(\ell)}$. For each such $\mathcal{C}^{(\ell)}_{\mathrm{con}}$ all diagram lines are now understood to represent the functions $C_{\delta_i\delta_j}$, $c_{\delta_ip_j}$, $c_{p_ip_j}$ defined with the sets $\{s\}_j$ of external labels that define the shift vectors $\mathbf{L}_j$ of the respective term.

Just like for the $\hat{b}$ operators, knowing the exact form of the results of the application of the correlation operators allows us to derive a helpful theorem concerning the individual terms arising from the product of collective field operators in a general cumulant like (4.23).

Theorem 3. *If in a term contributing to a general $G^{(0,\ell)}_{\Phi_{\alpha_1}\dots\Phi_{\alpha_n}}$ some particle 'j' carries no external labels, i.e. no $\hat{\phi}_{\rho_a}$ has been applied, then the term vanishes.*

Proof. Since the particle j is involved in the cumulant it must be present in the correlation operator $\hat{\mathcal{C}}^{(\ell)}_{\mathrm{con}}$. It must thus be connected with one of the three line types •——•, •—--•, •------•.

If the particle is 'inside the diagram', i. e. connected to more than one line, then the δ-line rule demands that at least one of the lines connects to j with a dashed p-side. Thus either a factor of $c_{\delta_ip_j}$ or $c_{p_ip_j}$ is present. But since j carries no external labels the set $\{s\}_j$ in the transport vector (4.36) is empty and thus $c_{\delta_ip_a} = 0 = c_{p_ip_a}$ and the term vanishes.

If the particle is 'at the boundary of the diagram', i. e. connected to only one line, then we need to distinguish three different cases.

- The particle is connected to a dashed p-type line and we thus can apply the same argument as above.
- It is connected by a $C_{\delta_j\delta_i}$ line. Since the set $\{s\}_j$ is empty we have

$$Z_0^{(\ell)}[\mathbf{L},\mathbf{0}] \propto \exp\left\{-\mathrm{i}\sum_{s\in\{s\}_j}\vec{k}_s\cdot\vec{q}^{\,(\mathrm{i})}_j\right\} = \exp(0) = 1\,.$$

Consequently the term has only one quantity left that depends on $\vec{q}_j^{\,(\mathrm{i})}$ which is $C_{\delta_j\delta_i}$. This leaves us with

$$\int \mathrm{d}\vec{q}_j^{\,(\mathrm{i})}\, C_{\delta_j\delta_i} = \left\langle \int \mathrm{d}\vec{q}_j^{\,(\mathrm{i})}\, \delta^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})})\, \delta^{(\mathrm{i})}(\vec{q}_i^{\,(\mathrm{i})}) \right\rangle = 0$$

where we used (3.29).

- It is connected to the solid δ-side of a $\vec{C}_{\delta_j p_i}$. With the arguments from the previous case we have

$$\int \mathrm{d}\vec{q}_j^{\,(\mathrm{i})}\, \vec{C}_{\delta_j p_i} = \left\langle \int \mathrm{d}\vec{q}_j^{\,(\mathrm{i})}\, \delta^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})})\, \vec{\Pi}^{(\mathrm{i})}(\vec{q}_i^{\,(\mathrm{i})}) \right\rangle = 0$$

□

Combining Theorems 1 and 3 we can derive yet another corollary.

Corollary 4. *For all $\ell > n$, the cumulant $G^{(0,\ell)}_{\Phi_{\rho_1}\dots\Phi_{\rho_n}\Phi_{B_{n+1}}\dots\Phi_{B_{n+m}}} = 0$.*

Proof. We begin by first considering density-only cumulants $G^{(0,\ell)}_{\Phi_{\rho_1}\dots\Phi_{\rho_n}}$ whose principal form is given in (4.23). Each term coming from the product of collective operators $\hat{\Phi}^{(\ell)}_\rho$ is a product of n single particle operators such that each external label appears exactly once in them. For $\ell > n$, there will thus be at least one particle in each term that will not carry an external label. According to Theorem 3 all terms must then vanish. Next we can add any number m of Φ_B-fields to the cumulant. This leads to terms with $n+m$ factors. But as $\ell > n$ for every term, we still have at least one particle which either carries no external label which causes the term to vanish due to Theorem 3 or it only carries Φ_B-field labels which also makes the term vanish according to Theorem 1. □

This corollary is the reason that the sum over representative particle numbers ℓ in (4.18) truncates at the number of density fields present in the cumulant.

4.2.4 *The combinatorial hierarchy of external labels*

By now we know the effects of all operators that appear in a general free n-point ℓ-particle cumulant as shown in (4.23). Before we start to calculate any explicit density-only cumulants it will be advantageous to find a way to organize the many terms containing products of the single particle density operators $\hat{\phi}_{\rho_j}$. Their form will determine the makeup of the subsets $\{s\}_j$ of external labels which in turn dictate the form of all other parts of the cumulant. Our organisational scheme is a hierarchy of three levels. From top to bottom they are:

LABEL DISTRIBUTION This category determines how many of the n external labels each of the ℓ particles carries. We denote them by $\#_1|\dots|\#_\ell$. Take for example an $(n=4)$-point $(\ell=3)$-particle cumulant. A possible distribution would then be $1|1|2$. This means that two particles carry one label each and the third carries

two labels. Note that we do not specify which particle carries which label. We also do not specify which of the three particles carries two labels, all three possibilities are in the same distribution.

LABEL GROUPING In this category we specify which labels are grouped together into subsets $\{s\}$ due to being carried by a single particle. We denote this by $(\{s\}_1;\ldots;\{s\}_m)$. Note that we do *not* specify which exact particle carries which subset $\{s\}_j$, i. e. here the numbers on the subsets in the grouping are *not* the particle indices but just enumerate the subsets. Two examples of groupings for an $(n = 4)$-point $(\ell = 3)$-particle cumulant would be $(1;2;3,4)$ and $(1;3;2,4)$. Both of these belong to the $1|1|2$ distribution.

LABELING This lowest level of the hierarchy represents one explicit term in (4.23). Its notation is best explained in terms of an example. We again consider an $(n = 4)$-point $(\ell = 3)$-particle cumulant with particles a, b, c and external labels $1, 2, 3, 4$. Consider the grouping $(2;3;1,4)$ in the distribution $1|1|2$ with subsets $\{s\}_1 = \{2\}$,$\{s\}_2 = \{3\}, \{s\}_3 = \{1,4\}$. The actual labelings or terms belonging to this grouping are then denoted as $a_{\{s\}_{i_1}} b_{\{s\}_{i_2}} c_{\{s\}_{i_3}}$, for example $a_2 b_3 c_{1,4}$ or $a_3 c_2 b_{1,4}$ and so on.

A visual representation of this hierarchy can be seen in Fig. 5. With this hierarchy es-

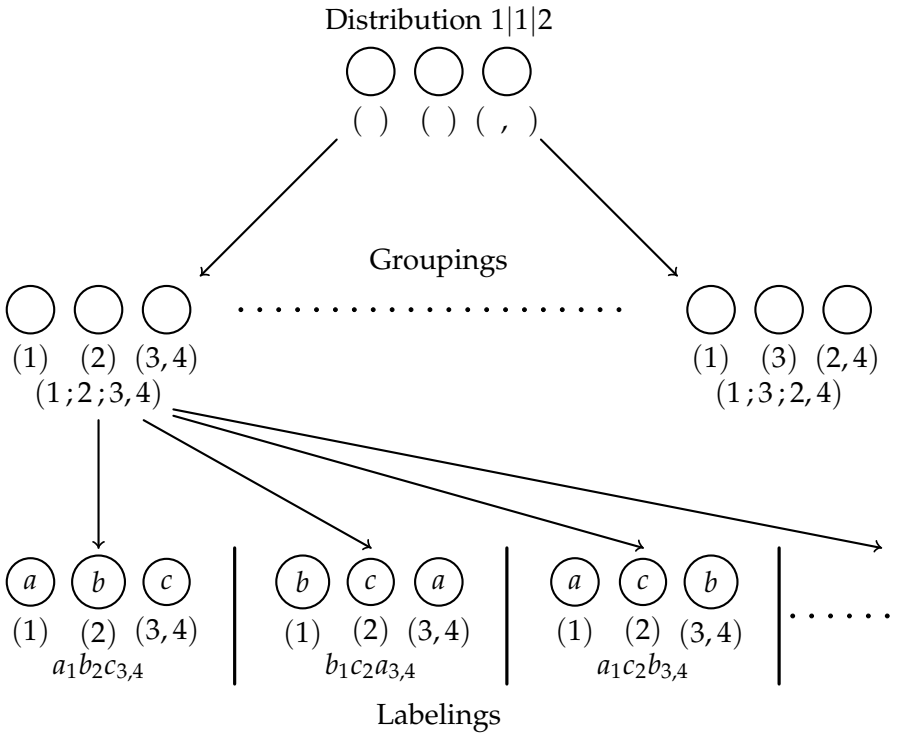


Figure 5: The hierarchy of terms in an $(n = 4)$-point $(\ell = 3)$-particle cumulant sorted by external labels.

tablished we now have to realise that the result of the integral over initial momenta for any cumulant will only depend on the *grouping* and not on the actual labeling, since

the initial momenta only appear in the unaveraged generating functional $Z_0^{(\ell)}[\mathbf{L},\mathbf{0}]$ of (4.30). This is yet another consequence of using a momentum field to specify the initial momenta of particles, which makes the initial correlations only depend on the initial positions of particles. The integral over initial momenta results in a Gaussian damping factor which we define as

$$\begin{aligned}\mathfrak{D}(\{s\}_1\dots\{s\}_\ell) &:= \prod_{j=1}^{\ell}\int \mathrm{d}\vec{p}_j^{\,(\mathrm{i})}\, P_{\sigma_p}(\vec{p}_j^{\,(\mathrm{i})}) \exp\left\{-\mathrm{i}\sum_{s\in\{s\}_j}\vec{p}_j^{\,(\mathrm{i})}\cdot\vec{k}_s\,\mathrm{g}_s\right\}\\ &= \prod_{j=1}^{\ell}\exp\left\{-\frac{\sigma_p^2}{2}\,\vec{T}^2_{\{s\}_j}\right\}\,. \end{aligned} \tag{4.39}$$

We used the freedom afforded to us by the integrals over all momenta of the representative ℓ-particle set to renumber the momenta such that their indices match with the arbitrarily chosen enumeration of the grouping subsets. We can always do this since any grouping with less than ℓ subsets has a particle not carrying an index and thus all of its terms vanish due to Theorem 3. The physical interpretation of this damping factor is obvious. The random free motion of particles set up by the ideal gas part of the momentum distribution will wash out any kind of correlation over time. For a given width σ_p of this distribution, due to the propagators g_i this will happen the sooner, the smaller the length scale $1/k_i$ is that one considers.

With the common factor (4.39) for all terms of a grouping identified we can write the general n-point ℓ-particle cumulant of (4.23) as

$$G^{(0,\ell)}_{\Phi_{\alpha_1}\dots\Phi_{\alpha n}} = \bar{\rho}^{\ell}\sum_{(\{s\}_1\dots\{s\}_\ell)}\mathfrak{D}(\{s\}_1;\dots;\{s\}_\ell)\sum_{\substack{\text{labelings}\in\\(\{s\}_1\dots\{s\}_\ell)}}\int \mathrm{d}\mathbf{q}^{(\mathrm{i})}\,\mathcal{C}^{(\ell)}_{\mathrm{con}}\prod_{j=1}^{\ell}\mathrm{e}^{-\mathrm{i}\vec{q}_j^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_j}}\,, \tag{4.40}$$

where we have introduced the sum of mode vectors over a set of external labels carried by a particle j as

$$\vec{k}_{\{s\}_j} := \sum_{s\in\{s\}_j}\vec{k}_s\,. \tag{4.41}$$

It is now good practice to adopt the following strategy for calculating a general free n-point ℓ-particle density-only cumulant $G^{(0,\ell)}_{\Phi_{\rho_1}\dots\Phi_{\rho_n}}$:

- Find all possible label distributions $\#_1|\dots|\#_\ell$, where all particles carry at least one external label.
- For each of these distributions find all possible label groupings and then pick a general representative grouping with general label sets $(\{s\}_1;\dots;\{s\}_\ell)$.
- Go through all labelings belonging to this representative grouping and for each labeling execute the integral over initial positions of the particles taking into account the diagrams contained in $\hat{\mathcal{C}}_{\mathrm{con}}$ up to some desired order. Gather the results into a single function $\mathcal{T}^{(\ell)}_{\#_1|\dots|\#_\ell}$. We obtain the contribution from any label distributions $\#_1|\dots|\#\ell$ by summing the respective $\mathcal{T}^{(\ell)}_{\#_1|\dots|\#_\ell}$ evaluated with all groupings $(\{s\}_1;\dots;\{s\}_\ell)$ belonging to that distribution.

The general density-only cumulant will then be of the form

$$G^{(0,\ell)}_{\Phi_{\rho_1}\dots\Phi_{\rho_n}} = \bar{\rho}^{\ell} \sum_{\#_1|\dots|\#_\ell} \sum_{\substack{(\{s\}_1\dots\{s\}_\ell)\in \\ \#_1|\dots|\#_\ell}} \mathcal{T}^{(\ell)}_{\#_1|\dots|\#_\ell}(\{s\}_1;\dots;\{s\}_\ell) \,. \tag{4.42}$$

This strategy has the clear advantage that for every cumulant we only have to calculate a single function $\mathcal{T}^{(\ell)}_{\#_1|\dots|\#_\ell}$ once. When we calculate the general $(\ell = 2)$-particle cumulants we will also see that deriving the mixed cumulants between the density field Φ_ρ and the response field Φ_B will become a straightforward task since the b_j factors of (4.31) also only depend on the grouping.

4.2.5 *Initial correlations in Fourier space*

In order to give explicit expressions for general cumulants we need to express the initial two-point correlation functions in terms of their Fourier transforms. We start with the density correlation and find

$$\begin{aligned} C_{\delta_i\delta_j} &= \left\langle \delta^{(\mathrm{i})}(\vec{q}_i^{\,(\mathrm{i})})\, \delta^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})}) \right\rangle \\ &= \left\langle \left(\int \frac{\mathrm{d}\vec{h}_1}{(2\pi)^d}\, \mathrm{e}^{\mathrm{i}\vec{h}_1\cdot\vec{q}_i^{\,(\mathrm{i})}} \delta^{(\mathrm{i})}(\vec{h}_1) \right) \left(\int \frac{\mathrm{d}\vec{h}_2}{(2\pi)^d}\, \mathrm{e}^{\mathrm{i}\vec{h}_2\cdot\vec{q}_j^{\,(\mathrm{i})}} \delta^{(\mathrm{i})}(\vec{h}_2) \right) \right\rangle \\ &= \int \frac{\mathrm{d}\vec{h}_1}{(2\pi)^d} \int \frac{\mathrm{d}\vec{h}_2}{(2\pi)^d}\, \mathrm{e}^{\mathrm{i}\vec{h}_1\cdot\vec{q}_i^{\,(\mathrm{i})}+\mathrm{i}\vec{h}_2\cdot\vec{q}_j^{\,(\mathrm{i})}} \left\langle \delta^{(\mathrm{i})}(\vec{h}_1)\, \delta^{(\mathrm{i})}(\vec{h}_2) \right\rangle \,. \end{aligned} \tag{4.43}$$

Statistical homogeneity and isotropy now dictates that the two-point correlation of the Fourier transform or *power spectrum* of the density contrast has the following form

$$\left\langle \delta^{(\mathrm{i})}(\vec{h}_1)\, \delta^{(\mathrm{i})}(\vec{h}_2) \right\rangle = (2\pi)^d\, \delta_{\mathrm{D}}(\vec{h}_1+\vec{h}_2)\, P_\delta(h_1) \,, \tag{4.44}$$

which means that it is determined by a function P_δ which only depends on the modulus of the mode h_1. In cosmological structure formation it is conventional to call P_δ itself *the* power spectrum. Inserting this back into (4.43) we find

$$C_{\delta_i\delta_j} = \int \frac{\mathrm{d}\vec{h}}{(2\pi)^d}\, \mathrm{e}^{\mathrm{i}\vec{h}\cdot\left(\vec{q}_i^{\,(\mathrm{i})}-\vec{q}_j^{\,(\mathrm{i})}\right)} P_\delta(h) \,, \tag{4.45}$$

where we renamed $\vec{h}_1 \to \vec{h}$. In the general case we would repeat the same for $\vec{C}_{\delta_i p_j}$ and $C^{\times}_{p_i p_j}$ leading to two additional powerspectra to consider. However, for the sake of simplicity we will adopt the following scenario. The initial momentum field is assumed to be irrotational such that we can express it as the gradient of some momentum potential field

$$\vec{\Pi}^{(\mathrm{i})}(\vec{q}) = \nabla_q \psi(\vec{q}) \quad \Longrightarrow \quad \vec{\Pi}(\vec{h}) = \mathrm{i}\vec{h}\,\psi(\vec{h}) \,, \tag{4.46}$$

where we used (1.29) to translate this relation into Fourier space. With the help of the continuity equation, we may then link this momentum potential to the initial density contrast field as

$$\delta^{(\mathrm{i})}(\vec{q}) = -\nabla_q^2 \psi(\vec{q}) \quad \Longrightarrow \quad \delta^{(\mathrm{i})}(\vec{h}) = h^2 \psi(\vec{h}) \,. \tag{4.47}$$

We will motivate why this scenario is precisely the one we encounter in cosmological structure formation in part ii. Both $\vec{C}_{\delta_i p_j}$ and $C^{\times}_{p_i p_j}$ can now be expressed in terms of P_δ.

$$\begin{aligned}
\vec{C}_{\delta_i p_j} &= \left\langle \delta^{(\mathrm{i})}(\vec{q}_i^{\,(\mathrm{i})})\, \vec{\Pi}^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})}) \right\rangle \\
&= \int \frac{\mathrm{d}\vec{h}_1}{(2\pi)^d} \int \frac{\mathrm{d}\vec{h}_2}{(2\pi)^d}\, \mathrm{e}^{\mathrm{i}\vec{h}_1\cdot\vec{q}_i^{\,(\mathrm{i})} + \mathrm{i}\vec{h}_2\cdot\vec{q}_j^{\,(\mathrm{i})}} \left\langle \delta^{(\mathrm{i})}(\vec{h}_1)\, \vec{\Pi}(\vec{h}_2) \right\rangle \\
&= \int \frac{\mathrm{d}\vec{h}_1}{(2\pi)^d} \int \frac{\mathrm{d}\vec{h}_2}{(2\pi)^d}\, \mathrm{e}^{\mathrm{i}\vec{h}_1\cdot\vec{q}_i^{\,(\mathrm{i})} + \mathrm{i}\vec{h}_2\cdot\vec{q}_j^{\,(\mathrm{i})}} \left\langle \delta^{(\mathrm{i})}(\vec{h}_1)\, \frac{\mathrm{i}\vec{h}_2}{h_2^2}\, \delta^{(\mathrm{i})}(\vec{h}_2) \right\rangle \\
&= \mathrm{i} \int \frac{\mathrm{d}\vec{h}_1}{(2\pi)^d} \int \frac{\mathrm{d}\vec{h}_2}{(2\pi)^d}\, \mathrm{e}^{\mathrm{i}\vec{h}_1\cdot\vec{q}_i^{\,(\mathrm{i})} + \mathrm{i}\vec{h}_2\cdot\vec{q}_j^{\,(\mathrm{i})}} \frac{\vec{h}_2}{h_2^2}\, (2\pi)^d\, \delta_{\mathrm{D}}(\vec{h}_1 + \vec{h}_2)\, P_\delta(h_1) \\
&= -\mathrm{i} \int \frac{\mathrm{d}\vec{h}}{(2\pi)^d}\, \mathrm{e}^{\mathrm{i}\vec{h}\cdot\left(\vec{q}_i^{\,(\mathrm{i})} - \vec{q}_j^{\,(\mathrm{i})}\right)} \frac{\vec{h}}{h^2}\, P_\delta(h)\,.
\end{aligned} \tag{4.48}$$

In the third line we have combined (4.46) and (4.47) in order to express the Fourier transform of the momentum field in terms of the density contrast. In analogy we find

$$\begin{aligned}
C^{\times}_{p_i p_j} &= \left\langle \vec{\Pi}^{(\mathrm{i})}(\vec{q}_i^{\,(\mathrm{i})}) \otimes \vec{\Pi}^{(\mathrm{i})}(\vec{q}_j^{\,(\mathrm{i})}) \right\rangle \\
&= \int \frac{\mathrm{d}\vec{h}_1}{(2\pi)^d} \int \frac{\mathrm{d}\vec{h}_2}{(2\pi)^d}\, \mathrm{e}^{\mathrm{i}\vec{h}_1\cdot\vec{q}_i^{\,(\mathrm{i})} + \mathrm{i}\vec{h}_2\cdot\vec{q}_j^{\,(\mathrm{i})}} \left\langle \frac{\mathrm{i}\vec{h}_1}{h_1^2}\, \delta^{(\mathrm{i})}(\vec{h}_1) \otimes \frac{\mathrm{i}\vec{h}_2}{h_2^2}\, \delta^{(\mathrm{i})}(\vec{h}_2) \right\rangle \\
&= \int \frac{\mathrm{d}\vec{h}}{(2\pi)^d}\, \mathrm{e}^{\mathrm{i}\vec{h}\cdot\left(\vec{q}_i^{\,(\mathrm{i})} - \vec{q}_j^{\,(\mathrm{i})}\right)} \frac{\vec{h}\otimes\vec{h}}{h^4}\, P_\delta(h)\,.
\end{aligned} \tag{4.49}$$

Since all three correlation functions are now expressed as Fourier integrals involving the power spectrum linearly, P_δ presents itself as a convenient order parameter for doing perturbative expansions in the initial correlations. We will show this explicitly for the two-particle and three-particle cumulants. Doing this is well justified especially when the initial correlations are weak and the powerspectrum can thus be considered to be small. We will clarify in section 8.1 how to quantify this statement.

4.2.6 *One-particle cumulants*

The one-particle cumulants $G^{(0,1)}_{\Phi_{\alpha_1}\dots\Phi_{\alpha_n}}$ can be written down directly to any desired order in n. This was already shown in the original papers [22, 39] on this kind of field theory. Initial correlations have no effect due to $\hat{\mathcal{C}}^{(1)}_{\mathrm{con}} = 1$ in (4.23). Since there is only one particle, the only possible grouping of external labels is their entirety, i. e. $\{s\} = \{1,\dots,n\}$. This means that integrating the spatial part of the non-averaged ℓ-particle generating functional (4.30) over the initial position of the single particle gives

$$\int \mathrm{d}\vec{q}^{\,(\mathrm{i})}\, \bar{\rho} \exp\left\{ -\vec{q}^{\,(\mathrm{i})} \cdot \sum_{s\in\{s\}} \vec{k}_s \right\} = \bar{\rho}\,(2\pi)^d\, \delta_{\mathrm{D}}\left(\sum_{s=1}^{n} \vec{k}_s \right)\,. \tag{4.50}$$

Combining this with the Gaussian cutoff, the one-particle contribution to the n-point density-only cumulant is given by

$$G^{(0,1)}_{\Phi_{\rho_1}\dots\Phi_{\rho n}} = \bar{\rho}\,(2\pi)^d\,\delta_{\mathrm{D}}\left(\sum_{s=1}^{n}\vec{k}_s\right)\exp\left\{-\frac{\sigma_p^2}{2}\sum_{s=1}^{n}\mathrm{g}_s\,\vec{k}_s\right\}\,. \tag{4.51}$$

Any cross correlator between Φ_ρ and Φ_B is obtained by applying the appropriate $b_j(s) = b(s)$ factor

$$G^{(0,1)}_{\Phi_{\rho_1}\dots\Phi_{\rho n}\Phi_{B_{n+1}}\dots\Phi_{B_{n+m}}} = b(n+1)\,\dots\,b(n+m)\,G^{(0,1)}_{\Phi_{\rho_1}\dots\Phi_{\rho n}}\,. \tag{4.52}$$

The most interesting cases are the one- and two-point cumulants

$$G^{(0,1)}_{\Phi_{\rho_1}} = \bar{\rho}\,(2\pi)^d\,\delta_{\mathrm{D}}\left(\vec{k}_1\right)\,. \qquad G^{(0,1)}_{\Phi_{B_1}} = 0\,. \tag{4.53}$$

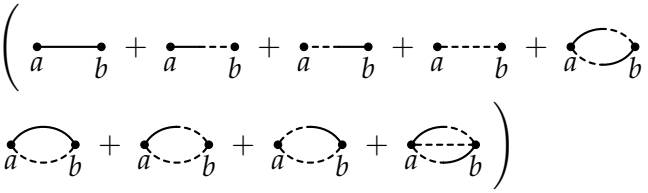
As expected the one-point cumulant of Φ_ρ just gives the mean particle density and the one-point cumulant of the Φ_B-field vanishes according to Corollary 2.

$$\begin{aligned}
G^{(0,1)}_{\Phi_{\rho_1}\Phi_{\rho_2}} &= \bar{\rho}\,(2\pi)^d\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\exp\left\{-\frac{\sigma_p^2}{2}\,k_1^2(\mathrm{g}_1-\mathrm{g}_2)^2\right\}\\
G^{(0,1)}_{\Phi_{\rho_1}\Phi_{B_2}} &= \left(\mathrm{i}\vec{k}_2\cdot\vec{k}_1\,\mathrm{g}_{12}\right)\bar{\rho}\,(2\pi)^d\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\mathfrak{D}(1,2) = -\mathrm{i}\,k_1^2\,\mathrm{g}_{12}\,G^{(0,1)}_{\Phi_{\rho_1}\Phi_{\rho_2}}\\
G^{(0,1)}_{\Phi_{B_1}\Phi_{\rho_2}} &= \left(\mathrm{i}\vec{k}_1\cdot\vec{k}_2\,\mathrm{g}_{21}\right)\bar{\rho}\,(2\pi)^d\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\mathfrak{D}(1,2) = -\mathrm{i}\,k_1^2\,\mathrm{g}_{21}\,G^{(0,1)}_{\Phi_{\rho_1}\Phi_{\rho_2}}\\
G^{(0,1)}_{\Phi_{B_1}\Phi_{B_2}} &= 0
\end{aligned} \tag{4.54}$$

We used the Dirac delta distribution to set $\vec{k}_2 = -\vec{k}_1$. The interpretation of the two-point density cumulant as an exponentially damped shot-noise contribution will be motivated in section 4.3.4. Following Theorem 1, we already argued why $G^{(0,1)}_{\Phi_{\rho_1}\Phi_{B_2}}$ and $G^{(0,1)}_{\Phi_{B_1}\Phi_{\rho_2}}$ can be understood as propagators for the density field Φ_ρ in a statistical sense. This will become clearer once we take a look at perturbation theory.

4.2.7 *Two-particle cumulants*

As in the one-particle case the two-particle cumulants can be written down to any desired order of external labels n. The correlation function $\mathcal{C}^{(2)}_{\mathrm{con}}$ can be seen in its diagrammatic form as the two-particle sum in (3.91). We now apply the reasoning used in (3.117) that once the trace operators are applied diagrams of equal topology give the same result to combine these and find

$\mathcal{C}^{(2)}_{\mathrm{con}} = \frac{1}{2!}\Big($  $\Big)$

$$= \frac{1}{2}\Bigg(\underset{a}{\bullet}\!\!-\!\!\!-\!\!\underset{b}{\bullet} + 2\,\underset{a}{\bullet}\!\!-\!\!\!-\!\!\underset{b}{\bullet} + \underset{a}{\bullet}\!\!\cdots\!\!\underset{b}{\bullet} + \underset{a}{\bullet}\!\!\circlearrowright\!\!\underset{b}{\bullet} + \underset{a}{\bullet}\!\!\circlearrowright\!\!\underset{b}{\bullet} + 2\,\underset{a}{\bullet}\!\!\circlearrowright\!\!\underset{b}{\bullet} + \underset{a}{\bullet}\!\!\circlearrowright\!\!\underset{b}{\bullet} \Bigg) \,. \tag{4.55}$$

Next we need to consider that the $\bullet\cdots\bullet$ line actually represents an exponential of the momentum correlations according to (4.37) and thus through (4.49) contains arbitrary orders of the initial power spectrum P_δ. We thus have to truncate at some order of P_δ and for the sake of keeping the length of expressions managable we choose to truncate at quadratic order. This means that the last diagram in (4.55) containing three lines is excluded. The $c_{p_a p_b}$ factors coming from any $\bullet\cdots\bullet$ are approximated as

$$c_{p_a p_b} \approx -\vec{T}^{\mathrm{T}}_{\{s\}_a} C^{\times}_{p_a p_b} \vec{T}_{\{s\}_b} + \frac{1}{2}\left(\vec{T}^{\mathrm{T}}_{\{s\}_a} C^{\times}_{p_a p_b} \vec{T}_{\{s\}_b}\right)^2 \,. \tag{4.56}$$

In terms of diagrams we write this as

$$\mathcal{C}^{(2)}_{\mathrm{con}} = \frac{1}{2}\Bigg(\underset{a}{\bullet}\!\!-\!\!\!-\!\!\underset{b}{\bullet} + 2\,\underset{a}{\bullet}\!\!-\!\!\!-\!\!\underset{b}{\bullet} + \overset{(1)}{\underset{a}{\bullet}\!\!\cdots\!\!\underset{b}{\bullet}} \Bigg) + \frac{1}{2}\Bigg(\overset{(2)}{\underset{a}{\bullet}\!\!\cdots\!\!\underset{b}{\bullet}} + \underset{a}{\bullet}\!\!\circlearrowright\!\!\underset{b}{\bullet} + \overset{(1)}{\underset{a}{\bullet}\!\!\circlearrowright\!\!\underset{b}{\bullet}} + 2\,\overset{(1)}{\underset{a}{\bullet}\!\!\circlearrowright\!\!\underset{b}{\bullet}} \Bigg) = \mathcal{C}^{(2,1)}_{\mathrm{con}} + \mathcal{C}^{(2,2)}_{\mathrm{con}} \,, \tag{4.57}$$

where $\overset{(1)}{\bullet\cdots\bullet}$ means the first order contribution in (4.56) and so on. We now want to calculate the general n-point density-only cumulant with the correlations shown in (4.57). For this we implement the general strategy for organising the terms originating from the product of single-particle density operators $\hat{\phi}_\rho$ that we discussed in section 4.2.4. We have $\ell = 2$ particles a and b and thus all non-vanishing label distributions are given by $m|(n-m)$ with $1 \leq m \leq \lfloor n/2 \rfloor$. All label groupings $(\{s_1\};\{s_2\}) = (i_1,\ldots,i_m;j_1,\ldots,j_{n-m})$ only include two labelings $a_{i_1\ldots i_m} b_{j_1\ldots j_{n-m}}$ and $a_{j_1\ldots j_{n-m}} b_{i_1\ldots i_m}$. We pick such a general grouping $(\{s_1\};\{s_2\})$ and first calculate the damping function coming from the integration over the initial momenta. With (4.39) we easily find

$$\mathfrak{D}(\{s_1\};\{s_2\}) = \exp\left\{-\frac{\sigma_p^2}{2}\left(\vec{T}^2_{\{s\}_1} + \vec{T}^2_{\{s\}_2}\right)\right\} \,. \tag{4.58}$$

We now need to evaluate the second sum in (4.40) for the grouping we have chosen in order to find the general $\mathcal{T}^{(2)}_{\#\{s\}_1|\#\{s\}_2}$ function. Since we only include first and second order effects in the power spectrum P_δ we also define the $\mathcal{T}$ to these orders as

$$\begin{aligned} &(2\pi)^d\,\delta_{\mathrm{D}}\left(\sum_{s=1}^n \vec{k}_s\right) \mathcal{T}^{(2,1)}_{\#\{s\}_1|\#\{s\}_2}(\{s_1\};\{s_2\}) \\ &:= (2\pi)^d\,\delta_{\mathrm{D}}\left(\sum_{s=1}^n \vec{k}_s\right) \mathfrak{D}(\{s_1\};\{s_2\}) \times \\ &\int \mathrm{d}\vec{q}^{\,(\mathrm{i})}_a \int \mathrm{d}\vec{q}^{\,(\mathrm{i})}_b \left(\mathcal{C}^{(2,1)}_{\mathrm{con}} \mathrm{e}^{-\mathrm{i}\vec{q}^{\,(\mathrm{i})}_a \cdot \vec{k}_{\{s\}_1}} \mathrm{e}^{-\mathrm{i}\vec{q}^{\,(\mathrm{i})}_b \cdot \vec{k}_{\{s\}_2}} + \mathcal{C}^{(2,1)}_{\mathrm{con}} \mathrm{e}^{-\mathrm{i}\vec{q}^{\,(\mathrm{i})}_a \cdot \vec{k}_{\{s\}_2}} \mathrm{e}^{-\mathrm{i}\vec{q}^{\,(\mathrm{i})}_b \cdot \vec{k}_{\{s\}_1}} \right) \end{aligned} \tag{4.59}$$

and analogously for the second order function. The role of the Dirac delta distribution in front of the $\mathcal{T}$ function will become clear in a moment. We start evaluating the simplest of all diagrams in (4.57), the $\bullet\!\!-\!\!-\!\!\bullet$ line. The integral over initial positions is then

$$\begin{aligned}
&\frac{1}{2}\int \mathrm{d}\vec{q}_a^{\,(\mathrm{i})} \int \mathrm{d}\vec{q}_b^{\,(\mathrm{i})} \; \overset{a}{\bullet}\!\!-\!\!-\!\!\overset{b}{\bullet} \left(\mathrm{e}^{-\mathrm{i}\vec{q}_a^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_1}} \mathrm{e}^{-\mathrm{i}\vec{q}_b^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_2}} + \mathrm{e}^{-\mathrm{i}\vec{q}_a^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_2}} \mathrm{e}^{-\mathrm{i}\vec{q}_b^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_1}} \right) \\
&= \frac{1}{2}\int \mathrm{d}\vec{q}_a^{\,(\mathrm{i})} \int \mathrm{d}\vec{q}_b^{\,(\mathrm{i})}\, 2\, C_{\delta_a\delta_b}(\vec{q}_a^{\,(\mathrm{i})}, \vec{q}_b^{\,(\mathrm{i})})\, \mathrm{e}^{-\mathrm{i}\vec{q}_a^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_1}} \mathrm{e}^{-\mathrm{i}\vec{q}_b^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_2}} \\
&= \int \mathrm{d}\vec{q}_a^{\,(\mathrm{i})} \int \mathrm{d}\vec{q}_b^{\,(\mathrm{i})} \int \frac{\mathrm{d}\vec{h}}{(2\pi)^d} \mathrm{e}^{\mathrm{i}\vec{h}\cdot\left(\vec{q}_a^{\,(\mathrm{i})}-\vec{q}_b^{\,(\mathrm{i})}\right)} P_\delta(h)\, \mathrm{e}^{-\mathrm{i}\vec{q}_a^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_1}} \mathrm{e}^{-\mathrm{i}\vec{q}_b^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_2}} \\
&= (2\pi)^d \int \mathrm{d}\vec{h}\, P_\delta(h) \int \frac{\mathrm{d}\vec{q}_a^{\,(\mathrm{i})}}{(2\pi)^d} \mathrm{e}^{\mathrm{i}\vec{q}_a^{\,(\mathrm{i})}\cdot\left(\vec{h}-\vec{k}_{\{s\}_1}\right)} \int \frac{\mathrm{d}\vec{q}_b^{\,(\mathrm{i})}}{(2\pi)^d} \mathrm{e}^{-\mathrm{i}\vec{q}_b^{\,(\mathrm{i})}\cdot\left(\vec{h}+\vec{k}_{\{s\}_1}\right)} \\
&= (2\pi)^d \int \mathrm{d}\vec{h}\, P_\delta(h)\, \delta_\mathrm{D}(\vec{h}-\vec{k}_{\{s\}_1})\, \delta_\mathrm{D}(\vec{h}+\vec{k}_{\{s\}_1}) \\
&= (2\pi)^d\, \delta_\mathrm{D}(\vec{k}_{\{s\}_1}+\vec{k}_{\{s\}_2})\, P_\delta(|\vec{k}_{\{s\}_1}|) = (2\pi)^d\, \delta_\mathrm{D}\left(\sum_{s=1}^{n}\vec{k}_s\right) P_\delta(|\vec{k}_{\{s\}_1}|)\,. \qquad (4.60)
\end{aligned}$$

In the first line we already used the fact that the diagram does not actually depend on the sets of external labels $\{s\}_1$ and $\{s\}_2$ to pull it out in front of the two explicit labeling terms. In the second line we used the symmetry of the diagram in order to combine both terms by renaming the particles in the second term. We then inserted (4.45) and used the relation (1.26) for the Fourier transform of the Dirac delta distribution. In the last line we used that the union of both sets $\{s\}_1$ and $\{s\}_2$ must be the entirety of all external labels. The fact that we find a Dirac delta distribution with the sum of modes as its arguments is a clear sign that this is a *connected* contribution to the correlation of the collective fields $\Phi_{\rho_1}\ldots\Phi_{\rho_n}$ in a statistically homogeneous and isotropic system. Note that using this Dirac delta distribution we may always exchange the argument of the power spectrum P_δ between $\vec{k}_{\{s\}_1}$ and $\vec{k}_{\{s\}_2}$.

The above calculation already shows most of the features that we encounter in the calculation of all the other diagrams of (4.57). We will do the explicit calculation for two more diagrams to show the remaining features. First up is the $\bullet\!\!-\!\!-\!\!\bullet$ line.

$$\begin{aligned}
&\frac{1}{2}\int \mathrm{d}\vec{q}_a^{\,(\mathrm{i})} \int \mathrm{d}\vec{q}_b^{\,(\mathrm{i})}\, 2\; \overset{a}{\bullet}\!\!-\!\!-\!\!\overset{b}{\bullet}\; \mathrm{e}^{-\mathrm{i}\vec{q}_a^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_1}} \mathrm{e}^{-\mathrm{i}\vec{q}_b^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_2}} \\
&+ \frac{1}{2}\int \mathrm{d}\vec{q}_a^{\,(\mathrm{i})} \int \mathrm{d}\vec{q}_b^{\,(\mathrm{i})}\, 2\; \overset{a}{\bullet}\!\!-\!\!-\!\!\overset{b}{\bullet}\; \mathrm{e}^{-\mathrm{i}\vec{q}_a^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_2}} \mathrm{e}^{-\mathrm{i}\vec{q}_b^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_1}} \\
&= (-\mathrm{i})^2 \int \mathrm{d}\vec{q}_a^{\,(\mathrm{i})} \int \mathrm{d}\vec{q}_b^{\,(\mathrm{i})} \int \frac{\mathrm{d}\vec{h}}{(2\pi)^d} \mathrm{e}^{\mathrm{i}\vec{h}\cdot\left(\vec{q}_a^{\,(\mathrm{i})}-\vec{q}_b^{\,(\mathrm{i})}\right)} P_\delta(h)\, \frac{\vec{h}\cdot\vec{T}_{\{s\}_2}}{h^2}\, \mathrm{e}^{-\mathrm{i}\vec{q}_a^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_1}-\mathrm{i}\vec{q}_b^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_2}} \\
&+ (-\mathrm{i})^2 \int \mathrm{d}\vec{q}_a^{\,(\mathrm{i})} \int \mathrm{d}\vec{q}_b^{\,(\mathrm{i})} \int \frac{\mathrm{d}\vec{h}}{(2\pi)^d} \mathrm{e}^{\mathrm{i}\vec{h}\cdot\left(\vec{q}_a^{\,(\mathrm{i})}-\vec{q}_b^{\,(\mathrm{i})}\right)} P_\delta(h)\, \frac{\vec{h}\cdot\vec{T}_{\{s\}_1}}{h^2}\, \mathrm{e}^{-\mathrm{i}\vec{q}_a^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_2}-\mathrm{i}\vec{q}_b^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_1}}
\end{aligned}$$

$$
\begin{aligned}
&= -(2\pi)^d \int \mathrm{d}\vec{h}\, P_\delta(h)\, \frac{\vec{h}\cdot\vec{T}_{\{s\}_2}}{h^2}\, \delta_\mathrm{D}(\vec{h}-\vec{k}_{\{s\}_1})\, \delta_\mathrm{D}(\vec{h}+\vec{k}_{\{s\}_2}) \\
&\quad - (2\pi)^d \int \mathrm{d}\vec{h}\, P_\delta(h)\, \frac{\vec{h}\cdot\vec{T}_{\{s\}_1}}{h^2}\, \delta_\mathrm{D}(\vec{h}-\vec{k}_{\{s\}_2})\, \delta_\mathrm{D}(\vec{h}+\vec{k}_{\{s\}_1}) \\
&= -(2\pi)^d\, \delta_\mathrm{D}\left(\sum_{s=1}^{n}\vec{k}_s\right)\left(P_\delta(|\vec{k}_{\{s\}_1}|)\, \frac{\vec{k}_{\{s\}_1}\cdot\vec{T}_{\{s\}_2}}{\vec{k}^2_{\{s\}_1}} + P_\delta(|\vec{k}_{\{s\}_2}|)\, \frac{\vec{k}_{\{s\}_2}\cdot\vec{T}_{\{s\}_1}}{\vec{k}^2_{\{s\}_2}}\right) \\
&= (2\pi)^d\, \delta_\mathrm{D}\left(\sum_{s=1}^{n}\vec{k}_s\right) P_\delta(|\vec{k}_{\{s\}_1}|)\left(\frac{\vec{k}_{\{s\}_1}\cdot\vec{T}_{\{s\}_1}}{\vec{k}^2_{\{s\}_1}} + \frac{\vec{k}_{\{s\}_2}\cdot\vec{T}_{\{s\}_2}}{\vec{k}^2_{\{s\}_2}}\right)
\end{aligned}
\tag{4.61}
$$

We see that due to the •---• line not being symmetric we have to consider both labelings separately. In the first step we used both (4.35) and (4.48). The second step is then just a repetition of the calculation in (4.59). In the last line we used the overall Dirac delta distribution to exchange $\vec{k}_{\{s\}_1}$ and $\vec{k}_{\{s\}_2}$ in such a way as to simplify the expression as much as possible.

The last diagram we calculate explicitly is $\overset{(1)}{\circlearrowright}$. Just like in the case of the •—• line, the symmetry of the diagram leads to both labelings giving the same contribution. We thus only calculate one of them and take a factor of 2 into account from the beginning. With the help of (4.29) we find

$$
\begin{aligned}
&2\frac{1}{2}\int \mathrm{d}\vec{q}_a^{\,(\mathrm{i})} \int \mathrm{d}\vec{q}_b^{\,(\mathrm{i})}\; \overset{(1)}{\underset{a}{\circlearrowright}}\!\!{}_{b}\; \mathrm{e}^{-\mathrm{i}\vec{q}_a^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_1}}\, \mathrm{e}^{-\mathrm{i}\vec{q}_b^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_2}} \\
&= -\int \mathrm{d}\vec{q}_a^{\,(\mathrm{i})} \int \mathrm{d}\vec{q}_b^{\,(\mathrm{i})} \int \frac{\mathrm{d}\vec{h}_1}{(2\pi)^d}\, P_\delta(h_1)\, \mathrm{e}^{\mathrm{i}\vec{h}_1\cdot\left(\vec{q}_a^{\,(\mathrm{i})}-\vec{q}_b^{\,(\mathrm{i})}\right)}\, \vec{T}^{\,\mathrm{T}}_{\{s\}_1}\left(\frac{\vec{h}_1\otimes\vec{h}_1}{h_1^4}\right)\vec{T}_{\{s\}_1}\times \\
&\quad \int \frac{\mathrm{d}\vec{h}_2}{(2\pi)^d}\, P_\delta(h_2)\, \mathrm{e}^{\mathrm{i}\vec{h}_2\cdot\left(\vec{q}_a^{\,(\mathrm{i})}-\vec{q}_b^{\,(\mathrm{i})}\right)}\, \mathrm{e}^{-\mathrm{i}\vec{q}_a^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_1}}\, \mathrm{e}^{-\mathrm{i}\vec{q}_b^{\,(\mathrm{i})}\cdot\vec{k}_{\{s\}_2}} \\
&= -(2\pi)^{2d} \int \frac{\mathrm{d}\vec{h}_1}{(2\pi)^d} \int \frac{\mathrm{d}\vec{h}_2}{(2\pi)^d}\, \delta_\mathrm{D}(\vec{h}_1+\vec{h}_2-\vec{k}_{\{s\}_1})\, \delta_\mathrm{D}(\vec{h}_1+\vec{h}_2+\vec{k}_{\{s\}_2})\times \\
&\quad P_\delta(h_1)\, P_\delta(h_2)\, \frac{\vec{T}_{\{s\}_1}\cdot\vec{h}_1}{h_1^2}\, \frac{\vec{T}_{\{s\}_2}\cdot\vec{h}_1}{h_1^2} \\
&= -(2\pi)^d\, \delta_\mathrm{D}\left(\sum_{s=1}^{n}\vec{k}_s\right) \int \frac{\mathrm{d}\vec{h}}{(2\pi)^d}\, P_\delta(h)\, P_\delta(|\vec{h}-\vec{k}_{\{s\}_1}|)\, \frac{\vec{T}_{\{s\}_1}\cdot\vec{h}}{h^2}\, \frac{\vec{T}_{\{s\}_2}\cdot\vec{h}}{h^2}\,.
\end{aligned}
\tag{4.62}
$$

Going from the third and fourth to the last line we executed the integral over $\vec{h}_2$ and then renamed $\vec{h}_1 \to \vec{h}$. All other steps should by now be familiar from the previous two calculations. Note that as soon as we have more than one correlation line and thus a loop-like structure[1] we retain one Fourier integral which we cannot perform analytically. It mixes contributions of the power spectrum from different modes. This

1 Note that the $\overset{(2)}{\bullet\!\!-\!\!-\!\!-\!\!\bullet}$ line actually stands for the loop like diagram $\overset{(1)}{\underset{(1)}{\circlearrowright}}$. We have drawn it as single second order line to clarify its origin.

phenomenon is often called *mode coupling*. Once all diagrams of (4.57) have been evaluated for the general grouping under consideration, i. e. $(\{s\}_1;\{s\}_2)$, we can write down both the first and second order $\mathcal{T}$ functions.

$$\mathcal{T}^{(2,1)}_{\#\{s_1\}|\#\{s_2\}}(\{s_1\};\{s_2\}) = \mathfrak{D}(\{s_1\},\{s_2\})\, P_\delta(|\vec{k}_{\{s_1\}}|) \left\{ 1 + \frac{\vec{T}_{\{s\}_1}\cdot\vec{k}_{\{s\}_1}}{\vec{k}^2_{\{s\}_1}} + \frac{\vec{T}_{\{s\}_2}\cdot\vec{k}_{\{s\}_2}}{\vec{k}^2_{\{s\}_2}} + \frac{\vec{T}_{\{s\}_1}\cdot\vec{k}_{\{s\}_1}}{\vec{k}^2_{\{s\}_1}}\,\frac{\vec{T}_{\{s\}_2}\cdot\vec{k}_{\{s\}_2}}{\vec{k}^2_{\{s\}_2}} \right\} . \tag{4.63}$$

$$\begin{aligned}\mathcal{T}^{(2,2)}_{\#\{s_1\}|\#\{s_2\}}(\{s_1\};\{s_2\}) = \mathfrak{D}(\{s_1\},\{s_2\}) \int \frac{\mathrm{d}\vec{h}}{(2\pi)^d}\, P_\delta(h)\, P_\delta(|\vec{k}_{\{s_1\}}-\vec{h}|) \\ \left\{ \frac{\vec{T}_{\{s\}_1}\cdot\vec{h}}{h^2}\,\frac{\vec{T}_{\{s\}_2}\cdot\left(\vec{k}_{\{s\}_1}-\vec{h}\right)}{\left(\vec{k}_{\{s\}_1}-\vec{h}\right)^2} - \frac{\vec{T}_{\{s\}_1}\cdot\vec{h}}{h^2}\,\frac{\vec{T}_{\{s\}_2}\cdot\vec{h}}{h^2} \times \right. \\ \left(1 + \frac{\vec{T}_{\{s\}_1}\cdot\left(\vec{k}_{\{s\}_1}-\vec{h}\right)}{\left(\vec{k}_{\{s\}_1}-\vec{h}\right)^2} - \frac{\vec{T}_{\{s\}_2}\cdot\left(\vec{k}_{\{s\}_1}-\vec{h}\right)}{\left(\vec{k}_{\{s\}_1}-\vec{h}\right)^2} \right. \\ \left. \left. -\frac{1}{2}\frac{\vec{T}_{\{s\}_1}\cdot\left(\vec{k}_{\{s\}_1}-\vec{h}\right)}{\left(\vec{k}_{\{s\}_1}-\vec{h}\right)^2}\,\frac{\vec{T}_{\{s\}_2}\cdot\left(\vec{k}_{\{s\}_1}-\vec{h}\right)}{\left(\vec{k}_{\{s\}_1}-\vec{h}\right)^2} \right) \right\}\end{aligned} \tag{4.64}$$

With these two functions the general n-point ℓ-particle density-only cumulant up to second order in the initial powerspectrum can then be written down as

$$G^{(0,2)}_{\Phi_{\rho_1}\dots\Phi_{\rho_n}} = \bar{\rho}^2(2\pi)^d\,\delta_{\mathrm{D}}\left(\sum_{s=1}^{n}\vec{k}_s\right)\sum_{m=1}^{\lfloor n/2\rfloor}\sum_{\substack{\{s_1\},\{s_2\}\\ \#\{s_1\}=m\\ \#\{s_2\}=n-m}}\sum_{p=1}^{2}\mathcal{T}^{(2,p)}_{\#\{s_1\}|\#\{s_2\}}(\{s_1\};\{s_2\})\,. \tag{4.65}$$

Although both $\mathcal{T}^{(2)}$ functions might look somewhat intimidating due to their extensive length, they reduce in size if we consider the most interesting cases of lower n-point cumulants. For the $(n=1)$-point case we can immediately infer from Theorem 3 that

$$G^{(0,2)}_{\Phi_{\rho_1}} = 0 \quad \text{and} \quad G^{(0,2)}_{\Phi_{B_1}} = 0\,. \tag{4.66}$$

This is not very surprising since the mean density of a statistically homogeneous and isotropic system must be spatially constant. Thus the correlations of two particles may not influence it. Moving on to the $(n=2)$-point case the only possible label distribution is $1|1$ and it trivially contains only the grouping $(1;2)$. The overall Dirac delta distribution in (4.65) then allows us to set $\vec{k}_2 = -\vec{k}_1$. The two $\mathcal{T}^{(2)}$ functions have the explicit form

$$\mathcal{T}^{(2,1)}_{1|1}(1;2) = P_\delta(k_1)\,(1+\mathrm{g}_1)\,(1+\mathrm{g}_2)\exp\left\{-\frac{\sigma_p^2}{2}\,k_1^2\,(\mathrm{g}_1^2+\mathrm{g}_2^2)\right\} \tag{4.67}$$

$$\mathcal{T}^{(2,2)}_{1|1}(1;2) = \exp\left\{-\frac{\sigma_p^2}{2}\,k_1^2\,(g_1^2+g_2^2)\right\}\int\frac{d\vec{h}}{(2\pi)^d}\,P_\delta(|\vec{k}_1-\vec{h}|)\,P_\delta(h)\times$$
$$\left\{g_1g_2\left(\frac{\vec{k}_1\cdot\vec{h}}{h^2}\right)^2\left(1+(g_1+g_2)\frac{\vec{k}_1\cdot\left(\vec{k}_1-\vec{h}\right)}{\left(\vec{k}_1-\vec{h}\right)^2}\right.\right.$$
$$\left.\left.+\frac{g_1g_2}{2}\left(\frac{\vec{k}_1\cdot\left(\vec{k}_1-\vec{h}\right)}{\left(\vec{k}_1-\vec{h}\right)^2}\right)^2\right)+g_1g_2\left(\frac{\vec{k}_1\cdot\vec{h}}{h^2}\right)\left(\frac{\vec{k}_1\cdot\left(\vec{k}_1-\vec{h}\right)}{\left(\vec{k}_1-\vec{h}\right)^2}\right)\right\} \tag{4.68}$$

We will comment on the physical meaning of these two terms in part ii. Completing our discussion of $(\ell = 2)$-particle cumulants we will now show a general scheme how one can easily derive mixed cumulants between the density field Φ_ρ and the response field Φ_B once the density-only cumulants are known. In the $(n = 2)$-point case Corollary 4 directly tells us that there are no mixed cumulants

$$G^{(0,2)}_{\Phi_{\rho_1}\Phi_{B_2}} = 0 = G^{(0,2)}_{\Phi_{B_1}\Phi_{\rho_2}}\,. \tag{4.69}$$

We must thus at least consider the $(n = 3)$-point cumulants. The only possible label distribution is $1|2$ and without specifying the $\mathcal{T}^{(2)}_{1|2}$ function the density-only cumulant reads

$$G^{(0,2)}_{\Phi_{\rho_1}\Phi_{\rho_2}\Phi_{\rho_3}} = \bar{\rho}^2(2\pi)^d\,\delta(\vec{k}_1+\vec{k}_2+\vec{k}_3)\left(\mathcal{T}^{(2)}_{1|2}(1;2,3)+\mathcal{T}^{(2)}_{1|2}(2;1,3)+\mathcal{T}^{(2)}_{1|2}(3;1,2)\right). \tag{4.70}$$

We now replace the Φ_{ρ_3} field with a Φ_{B_3} field. The only thing we have to change is that each of the $\mathcal{T}^{(2)}_{1|2}$ functions must now be multiplied with the appropriate $b(3)$ factor. Remember that these only depend on the grouping and not on the actual labeling. With the help of (4.31) we easily find

$$G^{(0,2)}_{\Phi_{\rho_1}\Phi_{\rho_2}\Phi_{B_3}} = i\bar{\rho}^2(2\pi)^d\delta(\vec{k}_1+\vec{k}_2+\vec{k}_3)\left(\vec{k}_3\cdot\vec{k}_2\,g_{23}\,\mathcal{T}^{(2)}_{1|2}(1;2,3)+\vec{k}_3\cdot\vec{k}_1\,g_{13}\,\mathcal{T}^{(2)}_{1|2}(2;1,3)\right). \tag{4.71}$$

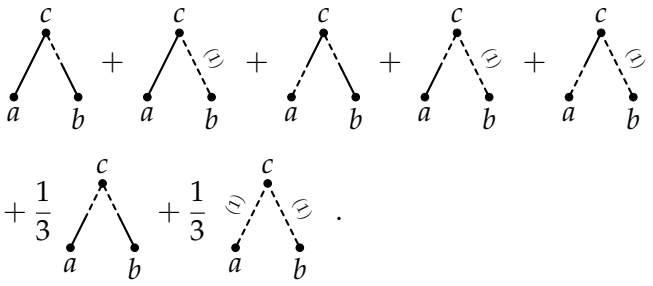
Note that the third term $\mathcal{T}^{(2)}_{1|2}(3;1,2)$ vanishes due to Theorem 1 because here one of the two particles only carries the Φ_B-field index 3. If we also exchange $\Phi_{\rho_2}\to\Phi_{B_2}$ the same situation will hold for all three terms and thus $G^{(0,2)}_{\Phi_{\rho_1}\Phi_{B_2}\Phi_{B_3}} = 0$ as required by Corollary 4. We now infer a general strategy for finding arbitrary mixed cumulants.

- First one calculates the $\mathcal{T}^{(\ell)}$ functions for the corresponding density-only cumulant.
- Then one replaces density fields by response fields as desired. We then identify those label groupings where we have particles that only carry Φ_B-field labels and drop their $\mathcal{T}^{(\ell)}$ functions.
- For the surviving $\mathcal{T}^{(\ell)}$ functions we place the appropriate number of b factors in front of them. The form of those b factors can be read off directly from the label grouping.

4.2.8 *Three-particle cumulants*

The one- and two-particle cumulants are unique in the sense that they are the only ℓ-particle contributions to a general non-interacting cumulant (4.18) where the number of labelings $\ell!$ per label grouping is still fairly manageable. We will confine ourselves to the $(n = 3)$-case in order to give a quick example of how one should in principle approch calculating cumulants for $\ell \geq 3$ and to show an interesting consequence of initial momentum correlations.

The correlation function $\mathcal{C}^{(3)}_{\text{con}}$ can be seen in its diagrammatic form as the three-particle sum in (3.91) and consists of an enormous number of diagrams. Just like in the $(\ell = 2)$-particle case we will only consider terms of quadratic order in P_δ. This reduces the number of diagrams down to 36 and once we combine those of equivalent topology we are left with

$\mathcal{C}^{(3,2)}_{\text{con}} =$  (4.72)

In the $(n = 3)$-point case the only possible label distribution is trivially $1|1|1$ which contains the single grouping $(1;2;3)$. The cumulant will thus consist of only one $\mathcal{T}^{(3,2)}_{1|1|1}$ function. However, the grouping contains $\ell! = 3! = 6$ labelings which have to be evaluated for each of the 7 diagrams. Thus, we still have to calculate 42 individual contributions. In the end one finds that they can be combined into

$$\mathcal{T}^{(3,2)}_{1|1|1}(1;2;3) = \exp\left\{-\frac{\sigma_p^2}{2}\left(\vec{T}_1^2+\vec{T}_2^2+\vec{T}_3^2\right)\right\}\left\{P_\delta(k_1)\,P_\delta(k_2)\,(1+g_1)(1+g_2)\times \left[\frac{\vec{T}_3\cdot\vec{k}_1}{k_1^2}\frac{\vec{T}_3\cdot\vec{k}_2}{k_2^2}-\vec{T}_3\cdot\left(\frac{\vec{k}_1}{k_1^2}+\frac{\vec{k}_2}{k_2^2}\right)\right]+\text{cyc. perm.}\right\}, \tag{4.73}$$

where $\vec{T}_3 = g_3\vec{k}_3$ is the special case of the transport vector for label sets containing only one label. From Corollary 4 it immediately follows that the pure density cumulant is the only non-vanishing $(n = 3)$-point $(\ell = 3)$-particle cumulant which reads

$$G^{(0,3)}_{\Phi_{\rho_1}\Phi_{\rho_2}\Phi_{\rho_3}} = \bar{\rho}^3(2\pi)^d\,\delta_{\text{D}}(\vec{k}_1+\vec{k}_2+\vec{k}_3)\,\mathcal{T}^{(3,2)}_{1|1|1}(1;2;3)\,. \tag{4.74}$$

This cumulant is usually called the *bispectrum*. Note that since every diagram in (4.72) involves some kind of momentum correlation the bispectrum vanishes for $t_1 = t_2 = t_3 = t_{\text{i}}$, as is required by the Gaussianity of the initial density-momentum random field. However, once the field evolves over time it will necessarily become non-Gaussian even in the absence of interactions due to initial momentum correlations.

4.3 PERTURBATION THEORY

In this section we will show how one can obtain a perturbative expansion of the full interacting cumulants in terms of the non-interacting ones and the interaction potential $\sigma_{\mu\nu}$. We first derive what we call the exact *master equation* of perturbation theory and then expand it in orders of the interaction. While this form of perturbation theory will have desirable advantages over the canonical case (2.58), we will also argue why it is problematic to use it in a consistent fashion. We then introduce another diagrammatic language different from that for the initial correlations in order to better organize the terms of perturbation theory visually. This will allow us to make the advantages of the grand canonical approach apparent more easily. Furthermore, we will use the diagrammatic language to point out how one might cure the consistency problems by identifying the first order solution for the $G_{\Phi_\rho \Phi_B}$ cumulant as the basic building block of a propagator for the statistics of the density field Φ_ρ.

Since we will encounter equations containing many cumulants, we will streamline their notation by writing $G_{\Phi_{\alpha_1} \dots \Phi_{\alpha_n}} = G_{\alpha_1 \dots \alpha_n}$ and using the reduced notation explained at the end of section 1.2.2, where greek indices encode both the field type and the external label, i. e. $\alpha \equiv \alpha_1$.

4.3.1 *The master equation*

We will derive the central or master equation of perturbation theory by basically repeating the calculations of Mazenko [39]. However, these were done for a system without any initial correlations. In our case these correlations will introduce a seemingly small deviation from Mazenko's calculation, which nonetheless introduces a whole new class of terms into the perturbation theory. It is this class of terms which will make it hard to order the perturbation series in a consistent way.

The general definition of a full interacting cumulant $G_{\alpha_1 \dots \alpha_n}$ can be found in (4.14). In the following we will suppress the $\big|_0$ and always assume that all sources are only turned off once all functional derivatives have been executed. Since we have to deal with a lot of functional derivatives w. r. t. to the collective source field H we introduce the shorthand notation

$$\hat{H}_{\alpha_1} := \frac{\delta}{\mathrm{i}\delta H_{\alpha_1}} \,. \tag{4.75}$$

We begin by looking at the one-point cumulant. If we recall that the interaction operator (2.48) is defined in terms of the functional derivatives $\hat{H}_\alpha$ and that such derivatives commute we find

$$\begin{aligned} G_\alpha &= \hat{H}_\alpha \ln \left(\mathrm{e}^{\mathrm{i}\hat{S}_I} \exp\left\{ \sum_{\ell=1}^{\infty} \Sigma_0^{(\ell)}[H] \right\} \right) \\ &= \frac{1}{Z_{\mathrm{GC}}[H]} \mathrm{e}^{\mathrm{i}\hat{S}_I} \left[\left(\sum_{\ell=1}^{\infty} \hat{H}_\alpha \, \Sigma_0^{(\ell)}[H] \right) \exp\left\{ \sum_{\ell=1}^{\infty} \Sigma_0^{(\ell)}[H] \right\} \right] \\ &= \frac{1}{Z_{\mathrm{GC}}[H]} \mathrm{e}^{\mathrm{i}\hat{S}_I} \left[\left(\sum_{\ell=1}^{\infty} \mathrm{Tr}^{(\ell)}[H] \, \mathcal{C}_{\mathrm{con}}^{(\ell)} \, \Phi_\alpha^{(\ell)} \right) \exp\left\{ \sum_{\ell=1}^{\infty} \Sigma_0^{(\ell)}[H] \right\} \right] . \end{aligned} \tag{4.76}$$

We have used that the connected and free ℓ-particle generating functional may be written as

$$\Sigma_0^{(\ell)}[H] = \mathrm{Tr}^{(\ell)}[H]\,\mathcal{C}_{\mathrm{con}}^{(\ell)} \quad \text{with} \quad \mathrm{Tr}^{(\ell)}[H] = \prod_{j=1}^{\ell} \mathrm{Tr}_j \propto \prod_{j=1}^{\ell} \mathrm{e}^{\mathrm{i}H\cdot\phi_j} = \mathrm{e}^{\mathrm{i}H\cdot\Phi^{(\ell)}}\,, \tag{4.77}$$

where the single-particle trace is defined through the combination of (3.101) and (3.118). We also made all dependences on H explicit. We now want to commute the interaction operator through the first instance of H in the terms of the sum over representative particle numbers which has been taken down from the exponential function by the single $\hat{H}_\alpha$. For this we remind ourselves that by definition

$$\mathrm{e}^{\mathrm{i}\hat{S}_I} = \sum_{n=1}^{N} \frac{\mathrm{i}^n}{n!}\,\hat{S}_I^n = \sum_{n=1}^{N} \frac{\mathrm{i}^n}{n!} \left(\frac{1}{2}\,\hat{H}_\mu \sigma_{\mu\nu} \hat{H}_\nu\right)^n . \tag{4.78}$$

The commutation of a single $\hat{S}_I$ operator with the source term contained in the $\mathrm{Tr}^{(\ell)}$ is given by

$$\begin{aligned}
&\hat{H}_\mu \sigma_{\mu\nu} \hat{H}_\nu\, \mathrm{e}^{\mathrm{i}\,H\cdot\Phi^{(\ell)}} \\
&= \sigma_{\mu\nu} \hat{H}_\mu \left(\Phi_\nu^{(\ell)} \mathrm{e}^{\mathrm{i}H\cdot\Phi^{(\ell)}} + \mathrm{e}^{\mathrm{i}H\cdot\Phi^{(\ell)}} \hat{H}_\nu\right) \\
&= \sigma_{\mu\nu} \left(\Phi_\mu^{(\ell)} \Phi_\nu^{(\ell)} \mathrm{e}^{\mathrm{i}H\cdot\Phi^{(\ell)}} + \Phi_\nu^{(\ell)} \mathrm{e}^{\mathrm{i}H\cdot\Phi^{(\ell)}} \hat{H}_\mu + \Phi_\mu^{(\ell)} \mathrm{e}^{\mathrm{i}H\cdot\Phi^{(\ell)}} \hat{H}_\nu + \mathrm{e}^{\mathrm{i}H\cdot\Phi^{(\ell)}} \hat{H}_\mu \hat{H}_\nu\right) \\
&= e^{\mathrm{i}H\cdot\Phi^{(\ell)}} \left(\Phi_\mu^{(\ell)} \sigma_{\mu\nu} \Phi_\nu^{(\ell)} + 2\,\Phi_\mu^{(\ell)} \sigma_{\mu\nu} \hat{H}_\nu + \hat{H}_\mu \sigma_{\mu\nu} \hat{H}_\nu\right)\,,
\end{aligned} \tag{4.79}$$

where we have used the symmetry property $\sigma_{\mu\nu} = \sigma_{\nu\mu}$ in the last line. Since this commutation does not generate any new instances of H, we can perform it for each term in the series of (4.78) and find the following commutation relation for the complete interaction operator

$$\mathrm{e}^{\mathrm{i}\hat{S}_I} \mathrm{e}^{\mathrm{i}H\cdot\Phi^{(\ell)}} = \mathrm{e}^{\mathrm{i}H\cdot\Phi^{(\ell)}}\, \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi_\mu^{(\ell)}\sigma_{\mu\nu}\Phi_\nu^{(\ell)}}\, \mathrm{e}^{\mathrm{i}\Phi_\mu^{(\ell)}\sigma_{\mu\nu}\hat{H}_\nu}\, \mathrm{e}^{\mathrm{i}\hat{S}_I}\,. \tag{4.80}$$

With the help of this relation the one-point cumulant now reads

$$\begin{aligned}
G_\alpha &= \frac{1}{Z_{\mathrm{GC}}[H]} \sum_{\ell=1}^{\infty} \left(\mathrm{Tr}^{(\ell)} \mathcal{C}_{\mathrm{con}}^{(\ell)}\, \Phi_\alpha^{(\ell)} \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi_\mu^{(\ell)}\sigma_{\mu\nu}\Phi_\nu^{(\ell)}}\right) \mathrm{e}^{\mathrm{i}\Phi_\mu^{(\ell)}\sigma_{\mu\nu}\hat{H}_\nu} \mathrm{e}^{\mathrm{i}\hat{S}_I} \exp\left\{\sum_{\ell=1}^{\infty} \Sigma_0^{(\ell)}[H]\right\} \\
&= \sum_{\ell=1}^{\infty} \left(\mathrm{Tr}^{(\ell)} \mathcal{C}_{\mathrm{con}}^{(\ell)}\, \Phi_\alpha^{(\ell)} \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi_\mu^{(\ell)}\sigma_{\mu\nu}\Phi_\nu^{(\ell)}}\right) \frac{1}{Z_{\mathrm{GC}}[H]}\, \mathrm{e}^{\mathrm{i}\Phi_\mu^{(\ell)}\sigma_{\mu\nu}\hat{H}_\nu} Z_{\mathrm{GC}}[H]\,.
\end{aligned} \tag{4.81}$$

Next we define the *force* term

$$F_\mu^{(\ell)} := \Phi_\nu^{(\ell)} \sigma_{\nu\mu} \tag{4.82}$$

whose physical meaning will become clear shortly. Next we define another trace operator as

$$\mathrm{Tr}_0^{(N)}[H] := \frac{(\bar{\rho}V)^N}{N!} \int \mathrm{d}\mathbf{x}^{(\mathrm{i})} \int_{\mathrm{i}} \mathcal{D}\mathbf{x}(t) \int \mathcal{D}\boldsymbol{\chi}(t)\, \mathrm{e}^{\mathrm{i}S_0 + \mathrm{i}\mathbf{J}\cdot\mathbf{x} + \mathrm{i}\mathbf{K}\cdot\boldsymbol{\chi}}\, \mathrm{e}^{\mathrm{i}H\cdot\Phi^{(N)}}\,, \tag{4.83}$$

which is the N-particle equivalent of $\mathrm{Tr}^{(\ell)}$ but without the phase-space probability distribution of the ideal gas. We also wrote $\Phi^{(N)}$ to explicitly mark the collective field made up of all N particles of the canonical systems one averages over when calculating the grand canonical generating functional as

$$Z_{\mathrm{GC}}[H] = \sum_{N=0}^{\infty} \mathrm{Tr}_0^{(N)}[H]\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \exp\left\{ \frac{\mathrm{i}}{2} \Phi_\mu^{(N)} \sigma_{\mu\nu} \Phi_\nu^{(N)} \right\} . \tag{4.84}$$

From (4.83) it now follows easily that

$$\mathrm{e}^{\mathrm{i}F_\mu^{(\ell)}\hat{H}_\mu}\, \mathrm{Tr}_0^{(N)}[H] = \mathrm{Tr}_0^{(N)}[H]\, \mathrm{e}^{\mathrm{i}F^{(\ell)}\Phi_\mu^{(N)}} = \mathrm{Tr}_0^{(N)}[H + F^{(\ell)}] . \tag{4.85}$$

It is important here to keep in mind that the microscopic phase-space coordinates on which $F_\mu^{(\ell)}$ depends through the collective field $\Phi_\nu^{(\ell)}$ in (4.82) are *not* traced over by $\mathrm{Tr}_0^{(N)}$ but by the $\mathrm{Tr}^{(\ell)}$ in (4.81). If we combine this with (4.84), we can define

$$\begin{aligned}
\mathrm{e}^{\Delta W^{(\ell)}} &:= \frac{1}{Z_{\mathrm{GC}}[H]}\, \mathrm{e}^{\mathrm{i}\Phi_\mu^{(\ell)}\sigma_{\mu\nu}\hat{H}_\nu} Z_{\mathrm{GC}}[H] = \frac{1}{Z_{\mathrm{GC}}[H]}\, \mathrm{e}^{\mathrm{i}F_\mu^{(\ell)}\hat{H}_\mu} Z_{\mathrm{GC}}[H] \\
&= \frac{1}{Z_{\mathrm{GC}}[H]} \sum_{N=0}^{\infty} \mathrm{Tr}_0^{(N)}[H + F^{(\ell)}]\, \mathcal{P}(\mathbf{x}^{(\mathrm{i})})\, \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi_\mu^{(N)}\sigma_{\mu\nu}\Phi_\nu^{(N)}} \\
&= \frac{Z_{\mathrm{GC}}[H + F^{(\ell)}]}{Z_{\mathrm{GC}}[H]} = \frac{\mathrm{e}^{W_{\mathrm{GC}}[H+F^{(\ell)}]}}{\mathrm{e}^{W_{\mathrm{GC}}[H]}} = \mathrm{e}^{W_{\mathrm{GC}}[H+F^{(\ell)}] - W_{\mathrm{GC}}[H]} .
\end{aligned} \tag{4.86}$$

The full one-point cumulant thus has the concise form

$$G_\alpha = \sum_{\ell=1}^{\infty} \mathrm{Tr}^{(\ell)} \mathcal{C}_{\mathrm{con}}^{(\ell)}\, \Phi_\alpha^{(\ell)} \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi_\mu^{(\ell)}\sigma_{\mu\nu}\Phi_\nu^{(\ell)}} \mathrm{e}^{\Delta W^{(\ell)}} . \tag{4.87}$$

This is our so-called *master equation* since one can now easily generate the full higher order cumulants by taking additional functional derivatives w. r. t. H. A few comments are in order at this point.

- First we like to point out the difference of our result when compared to the calculation in Mazenko [39]. His original calculation concerned a system without initial correlations. This case is contained in our result as the special case where one sets $\mathcal{C}_{\mathrm{con}}^{(\ell)} = 0$ for all $\ell \geq 2$. With $\mathcal{C}_{\mathrm{con}}^{(1)} = 1$ one then finds that (4.87) reduces to

  $$G_\alpha = \mathrm{Tr}^{(1)} \Phi_\alpha^{(1)} \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi_\mu^{(1)}\sigma_{\mu\nu}\Phi_\nu^{(1)}} \mathrm{e}^{\Delta W^{(1)}} = \mathrm{Tr}^{(1)} \Phi_\alpha^{(1)} \mathrm{e}^{\Delta W^{(1)}} . \tag{4.88}$$

  We have used that our particles should have no self-interaction, i. e. we require that the interaction potential satisfies[2] $v(\vec{q}, \vec{q}')|_{\vec{q}=\vec{q}'} = 0$. From this it directly follows that the 'self-interaction' term evaluates to unity as

  $$\mathrm{e}^{\frac{\mathrm{i}}{2}\Phi_\mu^{(1)}\sigma_{\mu\nu}\Phi_\nu^{(1)}} = 1 . \tag{4.89}$$

  In our case this is no longer the case since we have to consider arbitrary representative particle numbers ℓ and these particles may then of course interact.

2 To be more precise one also has to require $\nabla_q v(\vec{q}, \vec{q}')|_{\vec{q}=\vec{q}'} = 0$, due to the gradient contained in the Φ_B field.

- One can also give a physical interpretation of (4.87). One picks some set of ℓ representative particles from the system which are grouped into a cluster due to their *connected* initial correlations $\mathcal{C}^{(\ell)}_{\text{con}}$. Considering interactions $\mathrm{e}^{\frac{\mathrm{i}}{2}\Phi^{(\ell)}_\mu \sigma_{\mu\nu}\Phi^{(\ell)}_\nu}$ amongst the particles of the cluster one calculates their contribution to the one-point cumulant. It is these 'intra-cluster' interactions, where the potential appears together with quantities which are directly coupled to a specific number of particles, that will lead to the perturbation series being generated in a non-consistent way.

- The fact that this cluster of particles also interacts with the rest of the system is expressed by the weight factor $\mathrm{e}^{\Delta W^{(\ell)}}$. From (4.86) we see that it is given by the ratio of the generating functional of the entire system under the effect of an additional external force $F^{(\ell)}_\mu$ to that of the system without such a force. This external force leads to an additional interaction term

$$\mathrm{e}^{\mathrm{i}\,F^{(\ell)}\Phi^{(N)}_\mu} = \mathrm{e}^{\mathrm{i}\,\Phi^{(\ell)}_\mu \sigma_{\mu\nu}\Phi^{(N)}_\nu}\,, \tag{4.90}$$

  as one can see from (4.85). Here we directly see that it contains the interactions of the cluster particles with all other particles. To obtain the complete one-point cumulant one then sums such contributions from clusters of all sizes ℓ.

- We stress that (4.87) is *exact*. Up to this point no approximations have been made. So far the sum over particle numbers is also in no way tied to the order of interactions considered. Its truncation is only controlled by the order of initial correlations one is willing to consider, as we explained following (4.18). How and why this will change once we consider individual terms in the perturbation series of certain order in the interaction $\sigma_{\mu\nu}$ will be explained in the next section.

The quantity we are actually interested in is the two-point cumulant. As already mentioned, we obtain an exact expression for it by taking another functional derivative of the master equation (4.87). We find

$$\begin{aligned}
G_{\alpha\beta} &= \hat{H}_\beta G_\alpha \\
&= \sum_{\ell=1}^{\infty} \Big[\Big(\hat{H}_\beta \mathrm{Tr}^{(\ell)}[H] \Big)\, \mathcal{C}^{(\ell)}_{\text{con}}\, \Phi^{(\ell)}_\alpha\, \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi^{(\ell)}_\mu \sigma_{\mu\nu}\Phi^{(\ell)}_\nu}\, \mathrm{e}^{\Delta W^{(\ell)}} \\
&\qquad + \mathrm{Tr}^{(\ell)}[H]\, \mathcal{C}^{(\ell)}_{\text{con}}\, \Phi^{(\ell)}_\alpha\, \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi^{(\ell)}_\mu \sigma_{\mu\nu}\Phi^{(\ell)}_\nu}\, \hat{H}_\beta\, \mathrm{e}^{\Delta W^{(\ell)}} \Big] \\
&= \sum_{\ell=1}^{\infty} \Big[\mathrm{Tr}^{(\ell)}[H]\, \mathcal{C}^{(\ell)}_{\text{con}}\, \Phi^{(\ell)}_\alpha\, \Phi^{(\ell)}_\beta\, \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi^{(\ell)}_\mu \sigma_{\mu\nu}\Phi^{(\ell)}_\nu}\, \mathrm{e}^{\Delta W^{(\ell)}} \\
&\qquad + \mathrm{Tr}^{(\ell)}[H]\, \mathcal{C}^{(\ell)}_{\text{con}}\, \Phi^{(\ell)}_\alpha\, \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi^{(\ell)}_\mu \sigma_{\mu\nu}\Phi^{(\ell)}_\nu}\, \hat{H}_\beta\, \mathrm{e}^{\Delta W^{(\ell)}} \Big]\,.
\end{aligned} \tag{4.91}$$

Mazenko [39] then rewrites this into a form that has the same structure as the so-called *Dyson equation* known from QFT. For this we use the chain rule

$$\hat{H}_\beta\, \mathrm{e}^{\Delta W^{(\ell)}} = \frac{\delta G_\gamma}{\mathrm{i}\delta H_\beta} \frac{\delta}{\delta G_\gamma} \mathrm{e}^{\Delta W^{(\ell)}} = \left(\frac{\delta}{\delta G_\gamma} \mathrm{e}^{\Delta W^{(\ell)}} \right) G_{\gamma\beta}\,. \tag{4.92}$$

If one then identifies the cluster self-correlation[3]

$$\mathcal{G}_{\alpha\beta} = \sum_{\ell=1}^{\infty} \mathrm{Tr}^{(\ell)}[H]\, \mathcal{C}_{\mathrm{con}}^{(\ell)}\, \Phi_{\alpha}^{(\ell)}\, \Phi_{\beta}^{(\ell)}\, \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi_{\mu}^{(\ell)}\sigma_{\mu\nu}\Phi_{\nu}^{(\ell)}}\, \mathrm{e}^{\Delta W^{(\ell)}} \tag{4.93}$$

and

$$\Sigma_{\alpha\gamma} = \sum_{\ell=1}^{\infty} \mathrm{Tr}^{(\ell)}[H]\, \mathcal{C}_{\mathrm{con}}^{(\ell)}\, \Phi_{\alpha}^{(\ell)}\, \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi_{\mu}^{(\ell)}\sigma_{\mu\nu}\Phi_{\nu}^{(\ell)}}\, \frac{\delta}{\delta G_{\gamma}}\, \mathrm{e}^{\Delta W^{(\ell)}}\,, \tag{4.94}$$

then (4.91) would be written as

$$G_{\alpha\beta} = \mathcal{G}_{\alpha\beta} + \Sigma_{\alpha\gamma} G_{\gamma\beta}\,. \tag{4.95}$$

In comparison to the QFT case $\mathcal{G}_{\alpha\beta}$ has the same role as the so-called *bare propagator* and $\Sigma_{\alpha\gamma}$ is this theory's version of the *self-energy*. In QFT the bare propagator describes the propagation of a quantized contribution to the field, i. e. a particle, through space-time without taking into account its interaction with its 'vacuum' environment. In our theory for classical particles this role is taken by initially correlated clusters of particles of all sizes which of course may interact inside the cluster. If we had no initial correlations like in equilibrium QFT this would reduce to the trivial case of one-particle clusters only. The interaction of a particle with the QFT vacuum is encoded in the self-energy. In our case however the interaction of the cluster with the surrounding environment of all other particles is encoded in $\mathrm{e}^{\Delta W^{(\ell)}}$ which appears in both $\mathcal{G}_{\alpha\beta}$ and $\Sigma_{\alpha\gamma}$ and thus the physical analogy breaks down at this point.

We will see in the next sections that while we can write the perturbation expansion in a form that is structurally similar to QFT when expressed in diagrams, as is hinted at by (4.95), it is however not generated in such a way that it is consistent in the orders of the interaction $\sigma_{\mu\nu}$. We also like to mention that the formulation of perturbation theory in terms of integral equations is not confined to the grand-canonical ensemble. In Appendix B we show that up to second order the same structure as found in the next section emerges in the canonical ensemble, however purely in terms of free cumulants and the interaction potential. Proving the canonical analogue (4.87) generally is somewhat hard, since the free generating functional (3.115) of the canonical ensemble does not have the exponential form of its grand canonical counterpart.

4.3.2 *Perturbation expansion up to second order*

The main order parameter for doing perturbative expansions of both the one- and two-point functions (4.87) and (4.91) is the interaction potential $\sigma_{\mu\nu}$. In both cases there are two separate instances of the potential present which lead to different kinds of expansions.

The first instance is the intra-cluster interaction contained in the $\mathrm{e}^{\frac{\mathrm{i}}{2}\Phi_{\mu}^{(\ell)}\sigma_{\mu\nu}\Phi_{\nu}^{(\ell)}}$ factors. Since it is impossible to obtain the trajectories of even two interacting particles in a

3 This quantity must not be confused with the free phase-space propagator.

non-parametric way our only option for performing explicit calculations is to expand the exponential function and thus define the *interacting ℓ-particle cluster cumulant*

$$\begin{aligned} G^{(\ell)}_{\alpha_1\dots\alpha_n} &:= \mathrm{Tr}^{(\ell)}\, \mathcal{C}^{(\ell)}_{\mathrm{con}}\, \Phi^{(\ell)}_{\alpha_1}\dots\Phi^{(\ell)}_{\alpha_n}\, \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi^{(\ell)}_\mu\,\sigma_{\mu\nu}\,\Phi^{(\ell)}_\nu} \\ &= \sum_{j=0}^{\infty} \frac{\mathrm{i}^j}{2^j j!}\, \mathrm{Tr}^{(\ell)}\, \mathcal{C}^{(\ell)}_{\mathrm{con}}\, \Phi^{(\ell)}_{\alpha_1}\dots\Phi^{(\ell)}_{\alpha_n} \prod_{n=1}^{j} \Phi^{(\ell)}_{\mu_n}\Phi^{(\ell)}_{\nu_n}\sigma_{\mu_n\nu_n} \\ &= \sum_{j=0}^{\infty} \frac{\mathrm{i}^j}{2^j j!}\, G^{(0,\ell)}_{\alpha_1\dots\alpha_n\mu_1\nu_1\dots\mu_j\nu_j}\sigma_{\mu_1\nu_1}\dots\sigma_{\mu_j\nu_j} \\ &= \sum_{j=0}^{\infty} \frac{\mathrm{i}^j}{j!}\, G^{(0,\ell)}_{\alpha_1\dots\alpha_n\rho_1 B_1\dots\rho_j B_j}\sigma_{\rho_1 B_1}\dots\sigma_{\rho_j B_j}\,. \end{aligned} \tag{4.96}$$

In the last line we used the symmetry property $\sigma_{\rho B} = \sigma_{B\rho}$. The second and more important instance is the interaction potential contained in the force $F^{(\ell)}_\mu$ which defines $\Delta W^{(\ell)}$. Just like Mazenko we expand this into a functional Taylor series around $H = 0$ and find

$$\begin{aligned} \Delta W^{(\ell)} &= W[H + F^{(\ell)}] - W[H] \\ &= \mathrm{i}\, F^{(\ell)}_\mu \hat{H}_\mu W[H]\big|_{H=0} + \frac{\mathrm{i}^2}{2!} F^{(\ell)}_\mu F^{(\ell)}_\nu \hat{H}_\mu\hat{H}_\nu W[H]\big|_{H=0} + \dots \\ &= \mathrm{i}\, F^{(\ell)}_\mu G_\mu + \frac{\mathrm{i}^2}{2!} F^{(\ell)}_\mu F^{(\ell)}_\nu G_{\mu\nu} + \dots\,, \end{aligned} \tag{4.97}$$

where we have restricted ourselves to the second order since this will already suffice to see all important features of the perturbation theory. If we insert this into the series expansion of $\mathrm{e}^{\Delta W^{(\ell)}}$ we find again up to second order

$$\mathrm{e}^{\Delta W^{(\ell)}} = 1 + \mathrm{i}F^{(\ell)}_\mu G_\mu + \frac{\mathrm{i}^2}{2} F^{(\ell)}_\mu F^{(\ell)}_\nu \left(G_\mu G_\nu + G_{\mu\nu}\right) + \dots\,. \tag{4.98}$$

We now insert this into our expression (4.87) for the one-point cumulant and find

$$\begin{aligned} G_\alpha &= \sum_{\ell=1}^{\infty} \mathrm{Tr}^{(\ell)} \Phi^{(\ell)}_\alpha \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi^{(\ell)}_\mu\,\sigma_{\mu\nu}\,\Phi^{(\ell)}_\nu} \left(1 + \mathrm{i}\, F^{(\ell)}_\beta G_\beta + \frac{\mathrm{i}^2}{2} F^{(\ell)}_\beta F^{(\ell)}_\gamma \left(G_\beta G_\gamma + G_{\beta\gamma}\right)\right) + \dots \\ &= \sum_{\ell=1}^{\infty} \Big(G^{(\ell)}_\alpha + \mathrm{i}\mathrm{Tr}^{(\ell)} \Phi^{(\ell)}_\alpha \Phi^{(\ell)}_\gamma \mathrm{e}^{\frac{\mathrm{i}}{2}\Phi^{(\ell)}_\mu\,\sigma_{\mu\nu}\,\Phi^{(\ell)}_\nu} \sigma_{\gamma\beta} G_\beta \\ &\qquad + \frac{\mathrm{i}^2}{2} \mathrm{Tr}^{(\ell)} \Phi^{(\ell)}_\alpha \Phi^{(\ell)}_\delta \Phi^{(\ell)}_\lambda \mathrm{e}^{\frac{\mathrm{i}^2}{2}\Phi^{(\ell)}_\mu\,\sigma_{\mu\nu}\,\Phi^{(\ell)}_\nu} \sigma_{\delta\beta}\sigma_{\lambda\gamma} \left(G_\beta G_\gamma + G_{\beta\gamma}\right) \Big) + \dots \\ &= \sum_{\ell=1}^{\infty} \left(G^{(\ell)}_\alpha + \mathrm{i} G^{(\ell)}_{\alpha\gamma}\sigma_{\gamma\beta} G_\beta + \frac{\mathrm{i}^2}{2} G^{(\ell)}_{\alpha\delta\lambda}\sigma_{\delta\beta}\sigma_{\lambda\gamma} \left(G_\beta G_\gamma + G_{\beta\gamma}\right) \right) + \dots\,. \end{aligned} \tag{4.99}$$

Since all dependences on the representative particle number ℓ can now be written out in terms of non-interacting cumulants we can use (4.96) to define

$$G^{(\mathrm{c})}_{\alpha_1\dots\alpha_n} = \sum_{\ell=1}^{\infty} G^{(\ell)}_{\alpha_1\dots\alpha_n} = \sum_{j=0}^{\infty} \sum_{\ell=1}^{r+j} \frac{\mathrm{i}^j}{j!}\, G^{(0,\ell)}_{\alpha_1\dots\alpha_n\rho_1 B_1\dots\rho_j B_j}\sigma_{\rho_1 B_1}\dots\sigma_{\rho_j B_j}\,. \tag{4.100}$$

Here we used Corollary 4 to truncate the series over particle numbers, where r is the number of ρ-labels in $\alpha_1 \dots \alpha_n$. Since each order of the interaction adds another such label to the cumulant it extends the range of possible cumulants. With this definition we finally arrive at

$$G_\alpha = G^{(c)}_\alpha + \mathrm{i} G^{(c)}_{\alpha\beta} \sigma_{\beta\gamma} G_\gamma + \frac{\mathrm{i}^2}{2} G^{(c)}_{\alpha\beta\gamma} \sigma_{\beta\mu} \sigma_{\gamma\nu} \left(G_\mu G_\nu + G_{\mu\nu} \right) + \dots \,. \tag{4.101}$$

The second order expansion for $G_{\alpha\beta}$ can be derived in two different ways depending on whether we start from (4.91) or (4.95). We first look at the former option. The first of the two terms works exactly like the one-point case and can be obtained by just adding another external label to (4.101). For the second term we need to calculate

$$\begin{aligned} \hat{H}_\beta \mathrm{e}^{\Delta W^{(\ell)}} &= \mathrm{i} F^{(\ell)}_\mu \hat{H}_\beta G_\mu + \frac{\mathrm{i}^2}{2} F^{(\ell)}_\mu F^{(\ell)}_\nu \hat{H}_\beta \left(G_\mu G_\nu + G_{\mu\nu} \right) + \dots \\ &= \mathrm{i} F^{(\ell)}_\mu G_{\mu\beta} + \frac{\mathrm{i}^2}{2} F^{(\ell)}_\mu F^{(\ell)}_\nu \left(2 G_\mu G_{\nu\beta} + G_{\mu\nu\beta} \right) + \dots \,. \end{aligned} \tag{4.102}$$

If we insert this back into the second term of (4.91) and perform calculations analoguous to (4.99) we find that the complete second order expansion of the two-point cumulant is

$$\begin{aligned} G_{\alpha\beta} = G^{(c)}_{\alpha\beta} &+ \mathrm{i} G^{(c)}_{\alpha\beta\mu} \sigma_{\mu\nu} G_\nu + \mathrm{i} G^{(c)}_{\alpha\mu} \sigma_{\mu\nu} G_{\nu\beta} + \frac{\mathrm{i}^2}{2} G^{(c)}_{\alpha\beta\mu\nu} \sigma_{\mu\gamma} \sigma_{\nu\delta} \left(G_\gamma G_\delta + G_{\gamma\delta} \right) \\ &+ \frac{\mathrm{i}^2}{2} G^{(c)}_{\alpha\mu\nu} \sigma_{\mu\gamma} \sigma_{\nu\delta} \left(2 G_\gamma G_{\delta\beta} + G_{\gamma\delta\beta} \right) + \dots \,. \end{aligned} \tag{4.103}$$

At this point we can now make some interesting observations.

- The expansion of the second instance of the interaction potential in $\mathrm{e}^{\Delta W^{(\ell)}}$ has led to a *self-consistent* perturbation expansion where the full interacting cumulants are defined in terms of themselves. In mathematical terms this means that we no longer have a simple series expansion where we add more and more independent terms, but non-linear integral equations. Once we introduce a diagrammatic language in section 4.3.5 it will be easy to see that this amounts to the inclusion of whole infinite classes of terms found in the canonical perturbation series (2.58) even at the first order expansion of $\mathrm{e}^{\Delta W^{(\ell)}}$. Consequently, the exact solution to this first order expansion will include effects of infinite orders in $\sigma_{\mu\nu}$.

- Once we expand $\mathrm{e}^{\Delta W^{(\ell)}}$ up to second order, n-point cumulants depend on all cumulants up to $(n+1)$-point order. This is reminiscent of the BBGKY hierarchy. However, as explained in section 2.6 in this hierarchy the evolution for the n-point distribution function only depend on themselves and the $(n+1)$-point distribution function. By truncating the hierarchy at some n-point level it is thus in principle possible to solve the problem going down level by level. This is no longer possible in our case where one has to solve the equations for all n-point cumulants present in the perturbation expansion at the same time. Especially for non-linear integral equations this is a daunting task. One would like to be able to disentangle the equations from one another.

- The structure of the equations seems to suggest that the natural quantities in which perturbation theory should be expressed are the full n-point cumulants $G_{\alpha_1\dots\alpha_n}$, the interaction potential $\sigma_{\mu\nu}$ and the quantities $G^{(\mathrm{c})}_{\alpha_1\dots\alpha_n}$, which themselves can be expressed through $\sigma_{\mu\nu}$ and the non-interacting cumulants $G^{(0,\ell)}_{\alpha_1\dots\alpha_n}$. This is preferable to the canonical perturbation theory since we directly generate a formulation in terms of quantities, which themselves cannot be factorized any further.

- These seemingly natural quantities however make a consistent treatment of the perturbation theory complicated. First, it is not in any way clear up to which order in $\sigma_{\mu\nu}$ one should include terms in the $G^{(\mathrm{c})}_{\alpha_1\dots\alpha_n}$ depending on the order of $\sigma_{\mu\nu}$ one has chosen for the expansion of $\mathrm{e}^{\Delta W^{(\ell)}}$, since these expansions are completely different in nature as explained above. In the original papers [22, 39, 40] this problem does not exist since the system under consideration does not have initial correlations. Then $G^{(\mathrm{c})}_{\alpha_1\dots\alpha_n} = G^{(0)}_{\alpha_1\dots\alpha_n}$ and the interaction potential becomes a solid order parameter since it only appears in the expansion of $\mathrm{e}^{\Delta W^{(\ell)}}$.

- Second, in order to apply methods known from QFT one would like to have a formulation of perturbation theory in terms of a two-point correlator quantity or 'statistical field propagator' and $(n > 2)$-point vertices. Since $\sigma_{\mu\nu}$ is also a two-point quantity it seems natural that it should be possible to incorporate all its instances into this field propagator. One could then organize perturbation theory in terms of loop orders just like in QFT. We will identify a candidate for the field propagator in section 4.3.5.

We can partly disentangle the equations for the different n-point cumulants by introducing the concept of an *effective action* Γ. In QFT it is the quantum-mechanical counterpart of the classical action in the sense that the equations of motion for the expectation value of the fields can be derived from it by the principle of stationary action. These equations of motion will include all quantum-mechanical corrections. We can define it in just the same way as in QFT as the Legendre transform of the cumulant generating functional

$$\Gamma[\varphi] = W_{\mathrm{GC}}[H] - \mathrm{i}\varphi_\mu H_\mu \,, \tag{4.104}$$

where we have defined the expectation value of the collective field in the presence of the source H as

$$\varphi_\mu[H] := \frac{\delta}{\mathrm{i}\delta H_\mu} W_{\mathrm{GC}}[H] \,. \tag{4.105}$$

From this one easily shows that

$$\frac{\delta\Gamma}{\mathrm{i}\delta\varphi_\mu} = -H_\mu \tag{4.106}$$

which at $H = 0$ can be seen as the equations of motion for the expectation value of the collective field Φ which incorporates both the effects of all particle interactions and

the fluctuations which are due to the fact that the initial conditions have a statistical distribution. Using the chain rule

$$\frac{\delta}{\mathrm{i}\delta H_\mu} = \mathrm{i}\frac{\delta\varphi_\nu}{\mathrm{i}\delta H_\mu}\frac{\delta}{\mathrm{i}\delta\varphi_\nu} = \left(\frac{\delta}{\mathrm{i}\delta H_\mu}\frac{\delta}{\mathrm{i}\delta H_\nu}W_{\mathrm{GC}}[H]\right)\mathrm{i}\frac{\delta}{\mathrm{i}\delta\varphi_\nu} = G_{\mu\nu}\mathrm{i}\frac{\delta}{\mathrm{i}\delta\varphi_\nu} \tag{4.107}$$

we can take another functional derivative of (4.106) to find

$$G_{\alpha_1\gamma_3}\Gamma_{\gamma_3\beta_2} = \delta_{\alpha\beta}\,\delta_{\mathrm{D}}\,(1-2) \equiv \delta_{\alpha_1\beta_2} \quad \text{where} \quad \Gamma_{\mu_1\nu_2} = \frac{\delta}{\mathrm{i}\delta\varphi_\mu(1)}\frac{\delta}{\mathrm{i}\delta\varphi_\nu(2)}\Gamma\,. \tag{4.108}$$

This means that the second derivative of Γ is functionally inverse to the full two-point cumulant. For the three-point cumulant we find

$$\begin{aligned} G_{\alpha\beta\gamma} &= \frac{\delta}{\mathrm{i}\delta H_\gamma}G_{\alpha\beta} = G_{\gamma\delta}\mathrm{i}\frac{\delta}{\mathrm{i}\delta\varphi_\delta}\Gamma^{-1}_{\alpha\beta} = -\mathrm{i}G_{\gamma\delta}\Gamma^{-1}_{\alpha\mu}\left(\frac{\delta}{\mathrm{i}\delta\varphi_\delta}\Gamma_{\mu\nu}\right)\Gamma^{-1}_{\nu\beta} \\ &= -\mathrm{i}G_{\alpha\mu}G_{\beta\nu}G_{\gamma\delta}\Gamma_{\mu\nu\delta}\,. \end{aligned} \tag{4.109}$$

Doing this inductively for all higher n-point cumulants one sees that the effective action Γ is the generating functional of the so-called *amputated Green's functions* which are one-particle irreducible (1PI). If one expresses the perturbation expansion for the correlation functions of a field theory in terms of diagrams, the term 1PI designates those diagrams and subdiagrams which cannot be made into disconnected diagrams by cutting only a single line. In terms of correlation functions this means that the term represented by this subdiagram cannot be written into a form that schematically looks like $(1PI)\times G_{\alpha\beta}\times(1PI)$, where $G_{\alpha\beta}$ would be the two-point propagator of that particular theory.

The term *amputated* means that if in a general diagram we can identify a subdiagram which is connected to the rest of the overall diagram with n legs, we can cut off these legs and consider this subdiagram individually. If it is 1PI, one can then show that it is contained in the n-th derivative $\Gamma_{\alpha_1\ldots\alpha_n}$. By organising all diagrams contributing to some n-point cumulant $G_{\alpha_1\ldots\alpha_n}$ in terms of these amputated 1PI subdiagrams and the contributions to the full two-point cumulant $G_{\alpha_1\alpha_2} = \Gamma^{-1}_{\alpha_1\alpha_2}$ connecting them, one then sees that $G_{\alpha_1\ldots\alpha_n}$ will be written purely in terms of tree-level diagrams assembled from $G_{\alpha_1\alpha_2}$ and the $\Gamma_{\alpha_1\ldots\alpha_n}$. This is why the latter are often called *effective vertices* since they allow the computation of arbitrary cumulants in terms of expressions like (4.109) that have no loop-like integrals, i. e. all loop corrections to subdiagrams with more than two external legs are contained in the $\Gamma_{\alpha_1\ldots\alpha_n}$.

We now return to (4.95) and rederive the perturbation expansion for the two-point function. From (4.94) we see that we need to compute

$$\begin{aligned} \frac{\delta}{\delta G_\gamma}\mathrm{e}^{\Delta W^{(\ell)}} &= \frac{\delta}{\delta G_\gamma}\left(1 + \mathrm{i}F^{(\ell)}_\mu G_\mu + \frac{\mathrm{i}^2}{2}F^{(\ell)}_\mu F^{(\ell)}_\nu\left(G_\mu G_\nu + G_{\mu\nu}\right) + \mathcal{O}(\sigma^3)\right) \\ &= \mathrm{i}F^{(\ell)}_\gamma + \frac{\mathrm{i}^2}{2}2\,F^{(\ell)}_\gamma F^{(\ell)}_\mu G_\mu + \frac{\mathrm{i}^2}{2}F^{(\ell)}_\mu F^{(\ell)}_\nu\frac{\delta}{\delta G_\gamma}G_{\mu\nu}\,. \end{aligned} \tag{4.110}$$

Since $G_\gamma = \varphi_\gamma$ in the presence of H we have

$$\frac{\delta}{\delta G_\gamma}G_{\mu\nu} = \mathrm{i}\frac{\delta}{\mathrm{i}\delta\varphi_\gamma}\Gamma^{-1}_{\mu\nu} = -\mathrm{i}G_{\mu\delta}G_{\nu\lambda}\Gamma_{\delta\lambda\gamma}\,. \tag{4.111}$$

The first term of (4.95) is exactly the same as the first term (4.91) and thus we find the following expression for the two-point cumulant

$$G_{\alpha\beta} = G^{(c)}_{\alpha\beta} + \mathrm{i}G^{(c)}_{\alpha\beta\mu}\,\sigma_{\mu\nu}G_{\nu} + \mathrm{i}G^{(c)}_{\alpha\mu}\sigma_{\mu\nu}G_{\nu\beta} + \frac{\mathrm{i}^2}{2}G^{(c)}_{\alpha\beta\mu\nu}\,\sigma_{\mu\gamma}\sigma_{\nu\delta}\left(G_{\gamma}G_{\delta} + G_{\gamma\delta}\right) + \frac{\mathrm{i}^2}{2}G^{(c)}_{\alpha\mu\nu}\,\sigma_{\mu\gamma}\sigma_{\nu\delta}\left(2\,G_{\gamma}G_{\delta\beta} - \mathrm{i}G_{\gamma\lambda}G_{\delta\theta}\Gamma_{\lambda\theta\omega}G_{\omega\beta}\right) + \mathcal{O}(\sigma^3)\,. \tag{4.112}$$

The same result would of course be found by inserting (4.109) into (4.103). This resolves the problem that we needed the three-point cumulant in order to calculate the two-point cumulant. We payed for this with the introduction of a cubic term in $G_{\alpha\beta}$ and the effective three-point vertex $\Gamma_{\lambda\theta\omega}$. Given some expression for Γ the equations (4.101) for the one-point and (4.112) for the two-point cumulant then again form a closed system even at second order of the expansion of $\mathrm{e}^{\Delta W^{(\ell)}}$. In QFT formulae exist for deriving approximations for Γ from the classical action S. However, they cannot be transferred directly to our theory in its present form since our action only describes interactions in terms of the collective field Φ but not the free dynamics. Another approach taken by Mazenko [40] is to use (4.108) with the non-interacting cumulants to find a non-interacting approximation for the effective vertices. The necessary functional inversion however has so far only been done analytically for Smoluchowski dynamics, and seems impossible to be performed in a closed form for Newtonian dynamics, let alone for a system with initial correlations like ours. All in all, applying the effective action approach to our theory in the present form does not provide any significant advantages.

4.3.3 *General form of the interaction potential*

Before we progress further it will be very advantageous to have some more explicit information about the form of the two-particle interaction potential $v(\vec{q},\vec{q}')$, especially about its Fourier transform. Aside from the assumptions made in section 2.4.1, we can make one more important statement in a system which is statistically homogeneous and isotropic. For such a system the interaction potential may only depend on the modulus $|\vec{q}-\vec{q}'|$ of the separation vector. If it would depend on the absolute position of the two particles involved, then particle pairs at equal distance but in different subparts of the system would experience different forces in all members of the ensemble. Consequently, even when we average over the ensemble we would always find over- or underdensities in the system at the same positions, depending on the sign of the interaction. This obviously violates statistical homogeneity. If the potential did depend not only on the modulus but also on the direction of the separation vector this would lead to a preferred streaming direction of the particles across all ensemble members. This would then break the statistical isotropy of the velocity field. With this new information we find for the Fourier transform of the potential

$$\begin{aligned} v(\vec{k},\vec{k}') &= \int \mathrm{d}\vec{q}\,\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{k}} \int \mathrm{d}\vec{q}'\,\mathrm{e}^{-\mathrm{i}\vec{q}'\cdot\vec{k}'}\,v(|\vec{q}-\vec{q}'|) \\ &= \int \mathrm{d}\vec{q}\,\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{k}} \int \mathrm{d}\Delta\vec{q}'\,\mathrm{e}^{-\mathrm{i}(\vec{q}+\Delta\vec{q})\cdot\vec{k}'}\,v(|\Delta\vec{q}|) \end{aligned}$$

$$= \int \mathrm{d}\vec{q}\, \mathrm{e}^{-\mathrm{i}\vec{q}\cdot(\vec{k}+\vec{k}')} \int \mathrm{d}\Delta\vec{q}'\, \mathrm{e}^{-\mathrm{i}\Delta\vec{q}\cdot\vec{k}'} v(|\Delta\vec{q}|)$$
$$= (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}+\vec{k}')\, v(k') = (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}+\vec{k}')\, v(k)\,. \tag{4.113}$$

We have defined $\Delta\vec{q} = \vec{q}' - \vec{q}$ in the second line. Consequently, the interaction matrix in Fourier space reads

$$\sigma(1,2) = -(2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\, \delta_{\mathrm{D}}(t_1-t_2) \begin{pmatrix} 0 & v(k_1) \\ v(k_1) & 0 \end{pmatrix}. \tag{4.114}$$

With the help of (1.28) any interaction term in Fourier space then reads as

$$\Phi_{\mu_1}\sigma_{\mu_1\nu_2}\Phi_{\nu_2} = \Phi_\mu(1)\sigma_{\mu\nu}(-1,-2)\Phi_\nu(2) = \Phi_\mu(1)\sigma_{\mu\nu}(1,2)\Phi_\nu(2) = \Phi_\mu\sigma_{\mu\nu}\Phi_\nu\,, \tag{4.115}$$

where we have used the form (4.114) in the third step. We thus do not have to take any minus signs into account when writing down general interaction terms. We will also demand that the potential $v(q)$ drops off fast enough for $q \to \infty$ such that the value of the Fourier transform at $k = 0$ is well defined in the sense of

$$v(k)\big|_{k=0} = \int \mathrm{d}\vec{q}\, \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{k}} v(q)\big|_{k=0} = \frac{2\pi^{n/2}}{\Gamma(n/2)} \int_0^\infty \mathrm{d}q\, q^{n-1} v(q) < \infty\,. \tag{4.116}$$

From this we can conclude the identity

$$\delta_{\mathrm{D}}(\vec{k})\, k^n\, v(k) = 0 \quad \forall\, n > 0\,. \tag{4.117}$$

This identity is important because it allows us to drop all diagrams that contain a 'tadpole'[4] of any order in the interaction connecting to a non-interacting cumulant. For this we use that $G_B = 0$ to any order in the interaction (see Appendix A). This leads to

$$G^{(0,\ell)}_{\alpha_1\ldots\alpha_{n-1}\alpha_n}\sigma_{\alpha_n\mu}G_\mu = G^{(0,\ell)}_{\alpha_1\ldots\alpha_{n-1}B_n}\sigma_{B_n\rho}G_\rho\,. \tag{4.118}$$

We also need that due to statistical homogeneity and isotropy any general n-point cumulant has the following form in Fourier space

$$G_{\alpha_1\ldots\alpha_n} = (2\pi)^d\, \delta_{\mathrm{D}}\left(\sum_{j=1}^n \vec{k}_j\right) \bar{G}_{\alpha_1\ldots\alpha_n}\,. \tag{4.119}$$

For the one-point cumulant we thus have $G_\rho = (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k})\, \bar{G}_\rho$ where $\bar{G}_\rho$ must be constant in $\vec{k}$, because it must be constant in configuration space. We thus find

$$\begin{aligned} G^{(0,\ell)}_{\alpha_1\ldots\alpha_{n-1}B_n}\sigma_{B_n\rho_m}G_{\rho_m} &= -(2\pi)^{2d} \int \mathrm{d}n \int \mathrm{d}m\, G^{(0,\ell)}_{\alpha_1\ldots\alpha_{n-1}B_n}\, \delta_{\mathrm{D}}(\vec{k}_m)\, \bar{G}_\rho(t_m) \times \\ &\qquad \Big(\delta_{\mathrm{D}}(\vec{k}_n+\vec{k}_m)\, \delta_{\mathrm{D}}(t_n-t_m)\, v(k_n)\Big) \\ &= -\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t_n\, G^{(0,\ell)}_{\alpha_1\ldots\alpha_{n-1}B_n}\delta_{\mathrm{D}}(\vec{k}_n)\, v(k_n)\, \bar{G}_\rho(t_n) \\ &\propto \delta_{\mathrm{D}}(\vec{k}_n)\, b(n)\, v(k_n) \propto \delta_{\mathrm{D}}(\vec{k}_n)\, \vec{k}_n\, v(k_n) = 0\,. \end{aligned} \tag{4.120}$$

4 This is a common nomenclature for these kinds of terms in QFT. It will become more obvious once we write these terms as diagrams.

All other factors must be finite at $k_n = 0$. The only possible source of any inverse powers of k_n would be the non-interacting cumulant. If one goes through their derivation in section 4.2, one finds that $\vec{k}_n$ would need to be the sole mode put into the denominator of either $\vec{C}_{\delta_i p_j}$ or $C_{p_i p_j}$ by a Dirac delta distribution. In order for this to happen the external label 3 must be the only label carried by some particle. But since it is a Φ_B-field label, Theorem 1 dictates that the cumulant vanishes due to causality in the first place.

The two Dirac delta distributions in (4.114) also allow us to drop certain terms from non-interacting cumulants whose fields are contracted with $\sigma_{\mu\nu}$. These are the quantities appearing in (4.96). The effect of a contraction is in general

$$G^{(0,\ell)}_{\alpha_1\dots\alpha_n\alpha_m}\sigma_{\alpha_n\alpha_m} = -2\int \mathrm{d}n\, G^{(0,\ell)}_{\alpha_1\dots\rho_n B_{-n}}\, v(k_n)\ . \tag{4.121}$$

Remember that $-n = (-\vec{k}_n, t_n)$. Now consider a label grouping where both external labels that have been contracted are carried by the same particle, i. e. we now look at the interaction between contributions to two different fields coming from the same particle or simpler said a self-interaction of the particle. Since now

$$\begin{aligned} \vec{k}_n + \vec{k}_m &\to \vec{k}_n - \vec{k}_n = 0 \\ \mathrm{g}_n\vec{k}_n + \mathrm{g}_m\vec{k}_m &\to g_n(\vec{k}_n - \vec{k}_n) = 0 \\ \vec{k}_n\mathrm{g}_{nm} &\to \vec{k}_n\mathrm{g}_{nn} = 0 \\ \vec{k}_m\mathrm{g}_{mn} &\to -\vec{k}_n\mathrm{g}_{nn} = 0\ , \end{aligned} \tag{4.122}$$

we see from (4.30) and (4.31) that the only remaining instance of $\vec{k}_n$ left in the contribution from this grouping is the leading factor in $b(n)$. The contribution thus has an overall factor

$$\int \frac{\mathrm{d}\vec{k}_n}{(2\pi)^d}\,\vec{k}_n\, v(k_n) = 0 \tag{4.123}$$

due to the angular integration and can consequently be dropped. This shows that the requirement of statistical homogeneity and isotropy automatically ensures that particle self-interactions do not contribute to any kind of cumulant.

Another important feature of the potential is its scaling with the mean particle number density $\bar{\rho}$. Since the case of the gravitational potential of a collection of identical particles of mass m will be the relevant one in part ii we use it as an example here. The potential $v_j(\vec{q})$ generated by the particle j is proportional to its mass. The physical system we are describing is some distribution of the total mass M distributed over some volume V. As explained in section 3.1, the particles of our field theory are just tracer particles whose number N and mass m we are free to choose as long as we fulfil the constraint $M = Nm$. Since we also fix the volume, the quantity that characterises our system is the mean mass density $\bar{\rho}_\mathrm{m} = M/V$. As long as we keep it fixed, we are describing the same system, no matter what the number N of particles is we use to represent it with. For the potential it thus follows that

$$v_j(\vec{q}) \propto m = \frac{M}{N} = \frac{M}{V}\frac{V}{N} = \frac{\bar{\rho}_\mathrm{m}}{\bar{\rho}} \propto \frac{1}{\bar{\rho}}\ . \tag{4.124}$$

Analoguous reasonings can be found for any interaction which is proportional to some 'charge' property of the particles. We only require that the respective charge density is fixed.

4.3.4 *Shot-noise and relevance of terms*

We just saw that the interaction potential scales with the inverse of the mean particle number density $\bar{\rho}$ if we keep the characteristic 'charge' or mass density fixed. On the other hand we also have for a general non-interacting cumulant $G^{(0,\ell)}_{\alpha_1\dots\alpha_n} \propto \bar{\rho}^\ell$. Our perturbation theory will thus produce a multitude of terms all scaling differently with $\bar{\rho}$ due to the combination of factors coming from the two aforementioned sources. We thus need to ask ourselves whether we actually need to consider all of them.

The statistical quantities we are ultimately interested in are n-point cumulants of a *continuous* mass density field ρ_m. The description in terms of particles is after all just due to a discrete sampling of this continuous density field at the initial time. In the end we only want to keep those terms that would also appear in a continuous field description and we can identify those terms through their scaling with $\bar{\rho}$.

Let us first consider a statistically homogeneous and isotropic mass density field $\rho_\mathrm{m}(\vec{q}) = \bar{\rho}_\mathrm{m}(1+\delta(\vec{q}))$ at some instant in time. In Fourier space we then have $\rho_\mathrm{m}(\vec{k}_1) = \bar{\rho}_\mathrm{m}(\hat{1} + \delta(\vec{k}_1))$ where $\hat{1} = (2\pi)^d\,\delta_\mathrm{D}(\vec{k}_1)$ is the Fourier transformed unity. Its two-point cumulant is given by

$$\begin{aligned}
&\left\langle \rho_\mathrm{m}(\vec{k}_1)\,\rho_\mathrm{m}(\vec{k}_2)\right\rangle - \left\langle \rho_\mathrm{m}(\vec{k}_1)\right\rangle \left\langle \rho_\mathrm{m}(\vec{k}_2)\right\rangle \\
&= \bar{\rho}_\mathrm{m}^2 \left(\hat{1}\hat{2} + \hat{1}\left\langle \delta(\vec{k}_2)\right\rangle + \hat{2}\left\langle \delta(\vec{k}_1)\right\rangle + \left\langle \delta(\vec{k}_1)\delta(\vec{k}_2)\right\rangle\right) - \bar{\rho}_\mathrm{m}^2\hat{1}\hat{2} \\
&= m^2\bar{\rho}^2(2\pi)^d\,\delta_\mathrm{D}(\vec{k}_1+\vec{k}_2)\,P(k_1)\;. \qquad (4.125)
\end{aligned}$$

We have used that $\langle\delta\rangle = 0$ in the third line and written the mass density in terms of a particle mass m and particle number density $\bar{\rho}$ in the last line. We see that we only have a term which scales as $\bar{\rho}^2$. It is not difficult to see from this simple example that any n-point cumulant of the continuous field ρ_m will consist only of terms which scale as $\bar{\rho}^n$.

In contrast let us now consider our collective density field (4.19) made up of single particle contributions in the canonical ensemble. For an instantaneous discrete sampling of a Gaussian random density field one can easily obtain the joint probability for two particles i and j to be found at positions $\vec{q}_i$ and $\vec{q}_j$ by marginalizing the phase-space probability density (3.49) over all momenta and the positions of all other particles. One finds

$$\mathcal{P}\left(\vec{q}_i,\vec{q}_j\right) = \frac{1}{V^2}\left(1+\xi\left(\vec{q}_i,\vec{q}_j\right)\right)\;, \qquad (4.126)$$

where ξ is the two-point correlation function, the Fourier conjugate of the powerspectrum of the density field. The probability to find a single particle then is $\mathcal{P}(\vec{q}_j) = 1/V$ and thus the one-point cumulant of the discrete density field is

$$\left\langle \Phi_\rho(\vec{k}_1)\right\rangle = \sum_{j=1}^{N}\int \mathrm{d}\vec{q}_j\,\frac{1}{V}\mathrm{e}^{-\mathrm{i}\vec{k}_1\cdot\vec{q}_j} = \frac{N}{V}(2\pi)^d\,\delta_\mathrm{D}(\vec{k}_1) = \bar{\rho}\,\hat{1}\;. \qquad (4.127)$$

We thus find for the instantaneous two-point cumulant of the discrete density field

$$\begin{aligned}
&\left\langle \Phi_\rho(\vec{k}_1)\, \Phi_\rho(\vec{k}_2) \right\rangle - \left\langle \Phi_\rho(\vec{k}_1) \right\rangle \left\langle \Phi_\rho(\vec{k}_2) \right\rangle \\
&= \sum_{i=1}^{N} \sum_{j=1}^{N} \left\langle \mathrm{e}^{-\mathrm{i}\vec{k}_1\cdot\vec{q}_i} \mathrm{e}^{-\mathrm{i}\vec{k}_2\cdot\vec{q}_j} \right\rangle - \bar{\rho}^2 \hat{1}\hat{2} \\
&= \sum_{i=j} \int \mathrm{d}\vec{q}_i \, \frac{1}{V} \, \mathrm{e}^{-\mathrm{i}\left(\vec{k}_1+\vec{k}_2\right)\cdot\vec{q}_i} + \sum_{i\neq j} \int \mathrm{d}\vec{q}_i \int \mathrm{d}\vec{q}_j \, \frac{1}{V^2} \left(1 + \xi\left(\vec{q}_i, \vec{q}_j\right)\right) \left\langle \mathrm{e}^{-\mathrm{i}\vec{k}_1\cdot\vec{q}_i} \mathrm{e}^{-\mathrm{i}\vec{k}_2\cdot\vec{q}_j} \right\rangle \\
&\quad - \bar{\rho}^2 \hat{1}\hat{2} \\
&= \frac{N}{V} (2\pi)^d \, \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_2) + \frac{N(N-1)}{V^2} \left(\hat{1}\hat{2} + \int \mathrm{d}\vec{q}_i \int \mathrm{d}\vec{q}_j \, \xi\left(\vec{q}_i, \vec{q}_j\right) \mathrm{e}^{-\mathrm{i}\vec{k}_1\cdot\vec{q}_i} \mathrm{e}^{-\mathrm{i}\vec{k}_2\cdot\vec{q}_j} \right) \\
&\quad - \bar{\rho}^2 \hat{1}\hat{2} \\
&= (2\pi)^d \, \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_2) \left(\bar{\rho} + \bar{\rho}^2 P(k_1)\right) \, .
\end{aligned} \tag{4.128}$$

In the third step we separated the double sum into those terms which come from one and the same particle and those which come from truly different particles. In the final step we used that $N \gg 1$. We see that due to the discrete particle nature of our system the former case has led to a *shot-noise* term which scales with a smaller power than $n = 2$. Just like in the continuous case one can easily convince oneself that for a general n-point cumulant of Φ_ρ there will arise such shot-noise terms of all scalings $\bar{\rho}^m$ with $1 \leq m < n$ due to the identification of all possible numbers of particles. Only from those terms where all n particles are actually distinct do we get a contribution equivalent to the continuous case which scales as $\bar{\rho}^n$. In the grand-canonical ensemble we find the same structure even for non-instantaneous density-only cumulants if we combine (4.18) with Corollary 4.

Let us now consider mixed cumulants between Φ_ρ and Φ_B at the same n-point level. We start with the density-only cumulant and then replace one Φ_ρ with a Φ_B field. Now Corollary 4 dictates that only terms with scaling up to $\bar{\rho}^{n-1}$ are left and for each additional Φ_B field we lose another power of $\bar{\rho}$. The presence of the Φ_B field thus leads to particles being identified. In light of the considerations we gave after Theorem 1 this is not surprising as the Φ_B field encodes how effects of interactions at one external label are transported forward to another label by *single* particles.

We now want to consider the 'thermodynamic' limit where $N \to \infty$ and thus also $\bar{\rho} \to \infty$. In this 'infinite resolution' limit we have to recover the continuum case. But to make sure that we describe the same physical system throughout we must keep the mean mass density $\bar{\rho}_{\mathrm{m}} = m\bar{\rho}$ fixed. Thus, we multiply (4.128) by m^2 to find

$$\left\langle \Phi_{\rho_m}(\vec{k}_1)\, \Phi_{\rho_m}(\vec{k}_2) \right\rangle - \left\langle \Phi_{\rho_m}(\vec{k}_1) \right\rangle \left\langle \Phi_{\rho_m}(\vec{k}_2) \right\rangle = (2\pi)^d \, \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_2) \, \bar{\rho}_{\mathrm{m}}^2 \left(\frac{1}{\bar{\rho}} + P(k_1) \right) \, , \tag{4.129}$$

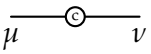
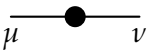
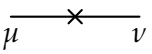
where Φ_{ρ_m} is now the discrete version of the mass density field. We see that in the above 'thermodynamic' limit the shot noise term will become irrelevant compared to the actual power spectrum, which is the dominant $\bar{\rho}^2$ term. We will thus just drop the shot-noise term. Then we get the same result (4.125) as in the continuum case. It is

straightforward to extend this argument to arbitrary n-point cumulants, i. e. we only ever keep the leading order term in $\bar{\rho}$.

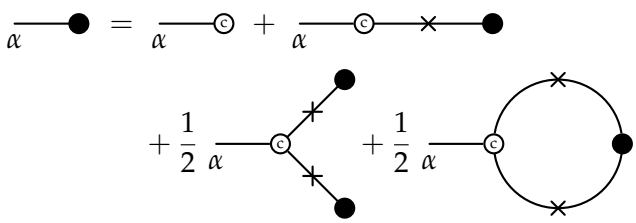
In the case of perturbative expansions of some cumulant we first have to identify its leading contribution in $\bar{\rho}$. Then for each term in the perturbative expansion we gather all factors of $\bar{\rho}$ coming either from free cumulants or the interaction potential and then drop all terms which do not have the same scaling as the leading contribution.

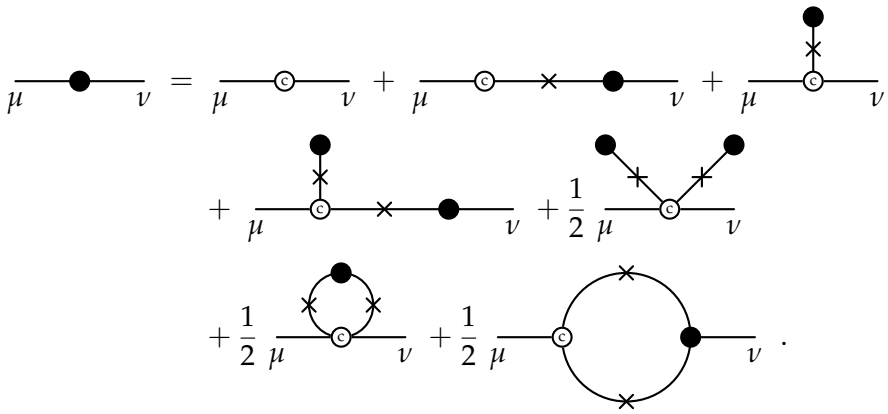
4.3.5 *Diagrammatic language for perturbation theory*

With the general form of the interaction and the relevance of individual terms in the perturbation series clarified, we now want to get into some more detailed calculations. As in the case of managing the initial correlations, it will be a lot more convenient to do this in terms of a diagram language. We will first introduce a top-level language for the quantities $G^{(c)}_{\alpha_1\dots\alpha_n}$, the full cumulants $G_{\alpha_1\dots\alpha_n}$ and the interaction potential $\sigma_{\mu\nu}$. We define:

$G^{(c)}_{\mu\nu} :=$  $G_{\mu\nu} :=$  $\mathrm{i}\sigma_{\mu\nu} :=$  (4.130)

The extension to the generic n-point case is then obtained by appending the appropriate number of lines to the circles. We use the solid line for both field types ρ and B at this top-level and summation over both types is implied for internal lines. With this language we can now easily write down both the second order one-point equation (4.101) and two-point equation (4.103) as

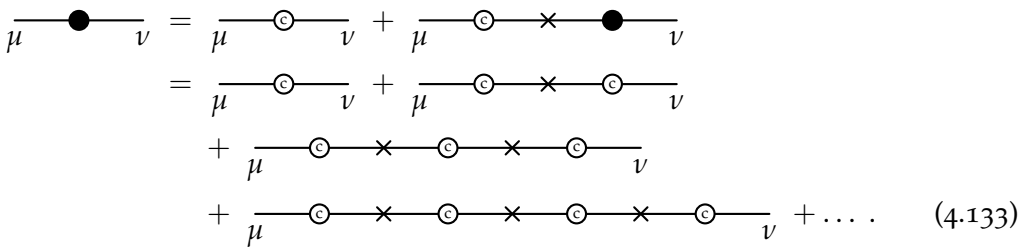

(4.131)


(4.132)

Concerning the one-point equation we can now use our findings from section 4.3.3 to drop the second and third diagram since both of them contain *tadpoles*, i. e. full one-point cumulants attached to some $G^{(c)}$. Since the latter are made up of $G^{(0,\ell)}$

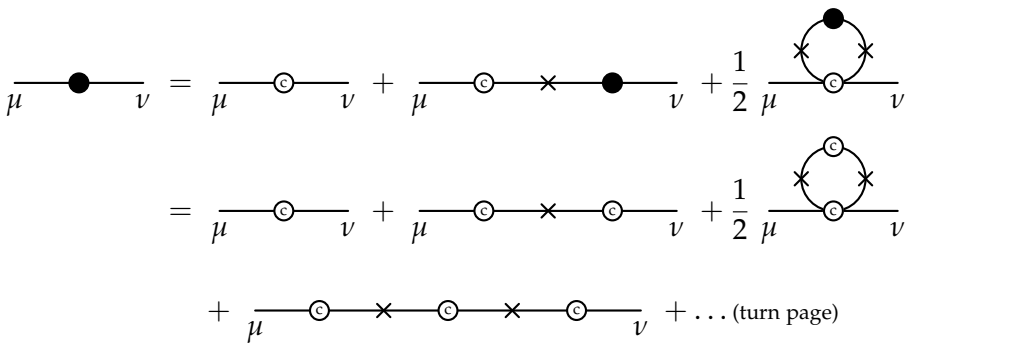
(4.120) also applies here. Furthermore, since we fixed the mean particle number density when we defined our grand canonical ensemble in the first place, we expect it to be unchanged by interactions between the particles. We show in Appendix C that indeed all remaining contributions vanish if we consider only terms where $\sigma_{\mu\nu}$ appears explicitly up to second order. A general proof of this seems hard at least in the grand canonical formulation of perturbation theory due to its self-consistent form. We like to mention that in [22, 39, 40] Das and Mazenko actually do find a correction to the one-point cumulant, i. e. the mean density. How and why this comes about there is also discussed in Appendix C. For the remainder of this work however, the one-point cumulant will no longer be of any concern.

Dropping all tadpole diagrams also reduces the two-point equation as we may drop the third, fourth and fifth diagram. In order to see which kind of diagram structures found in the canonical perturbation series are 'resummed' as solutions to integral equations in this self-consistent formulation we now restrict ourselves to the remaining first order term coming from the expansion of $e^{\Delta W^{(\ell)}}$. This equation now again looks similiar to the Dyson equation of QFT and can be formally solved iteratively



(4.133)

From this we see that the first order solution contains all straight line diagrams obtained from gluing together the two-point quantity $G^{(c)}_{\mu\nu}$ with the interaction matrix $\sigma_{\mu\nu}$. In terms of the actual integral equation represented by these diagrams, this iterative solution is just the corresponding Neumann series. The exact first order solution to the self-consistent equation thus contains terms with arbitrary orders in the interaction. If in addition, we take into account the sixth diagram of (4.132), i. e. the simplest one-loop diagram, and again solve iteratively we also obtain all kinds of one-loop corrections that can be built with the four-point quantity $G^{(c)}_{\alpha_1\alpha_2\alpha_3\alpha_4}$



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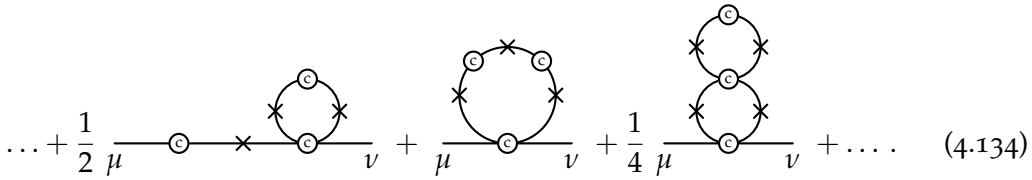
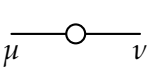


(4.134)

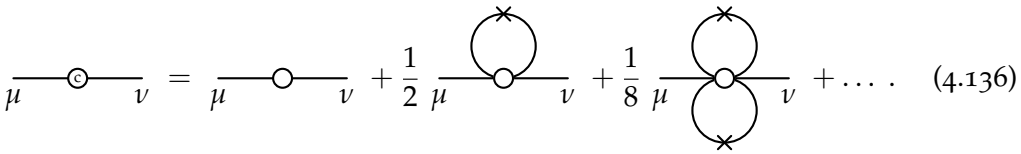
From this it becomes clear how to understand the grand canonical perturbation series. Taking into account higher orders in the expansion of $e^{\Delta W^{(\ell)}}$ leads to more complex loop structures in the self-consistent perturbation expansion. Solving these self-consistent equations iteratively we then get a series of diagrams of arbitrary loop order built from those loop-subdiagrams found in the full self-consistent equation but with the full cumulants exchanged for the $G^{(c)}_{\alpha_1\ldots\alpha_n}$. For higher loop orders this becomes cumbersome due to the coupling of the self-consistent equations between different n-point levels, because one has to do the iterative expansion of all these different equations at the same time.

It is in the above sense that the grand canonical perturbation theory resums classes of diagrams of the canonical perturbation theory. However, as we mentioned several times before, this way of organising the perturbation series has a serious drawback in the presence of initial correlations. It is obscure how to expand both $e^{\Delta W^{(\ell)}}$ and $G^{(c)}_{\alpha_1\ldots\alpha_n}$ in orders of $\sigma_{\mu\nu}$ consistently at the same time. The expansion of the $G^{(c)}_{\alpha_1\ldots\alpha_n}$ is not contained in the iterative solution to the self-consistent equations, rather it must in principle be known to all orders of $\sigma_{\mu\nu}$ as input. We can easily see why this is the case if we define a new diagram type

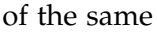
$G^{(0)}_{\mu\nu} :=$  .

(4.135)

With this new diagram type we can expand $G^{(c)}_{\alpha_1\ldots\alpha_n}$ as

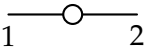


(4.136)

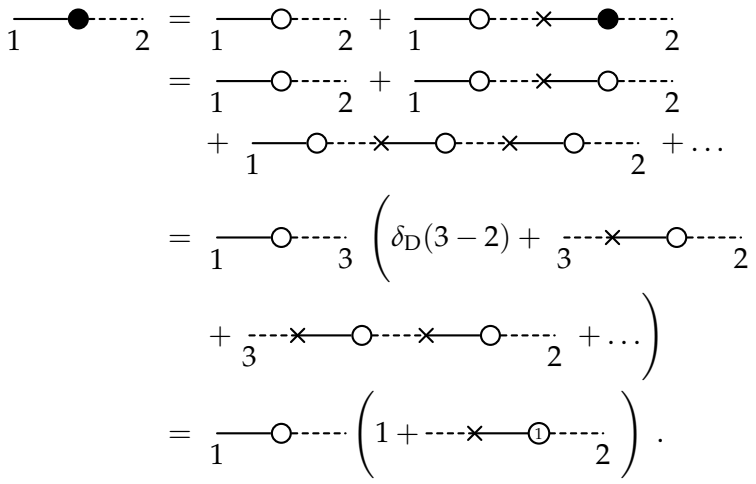
If we compare this with (4.133) we see that the diagrams in the iterative solution can be composed as multiple products of the same basic diagram  . One can see this as the functional analogue of a geometric series. No such thing is possible for the above expansion in (4.136) where each new term needs a free cumulant $G^{(0)}_{\alpha_1\ldots\alpha_n}$ two n-point levels higher than the term before. Thus, this expansion cannot be phrased as the iterative solution to a self-consistent equation.

From a purely diagrammatic perspective the terms in (4.136) look very similar to the loop contributions in (4.134). This suggests that we should reorganise our perturbative expansion in such a way that both of the terms are grouped together. For this we need to identify some new two-point quantity that gives both types of diagrams once we use it to build loop corrections with the free cumulants $G^{(0)}_{\alpha_1\ldots\alpha_n}$

as vertices. For this purpose we now make our diagram language more explicit by differentiating between Φ_ρ and Φ_B fields which we accomplish by

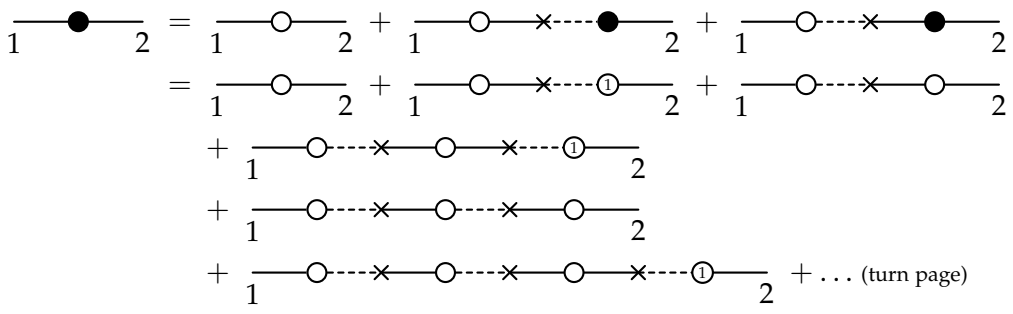
$G^{(0)}_{\rho_1 B_2} :=$  , $G^{(0)}_{\rho_1 \rho_2} :=$  , $\mathrm{i}\sigma_{\rho_1 B_2} :=$  , (4.137)

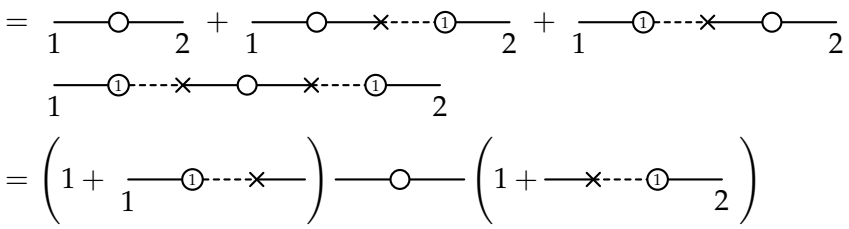
again with obvious extensions to higher n-point cases. Since $G^{(0)}_{B\dots B} = 0$ according to Corollary 2 there are no n-point diagrams of the above kind with only dashed legs. The interaction matrix (2.40) has only off-diagonal entries, so it only has a mixed diagram with one solid and one dashed line. We now consider the first order equation for $G_{\rho B}$ with none of the loop corrections in (4.136) taken into account, i. e. we reduce $G^{(c)}_{\alpha_1\dots\alpha_n} \to G^{(0)}_{\alpha_1\dots\alpha_n}$. Using that $G_{BB} = 0$ (see Appendix A) we can solve the equation in analogy to (4.133) to find



(4.138)

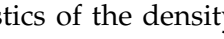
In the third step we factored out one instance of the free $G^{(0)}_{\rho_1 B_3}$ cumulant. In the final step we identified the infinite geometric series as the first order solution for $G_{\rho_1 B_2}$, which we indicate by the 1 inside the circle, times one instance of $\sigma_{B\rho}$. As we did in the last step, we will from now on always omit the inner labels and understand the integrations to be implicit as well as write unity for the Dirac delta distribution. We now take a look at the corresponding first order $G_{\rho_1\rho_2}$ equation and find





(4.139)

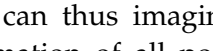
In the second line we have inserted the first order solution for $G_{B\rho}$, which is obtained iteratively in the same way as $G_{\rho B}$ and just gives the mirrored version of (4.138). We then proceeded to solve the $G_{\rho_1\rho_2}$ equation iteratively by using the first two diagrams in the second line as the starting zeroth order solution and then identified two instances of the infinite geometric series which defines the first order solution $G^{(1)}_{\rho B}$ of $G_{\rho B}$.

At this point we clearly see in which way $G_{\rho B}$ plays the role of a propagator for the statistics of the density field ρ. The quantity $(1 +$  $)$ can be seen as the sum of all particle interaction processes which transport a mode $\vec{k}$ of the density field contributing to the initial power spectrum $P_\delta(k)$ forward through time in a linear fashion, i. e. without any interaction with another mode of the density field.

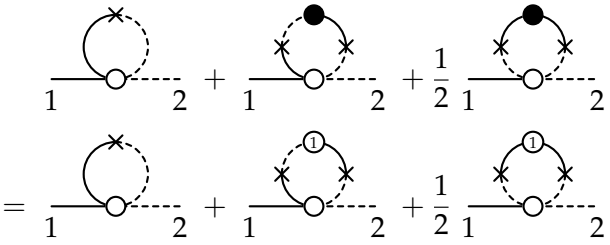
- The simplest such process represented by the leading unity is that there is no interaction and one particle carries the mode forward from the initial to the final time by means of the free particle propagator g_{qp} contained in $G^{(0)}_{\rho_1\rho_2}$, which is the result of the initial momentum correlations.

- The first interacting process is represented by the diagrammatic expression $= G^{(0)}_{\rho_1 B_3} i\sigma_{B_3\rho_2}$. Corollary 4 tells us that $G^{(0)}_{\rho_1 B_3} = G^{(0,1)}_{\rho_1 B_3}$ given in (4.54), and combining this with (4.114) we directly conclude that $G^{(0)}_{\rho_1 B_3} i\sigma_{B_3\rho_2} \propto \delta_{\mathrm{D}}(\vec{k}_1 - \vec{k}_2)\, g_{12}$. This process can thus be understood as the original particle carrying the mode $\vec{k}_2$ interacting with some other single particle at some intermediate time t_2, which then takes over this mode due to the Dirac delta distribution and transports it forward to the final time t_1 by virtue of g_{12}.

- The next higher process is then the same as the previous one, except that the second particle also interacts with some third particle which then takes over the propagation of the mode until the final time.

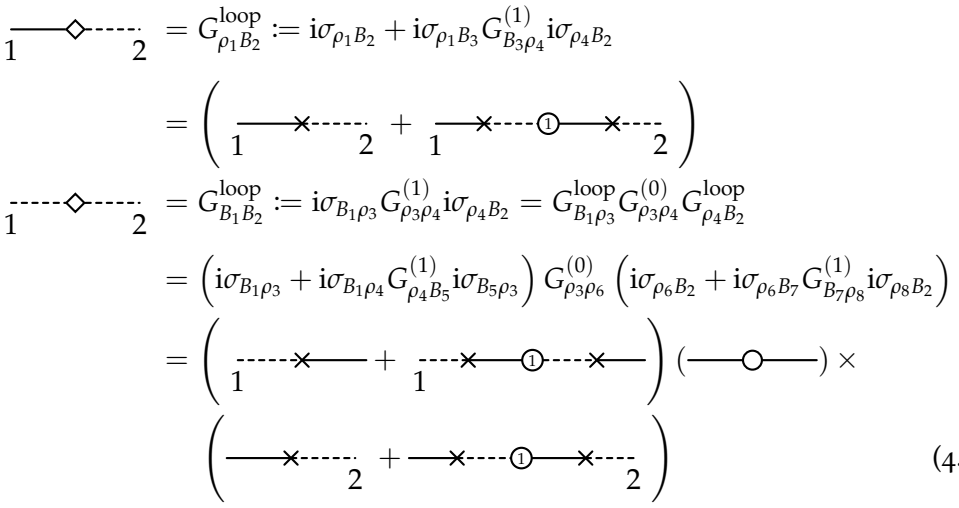
One can thus imagine the linear propagator quantity $(1 +$  $)$ as the summation of all possible 'bucket brigade' processes where the free propagation of a mode is 'handed over' from particle to particle by means of the interaction $\sigma_{\rho B}$. The Dirac delta distributions $\delta_{\mathrm{D}}(\vec{k}_j - \vec{k}_{j-1})$ ensure linearity and the propagators $g_{j(j-1)} \propto \Theta(t_j - t_{j-1})$ causality for each 'handover interaction' from particle $j-1$ to particle j in the chain. Furthermore, we note that $G^{(0,1)}_{\rho_1 B_3}\sigma_{B_3\rho_2} \propto \bar{\rho}^0$ holds for each term in the geometric series and thus $(1 +$  $) \propto \bar{\rho}^0$ as well. Hence, it leaves the $\bar{\rho}$-scaling of other quantities untouched reinforcing its interpretation as the linear propagator of field statistics.

With the linear propagator on the level of density field statistics identified we can finally turn to reorganising the loop structure of the perturbation expansion. For this purpose we consider the $G_{\rho B}$ version of the self-consistent second order equation (4.132) without tadpoles. We then identify all the one-loop diagrams which have the same form as the second diagram in (4.136) and after canceling the symmetry factors of $1/2$ against the sums of different possibilities to draw the diagrams we find



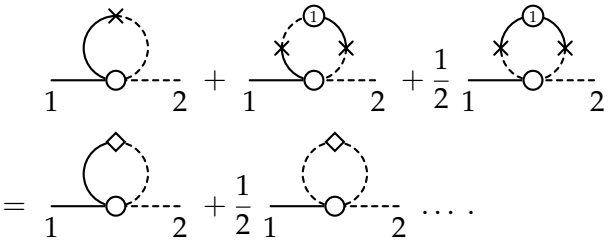
(4.140)

In the second line we have inserted the first order solutions $G^{(1)}_{B\rho}$ and $G^{(1)}_{\rho\rho}$. Let us a define two new two-point quantities:



(4.141)

With the help of these we can now write (4.140) as



(4.142)

This suggests that we can reformulate our perturbation expansions in terms of the linear field propagators appearing in (4.138), (4.139), the linear loop propagators of (4.141) and the free n-point cumulants. The interaction potential $\sigma_{\mu\nu}$ would then be completely contained in the basic two-point quantities and the number of loops in diagrams could serve as a clear-cut order parameter. Showing that this reformulation is possible for every order of the self-consistent expansion would however be a very

cumbersome task. A much better way to do this would be to reformulate the generating functional of the theory in such a way that this kind of perturbation expansion is generated automatically.

A possible hint to what one has to achieve can be gleaned from (4.76). The problem of the non-vanishing commutation (4.80) arises from the fact the collective fields used to describe the interaction in the system are the same fields that are used to calculate the free cumulants from the free motion of the individual particles. This suggests that we somehow have to separate these two instances of the collective fields into two separate classes when defining the generating functional, establishing a true separation between interactions and free motion.

If the perturbation expansion can indeed be reorganised in the way we described, the new generating functional would then need have a form completely analoguous to standard QFT. This would then allow us to directly transfer perturbative techniques from QFT, like e. g. Dyson resummation of the two-point cumulant with the 1PI-self-energy, over to our theory. However, finding this reformulation of the generating functional will be beyond the scope of this thesis.

4.3.6 *First order solution for the statistical field propagator*

With the solution of the first order self-consistent $G_{\rho B}$-equation identified as the core propagator quantity of the field theory, the question is in which cases we are able to obtain it analytically. We will see that under certain assumptions and approximations we can give a general closed form. We first write down the equation explicitly as

$$G^{(1)}_{\rho B}(1,2) = G^{(0,1)}_{\rho B}(1,2) + \int \mathrm{d}3 \int \mathrm{d}4\, G^{(0,1)}_{\rho B}(1,3)\, \mathrm{i}\sigma_{B\rho}(3,4)\, G^{(1)}_{\rho B}(4,2)\,. \tag{4.143}$$

We can make (4.119) more explicit for two-point cumulants

$$G_{\alpha\beta}(1,2) = (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_2)\, \bar{G}_{\alpha\beta}(k_1, t_1, t_2)\,. \tag{4.144}$$

We use this as well as the explicit forms of $G^{(0,1)}_{\rho B}(1,2)$ given in (4.54) and the interaction potential $\sigma_{\rho B}(1,2)$ given in (4.114) to simplify the integral

$$\begin{aligned}
&\int \mathrm{d}3 \int \mathrm{d}4 \left(-\mathrm{i}\bar{\rho}\, k_1^2\, \mathrm{g}_{13}\, (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_3)\, \mathfrak{D}(1,3)\right) \times \\
&\left(-\mathrm{i}(2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_3 + \vec{k}_4)\, \delta_{\mathrm{D}}(t_3 - t_4)\, v(k_3)\right) \left((2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_4 + \vec{k}_2)\, \bar{G}^{(1)}_{\rho B}(k_4, t_4, t_2)\right) \\
&= (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_2) \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t_3\, (-\bar{\rho}\, k_1^2\, v(k_1))\, \mathrm{g}_{13}\, \mathfrak{D}(1, (\vec{k}_2, t_3))\, \bar{G}^{(1)}_{\rho B}(k_2, t_3, t_2) \\
&= (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_2) \int_{t_2}^{t_1} \mathrm{d}t_3\, (-\bar{\rho}\, k_1^2\, v(k_1))\, \mathrm{g}_{13}\, \mathfrak{D}(k_1, t_1, t_3)\, \bar{G}^{(1)}_{\rho B}(k_1, t_3, t_2)\,.
\end{aligned} \tag{4.145}$$

In the last step we used that $\mathrm{g}_{13} \propto \Theta(t_1 - t_3)$ and $\bar{G}^{(1)}_{\rho B}(k_1, t_3, t_2) \propto \Theta(t_3 - t_2)$ in order to change the integral boundaries, assuming of course that $t_\mathrm{i} \leq t_1, t_2 \leq t_\mathrm{f}$. The

causality of $\bar{G}^{(1)}_{\rho B}$ is a consequence of the fact that every factor in the geometric series (4.138) obeys causality by itself. We abbreviate $\mathfrak{D}_{13} := \mathfrak{D}(k_1, t_1, t_3)$. We see that all terms in the integral equation have the same prefactor $(2\pi)^d \, \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_2)$ which we now drop to write

$$\bar{G}^{(1)}_{\rho B}(k_1, t_1, t_2) = -\mathrm{i}\bar{\rho}\, k_1^2 \, \mathrm{g}_{12} \, \mathfrak{D}_{12} + \int_{t_2}^{t_1} \mathrm{d}t_3 \, (-\bar{\rho}\, k_1^2 \, v(k_1)) \, \mathrm{g}_{13} \, \mathfrak{D}_{13} \, \bar{G}^{(1)}_{\rho B}(k_1, t_3, t_2) \; . \tag{4.146}$$

With regard to this integral equation the modulus of the mode k_1 and the potential $v(k_1)$ are just parameters. We now want to use the convolution theorem (1.36) of the Laplace transform. For this we first need to assume that the free particle propagator is invariant under time translation, i. e. $\mathrm{g}_{13} = \mathrm{g}_{qp}(t_1 - t_3)$. This will be true for most physical systems. Furthermore, the same must hold true for the damping factor as $\mathfrak{D}_{13} = \mathfrak{D}(k_1, t_1 - t_3)$. However, since the damping factor has the form

$$\mathfrak{D}(k_1, t_1, t_3) = \exp\left\{ -\frac{\sigma_p^2}{2} k_1^2 (g_1 - g_3)^2 \right\} \; , \tag{4.147}$$

we consequently need $g_1 - g_3 = \mathrm{g}_{qp}(t_1 - t_\mathrm{i}) - \mathrm{g}_{qp}(t_3 - t_\mathrm{i}) = f(t_1 - t_3)$, where f is some function. This directly implies $\mathrm{g}_1 \propto (t_1 - t_\mathrm{i})$. This is true for particles on inertial trajectories. In other cases we can still progress by approximating the damping factor by unity, i. e. $\mathfrak{D}_{13} \approx 1$. The solution for $\bar{G}^{(1)}_{\rho B}(k_1, t_1, t_2)$ is then of course only valid in a certain range of values for (k_1, t_1, t_2) one has to specify. We will see an example for this in part ii. Under these assumptions we can define

$$\begin{aligned} g(k_1, t_1 - t_2) &:= -\mathrm{i}\bar{\rho}\, k_1^2 \, \mathrm{g}_{12} \, \mathfrak{D}_{12} \\ K(k_1, t_1 - t_3) &:= (-\bar{\rho}\, k_1^2 \, v(k_1)) \, \mathrm{g}_{13} \, \mathfrak{D}_{13} \; , \end{aligned} \tag{4.148}$$

where K designates the kernel of the integral equation and is not to be confused with the source term $\mathbf{K}$. We now define two new time variables by $t = t_1 - t_2$ and $t' = t_3 - t_2$ which allow us to write the integral equation as

$$\bar{G}^{(1)}_{\rho B}(k_1, t + t_2, t_2) = g(k_1, t) + \int_0^t \mathrm{d}t' \, K(k_1, t - t') \, \bar{G}^{(1)}_{\rho B}(k_1, t' + t_2, t_2) \; . \tag{4.149}$$

In this form we may now apply the Laplace transform $\mathcal{L}_{t\to s}$ to the equation and use the convolution theorem (1.36) to find

$$\begin{aligned} \mathcal{L}_{t\to s}\left[\bar{G}^{(1)}_{\rho B}(k_1, t + t_2, t_2) \right] &= \mathcal{L}_{t\to s}\left[g(k_1, t) \right] \\ &\quad + \mathcal{L}_{t\to s}\left[K(k_1, t) \right] \mathcal{L}_{t'\to s}\left[\bar{G}^{(1)}_{\rho B}(k_1, t' + t_2, t_2) \right] \; . \end{aligned} \tag{4.150}$$

Since the time variable which we transform is now just an integration variable, we may rename $t' \to t$ in the second term on the RHS. We now use (1.35) to rewrite

$$\mathcal{L}_{t\to s}\left[\bar{G}^{(1)}_{\rho B}(k_1, t + t_2, t_2) \right] = \mathrm{e}^{s t_2} \, \mathcal{L}_{t\to s}\left[\bar{G}^{(1)}_{\rho B}(k_1, t, t_2) \, \Theta(t - t_2) \right] \; . \tag{4.151}$$

Assuming that all transforms actually exist we can now solve this algebraic equation easily to find

$$\mathcal{L}_{t\to s}\left[\bar{G}^{(1)}_{\rho B}(k_1,t,t_2)\,\Theta(t-t_2)\right] = \mathrm{e}^{-st_2}\,\frac{\mathcal{L}_{t\to s}\left[g(k_1,t)\right]}{1-\mathcal{L}_{t\to s}\left[K(k_1,t)\right]}\,. \tag{4.152}$$

The full solution is then obtained by applying the inverse transform $\mathcal{L}^{-1}_{t_1\leftarrow s}$. Restoring the Dirac delta distribution prefactor we dropped earlier we have as our general solution

$$G^{(1)}_{\rho_1 B_2} = (2\pi)^d\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\,\mathcal{L}^{-1}_{t_1\leftarrow s}\left[\mathrm{e}^{-st_2}\,\frac{\mathcal{L}_{t\to s}\left[g(k_1,t)\right]}{1-\mathcal{L}_{t\to s}\left[K(k_1,t)\right]}\right]\,. \tag{4.153}$$

From (1.34) we see that this solution will indeed respect causality, i. e. it will be proportional to $\Theta(t_1-t_2)$. Furthermore, because $v(k_1)\propto\bar{\rho}^{-1}$ the kernel is constant in the mean particle number density $K\propto\bar{\rho}^0$ and since $g\propto\bar{\rho}$ we see that also the solution scales as $G^{(1)}_{\rho_1 B_2}\propto\bar{\rho}$, as one would expect.

5

CONCLUSION ON PART I AND OUTLOOK

In the first part of this thesis we introduced a field-theoretical formulation of kinetic theory, dubbed Statistical Field Theory for Classical Particles (SFTCP) by us, pioneered in [39, 40, 22]. We went through the following steps:

- In chapter 2 we showed all the necessary steps that lead to the generating functional of the field theory already found in Mazenko [39]. We did this in the context of a system whose statistics are characterised by the number of particles N, its volume V and a probability distribution $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ for the initial phase-space coordinates of the particles, hence the denomination as a canonical statistical ensemble. We tried to emphasize where parallels of the concepts and central quantities of SFTCP can be found in standard equilibrium physics, but also how the latter is only a special case of the former. The separation of the theory into a 'free' and interacting part was discussed. We saw that the non-interacting free part can easily be treated analytically in terms of the individual particles. Under certain requirements on the Hamiltonian a general propagator for the motion of particles can be given. The interacting part is best handled in terms of macroscopic, collective fields Φ defined in terms of the phase-space coordinates of all particles. The two core fields which are required are the density Φ_ρ and an aptly defined response field Φ_B. Expressing these collective fields as operators directly leads to a straightforward perturbation theory for their correlators.

- A comparison with the standard formulation of kinetic theory showed that both approaches can indeed be understood as being based on the same core quantity, the N-particle phase-space distribution function. However, we argued that SFTCP posseses the advantage that actually applicable equations used for calculating macroscopic observables nominally retain the full phase-space information if all orders in the interaction are considered. Since this can be traced back to the use of the phase-space trajectories $\vec{x}_j$ of the individual particles as the basic variable of the field theory, we feel that it is an ingenius achievement on the part of Das and Mazenko to have come up with this idea.

- In chapter 3 we developed a general approach for how to set up the initial conditions $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ in terms of the phase-space coordinates of the N particles. We did this by sampling the macroscopic information known about the system at the initial time t_i in such a way that ensemble averages of the corresponding collective fields Φ become unbiased estimators for the actual macroscopic fields.

We looked at the simple example of Poisson sampling, but more complex sampling methods like e. g. 'hard-core' processes should also be compatible with the theory and are worth investigating.

- Building on top of this we allowed the initial macroscopic information to be given in terms of correlated random fields. For the central example of a statistically homogeneous and isotropic Gaussian random combined density-velocity field we then went on to derive the exact expression for $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$. By combining this with the explicit expression for the free generating functional we were able to rewrite the initial correlations imprinted on the phase-space distribution by this random field as an operator acting on the generating functional of an uncorrelated ideal gas. This operator was then analysed by introducing a diagram language for its basic constituents, the two-point correlations of the random field. With the help of the method known as the 'Mayer cluster expansion' we could then achieve a factorisation of the free generating functional into those terms which are 'connected' in the sense of the initial correlation diagrams. Since any probability distribution can formally be expanded around the Gaussian distribution given its cumulants, we expect that it should be possible to adapt the diagrammatic approach to arbitrary distributions.

- Finally, in chapter 4 we translated SFTCP into the grand-canonical ensemble for systems obeying statistical homogeneity and isotropy. This amounted to characterising the statistics of the system by its volume V, the phase-space probability distribution $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ for a fixed number N of particles and a probability distribution for finding N particles in the system, where the latter is only characterised by a mean particle number density $\bar{\rho}$. Using the result for the free generating functional of the canonical ensemble describing a Gaussian random field we could immediately show that its grand canonical counterpart is given by the exponentiated sum of those ℓ-particle generating functionals which are connected in the sense of the initial correlation diagrams. This result is very similar to QFT and stems from the fact that there is no fixed particle number in the system. It also establishes that free connected correlation functions or cumulants of any collective field can be obtained by considering only terms which are connected in the initial correlations, i. e. both conceptions are identical. Due to the supposed generality of the diagrammatic approach this relation should hold for initial random fields with arbitrary distributions and should be seen as one of the major achievements of this work.

- With a simple expression for the free generating functional found we calculated the cumulants of the two core collective fields Φ_ρ and Φ_B for the case of the initial Gaussian random field. We were able to give a general scheme for managing the various combinations of external labels of collective fields in the many terms contributing to the cumulants, which is helpful especially when considering high n-point orders or large numbers ℓ of connected particles. Together with some general theorems we were able to derive for the free cumulants, the scheme also helps in calculating terms in perturbation theory. We gave explicit

examples for one-, two- and three-particle cumulants, some of which will be used in ii.

- As a last step, we developed the self-consistent perturbation theory along the same lines as Das and Mazenko, resulting in a system of coupled non-linear integral equations. We showed how the presence of initial correlations modified the results of the original authors and led to the perturbation expansion suffering from an inconsistency problem. Introducing a diagrammatic language we could show that the first-order solution for the cumulant $G_{\rho B}$ could be understood as the field propagator for the statistics of the collective fields and already contained effects up to arbitrary order in the interaction. Using this first order solution we analysed the one-loop structure of the theory to find clues that hint at the possibility of reformulating the theory and thus the full generating functional in such a way as to cure the inconsistency problem. This new generating functional would then lead to a perturbation theory that is structurally equivalent to QFT, with the first order two-point solutions playing the role of the bare tree-level propagator and the free cumulants those of tree-level vertices. Under certain assumptions, we were able to give a general expression for the first order solution $G^{(1)}_{\rho B}$ of the field propagator in terms of Laplace transforms.

Despite the problems found in perturbation theory, we feel that in terms of what SFTCP is capable of, we only scratched the surface. There are certainly possibilities for future work in many different directions beside cosmological structure formation we would like to pursue. Without claim of completeness we list some of them here.

- The next big step is certainly finding the reformulation of the generating functional alluded to above. Efforts in this direction are underway and look very promising. This would effectively replace the complicated problem of the Liouville equation with the well-known perturbation theory of QFT.

- Using general cumulant expansions of probability distributions we would like to generalise the result (3.115) of the diagram based approach to initial conditions. Moving on from this one could investigate how to define grand canonical ensembles for general systems without the requirement of statistical homogeneity and isotropy. This should then allow us to find a general version of (4.11).

- Continuing on from the work done in Viermann et al. [55], it is worth investigating whether the SFTCP approach allows an easier investigation of fundamental properties of statistical physics in comparison to standard kinetic theory. It is especially interesting to see whether the equations of hydrodynamics can be derived directly from the theory itself, without the need to resort to heuristic arguments. The fact that in principle any macroscopic observable that can be derived from the phase-space trajectories of particles may easily be introduced into the theory by coupling the respective collective field to the collective source vector H, could potentially be of help here. Another point that might prove interesting in this regard is that dynamics containing statistical noise terms can be described by SFTCP without problems [39, 22].

- Having an operator that imprints the effects of initial correlations onto an ideal gas opens up the possibility to study the effects of such correlations on thermodynamical relations like equations of state. Kozlikin et al. [32] already found corrections to the pressure induced by initial correlations which in certain situations can be larger than those due to first order particle interactions.

Part II

APPLICATION TO COSMOLOGICAL STRUCTURE FORMATION

6

STRUCTURE FORMATION IN STANDARD COSMOLOGY

Before we start to apply the field theory approach we developed in part i to the problem of large scale structure (LSS) formation we first want to briefly set the stage. We assume that the reader is familiar with the basic principles of general relativity and cosmology in Friedmann-Lemaître-Robertson-Walker (FLRW) spacetime. A good introduction can be found in Carroll [17], more in-depth treatments are available in Straumann [54] and Weinberg [57]. We only introduce some basic equations common in cosmology. We will briefly discuss the scenario in which LSS formation is usually treated leading to the hydrodynamical picture of Standard Perturbation Theory (SPT). Since it is assumed that this description is accurate at least for the early matter-dominated phase of the universe we will use it to set up the initial conditions for our system. We will however also point out the approximations going into SPT and the shortcomings that result from this. We then argue why these problems should not be present in our approach of SFTCP.

6.1 COSMOLOGICAL MODEL

6.1.1 *FLRW universe*

We will operate under the assumption that our universe is well described by the standard ΛCDM-model of cosmology. This entails that when averaged on large enough scales the universe is homogeneous and isotropic and its spacetime geometry is described by the FLRW line element

$$\mathrm{d}s^2 = c^2\mathrm{d}t^2 - a^2(t)\left(\mathrm{d}q^2 + f_k^2(q)\,\mathrm{d}\Omega^2\right) \quad \text{with} \quad f_k(q) = \begin{cases} k^{-\frac{1}{2}}\sin\left(k^{\frac{1}{2}}q\right) & k>0 \\ q & k=0 \\ |k|^{-\frac{1}{2}}\sinh\left(|k|^{\frac{1}{2}}q\right) & k<0 \end{cases} \tag{6.1}$$

where k is a constant encoding the curvature of three-dimensional spatial hypersurfaces[1] which are described in terms of spherical *comoving coordinates*, where q is the radial coordinate. These coordinates are constant in time for objects without peculiar velocities, while the actual physical distances between such objects may change due

1 All results from part i we will use in this second part must thus be understood with the spatial dimension set to $d = 3$.

to the expansion and contraction of the universe encoded in the *scale factor* $a(t)$. Combining this line element with Einstein's field equations and the energy-momentum tensor of a perfect fluid the dynamics of this spacetime reduces to *Friedmann's equations*, which describe the time evolution of $a(t)$ by

$$\begin{aligned}\left(\frac{\dot{a}}{a}\right)^2 &= \frac{8\pi G}{3}\rho - \frac{kc^2}{a^2} + \frac{\Lambda}{3} \\ \frac{\ddot{a}}{a} &= -\frac{4\pi G}{3}\left(\rho + \frac{3p}{c^2}\right) + \frac{\Lambda}{3}\,,\end{aligned} \tag{6.2}$$

where $\rho(t)$ is the mean energy density of the universe in units of a mass density, $p(t)$ the mean pressure and Λ the cosmological constant. The energy content is usually split into non-relativistic matter and relativistic radiation as $\rho(t) = \rho_\mathrm{m}(t) + \rho_\mathrm{r}(t)$. The matter density evolves as $\rho_\mathrm{m}(t) = \rho_{\mathrm{m},0}\, a^{-3}(t)$ due to the expansion of volume elements with the scale factor a. The constant $\rho_{\mathrm{m},0}$ relates to some arbitrary point in time where $a = 1$ and this is usually chosen as the present cosmological epoch. The radiation density evolves as $\rho_\mathrm{r}(t) = \rho_{\mathrm{r},0}\, a^{-4}(t)$. The additional power of the scale factor comes from the fact that due to the expansion of the universe the wavelength of radiation gets stretched. Radiation emitted by some source at time t_e is thus observed by an observer at time t_o with a redshift of

$$z := \frac{\lambda_\mathrm{o} - \lambda_\mathrm{e}}{\lambda_\mathrm{e}} = \frac{a(t_\mathrm{o})}{a(t_\mathrm{e})} - 1 = \frac{\nu_\mathrm{e}}{\nu_\mathrm{o}} - 1\,. \tag{6.3}$$

Since the energy of radiation is related to its frequency by $E = h\nu$, where h is Planck's constant, we find the additional inverse scale factor. If we set $a(t_\mathrm{o}) = 1$ in (6.3) we obtain the usual expression $a = 1/(1+z)$, which makes it convenient to use the redshift as a time coordinate for past cosmological epochs. The first of Friedmann's equations in (6.2) is usually rewritten in parametric form. For this we introduce the *Hubble function*[2] $H(t) = \dot{a}(t)/a(t)$ and the *critical density*

$$\rho_\mathrm{crit}(t) := \frac{3H(t)^2}{8\pi G}\,. \tag{6.4}$$

The various Ω-parameters are then defined as:

$$\begin{aligned}\Omega_\mathrm{m}(t) &= \frac{\rho_\mathrm{m}(t)}{\rho_\mathrm{crit}(t)}\,, \quad \Omega_\mathrm{r}(t) = \frac{\rho_{\mathrm{r}(t)}}{\rho_\mathrm{crit}(t)}\,, \quad \Omega_k = -\frac{k\,c^2}{H_0^2}\,, \\ \Omega_\Lambda(t) &= \frac{\Lambda}{3H^2(t)} = \frac{8\pi G}{3H^2(t)}\frac{\Lambda}{8\pi G} = \frac{\widetilde{\Lambda}}{\rho_\mathrm{crit}(t)}\,.\end{aligned} \tag{6.5}$$

where H_0 is the Hubble function at the time where $a = 1$. In the second line, $\widetilde{\Lambda}$ has the units of a mass density showing that it can be understood as a contribution to the energy density of the universe. Friedmann's first equation can now be written as

$$1 = \Omega_\mathrm{m}(t) + \Omega_\mathrm{r}(t) + \Omega_\Lambda(t) - \frac{k\,c^2}{a^2H^2}\,. \tag{6.6}$$

2 The value of the Hubble function at the present time is often given as the reduced Hubble constant h defined by $H(t_\mathrm{today}) = h \times 100\frac{\mathrm{km}}{\mathrm{Mpc\,s}}$.

which clearly shows the meaning of the critical density. If the three energy density contributions fulfil the condition $\Omega_m + \Omega_r + \Omega_\Lambda = 1$ at any point in time then $k = 0$ follows at all times and the universe must be flat. If we evaluate all Ω-parameters at the time where $a = 1$ we arrive at the more practical equation

$$H^2(a) = H_0^2 \left(\Omega_{m,0}\, a^{-3} + \Omega_{r,0}\, a^{-4} + \Omega_{\Lambda,0} + \Omega_k\, a^{-2} \right) . \tag{6.7}$$

The combination of many observations like measurements of the cosmic microwave background (CMB) [28, 49] and LSS surveys [19, 18] have shown that if our universe can indeed be described by FLRW metric then its spatial curvature cannot be distinguished from being zero and thus we take $\Omega_k = 0$ to hold in all following considerations. For the cosmological epochs after the age of recombination at $z \approx 1100$ the radiation content of the universe quickly becomes negligible and since structure growth only starts in full earnest once matter comes to dominate we will assume that $\Omega_r \approx 0$ in all our calculations. We thus have $\Omega_{m,0} + \Omega_{\Lambda,0} = 1$ and the time-dependent parameters evolve in terms of the scale factor as

$$\begin{aligned} \Omega_m(a) &= \frac{8\pi G}{3H^2}\frac{\rho_{m,0}}{a^3} = \frac{8\pi G}{3H_0^2}\,\rho_{m,0}\,\frac{1}{a^3\left(\Omega_{m,0}\,a^{-3} + \Omega_{\Lambda,0}\right)} = \frac{\Omega_{m,0}}{\Omega_{m,0} + a^3(1-\Omega_{m,0})}\,, \\ \Omega_\Lambda(a) &= \frac{\Lambda}{3H^2(t)} = \frac{\Lambda}{3H_0^2}\,\frac{1}{\Omega_{m,0}\,a^{-3} + \Omega_{\Lambda,0}} = \frac{(1-\Omega_{m,0})}{\Omega_{m,0}\,a^{-3} + (1-\Omega_{m,0})}\,. \end{aligned} \tag{6.8}$$

In the ΛCDM-model the matter content is further split between two components, the baryonic matter with $\Omega_{bar,0} = 0.049$ and dark matter with $\Omega_{CDM,0} = 0.267$ [3]. The latter is a form of matter which does not interact with baryonic matter in a significant way other than through gravity[4]. It was originally proposed to explain a mismatch between the visible and dynamical masses of galaxies and galaxy clusters. Observations of their rotation curves leads one to derive a much higher mass compared to observations of the radiation emitted by them. By giving them additional mass that does not take part in electromagnetic interactions this problem is fixed. While a direct observation of dark matter particles has not succeeded so far, many other astronomical observations have delivered strong evidence for its existence, like for example the gravitational lensing of radiation due to the presence of galaxy clusters between source and observer, the CMB, direct observations of the LSS in redshift surveys of galaxies and the observed abundances of chemical elements in the universe. The variant favoured by most observations is called cold dark matter (CDM) since its constituents have a low velocity dispersion and thus allow for the 'bottom-up' formation of structure. What exactly it is composed of is so far unknown, the most popular candidate being some new kind of elementary particle like bosonic axions or fermionic weakly interacting massive particles (WIMP). Since dark matter makes up nearly 85% of the matter content in the universe we will concentrate on describing the evolution of a purely self-gravitating mass distribution for which the properties of the actual constituents are unimportant at the level of detail of our theory.

3 Values taken from the 2013 results of the Planck mission (cf. Planck Collaboration et al. [49]).

4 It is often assumed that it also interacts through the weak force, but this is insignificant due to its negligibly short range, especially compared to cosmological scales.

6.1.2 *Inflation and seeding of primordial structures*

The formation of structure in our universe is described as a hierachical process. One assumes that at the beginning of structure formation there a small perturbations in the overall homogeneous matter distribution of the universe. Through gravitational interaction overdense regions will attract more matter while underdense region have matter drained away from them. The overdense regions will eventually attract each other and merge into larger and larger structures, starting at galaxies, which then merge into clusters and superclusters. The question is where these initial perturbations came from. Today, their origin is usually explained in terms of a process called 'inflation' originally proposed by Guth [27]. While it is in no way fully understood or experimentally validated it has the appeal of solving several problems of cosmology. We need the concept of the *comoving Hubble radius* $x_H = \frac{c}{aH}$. Due to Hubble's law $v = Hr$ which gives the recession velocity in terms of physical distance r, two points which are at some time separated by $r \geq a\frac{c}{aH}$ recede from each other with $v \geq c$ and are thus out of causal contact at that point in time. The time evolution of this radius is governed by

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{c}{aH} = \frac{\mathrm{d}}{\mathrm{d}t}\frac{c}{\dot{a}} = -\frac{c\ddot{a}}{(aH)^2}\,. \tag{6.9}$$

According to the second of Friedmann's equations (6.2), a universe dominated by either matter or radiation will have negative acceleration and thus a growing comoving Hubble radius. The reasoning is now as follows:

- Observations of the CMB have shown it to be homogeneous and isotropic to a remarkable degree, i. e. the temperature of its radiation is nearly the same in each direction. However, when we observe it we are looking at patches of the universe with a comoving separation Δx that only entered the comoving Hubble horizon after the release of the CMB, i. e. $\Delta x < x_H$ at some time $t_{\text{enter}} > t_{\text{CMB}}$. If our universe is dominated by matter and radiation up to now, the comoving Hubble radius was always growing and in consequence $\Delta x > x_H$ for all times $t < t_{\text{enter}}$. This means that these patches were never in causal contact before the release of the CMB and could thus not interact in order to establish thermal equilibrium. This is already the case for angular separation scales $> 2°$.

- This problem is solved by assuming that very early in the history of the universe (approximately from 10^{-36}s to 10^{-33}s after the Big Bang) there was a short epoch of rapid exponential expansion with $\ddot{a} > 0$ called *inflation*. During this period, x_H will shrink according to (6.9) and thus patches of the universe that were in causal contact before inflation and could equilibrate are now moved outside of their relative comoving Hubble radius. After inflation ends, x_H begins to grow again and these patches of the universe will come into causal contact again already in a state of thermal equilibrium.

- Friedmann's second equation in (6.2) tells us that in order to drive inflation we need some dominating contribution to the energy content of the universe which has negative pressure below $p < -\rho c^2/3$. A very simple model would be

a scalar 'inflaton field' ϕ that is slowly settling into the minimum of its potential, i. e. its kinetic energy is much smaller than its potential energy as $\dot{\phi}^2 \ll V(\phi)$ during inflation.

- As a quantum field-theoretical object this inflaton field will undergo spatially extended quantum fluctuations with some comoving length scale ℓ. During inflation the comoving Hubble radius will shrink fast enough to $x_H < \ell$. Since they now lack causal contact the microscopic fluctuations are 'frozen in' and inflated to macroscopic proportions. Inflation ends once the field enters a phase where its energy is mostly stored in form of kinetic energy $\dot{\phi}^2$ and its equation of state approaches $p = \rho c^2$. Through some poorly understood coupling this energy then decays into the 'ordinary' constituents of the standard model of particle physics. Since most of the energy is believed to decay into photons, this process is also called *reheating* and starts the radiation dominated phase of the universe. Through this coupling the inflated quantum fluctuations are imprinted onto the distribution of the ordinary energy density.

- Since the resulting perturbations of the matter distribution are a superposition of many statistically independent fluctuations of the inflaton field, they should be Gaussian according to the central limit theorem. The latest measurements of the CMB by the Planck satellite [49] have confirmed the presence of tiny fluctuations in the temperature, with no indication of deviations from Gaussianity. Before the release of the CMB, matter and density were strongly coupled and one thus interprets these as echoes of small fluctuations in the matter density which are then identified with those coming from the inflaton field. In this way quantum fluctuations become the seeds for the formation of structure in the universe.

6.1.3 *Structure formation as a random process and the Newtonian approximation*

A fully deterministic description of how the matter distribution in the universe has evolved into its present state would require the exact knowledge of its initial configuration. Acquiring this information is impossible due to the enormous and supposedly infinite extension of the universe as well as the fact that due to the finite speed of light we will only ever be able to observe a fraction of the whole universe, let alone the actual limitations due to available technology and manpower. Instead of trying to model a deterministic system one thus turns to a statistical description. Observations clearly have shown matter to be distributed in a strongly clustered or 'clumped' way, but once these observations are averaged over large enough scales one indeed finds a homogeneous and isotropic distribution which is the basis for the FLRW world model. This has led to a system of assumptions which is sometimes collectively called the *Fair Sample Hypothesis* (cf. Peebles [44], Bernardeau et al. [13]).

- The matter distribution in the universe is a single realisation of a very complex random process. However, the fictitious random density field from which our universe was drawn is statistically homogeneous and isotropic as well as *ergodic*.

This means that any multi-point probability distribution defining the random field can be discerned from a single realisation. Thus, averages over the fictitious ensemble of field realisations can be exchanged for volume averages inside the single realisation we have at our disposal.

- Sufficiently separated patches of the universe can be seen as statistically independent realisations of this physical process.
- Our observable universe is a fair sample of the entire universe in the sense that it is large enough to contain many such independent sample patches. These can be taken to represent a statistical ensemble with which we can test the assumption of homogeneity and ergodicity, i. e. the statistics obtained from observations of different well-separated regions in the sky can themselves be checked for their statistical fluctuations.

One must make sure not to mix up the various levels of statistics involved when we apply SFTCP to this problem.

- The *dynamics* of the 'macroscopic' combined density-momentum field in a single patch of the universe are described by doing infinitely many Poisson samplings of the initial field into collections of tracer particles as shown in section 3.1. These particles are then transported forward through time with the help of their Hamiltonian equations of motion and the desired macroscopic information is reconstructed from the final phase-space configuration of the particles. The average over this ensemble of Poisson samplings, represented by all blocks with the same index j in the lower level of Fig. 3, then gives the evolution of the density-momentum field which at the 'macroscopic' scale looks deterministic.
- In the light of cosmological structure formation we however have to consider this macroscopic field in the patch itself as a random object. In order to describe its *statistics* we thus need to average over all of its possible inital configurations with some multi-point probability density $\mathcal{P}(\mathbf{d})$ as described in section 3.2. This corresponds to averaging over the ensemble of circles in the mid level of Fig. 3. It is this second averaging that imprints the initial correlations onto the density field.
- The correlation functions we obtain from our theoretical description of one patch are then nominally subject to their own statistics. This would correspond to introducing yet another level on top of Fig. 3, leading to an ensemble of the probability distributions $\mathcal{P}(\mathbf{d})$ for the initial random field represented by the ellipses. Under the assumption that the patches are uncorrelated we can however understand our theory to use a mean $\langle\mathcal{P}\rangle$, i. e. the probability distribution is already assumed to be the average over the ensemble of independent patches.

The theory of inflation implies that the initial density field should be a statistically homogeneous and isotropic Gaussian random field. As discussed in section 3.2.1, it is thus completely defined by its two-point correlation function $\xi(\Delta q)$ or its Fourier space counterpart, the power spectrum P_δ. We will soon see why also the momentum

field must then be assumed to be Gaussian and why P_δ is sufficient to describe the combined density-momentum field.

With the relation between the statistics of SFTCP and those of the cosmological density field established we still have to think about the actual particle dynamics. A rigorous discussion of how the fluctuations evolve after the end of inflation would need to employ the dynamical equations of general relativity, i. e. Einstein's field equations, which is a very hard task. However, if we consider a region of space where observers or objects move with non-relativistic relative velocities $\ll c$ and the metric perturbations are small enough in the sense that the gravitational potential fullfills $\Phi \ll c^2$ (cf. Peebles [44]), then the common assumption is that at least in the confines of the ΛCDM-model using Newtonian gravity is a good approximation (cf. Adamek et al. [1]). Let L be the size of that region with a mean density ρ and thus mass $M \approx \rho L^3$. The second of the above conditions then is

$$\Phi \approx \frac{GM}{L} = G\rho L^2 \ll c^2 \tag{6.10}$$

and according to Friedmann's first equation we have roughly $H \approx (G\rho)^{\frac{1}{2}}$ for a flat universe so that we find

$$L^2 \ll \frac{c^2}{H^2} \quad \Rightarrow \quad L \ll \frac{c}{H} \approx 3{-}4\,\mathrm{Gpc}\,. \tag{6.11}$$

If we combine this with Hubble's law $v = Hr$ and set $r = L$ we automatically get $v \ll c$. So for structures with extent smaller than the Hubble radius a Newtonian description is admissable. Since the typical correlation length for galaxy clusters, the largest gravitationally bound structures known today, found in the Sloan Digital Sky Survey is roughly somewhere between $10\,\mathrm{Mpc}/h$ and $20\,\mathrm{Mpc}/h$ (cf. Basilakos and Plionis [10]) we will adopt this approximation for the rest of this work.

6.2 STANDARD PERTURBATION THEORY

6.2.1 *Fluid description and single stream approximation*

The next step is to decide which theoretical tool is used to implement Newtonian dynamics and in SPT one chooses the hydrodynamic limit of kinetic theory. We again stress that while this is a statistical theory, one must be aware that these statistics are the theoretical tool used to describe the dynamics of macroscopic observables like the density and velocity field of some mass distribution in terms of the dynamics of a collection of particles representing this mass distribution. The statistics of the macroscopic observables must be introduced by averaging over their initial conditions. The formal starting point is the Boltzmann equation[5] which reads

$$\frac{\partial f(\vec{r},\vec{p},t)}{\partial t} + \dot{\vec{r}}\cdot\nabla_r f(\vec{r},\vec{p},t) + \dot{\vec{p}}\cdot\nabla_p f(\vec{r},\vec{p},t) = \mathcal{C}[f]\,. \tag{6.12}$$

5 If one wants to describe only dark matter, the collisionless Boltzmann equation, sometimes also called the Vlasov equation, without the the collision term $\mathcal{C}[f]$ may be used.

The hydrodynamical equations describing the macroscopic observables of a fluid are then derived by taking the momentum moments of this equation averaged over some intermediate length $\ell_{\text{micro}} \ll \ell_{\text{int}} \ll \ell_{\text{macro}}$ which is much larger than the microscopic scale where we would see the particle nature of the matter content and much smaller than the macroscopic scales of interest. If we can establish such a hierarchy, it is assumed that the collision terms $\mathcal{C}[f]$ drop out if we take moments of particle number, momentum and energy, which are assumed to be collisional invariants due to the huge number of collisions included. Since the one-particle distribution function is defined as the number

$$\mathrm{d}N = f(\vec{r},\vec{p},t)\,\mathrm{d}\vec{r}\,\mathrm{d}\vec{p} \tag{6.13}$$

of particles in the phase space cell around $\vec{r},\vec{p}$ we define the number density and the velocity field by

$$\begin{aligned} n(\vec{r},t) &= \int \mathrm{d}\vec{p} \int \mathrm{d}\vec{r}\,' \, W_{\ell_{\text{int}}}(\vec{r}-\vec{r}\,')f(\vec{r}\,',\vec{p},t) \\ \vec{v}(\vec{r},t) &= (n(\vec{r},t))^{-1} \int \mathrm{d}\vec{p} \int \mathrm{d}\vec{r}\,' \, W_{\ell_{\text{int}}}(\vec{r}-\vec{r}\,')\,\dot{\vec{r}}\, f(\vec{r}\,',\vec{p},t)\ , \end{aligned} \tag{6.14}$$

where $W_{\ell_{\text{int}}}$ is some window function of length ℓ_{int}. We then assume that the many different particle species which make up the cosmic fluid are strongly coupled to each other by their gravitational interaction. The cosmic fluid can then effectively be described as a single component fluid with some mean particle mass $\bar{m}_{\text{fluid}}$. During the matter dominated epoch, dark matter is much more abundant than baryonic matter and if dark matter is constituted of only one type of particle this should be reasonable. With this mean particle mass we define the mass density field $\rho_{\text{m}}(\vec{r},t) = \bar{m}_{\text{fluid}}\, n(\vec{r},t)$. After taking the zero and first order momentum moments of (6.12) we then arrive at the continuity and Euler's equation

$$\begin{aligned} &\partial_t\, \rho_{\text{m}}(\vec{r},t) + \nabla_r \left(\rho_{\text{m}}(\vec{r},t)\, \vec{v}(\vec{r},t)\right) = 0 \\ &\partial_t\, \vec{v}(\vec{r},t) + \left(\vec{v}(\vec{r},t)\cdot\nabla_r\right)\vec{v}(\vec{r},t) + \nabla_r \Phi(\vec{r},t) + \frac{\nabla_{r_j}\left(\rho_{\text{m}}(\vec{r},t)\left\langle \Delta v^i \Delta v^j \right\rangle\right)\vec{e}_i}{\rho_{\text{m}}(\vec{r},t)} = 0\ . \end{aligned} \tag{6.15}$$

The gravitational interaction of the particles has been expressed through an external force given by the gradient of the gravitational potential which is linked to this system of equations by Poisson's equation

$$\nabla_r^2 \Phi(\vec{r},t) = 4\pi G\, \rho_{\text{m}}(\vec{r},t) - \Lambda\ . \tag{6.16}$$

We also have introduced the random velocity components Δv^i of particles on top of the macroscopic velocity field $\vec{v}(\vec{r},t)$ and the *stress-energy tensor* $\epsilon^{ij} := \left\langle \Delta v^i \Delta v^j \right\rangle$. The latter thus characterizes how the macroscopic flow changes due to the motion of individual particles deviating from the 'single stream' defined by $\vec{v}$. In the next step we assume that the evolution of the cosmological background described by the FLRW-model is independent from the evolution of the perturbations on the scales of interest smaller than the Hubble radius. We can thus substract the evolution of

pure background quantities from the set of equations (6.15) and (6.16). For this we transform to *comoving coordinates* $\vec{q}$ defined by $\vec{r} = a(t)\,\vec{q}$. Since the velocity field $\vec{v}(\vec{r},t)$ gives the instantaneous change of position of a fluid element at $\vec{r}$ it must transform as

$$\vec{v}(\vec{r},t) = \partial_t \vec{r} = \partial_t\,(a\,\vec{q}) = \dot{a}\,\vec{q} + a\,\dot{\vec{q}} = H\,\vec{r} + a\,\dot{\vec{q}} = \vec{v}_{\mathrm{Hubble}}(\vec{q},t) + a\,\vec{v}_{\mathrm{pec}}(\vec{q},t)\ , \tag{6.17}$$

where we identified the Hubble flow and the *peculiar comoving velocity field* $\vec{v}_{\mathrm{pec}}$. We further use that due to homogeneity the mass density field can be split into a spatially constant mean density $\bar{\rho}_{\mathrm{m}}(t)$ and a density contrast as

$$\rho_{\mathrm{m}}(\vec{q},t) = \bar{\rho}_{\mathrm{m}}(t)\,(1+\delta(\vec{q},t)) \tag{6.18}$$

and identify $\bar{\rho}_{\mathrm{m}}$ with the homogeneous density field of the background cosmology. Last, we also split the gravitational potential as $\Phi = \Phi_0 + \varphi$ such that Φ_0 is the gravitational potential pertaining to the background. We will see in the next chapter that if we choose $\Phi_0 = -\frac{1}{2}a\ddot{a}\vec{q}^{\,2}$ the perturbation potential φ is only sourced by the density contrast. We insert these relations into (6.15), and then set the perturbations to zero as $\delta = 0$ and $\vec{v}_{\mathrm{pec}} = 0$. The resultant background evolution equations can now be substracted from the full equations and we arrive at the new set of equations for the perturbations

$$\begin{aligned}
&\partial_t\delta + \nabla_q\left((1+\delta)\,\vec{v}_{\mathrm{pec}}\right) = 0\ ,\\
&\partial_t\vec{v}_{\mathrm{pec}} + 2H\vec{v}_{\mathrm{pec}} + \left(\vec{v}_{\mathrm{pec}}\cdot\nabla_q\right)\vec{v}_{\mathrm{pec}} + \nabla_q\frac{\varphi}{a^2} + \frac{\nabla_{q_j}\left(\delta\,\epsilon^{ij}\vec{e}_i\right)}{1+\delta} = 0\ ,\\
&\nabla_q^2\frac{\varphi}{a^2} = \frac{3}{2}\Omega_{\mathrm{m}}H^2\delta\ .
\end{aligned} \tag{6.19}$$

In order to close the system of equations we need an ansatz for the stress-energy tensor ϵ^{ij}. If we wanted to treat this term exactly, we would need the information contained in the two-particle phase-space correlation function $f^{(2)}$, or under the approximation $f^{(2)} \approx f^{(1)}f^{(1)}$, in the one-particle version $f^{(1)}$. Standard considerations of fluid dynamics lead to a tensor containing a pressure term and viscosity terms written in terms of $\vec{v}_{\mathrm{pec}}$ (cf. Bernardeau et al. [13]).

Note that with this ansatz we assumed that the macroscopic motion of matter can at all times t be completely described at every point $\vec{q}$ by the 'single stream' $\vec{v}_{\mathrm{pec}}(\vec{q},t)$ which has an unambigious value. This means that at no time will macroscopic streams of matter cross each other. This is sometimes called the single-stream approximation (SSA). It will break down in the non-linear regime of $\delta \gg 1$ where matter coalesces into structures where virilisation and thus crossing of streams can take place. Since these structures will grow in size over time, the SSA will successively break down on larger and larger scales.

Another problem is the inverse density contrast multiplying the stress-energy tensor gradient. A formal expansion into a geometric series would add non-linear terms of arbitrary order in the density contrast. Any finite truncation of this series will also necessarily loose its validity in the non-linear regime of $\delta \gg 1$.

To circumvent the mathematical problems posed by the stress-energy tensor term, one usually assumes that CDM at least at the beginning of structure formation does

not have significant random velocities on top of its macroscopic flow, i. e. its initial velocity dispersion is low enough such that CDM particles do not move over large distances compared to the scales of interest before they start moving with the macroscopic flow $\vec{v}_{\rm pec}$. It is then a sensible approximation to set $\epsilon^{ij} \approx 0$, which solves both problems of hierarchy closure and the inverse δ. Note that one still operates under the SSA since velocities are only described by the single macroscopic flow $\vec{v}_{\rm pec}$. Since the virilisation of matter will lead to the creation of velocity dispersion this approximation will break down in the non-linear regime just like the SSA.

6.2.2 *The linear regime of SPT*

In the early stages of structure formation the perturbations around the background are assumed to be small in the sense of $\delta \ll 1$ and $|\vec{v}_{\rm pec}| \ll 1$. One may thus linearise the evolution equations (6.19) down to

$$\begin{aligned} &\partial_t \delta + \nabla_q \cdot \vec{v}_{\rm pec} = 0 \,, \\ &\partial_t \vec{v}_{\rm pec} + 2H\vec{v}_{\rm pec} + \nabla_q \frac{\varphi}{a^2} = 0 \,. \end{aligned} \tag{6.20}$$

In this limit we can give an analytical solution for the density contrast. For this purpose we take another time derivative of the continuity equation, insert Euler's equation and then use Poisson's equation to find

$$\ddot{\delta} + 2H\dot{\delta} = \frac{3}{2}\Omega_m H^2 \delta \quad \text{where} \quad \dot{} = \frac{\partial}{\partial t} \,. \tag{6.21}$$

Transforming this equation into Fourier space we see that each mode evolves independently as $\delta^{\rm lin}(\vec{k}, t) = D(t)\, \delta(\vec{k}, t_{\rm i})$ and with the same time behaviour given by the function $D(t)$ which is defined by the differential equation

$$\ddot{D} + 2H\dot{D} = \frac{3}{2}\Omega_m H^2 D \,. \tag{6.22}$$

The function $D(t)$ is called the *linear growth factor*. Since it follows a second order ordinary differential equation it has two solutions. In a simple Einstein de-Sitter (EdS) universe where $\Omega_{\rm m} = 1$ and $\Omega_\Lambda = 0$ at all times one finds the solutions $D(t) = (a(t)/a(t_{\rm i}))^n$ with $n = 1, -3/2$, i. e. one growing and one decaying solution. For all further purposes we only consider the growing solutions. In the general case of a flat ΛCDM universe we have to solve (6.22) numerically. For cosmologies where the dark energy density Ω_Λ is solely supplied by a cosmological constant, there however exists the excellent approximation formula

$$D(a) = \frac{5}{2}\, a\, \Omega_{\rm m}(a) \left(\Omega_{\rm m}(a)^{4/7} - \Omega_\Lambda(a) + \left(1 + \frac{\Omega_m(a)}{2}\right)\left(1 + \frac{\Omega_\Lambda(a)}{70}\right)\right)^{-1} \,, \tag{6.23}$$

which can be found in Bernardeau et al. [13]. The linear solution has been shown to accurately describe structure formation on large enough scales (depending on the cosmological epoch) by both observations and N-body simulations.

The linear equations (6.20) also allow the justification of another common approximation of SPT, which is that one assumes the velocity field to be irrotational, i. e. it has no vorticity $\nabla_q \times \vec{v}_{\text{pec}} = 0$. Taking the curl of the linearized version of Euler's equations one directly sees that if there is any initial vortitcity, it will be washed out by the cosmological expansion with $\propto a^{-1}$. Since the early evolution of structure is well described by the linear equations it is thus justified to assume that there is no initial vorticity if one places the initial time such that enough time has passed for it to be drained away. Furthermore, if there is no initial vorticity and one assumes $\epsilon^{ij} = 0$, vorticity cannot be produced by the dynamics [13]. However, for $\epsilon^{ij} \neq 0$ terms in Euler's equation can produce vorticity in the non-linear regime of $\delta \gg 1$ which further restricts the validity of SPT on small scales.

We now define the logarithmic derivative of the growth factor as

$$f := \frac{\mathrm{d}\ln D}{\mathrm{d}\ln a} = \frac{1}{D\frac{\dot{a}}{a}}\frac{\mathrm{d}D}{\mathrm{d}t} = \frac{\dot{D}}{HD} \quad \Rightarrow \quad Hf = \frac{\dot{D}}{D}\,. \tag{6.24}$$

We define a new time coordinate and see that the relation between its derivative and that w. r. t. to the cosmological time is given by

$$\tau := \ln D(t) \quad \Rightarrow \quad \mathrm{d}\tau = \mathrm{d}\ln D(t) = \frac{\mathrm{d}\ln D(t)}{\mathrm{d}t}\mathrm{d}t = \frac{\dot{D}}{D}\mathrm{d}t = Hf\,\mathrm{d}t\,. \tag{6.25}$$

We redefine our velocity field with respect to this new time coordinate

$$\vec{u}_{\text{pec}} := \frac{\mathrm{d}\vec{q}}{\mathrm{d}\tau} = \frac{1}{Hf}\frac{\mathrm{d}\vec{q}}{\mathrm{d}t} = \frac{1}{Hf}\vec{v}_{\text{pec}}\,. \tag{6.26}$$

We now return to the linearised continuity equation and use both the above relations and the linear solution for the density contrast to find

$$\begin{aligned} \partial_t\left(D(t)\,\delta(\vec{q},t_{\text{i}})\right) + Hf\,\nabla_q\cdot\vec{u}_{\text{pec}}(\vec{q},t) &= 0 \\ \dot{D}(t)\,\delta(\vec{q},t_{\text{i}}) + \frac{\dot{D}}{D}\,\nabla_q\cdot\vec{u}_{\text{pec}}(\vec{q},t) &= 0 \\ D(t)\,\delta(\vec{q},t_{\text{i}}) + \nabla_q\cdot\vec{u}_{\text{pec}}(\vec{q},t) &= 0\,. \end{aligned} \tag{6.27}$$

Under our assumption that the initial velocity field is irrotational we can write it as the gradient $\vec{u}_{\text{pec}}(\vec{q},t_{\text{i}}) = \nabla_q\psi(\vec{q})$ of some velocity potential. If we then normalise our growth factor such that $D(t_{\text{i}}) = 1$ we find

$$\delta(\vec{q},t_{\text{i}}) = -\nabla_q^2\psi(\vec{q})\,. \tag{6.28}$$

In the next chapter we will define the momentum variable of our field theory approach such that it coincides with the definition (6.26) of the velocity field. We already argued why the initial density perturbations are assumed to be a Gaussian random field. Due to the linearity of the Fourier transform, every derivative and integral of Gaussian random field is again such field (cf. Bardeen et al. [2]). The above equation (6.28) establishes such a relation between the initial density field and the initial velocity potential and in consequence justifies setting up the initial correlations of the combined density-momentum field as described in section 4.2.5.

6.2.3 *Path integral formulation of SPT*

If we knew to full solution $\delta(\vec{k},t)$ to the system of equations (6.19) we could use it to calculate the evolution of the initial power spectrum P_δ up to the present day. The simplest approximation to this is to use the solution to the linearised set of equations (6.20) which leads to the *linear* power spectrum

$$\begin{aligned}\left\langle \delta(\vec{k}_1,t_1)\delta(\vec{k}_2,t_2)\right\rangle &\approx \left\langle \delta^{\mathrm{lin}}(\vec{k}_1,t_1)\,\delta^{\mathrm{lin}}(\vec{k}_2,t_2)\right\rangle \\ &= (2\pi)^3\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\,D(t_1)\,D(t_2)\,P_\delta(k_1)\;. \end{aligned} \tag{6.29}$$

The principal idea of SPT is to expand the full solution as a power series in the linear solution. From the above equation we directly see that this will lead to an expansion of the 'full' power spectrum in powers of the linear and thus the initial power spectrum P_δ. This can be put into the same path integral based MSR framework as SFTCP as shown in Matarrese and Pietroni [37]. For this purpose we adopt $\epsilon^{ij}=0$, transform the set of five equations (6.19) to the time coordinate τ and consider only the divergence $\theta := \nabla\cdot\vec{u}_{\mathrm{pec}}$ of the velocity field, since we assume that it is vorticity-free as discussed above. Taking the divergence of Euler's equation and inserting Poisson's equation we reduce to two equations which we then transform into Fourier space. We define the field vector

$$\Psi(\vec{k},t) = \begin{pmatrix} \delta(\vec{k},t) \\ -\theta(\vec{k},t) \end{pmatrix} \tag{6.30}$$

and may then write the evolution equations in the compact form

$$(\delta_{ab}\partial_\tau + \omega_{ab})\,\Psi_b(\vec{k},\tau) = \int \frac{\mathrm{d}\vec{k}_1}{(2\pi)^3}\int \frac{\mathrm{d}\vec{k}_2}{(2\pi)^3}\,\lambda_{abc}(\vec{k},-\vec{k}_1,-\vec{k}_2)\Psi_b(\vec{k}_2,\tau)\Psi_c(\vec{k}_3,\tau)\;. \tag{6.31}$$

The linear evolution is encoded in the matrix

$$\omega_{ab} = \begin{pmatrix} 0 & -1 \\ -3/2 & 1/2 \end{pmatrix} \tag{6.32}$$

and the vertex tensor has three non-zero entries

$$\begin{aligned}\lambda_{112}(\vec{k},\vec{k}_1,\vec{k}_2) &= \lambda_{121}(\vec{k},\vec{k}_2,\vec{k}_1) = (2\pi)^3\,\delta_{\mathrm{D}}(\vec{k}+\vec{k}_1+\vec{k}_2)\,\frac{1}{2}\,\frac{\left(\vec{k}_1+\vec{k}_2\right)\cdot\vec{k}_2}{k_2^2} \\ \lambda_{222}(\vec{k},\vec{k}_1,\vec{k}_2) &= (2\pi)^3\,\delta_{\mathrm{D}}(\vec{k}+\vec{k}_1+\vec{k}_2)\,\frac{\left(\vec{k}_1+\vec{k}_2\right)^2\left(\vec{k}_1\cdot\vec{k}_2\right)}{k_1^2k_2^2}\;. \end{aligned} \tag{6.33}$$

Observe that the linear part of this equation contains the full gravitational interaction of the fluid encoded by the Poisson equation. The non-linear vertex terms describe

kinematic effects. The linear solution to this system is given in terms of the Green's function or linear propagator

$$\begin{aligned} g_{ab}(1,2) &= (2\pi)^3\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\,\Theta(\tau_1-\tau_2) \\ &\quad \left(\frac{\mathrm{e}^{\tau_1-\tau_2}}{5}\begin{pmatrix} 3 & 2 \\ 3 & 2 \end{pmatrix} + \frac{\mathrm{e}^{-\frac{3}{2}(\tau_1-\tau_2)}}{5}\begin{pmatrix} 2 & -2 \\ -3 & 3 \end{pmatrix}\right) \\ &= (2\pi)^3\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\,g_{ab}(\tau_1,\tau_2)\,. \end{aligned} \tag{6.34}$$

In complete analogy to SFTCP one can then define a generating functional for correlation functions of the field $\Psi_a(\vec{k},t)$ by introducing an auxiliary field $\chi_a(\vec{k},t)$ and with the equation of motion (6.31) abbreviated as $\mathcal{E}_a(\vec{k}_1,\tau_1)$ writing

$$\begin{aligned} Z[J,K] = \int \mathcal{D}\Psi_a \int \mathcal{D}\chi_a \exp\left\{-\frac{1}{2}\int \mathrm{d}1 \int \mathrm{d}2\,\Psi_a(1)\,C^{-1}_{ab}(1,2)\,\Psi_b(2)\right\} \\ \exp\left\{\mathrm{i}\left(\int \mathrm{d}1 \int \mathrm{d}2\,\chi_a(1)\,\mathcal{E}_a(1) + J_a(1)\,\Psi_a(1) + K_a(1)\,\chi_a(1)\right)\right\} \end{aligned} \tag{6.35}$$

where J,K are the usual source terms and $C^{-1}_{ab}(1,2)$ the inverse initial covariance matrix of the field Ψ_a. Writing the interaction part in terms of functional derivatives one can then solve the path integrals in the free generating functional to find

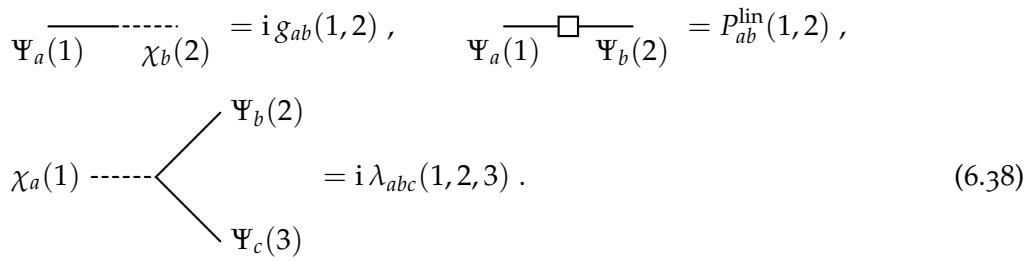
$$\begin{aligned} Z[J,K] = \exp\left\{\mathrm{i}\int \mathrm{d}1 \int \mathrm{d}2 \int \mathrm{d}3\,\frac{\delta}{\mathrm{i}\delta K_a(1)}\,\lambda_{abc}(1,-2,-3)\,\frac{\delta}{\mathrm{i}\delta J_b(2)}\,\frac{\delta}{\mathrm{i}\delta J_c(3)}\right\} \\ \exp\left\{-\int \mathrm{d}1 \int \mathrm{d}2\,\left(\frac{1}{2}J_a(1)\,P^{\mathrm{lin}}_{ab}(1,2)\,J_b(2) + \mathrm{i}\,J_a(1)\,g_{ab}(1,2)\,K_b(2)\right)\right\} \end{aligned} \tag{6.36}$$

where we defined the linear powerspectrum

$$\begin{aligned} P^{\mathrm{lin}}_{ab}(1,2) &= \int \mathrm{d}3 \int \mathrm{d}4\,g_{ac}(1,3)\,g_{bd}(2,4)\,(2\pi)^3\,\delta_{\mathrm{D}}(\vec{k}_3+\vec{k}_4) \\ &\quad \delta_{\mathrm{D}}(\tau_3-\tau_{\mathrm{i}})\,\delta_{\mathrm{D}}(\tau_4-\tau_{\mathrm{i}})\,P_\delta(k_3)\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \\ &= (2\pi)^3\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\,g_{ac}(\tau_1,\tau_{\mathrm{i}})\,g_{bd}(\tau_2,\tau_{\mathrm{i}})\,P_\delta(k_1)\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \\ &= (2\pi)^3\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\,\mathrm{e}^{\tau_1-\tau_{\mathrm{i}}}\,\mathrm{e}^{\tau_2-\tau_{\mathrm{i}}}\,P_\delta(k_1)\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \end{aligned} \tag{6.37}$$

where the form of the matrix follows from (6.28). Expanding both exponentials in (6.36) then leads to a perturbation expansion of the same form as in standard QFT.

When expressed in terms of Feynman diagrams any term is build from three basic 'tree-level' diagrams which are



(6.38)

Having a diagram language for SPT will make it easier to compare it against SFTCP later.

6.2.4 *Advantages of SFTCP over SPT*

As we saw in the last sections, setting up a generating functional for SPT can in principle be done with muss less effort when compared with SFTCP. This however comes at the price of some serious drawbacks. In section 2.6 we already elaborated on the loss of phase-space information one has to take when using the BBGKY hierarchy truncated at any finite level. We again stress that the problem is the unfortunate choice of variables for which one attempts to solve an evolution equation. We thus expect that at comparable levels in perturbation theory SFTCP will be able to include more effects of the underlying particle dynamics than SPT. This will become obvious once we solved the first order perturbation theory for both the field propagator $G_{\rho B}$ and the power spectrum $G_{\rho\rho}$. Throughout the derivation of the generating functional (6.35) numerous approximations had to be made.

- First we had to assume that one can establish a scale hierarchy that allowed the use of the fluid approximation. Considering the scales of interest in LSS formation this is not really a problem, but we still like to point out that this particular scale hierarchy is not needed in SFTCP since we directly work in terms of the particle dynamics.

- In terms of the BBGKY hierarchy the SSA can be seen as a truncation at the one-point level. We argued that in physical terms one can understand it as the assumption that streams in the matter fluid do not cross each other. Since this is expected to happen once structure formation enters the non-linear regime, the validity of SPT on small scales at late times is severely limited. With SFTCP using the phase-space trajectories of individual particles as the basic dynamic quantities it can describe the crossing of streams without the need for approximations to the dynamical equations of motion and should thus be valid over a much wider range of scales.

- In order to have a simple set of equations of motion, SPT assumes that the velocity or momentum field is irrotational throughout its entire evolution and this is only consistent with the equations of motion under the assumption $\epsilon^{ij} = 0$.

No such assumption is made in SFTCP and by including the momentum field as a collective field into the description the statistics of both its divergence and vorticity should be accessible. We only adopted the assumption of vanishing initial vorticity in order to make writing down explicit expressions for the initial density-momentum and momentum correlations easier. While this approximation is well founded, it is in no way necessary and could be given up if one is willing to introduce additional powerspectra for the initial correlations.

Regarding perturbation theory we like to point out that using the density contrast δ as an expansion parameter is actually a bad choice. This is immediately clear once we consider that one aims at evolving the system into the non-linear regime where $\delta \gg 1$ at the late stages of structure formation. Any non-resummed form of perturbation theory to a finite order must thus necessarily break down at those scales which have had enough time to evolve into the non-linear regime. On the other hand, SFTCP can describe large density contrasts even with small perturbations of its fundamental quantities which are the phase-space trajectories of particles. We illustrate this in Fig. 6.

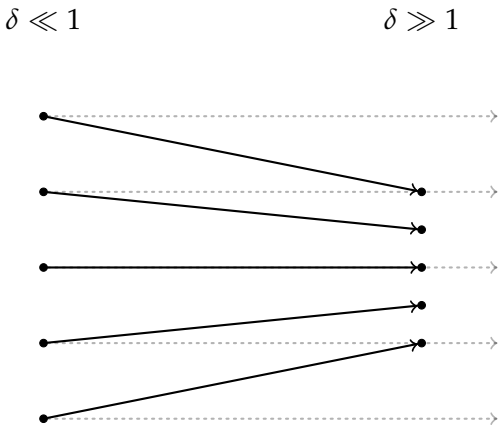


Figure 6: Schematic illustration of large density contrasts from small perturbations of particle trajectories. The dotted lines are the unperturbed free trajectories of the particles starting from a spatial configuration which corresponds to a small density contrast. The solid lines are the slightly perturbed trajectories due gravitational interaction which nonetheless lead to a large density contrast given enough time has passed.

Another problem of the naive version of SPT shown in section 6.2.3 is that individual loop-terms in the perturbative expansion of cumulants can exhibit both UV and IR divergences for certain forms of the initial power spectrum P_δ. It was shown that IR divergences should be canceled out by combining contributions from different terms (cf. Bernardeau et al. [13]). Whether similar effects are present in SFTCP is unclear at the moment and will be investigated in future work.

For regularizing the UV divergences in the case of general initial spectra various methods have been investigated. One prominent example is the variant of SPT called Resummed Perturbation Theory which was pioneered in Crocce and Scoccimarro [20, 21]. It leads to a resummed field propagator with a Gaussian cutoff very similar to that found for the free cumulants of SFTCP in section 4.2. The derivation is quite in-

volved and requires the by-hand resummation of an infinite sub-class of Feynman diagrams. A shorter derivation using Renormalisation Group techniques can be found in Matarrese and Pietroni [37]. It is yet another advantage of SFTCP that these cutoffs naturally appear already in the non-interacting theory due to the fact that the initial velocity dispersion of particles is correctly included.

Another benefit is that the time dependence of these damping factors is given by the free particle propagators g_{qp}, which must be bounded from above in an expanding spacetime as we will see in the next chapter (also cf. Bartelmann [4]). In contrast, the damping factor in the resummed propagator found in [21, 37] will evolve with the unbounded linear growth factor $D(t)$. They consequently lead to damping on much larger scales for late times which will reduce the generation of non-linear power at comparable levels of perturbation theory.

7

PARTICLE DYNAMICS IN STANDARD COSMOLOGY

Our goal is to set up the scenario that is usually explored in N-body simulations. We have a distribution of CDM mass over some volume V. Its mean mass density $\bar{\rho}_{\mathrm{m}}$ is taken to be the mean mass density of the decoupled background which is the standard flat ΛCDM-model of cosmology in the matter dominated epoch. The mass distribution is then sampled by tracer particles whose mass m and number N can be chosen freely, but under the constraint $\frac{mN}{V} = m\bar{\rho} \stackrel{!}{=} \bar{\rho}_{\mathrm{m}}$. Since the typical correlation length of galaxy clusters at the present day is two to three orders of magnitude smaller than the Hubble radius we can safely use the infinite volume limit of the grand canonical ensemble with fixed $\bar{\rho}$ and still apply the Newtonian approximation for the dynamics. We will derive the equations of motion for the particles starting from a Lagrange function. The general scheme of this calculation was taken from Peebles [44]. We will however adapt it to a different time coordinate which at the end will contain all effects of the background cosmology, making the resulting equations of motion very easy to work with.

7.1 THE HAMILTONIAN EQUATIONS OF MOTIONS

We start with the following standard Lagrange function for the Newtonian dynamics of a particle of mass m in a gravitational field with potential Φ

$$L = \frac{m}{2}\dot{\vec{r}}^2 - m\,\Phi(\vec{r},t)\ . \tag{7.1}$$

We use the dot notation for the total derivative $\frac{\mathrm{d}}{\mathrm{d}t}$ w. r. t. to the cosmological time and describe the position of the particle with physical coordinates $\vec{r}$. The gravitational potential is defined in terms of Poisson's equation (6.16) sourced by the mass density field ρ_{m}. We introduce *comoving coordinates* $\vec{r} = a(t)\,\vec{q}$ where the cosmological scale factor $a(t)$ obeys *Friedmann's equation* in the form

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}\bar{\rho}_{\mathrm{m}}(t) + \frac{\Lambda}{3}\ , \tag{7.2}$$

since for the dominating non-relativistc matter the pressure only gives negligible contributions to the energy density compared to the rest mass energy. The Lagrange function now has the form

$$L = \frac{m}{2}\left(\dot{a}\vec{q} + a\dot{\vec{q}}\right)^2 - m\Phi(\vec{q},t)\ . \tag{7.3}$$

Next we apply a gauge transformation $L \to L - \frac{\mathrm{d}\psi}{\mathrm{d}t}$ which leaves the Euler-Lagrange equations and thus the dynamics invariant. We choose $\psi = \frac{m}{2} a\dot{a}\vec{q}^2$ and find

$$\begin{aligned} L &= \frac{m}{2}\left(\dot{a}^2\vec{q}^2 + 2a\dot{a}\vec{q}\cdot\dot{\vec{q}} + a^2\dot{\vec{q}}^2\right) - \frac{m}{2}\left(\dot{a}^2\vec{q}^2 + a\ddot{a}\vec{q}^2 + 2a\dot{a}\vec{q}\cdot\dot{\vec{q}}\right) - m\Phi(\vec{q},t) \\ &= \frac{m}{2}a^2\dot{\vec{q}}^2 - m\underbrace{\left(\Phi(\vec{q},t) + \frac{1}{2}a\ddot{a}\vec{q}^2\right)}_{:=\varphi(\vec{q},t)} . \end{aligned} \tag{7.4}$$

Poisson's equation for the newly defined potential φ can be obtained from combining (6.16) with (7.2) to find

$$\begin{aligned} \nabla_q^2\,\varphi(\vec{q},t) &= a^2\nabla_r^2\,\Phi(\vec{q},t) + \frac{1}{2}a\ddot{a}\nabla_q^2\,\vec{q}^2 \\ &= 4\pi G\,a^2\rho_\mathrm{m}(\vec{q},t) - a^2\Lambda + 3a\ddot{a} \\ &= 4\pi G\,a^2\rho_\mathrm{m}(\vec{q},t) - a^2\Lambda - 4\pi G\,a^2\bar{\rho}_\mathrm{m}(t) + a^2\Lambda \\ &= \frac{4\pi G}{a}(\rho_\mathrm{m}(\vec{q},t) - \bar{\rho}_\mathrm{m}) , \end{aligned} \tag{7.5}$$

where we used that $\nabla_r = a^{-1}\nabla_q$. In the last line we also changed from densities defined w. r. t. volume elements $\mathrm{d}V_r$ in physical space to densities defined w. r. t. volume elements of comoving space which are related to the former by $\mathrm{d}V_q = a^{-3}\mathrm{d}V_r$. Note that the comoving mean mass density $\bar{\rho}_\mathrm{m}$ is now a constant in both space and time and coincides with the initial physical mean mass density $\bar{\rho}_\mathrm{m}(t_\mathrm{i})$. The above equation shows that in comoving coordinates the force acting on particles is only sourced by the density contrast. We now want to change to the time coordinate $\tau = \ln D(t)$, defined in (6.25). Note that this new time coordinate is dimensionless. The Euler-Lagrange equations are form-invariant under this change of time coordinate if the action S is invariant. We thus have

$$S = \int \mathrm{d}t\, L(\vec{q},\dot{\vec{q}},t) = \int \mathrm{d}\tau \underbrace{\frac{1}{Hf}\,L(\vec{q},\frac{\mathrm{d}\vec{q}}{\mathrm{d}\tau},\tau)}_{\widetilde{L}} . \tag{7.6}$$

Our new Lagrange function is then found to be

$$\widetilde{L} = \frac{1}{Hf}\left(\frac{m}{2}a^2\left(Hf\frac{\mathrm{d}\vec{q}}{\mathrm{d}\tau}\right)^2 - m\varphi(\vec{q},\tau)\right) = \frac{m}{2}a^2Hf\left(\frac{\mathrm{d}\vec{q}}{\mathrm{d}\tau}\right)^2 - \frac{m}{Hf}\varphi(\vec{q},\tau) . \tag{7.7}$$

We now make the standard transition to Hamiltonian mechanics with the help of a Legendre transformation. We first define the canonical momentum

$$\vec{p}_\mathrm{can} = \frac{\partial\widetilde{L}}{\partial\left(\frac{\mathrm{d}\vec{q}}{\mathrm{d}\tau}\right)} = ma^2Hf\frac{\mathrm{d}\vec{q}}{\mathrm{d}\tau} \tag{7.8}$$

and then easily find the Hamiltonian to be given by

$$\mathcal{H} = \vec{p}_\mathrm{can}\cdot\frac{\mathrm{d}\vec{q}}{\mathrm{d}\tau} - \widetilde{L} = \frac{\vec{p}_\mathrm{can}^2}{2ma^2Hf} + \frac{m}{Hf}\varphi(\vec{q},\tau) . \tag{7.9}$$

The resulting Hamiltonian equations of motion are then

$$\begin{aligned}\frac{\mathrm{d}\vec{q}}{\mathrm{d}\tau} &= \frac{\partial\mathcal{H}}{\partial\vec{p}_{\mathrm{can}}} = \frac{1}{ma^2Hf}\,\vec{p}_{\mathrm{can}}\,,\\ \frac{\mathrm{d}\vec{p}_{\mathrm{can}}}{\mathrm{d}\tau} &= -\frac{\partial\mathcal{H}}{\partial\vec{q}} = -\frac{m}{Hf}\nabla_q\varphi(\vec{q},\tau)\,.\end{aligned} \tag{7.10}$$

We now insert these into our field theory. If we normalise the growth factor such that it is $D(t_{\mathrm{i}}) = 1$ at the initial time, we have $\tau_{\mathrm{i}} = \ln D(t_{\mathrm{i}}) = 0$. The field theory action then has the form

$$S = \sum_{j=1}^{N} S_j = \sum_{j=1}^{N}\int_0^{\tau_{\mathrm{f}}}\mathrm{d}\tau\begin{pmatrix}\vec{\chi}_{q_j}(\tau)\\ \vec{\chi}_{p_{\mathrm{can},j}}(\tau)\end{pmatrix}^{\mathrm{T}}\begin{pmatrix}\vec{q}_j'(\tau) - \frac{1}{ma^2Hf}\,\vec{p}_{\mathrm{can},j}(\tau)\\ \vec{p}_{\mathrm{can},j}'(\tau) + \frac{m}{Hf}\nabla_{q_j}\varphi(\vec{q},\tau)\end{pmatrix}. \tag{7.11}$$

We stress again that it is important to use this canonical form of the equations of motion derived from the Hamiltonian to define the action and thus the generating functional of the field theory. Otherwise there might be a non-constant functional determinant one has to take into account (see section 2.3.2).

7.2 THE FREE PARTICLE PROPAGATOR

Before we attempt to use our findings in section 2.5.2 we will try to simplify the equations of motion such that no explicitly time dependent quantities are present besides the phase-space coordinates. We can easily achieve this for the equation of motion for the positions of the particles by defining a new momentum

$$\vec{p}_j = \frac{1}{ma^2Hf}\,\vec{p}_{\mathrm{can},j} = \frac{1}{ma^2Hf}\,ma^2Hf\,\frac{\mathrm{d}\vec{q}_j}{\mathrm{d}\tau} = \frac{1}{Hf}\,\dot{\vec{q}}\,. \tag{7.12}$$

This is a time dependent rescaling of the canonical momentum as well as of the actual peculiar velocity and simply has the dimension of a length. The velocity-momentum relation now has the very simple form $\vec{q}_j' - \vec{p}_j = 0$. The equation of motion for this new momentum is then

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}\tau}(ma^2Hf\vec{p}_j) + \frac{m}{Hf}\nabla_{q_j}\varphi(\vec{q},\tau)\\ &= ma^2Hf\,\frac{\mathrm{d}\vec{q}_j}{\mathrm{d}\tau} + m\frac{\mathrm{d}}{\mathrm{d}\tau}\left(a^2Hf\right)\vec{p}_j + \frac{m}{Hf}\nabla_{q_j}\varphi(\vec{q},\tau)\,.\end{aligned} \tag{7.13}$$

We need to execute the τ-derivative in the second term. Using (6.24), (6.25) and the differential equation (6.22) defining the growth factor we find

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(a^2Hf\right) &= Hf\frac{\mathrm{d}}{\mathrm{d}\tau}a^2 + a^2\frac{\mathrm{d}}{\mathrm{d}\tau}(Hf) = \frac{\mathrm{d}}{\mathrm{d}t}a^2 + a^2\frac{1}{Hf}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\dot{D}}{D}\\ &= 2a\dot{a} + a^2\frac{1}{Hf}\left(\frac{\ddot{D}}{D} - \frac{\dot{D}^2}{D^2}\right)\\ &= 2a^2H + a^2\frac{1}{Hf}\left(\frac{3}{2}\Omega_{\mathrm{m}}H^2 - 2H^2f - H^2f^2\right)\\ &= a^2Hf\left(\frac{3}{2}\frac{\Omega_{\mathrm{m}}}{f^2} - 1\right)\,.\end{aligned} \tag{7.14}$$

The first two terms of the equation of motion (7.13) now have a common prefactor of ma^2Hf. If we redefine the momentum part of the auxiliary field $\vec{\chi}_j$ of every particle as

$$\widetilde{\vec{\chi}}_{p_j}(\tau) \coloneqq ma^2Hf\vec{\chi}_{p_j}(\tau)\,, \tag{7.15}$$

then we can write the action (7.11) in terms of our new quantities as

$$S = \sum_{j=1}^{N}\int_0^{\tau_\mathrm{f}} \mathrm{d}\tau \begin{pmatrix} \vec{\chi}_{q_j}(\tau) \\ \widetilde{\vec{\chi}}_{p_j}(\tau) \end{pmatrix}^\mathrm{T} \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}\tau}\vec{q}_j(\tau) - \vec{p}_j(\tau) \\ \frac{\mathrm{d}}{\mathrm{d}\tau}\vec{p}_j(\tau) + \left(\frac{3}{2}\frac{\Omega_\mathrm{m}}{f^2} - 1\right)\vec{p}_j(\tau) + \frac{1}{a^2H^2f^2}\nabla_{q_j}\varphi(\vec{q},\tau) \end{pmatrix}. \tag{7.16}$$

In terms of the entire generating functional we also need to rescale the corresponding path integral measures as

$$\mathcal{D}\vec{p}_{\mathrm{can},j} = \mathcal{D}\vec{p}_j\,(ma^2Hf) \qquad \text{and} \qquad \mathcal{D}\vec{\chi}_{p_j} = \mathcal{D}\widetilde{\vec{\chi}}_{p_j}\frac{1}{ma^2Hf}\,. \tag{7.17}$$

As we see, these two factors cancel exactly. The single particle sources $\mathbf{J}$ and $\mathbf{K}$ can be chosen freely and may thus be defined directly w. r. t. to the new momentum and and the new auxiliary field. In the following we will drop the tildes and only work with these new quantities.

Regarding the initial conditions we can observe that our new momenta (7.12) at the initial time are precisely those that we obtain from the Poisson sampling process described in section 3.2 if we choose the initial momentum field to be given by the peculiar velocity field of (6.26) at the initial time, i. e. $\vec{\Pi}^{(\mathrm{i})}(\vec{q}) = \vec{u}_\mathrm{pec}(\vec{q},\tau_\mathrm{i})$. We argued in section 6.2.2 why this peculiar velocity field can be assumed to be irrotational and thus we arrive again at the situation shown in (4.46).

We now consider the free theory by neglecting the potential term in the equation of motion for the momentum. The only term preventing us from giving an analytic solution for the free particle propagator is the time dependent factor $\frac{\Omega_\mathrm{m}}{f^2}$. In an EdS universe with $\Omega_\mathrm{m} = 1$ the growth factor is given by $D = a$ and thus $f = 1$ and we do not have a problem. However, it also holds true for the more general flat ΛCDM case with $\Omega_\mathrm{m} + \Omega_\Lambda = 1$, that $\frac{\Omega_\mathrm{m}}{f^2} \approx 1$ throughout the matter dominated phase up to redshift $z = 0$ in very good approximation (cf. Bernardeau et al. [13]). We will thus set this factor to unity throughout our calculations. The action for the free theory then is

$$\begin{aligned} S_0 &= \sum_{j=1}^{N}\int_0^{\tau_\mathrm{f}} \mathrm{d}\tau\,\vec{\chi}_j^\mathrm{T}(\tau)\left[\left(\partial_\tau\mathcal{I}_6 + \begin{pmatrix} 0_3 & -\mathcal{I}_3 \\ 0_3 & \frac{1}{2}\mathcal{I}_3 \end{pmatrix}\right)\vec{x}_j(\tau)\right] \\ &= \sum_{j=1}^{N}\int_0^{\tau_\mathrm{f}} \mathrm{d}\tau\,\vec{\chi}_j^\mathrm{T}(\tau)\left[\left(\partial_\tau\mathcal{I}_6 + \mathcal{K}\right)\vec{x}_j(\tau)\right]\,. \end{aligned} \tag{7.18}$$

In the second step we identified the 'force matrix' $\mathcal{K}$ in analogy to (2.70). Using (2.79) we obtain the free particle propagator

$$\begin{aligned}\mathcal{G}(\tau,\tau') &= \exp\left\{-\int_{\tau'}^{\tau} \mathrm{d}\tau''\,\mathcal{K}\right\} = \exp\left\{-\mathcal{K}(\tau-\tau')\right\} \\ &= \mathcal{I}_6 + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!}\,(\tau-\tau')^n\,\mathcal{K}^n\,. \end{aligned} \tag{7.19}$$

It is straightforward to show that

$$\mathcal{K}^2 = \begin{pmatrix} 0_3 & -2^{-1}\,\mathcal{I}_3 \\ 0_3 & 2^{-2}\,\mathcal{I}_3 \end{pmatrix} \quad \underset{\text{induction}}{\Longrightarrow} \quad \mathcal{K}^n = \begin{pmatrix} 0_3 & -2^{-(n-1)}\,\mathcal{I}_3 \\ 0_3 & 2^{-n}\,\mathcal{I}_3 \end{pmatrix}\,. \tag{7.20}$$

The qp submatrix of $\mathcal{G}$ is then given by

$$\begin{aligned}\mathrm{g}_{qp}(\tau,\tau') &= \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{2^{n-1}n!}\,(\tau-\tau')^n = 2 - 2\sum_{n=0}^{\infty} \frac{(-1)^n}{2^n n!}\,(\tau-\tau')^n \\ &= 2\left(1-\mathrm{e}^{-\frac{1}{2}(\tau-\tau')}\right) \end{aligned} \tag{7.21}$$

and the pp submatrix by

$$\mathrm{g}_{pp}(\tau,\tau') = \sum_{n=1}^{\infty} \frac{(-1)^n}{2^n n!}\,(\tau-\tau')^n = \mathrm{e}^{-\frac{1}{2}(\tau-\tau')}\,. \tag{7.22}$$

The complete propagator then is given by

$$\begin{aligned}\mathcal{G}(\tau,\tau') &= \begin{pmatrix} \mathrm{g}_{qq}(\tau,\tau')\,\mathcal{I}_3 & \mathrm{g}_{qp}(\tau,\tau')\,\mathcal{I}_3 \\ \mathrm{g}_{pq}(\tau,\tau')\,\mathcal{I}_3 & \mathrm{g}_{pp}(\tau,\tau')\,\mathcal{I}_3 \end{pmatrix} \\ &= \begin{pmatrix} \mathcal{I}_3 & 2\left(1-\mathrm{e}^{-\frac{1}{2}(\tau-\tau')}\right)\mathcal{I}_3 \\ 0_3 & \mathrm{e}^{-\frac{1}{2}(\tau-\tau')}\,\mathcal{I}_3 \end{pmatrix} \Theta(\tau-\tau')\,. \end{aligned} \tag{7.23}$$

We see that due to the expanding background spacetime the initial momentum is exponentially drained away. In consequence particles on the trajectories $\vec{q}(\tau) = \vec{q}^{\,(\mathrm{i})} + 2\left(1-\mathrm{e}^{-\frac{\tau}{2}}\right)\vec{p}^{\,(\mathrm{i})}$ travel only a finite distance even over arbitrarily long times. Since the linear evolution of the power spectrum (4.67) in the non-interacting regime of SFTCP is only quadratic in g_{qp}, this cannot reproduce the linear growth behaviour we see in (6.37). This is not surprising, since the linear solution for the evolution of the density contrast in SPT already includes the full gravitational interaction. Rather, linear growth will occur once we apply the linear statistical field propagator to the non-interacting power spectrum as we will see in chapter 8. The upper bound on g_{qp} will actually be useful when we calculate this linear field propagator.

7.3 THE INTERACTION POTENTIAL

With the linear propagator found, we still need to determine the interaction potential in order to start doing perturbation theory. The general solution to Poisson's equation (7.5) is given in terms of a Green's function as

$$\varphi(\vec{q},\tau) = -\frac{G}{a}\int \mathrm{d}\vec{q}\,' \,\frac{\rho_\mathrm{m}(\vec{q}\,',\tau)-\bar{\rho}_\mathrm{m}}{|\vec{q}-\vec{q}\,'|}\,. \tag{7.24}$$

The force resulting from this potential is given by

$$\begin{aligned}
-\nabla_q\,\varphi(\vec{q},\tau) &= -\frac{G}{a}\int \mathrm{d}\vec{q}\,' \,\left(\rho_\mathrm{m}(\vec{q}\,',\tau)-\bar{\rho}_\mathrm{m}\right)\frac{\vec{q}-\vec{q}\,'}{|\vec{q}-\vec{q}\,'|^3}\\
&= -\frac{G}{a}\left(\int \mathrm{d}\vec{q}\,'\,\rho_\mathrm{m}(\vec{q}\,',\tau)\,\frac{\vec{q}-\vec{q}\,'}{|\vec{q}-\vec{q}\,'|^3}+\int \mathrm{d}\vec{q}\,''\,\bar{\rho}_\mathrm{m}\frac{\vec{q}\,''}{|\vec{q}\,''|^3}\right)\\
&= -\frac{G}{a}\int \mathrm{d}\vec{q}\,'\,\rho_\mathrm{m}(\vec{q}\,',\tau)\,\frac{\vec{q}-\vec{q}\,'}{|\vec{q}-\vec{q}\,'|^3}\,.
\end{aligned} \tag{7.25}$$

In the second step we shifted the integration variable to $\vec{q}\,'' = \vec{q}-\vec{q}\,'$ and then executed the integration over angles first to find that the mean density does not contribute to the force on any particle[1]. We may thus neglect the mean mass density in further calculations. The next step is to sample the mass density field with the collective number density field of our field theory such that we have

$$\rho_\mathrm{m}(\vec{q}\,',\tau) = m\sum_{j=1}^{N}\delta_\mathrm{D}\left(\vec{q}\,'-\vec{q}_j(\tau)\right) = m\,\Phi_\rho(\vec{q}\,',\tau)\,. \tag{7.26}$$

The potential term in the action (7.16) then has the form

$$\nabla_{q_j}\left(-\frac{mG}{a^3H^2f^2}\int \mathrm{d}\vec{q}\,'\,\frac{1}{|\vec{q}-\vec{q}\,'|}\,\Phi_\rho(\vec{q}\,',\tau)\right)\,, \tag{7.27}$$

from which we read off the two-particle interaction potential as

$$\begin{aligned}
v\left(\vec{q},\vec{q}\,'\right) &= -\frac{mG}{a^3H^2f^2}\frac{1}{|\vec{q}-\vec{q}\,'|} = -\frac{m}{\bar{\rho}_\mathrm{m}}\frac{3}{8\pi}\underbrace{\frac{\bar{\rho}_\mathrm{m}}{a^3}}_{\bar{\rho}_\mathrm{m}(t)}\underbrace{\frac{8\pi G}{3H^2}}_{1/\rho_\mathrm{crit}(t)}\frac{1}{f^2}\frac{1}{|\vec{q}-\vec{q}\,'|}\\
&= -\frac{3}{8\pi\bar{\rho}}\frac{\Omega_m}{f^2}\frac{1}{|\vec{q}-\vec{q}\,'|} = -\frac{3}{8\pi\bar{\rho}}\frac{1}{|\vec{q}-\vec{q}\,'|}\,,
\end{aligned} \tag{7.28}$$

where we have again used the very good approximation $\frac{\Omega_m}{f^2}=1$ in the second line. We have also used that we fix the mean particle number density $\bar{\rho}$ of our grand canonical system to fulfil the constraint $\bar{\rho}_m = m\bar{\rho}$. In this form the equations of motion are now only implicitly dependent on the background cosmology through our choice for the time variable $\tau = \ln D$.

1 One should note that for this symmetry argument to hold one must consider a flat mass distribution with infinite spatial extension. Since $\bar{\rho}_\mathrm{m}$ is identified with the homogeneous density of cosmological background model we can always extend the integration range in order to achieve this.

As a last step we need the Fourier transform of the two-particle potential. This is in principle a fairly simple calculation as we saw in (4.113). However, the infinite range of the gravitational potential or rather the fact that it does not drop off fast enough for $\Delta\vec{q} = |\vec{q} - \vec{q}\,'| \to \infty$ leads to a divergent oscillating integral. To amend this problem we regularize the Fourier integral by introducing a temporary Yukawa-like long-range cutoff

$$v\left(\vec{q},\vec{q}\,'\right) \to -\frac{3}{8\pi\bar{\rho}}\frac{1}{|\vec{q}-\vec{q}\,'|}\,\mathrm{e}^{-k_\mathrm{c}|\vec{q}-\vec{q}\,'|}\,, \tag{7.29}$$

where k_c is the inverse cutoff scale. With this regularization in place we can now execute the Fourier integral to find

$$\begin{aligned} v(k) &= -\frac{3}{8\pi\bar{\rho}}\int \mathrm{d}\Delta\vec{q}\,\mathrm{e}^{-\mathrm{i}\vec{k}\Delta\vec{q}}\frac{1}{|\Delta\vec{q}|}\,\mathrm{e}^{-k_\mathrm{c}|\Delta\vec{q}|} = -\frac{6\pi}{8\pi\bar{\rho}}\int_0^\infty \mathrm{d}\Delta q\,\Delta q\,\mathrm{e}^{-k_\mathrm{c}\Delta q}\int_{-1}^{1}\mathrm{d}\mu\,\mathrm{e}^{-\mathrm{i}\mu k\Delta q} \\ &= \frac{6\pi}{\mathrm{i}8\pi\bar{\rho}k}\int_0^\infty \mathrm{d}\Delta q\,\mathrm{e}^{-k_\mathrm{c}\Delta q}\left(\mathrm{e}^{-\mathrm{i}k\Delta q}-\mathrm{e}^{\mathrm{i}k\Delta q}\right) = \frac{6\pi}{\mathrm{i}8\pi\bar{\rho}k}\left(\frac{1}{\mathrm{i}k+k_\mathrm{c}}+\frac{1}{\mathrm{i}k-k_\mathrm{c}}\right) \\ &= \frac{6\pi}{\mathrm{i}8\pi\bar{\rho}k}\left(\frac{2\mathrm{i}k}{(\mathrm{i}k)^2-k_\mathrm{c}^2}\right) = \left(-\frac{3}{2\bar{\rho}}\frac{1}{k^2+k_\mathrm{c}^2}\right)\,. \end{aligned} \tag{7.30}$$

For all our purposes we want to work with this potential in the limit where we push the cutoff scale to infinity and thus the inverse scale to $k_\mathrm{c} \to 0$. Since the potential is finite for all modes $k \neq 0$ this is usually not a problem. Only when we evaluate terms at $k = 0$ we have to remember to take limits in such an order that

$$\lim_{k_\mathrm{c}\to 0}\delta_\mathrm{D}(\vec{k})\,\frac{k^n}{k^2+k_\mathrm{c}^2} = 0\,, \tag{7.31}$$

in order to retain the important property (4.117). Keeping this in mind we define the interaction matrix as

$$\sigma_{\mu_1\nu_2} = -(2\pi)^3\,\delta_\mathrm{D}(\vec{k}_1+\vec{k}_2)\,\delta_\mathrm{D}\left(\tau_1-\tau_2\right)\underbrace{\left(-\frac{3}{2\bar{\rho}}\frac{1}{k_1^2}\right)}_{v(k_1)}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\,. \tag{7.32}$$

8

LINEAR AND SLIGHTLY NON-LINEAR GROWTH OF THE POWER SPECTRUM

In this chapter we will combine all our findings in order to show that we can reproduce the linear growth of the power spectrum purely from particle dynamics. For this purpose we first calculate the linear statistical field propagator $G^{(1)}_{\rho B}$ employing the free particle propagators and the interaction potential derived in the previous chapter. With this propagator we then calculate the first order solution for the power spectrum taking into account both its non-interacting contributions which are linear and quadratic in the initial power spectrum.

8.1 THE LINEAR FIELD PROPAGATOR

In order to find the linear statistical field propagator $G^{(1)}_{\rho B}$ we only have to insert our findings for g_{qp} and $v(k)$ from the previous chapter into (4.148) and then use (4.153). Since our particles do not move on inertial trajectories the damping factor $\mathfrak{D}_{12}$ is not invariant under time translation. We thus have to approximate it as unity. This is a good approximation as long as the modulus of its argument fullfills

$$\frac{\sigma_p^2}{2} k_1^2 (g_1 - g_2)^2 \ll 1 \,. \tag{8.1}$$

We can now notice that the free particle propagators are bounded from above as $g_1 \leq 2$ and as such the above condition in the worst case $|(g_1 - g_2)| = 2$ is only a condition

$$k_1 \ll \frac{1}{\sqrt{2\sigma_p^2}} \tag{8.2}$$

on the modulus k_1 and thus on the range of spatial scales we can describe in good approximation. Since we are only interested in the linear evolution of the power spectrum we will not need to integrate over the mode of the field propagator and the above restriction is not too much of a problem. Furthermore, we will consider a starting time very early in the cosmological evolution when the power spectrum is 'small' in the sense that

$$\sigma_p^2 = \frac{1}{3} \int \frac{\mathrm{d}\vec{h}}{(2\pi)^3} \frac{P_\delta(h)}{h^2} \ll 1 \tag{8.3}$$

and thus the range of values for k_1 is fairly large. The above relation is derived in Appendix D. With $\mathfrak{D}_{12} \to 1$ the inhomogeneity and kernel of the $G^{(1)}_{\rho B}$ integral equation according to the combination of (4.148), (7.21) and (7.32) are given by

$$\begin{aligned} g(k_1,\tau) &= -\mathrm{i}\,\bar{\rho}\,k_1^2\,2\,(1-\mathrm{e}^{-\frac{1}{2}\tau}) \\ K(k_1,\tau) &= -\bar{\rho}\,k_1^2\left(-\frac{3}{2\bar{\rho}}\frac{1}{k_1^2}\right)2\,(1-\mathrm{e}^{-\frac{1}{2}\tau}) = 3\,(1-\mathrm{e}^{-\frac{1}{2}\tau})\,. \end{aligned} \tag{8.4}$$

Since the time-dependent part has the same functional form in both cases, the only Laplace transform we need to compute is

$$\mathcal{L}_{\tau,s}\left[\left(1-\mathrm{e}^{-\frac{1}{2}\tau}\right)\right] = \left(\frac{1}{s}-\frac{1}{s+\frac{1}{2}}\right)\,, \tag{8.5}$$

where we used (1.32). The argument of the inverse Laplace transform in (4.153) is then

$$\begin{aligned} \mathrm{e}^{-st_2}\frac{\mathcal{L}_{\tau\to s}\left[g(k_1,\tau)\right]}{1-\mathcal{L}_{\tau\to s}\left[K(k_1,\tau)\right]} &= -\mathrm{i}\,\bar{\rho}\,k_1^2\,\mathrm{e}^{-st_2}\,2\,\frac{\left(\frac{1}{s}-\frac{1}{s+\frac{1}{2}}\right)}{1-3\left(\frac{1}{s}-\frac{1}{s+\frac{1}{2}}\right)} \\ &= -\mathrm{i}\,\bar{\rho}\,k_1^2\,\mathrm{e}^{-s\tau_2}\,2\,\frac{s+\frac{1}{2}-s}{s(s+\frac{1}{2})-3\,(s+\frac{1}{2}-s)} \\ &= -\mathrm{i}\,\bar{\rho}\,k_1^2\,\mathrm{e}^{-s\tau_2}\,\frac{1}{s^2+\frac{3}{2}s-s-\frac{3}{2}} \\ &= -\mathrm{i}\,\bar{\rho}\,k_1^2\,\mathrm{e}^{-s\tau_2}\,\frac{1}{(s-1)(s+\frac{3}{2})} \\ &= -\mathrm{i}\,\bar{\rho}\,k_1^2\,\mathrm{e}^{-s\tau_2}\,\frac{2}{5}\left(\frac{1}{s-1}-\frac{1}{s+\frac{3}{2}}\right)\,. \end{aligned} \tag{8.6}$$

If we use (1.33) together with (1.34) we find

$$\begin{aligned} G^{(1)}_{\rho_1 B_2} &= -\mathrm{i}\,\bar{\rho}\,(2\pi)^3\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\,k_1^2\,\frac{2}{5}\,\mathcal{L}^{-1}_{\tau_1\leftarrow s}\left[\mathrm{e}^{-s\tau_2}\left(\frac{1}{s-1}-\frac{1}{s+\frac{3}{2}}\right)\right] \\ &= -\mathrm{i}\,\bar{\rho}\,(2\pi)^3\,\delta_{\mathrm{D}}(\vec{k}_1+\vec{k}_2)\,k_1^2\,\frac{2}{5}\left(\mathrm{e}^{\tau_1-\tau_2}-\mathrm{e}^{-\frac{3}{2}(\tau_1-\tau_2)}\right)\Theta(\tau_1-\tau_2)\,. \end{aligned} \tag{8.7}$$

Interestingly, the time dependent part is the same as the density-velocity-component of the linear propagator (6.34) in SPT. This makes sense if we recall our interpretation of the linear field propagator as the sum of all possible 'bucket brigade' processes, that we gave after (4.139). It contains all processes where a mode of the initial power spectrum is amplified or drained away in time by the piecewise free motion of particles through space. Between these sections of free motion, particles interact instantaneously and due to momentum conservation 'hand over' the propagation of the mode without any mode coupling taking place. Whether a mode is amplified or drained away depends on the initial conditions, but in our case we set them up such that only amplification will take place.

8.2 THE LINEAR POWER SPECTRUM

With our result (8.7) for the linear field propagator in hand we can now attempt to calculate the first order solution (4.139) for the power spectrum which reads

$$G^{(1)}_{\rho_1\rho_2} = \left(\delta_{\mathrm{D}}(1-3) + G^{(1)}_{\rho_1 B_4} \mathrm{i}\sigma_{B_4\rho_3}\right) G^{(0)}_{\rho_3\rho_5} \left(\delta_{\mathrm{D}}(5-2) + \mathrm{i}\sigma_{\rho_5 B_6} G^{(1)}_{B_6\rho_2}\right) . \tag{8.8}$$

We first look at the non-interacting power spectrum which can be separated as

$$\begin{aligned} G^{(0)}_{\rho_1\rho_2} &= G^{(0,1)}_{\rho_1\rho_2} + G^{(0,2)}_{\rho_1\rho_2} \\ &= (2\pi)^3 \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_2) \left(\bar{\rho}\, \mathfrak{D}(1,2) + \bar{\rho}^2 \left(\mathcal{T}^{(2,1)}_{1|1}(1;2) + \mathcal{T}^{(2,2)}_{1|1}(1;2)\right)\right) , \end{aligned} \tag{8.9}$$

where we used (4.54) for the one-particle contribution and (4.65) for the two-particle contribution. As argued in section 4.3.4 the one-particle contribution is just a shot-noise term due to its scaling with $\bar{\rho}^1$ and can thus be dropped. We see from (4.67) and (4.68) that both $\mathcal{T}$-functions are proportional to the damping factor

$$\mathfrak{D}(1;2) = \exp\left\{-\frac{\sigma_p^2}{2} k_1^2 \left(g_1^2 + g_2^2\right)\right\} . \tag{8.10}$$

In order to be able to carry out the calculations in an easy analytical way we will again restrict ourselves to the range of wave numbers k_1 where we can safely approximate the damping factor by unity. With $g_1, g_2 \leq 2$ we find the condition

$$k_1 \ll \frac{1}{2\sqrt{\sigma_p^2}} , \tag{8.11}$$

which is somewhat more restrictive than (8.2). We will later compare our analytical results against exact numerical ones to check the validity of this range. The $\mathcal{T}^{(2,1)}_{1|1}$ term represents the non-interacting and linear evolution of the power spectrum and we will concentrate on this term for now. First, we calculate

$$\begin{aligned} G^{(1)}_{\rho_1 B_3} \mathrm{i}\sigma_{B_3\rho_2} = \int \mathrm{d}3 \Bigg(& -\mathrm{i}\,\bar{\rho}\,(2\pi)^3\, \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_3)\, k_1^2 \frac{2}{5} \left(\mathrm{e}^{\tau_1-\tau_3} - \mathrm{e}^{-\frac{3}{2}(\tau_1-\tau_3)}\right) \times \\ & \Theta(\tau_1-\tau_3)\Bigg) \left(-\mathrm{i}(2\pi)^3 \delta_{\mathrm{D}}(\vec{k}_3 + \vec{k}_2)\, \delta_{\mathrm{D}}(\tau_3-\tau_2) \left(-\frac{3}{2\bar{\rho}} \frac{1}{k_3^2}\right)\right) \\ = {} & (2\pi)^3\, \delta_{\mathrm{D}}(\vec{k}_1 - \vec{k}_2) \frac{3}{5} \left(\mathrm{e}^{\tau_1-\tau_2} - \mathrm{e}^{-\frac{3}{2}(\tau_1-\tau_2)}\right) \Theta(\tau_1-\tau_2) \\ := {} & (2\pi)^3\, \delta_{\mathrm{D}}(\vec{k}_1 - \vec{k}_2)\, f(\tau_1-\tau_2)\, \Theta(\tau_1-\tau_2) . \end{aligned} \tag{8.12}$$

By straightforward calculations one shows that

$$\begin{aligned} \int_0^{\tau_1} \mathrm{d}\tau_2\, f(\tau_1-\tau_2) &= f(\tau_1) + \mathrm{e}^{-\frac{3}{2}\tau_1} - 1 , \\ \int_0^{\tau_1} \mathrm{d}\tau_2\, f(\tau_1-\tau_2)\, \mathrm{e}^{-\frac{1}{2}\tau_2} &= \mathrm{e}^{\tau_1} - f(\tau_1) - \mathrm{e}^{-\frac{1}{2}\tau} \end{aligned} \tag{8.13}$$

and by combining these we find

$$\begin{aligned}\int_0^{\tau_1} \mathrm{d}\tau_2\, f(\tau_1-\tau_2)\, g_2 &= \int_0^{\tau_1} \mathrm{d}\tau_2\, f(\tau_1-\tau_2)\, 2\left(1-\mathrm{e}^{-\frac{1}{2}\tau_2}\right)\\ &= 2\left(f(\tau_1)+\mathrm{e}^{-\frac{3}{2}\tau_1}-1-\mathrm{e}^{\tau_1}+f(\tau_1)+\mathrm{e}^{-\frac{1}{2}\tau_1}\right)\\ &= 2\left(2\,f(\tau_1)-\frac{5}{3}f(\tau_1)\right)-g_1 = \frac{2}{3}f(\tau_1)-g_1\,. \end{aligned} \tag{8.14}$$

Combining this again with (8.13) we finally find

$$\begin{aligned}\int_0^{\tau_1} \mathrm{d}\tau_2\, f(\tau_1-\tau_2)(1+g_2) &= f(\tau_1)+\mathrm{e}^{-\frac{3}{2}\tau_1}-1+\frac{2}{3}f(\tau_1)-g_1\\ &= \frac{5}{3}f(\tau_1)+\mathrm{e}^{-\frac{3}{2}\tau_1}-(1+g_1)\\ &= \mathrm{e}^{\tau_1}-(1+g_1)\,. \end{aligned} \tag{8.15}$$

With these relations we can now calculate the first order evolution of the contribution to the power spectrum which is linear in the *initial* power spectrum P_δ to be

$$\begin{aligned} G^{(1),\mathrm{lin}}_{\rho_1\rho_2} &= \int \mathrm{d}3 \int \mathrm{d}4\, \left(\delta_\mathrm{D}(1-3)+(2\pi)^3\,\delta_\mathrm{D}(\vec{k}_1-\vec{k}_3)\, f(\tau_1-\tau_3)\,\Theta(\tau_1-\tau_3)\right)\times\\ &\qquad \left(\delta_\mathrm{D}(2-4)+(2\pi)^3\,\delta_\mathrm{D}(\vec{k}_2-\vec{k}_4)\, f(\tau_2-\tau_4)\,\Theta(\tau_2-\tau_4)\right)\times\\ &\qquad \left(\bar{\rho}^2(2\pi)^3\,\delta_\mathrm{D}(\vec{k}_3+\vec{k}_4)\,(1+g_3)\,(1+g_4)\,P_\delta(k_3)\right)\\ &= \bar{\rho}^2(2\pi)^3\,\delta_\mathrm{D}(\vec{k}_1+\vec{k}_2)\,P_\delta(k_1)\left((1+g_1)+\int_0^{\tau_1}\mathrm{d}\tau_3\, f(\tau_1-\tau_3)\,(1+g_3)\right)\times\\ &\qquad \left((1+g_2)+\int_0^{\tau_2}\mathrm{d}\tau_4\, f(\tau_2-\tau_4)\,(1+g_4)\right)\\ &= \bar{\rho}^2(2\pi)^3\,\delta_\mathrm{D}(\vec{k}_1+\vec{k}_2)\,\mathrm{e}^{\tau_1}\,\mathrm{e}^{\tau_2}\,P_\delta(k_1)\\ &= \bar{\rho}^2(2\pi)^3\,\delta_\mathrm{D}(\vec{k}_1+\vec{k}_2)\,D(t_1)\,D(t_2)\,P_\delta(k_1)\,, \end{aligned} \tag{8.16}$$

where we used that $\mathrm{i}\sigma_{\rho_1 B_3} G^{(1)}_{B_3\rho_2} = G^{(1)}_{\rho_2 B_3}\mathrm{i}\sigma_{B_3\rho_1}$. This is exactly the same linear growth behaviour one also finds in SPT. It is very reassuring that our theory reproduces this well-known result. In order to show the validity of this result we compare it against the numerical solution for the following system of linear Volterra equations of the second kind

$$\begin{aligned} G^{(1)}_{B_1\rho_2} &= G^{(0,1)}_{B_1\rho_2} + G^{(0,1)}_{B_1\rho_3}\,\mathrm{i}\sigma_{\rho_3 B_4} G^{(1)}_{B_4\rho_2}\,,\\ G^{(1),\mathrm{lin}}_{\rho_1\rho_2} &= G^{(0,2),\mathrm{lin}}_{\rho_1\rho_2} + G^{(0,2),\mathrm{lin}}_{\rho_1\rho_3}\,\mathrm{i}\sigma_{\rho_3 B_4} G^{(1)}_{B_4\rho_2} + G^{(0,1)}_{\rho_1 B_3}\,\mathrm{i}\sigma_{B_3\rho_4} G^{(1),\mathrm{lin}}_{\rho_4\rho_2}\,. \end{aligned} \tag{8.17}$$

We used a simple 'forward-stepping' algorithm that can be found in Press et al. [51]. The background ΛCDM-cosmology is fixed by the reduced Hubble constant $h = 0.7$

and $\Omega_{\mathrm{m,today}} = 0.3$. The initial power spectrum P_δ is taken to be at redshift $z_\mathrm{i} = 100$ with a normalisation of $\sigma_8 = 0.8$ and then evolved to the present day at redshift $z = 0$ which translates to $\tau_{\mathrm{today}} = 4.364$. The necessary linear growth factor is calculated by combining (6.23) with (6.8) and using $a = 1/(1+z)$. The calculation of P_δ is explained in Appendix D. The momentum dispersion of the initial power spectrum is $\sigma_p^2 = 0.0054$ which means we should see the analytical solution starting to differ substantially from the exact numerical one somewhere around $k \approx 5 - 7\,h/\mathrm{Mpc}$ according to (8.11) and this matches well with the result shown in Fig. 7.

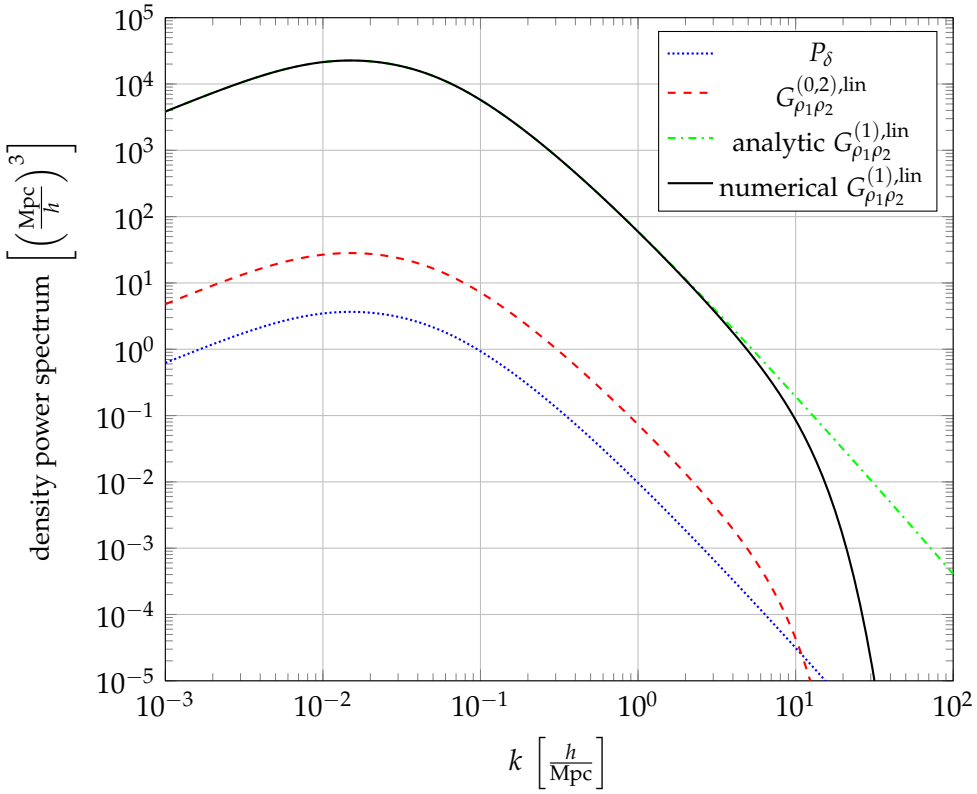


Figure 7: The initial power spectrum (dotted blue line) and its evolution up to redshift $z = 0$. The non-interacting evolution (red dashed line) and the first order evolution obtained from the analytic result (8.16) without damping (green dash-dotted line) and from numerical solutions (solid black line) of the integral equations (8.17) are shown.

8.3 FIRST CORRECTION TO THE LINEAR POWER SPECTRUM

Let us return to (8.9) and concentrate on the $\mathcal{T}^{(2,2)}_{1|1}$ term. It describes all initial correlation effects between two particles which are of quadratic order in the initial power spectrum P_δ and thus lead to the coupling of modes. The contribution of this mode coupling at the initial time is then transported forward by the free motion of the two particles. All these correlation effects must involve the momenta of both particles ac-

cording to (4.57) and thus the contribution vanishes at the initial time since the effects of momentum correlations need time evolution to have any effect.

We now want to apply the linear field propagator to this contribution as dictated by (8.8). For this purpose we state that

$$\delta_{\mathrm{D}}(1-2) + G^{(1)}_{\rho_1 B_3} \mathrm{i}\sigma_{B_3\rho_2} = (2\pi)^3 \delta_{\mathrm{D}}(\vec{k}_1 - \vec{k}_2) \left(\delta_{\mathrm{D}}(\tau_1 - \tau_2) + f(\tau_1 - \tau_2)\,\Theta(\tau_1 - \tau_2)\right) \tag{8.18}$$

according to (8.12). Combining this with (8.13) and (8.14) we find

$$\begin{aligned} &\int_0^\infty \mathrm{d}\tau_2 \, \left(\delta_{\mathrm{D}}(\tau_1 - \tau_2) + f(\tau_1 - \tau_2)\,\Theta(\tau_1 - \tau_2)\right) = f(\tau) + \mathrm{e}^{-\frac{3}{2}\tau} \\ &\int_0^\infty \mathrm{d}\tau_2 \, \left(\delta_{\mathrm{D}}(\tau_1 - \tau_2) + f(\tau_1 - \tau_2)\,\Theta(\tau_1 - \tau_2)\right) \mathrm{g}_2 = \frac{2}{3} f(\tau_1)\,. \end{aligned} \tag{8.19}$$

Notice that we pushed the global final time to $\tau_{\mathrm{f}} \to \infty$ for convenience, because then we do not always have to state explicitly that all times in the external labels of the fields are earlier than τ_{f}. We also encounter squares of the free particle propagator which we can rewrite as

$$\begin{aligned} \mathrm{g}_1^2 &= (\mathrm{g}_{qp}(\tau_1, 0))^2 = \left(2\left(1 - \mathrm{e}^{-\frac{1}{2}\tau_1}\right)\right)^2 \\ &= 4\left(1 - 2\mathrm{e}^{-\frac{1}{2}\tau_1} + \mathrm{e}^{-\tau_1}\right) = 4\left((\mathrm{g}_1 - 1) + \mathrm{e}^{-\tau_1}\right)\,. \end{aligned} \tag{8.20}$$

By straightforward calculation one finds

$$\int_0^{\tau_1} \mathrm{d}\tau_2 \, f(\tau_1 - \tau_2)\,\mathrm{e}^{-\tau_2} = \frac{3}{2}\mathrm{e}^{\tau_1} - 2f(\tau_1) - \frac{3}{2}\mathrm{e}^{-\tau_1} \tag{8.21}$$

and consequently also

$$\begin{aligned} &\int_0^\infty \mathrm{d}\tau_2 \, \left(\delta_{\mathrm{D}}(\tau_1 - \tau_2) + f(\tau_1 - \tau_2)\,\Theta(\tau_1 - \tau_2)\right) \mathrm{g}_2^2 \\ &= 4 \int_0^\infty \mathrm{d}\tau_2 \, \left(\delta_{\mathrm{D}}(\tau_1 - \tau_2) + f(\tau_1 - \tau_2)\,\Theta(\tau_1 - \tau_2)\right) \left((\mathrm{g}_2 - 1) + \mathrm{e}^{-\tau_2}\right) \\ &= 4\left(\frac{2}{3}f(\tau_1) - \left(f(\tau_1) + \mathrm{e}^{-\frac{3}{2}\tau_1}\right) + \frac{3}{2}\mathrm{e}^{\tau_1} - 2\,f(\tau_1) - \frac{1}{2}\mathrm{e}^{-\tau_1}\right) \\ &= 4\left(-\frac{7}{3}f(\tau_1) + \left(\mathrm{e}^{\tau_1} - \mathrm{e}^{-\frac{3}{2}\tau_1}\right) + \frac{1}{2}\mathrm{e}^{\tau_1} - \frac{1}{2}\mathrm{e}^{-\tau_1}\right) \\ &= 2\,\mathrm{e}^{\tau_1} - \frac{8}{3}f(\tau_1) - 2\,\mathrm{e}^{-\tau_1} = \frac{2}{3}f(\tau_1) - 2\left(\mathrm{e}^{-\tau_1} - \mathrm{e}^{-\frac{3}{2}\tau_2}\right)\,. \end{aligned} \tag{8.22}$$

One can easily check that this result is positive definite for $\tau_1 > 0$. The negative second term has a maximum value of $-8/27 \approx -0.3$ at $\tau_1 = 2 * \ln(3/2) \approx 0.8$ and

then quickly goes to zero. For $\tau_1 \geq 1$ the above result will thus nearly behave as $\frac{2}{3}f(\tau_1)$, which is the density-velocity-component of the linear propagator (6.34) of SPT as we discussed earlier. We define

$$X(\tau_1) = X_1 = \frac{2}{3}f(\tau_1) := \frac{2}{5}\left(\mathrm{e}^{\tau_1} - \mathrm{e}^{-\frac{3}{2}\tau_1}\right) = g_{\delta\theta}(\tau_1, 0) \tag{8.23}$$

and rewrite our result from (8.24) as

$$\frac{2}{3}f(\tau_1) - 2\left(\mathrm{e}^{-\tau_1} - \mathrm{e}^{-\frac{3}{2}\tau_2}\right) = X_1\left(1 - \frac{2\left(\mathrm{e}^{-\tau_1} - \mathrm{e}^{-\frac{3}{2}\tau_2}\right)}{\frac{2}{3}f(\tau_1)}\right) = X_1\,\Delta_1\,. \tag{8.24}$$

The Δ_1 function quantifies the difference to the normal linear growth and quickly goes to unity for $\tau_1 > 0$ as we have just discussed. Combining the above equations with (8.8), (8.9) and (4.68) we find that the first order evolution of the power spectrum contribution coming from terms quadratic in the initial power spectrum P_δ in the range specified in (8.11) is given by

$$\begin{aligned} G^{(1),\mathrm{quad}}_{\rho_1\rho_2} = \bar{\rho}^2(2\pi)^3\,\delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_2)\,X_1\,X_2 \int \frac{\mathrm{d}^3h}{(2\pi)^3}\,P_\delta\left(\left|\vec{k}_1 - \vec{h}\right|\right)\,P_\delta(h)\times \\ \left\{\left(\frac{\vec{k}_1\cdot\vec{h}}{h^2}\right)^2\left(1 + (\Delta_1+\Delta_2)\frac{\vec{k}_1\cdot\left(\vec{k}_1-\vec{h}\right)}{\left(\vec{k}_1-\vec{h}\right)^2}\right.\right. \\ \left.\left. + \frac{\Delta_1\,\Delta_2}{2}\left(\frac{\vec{k}_1\cdot\left(\vec{k}_1-\vec{h}\right)}{\left(\vec{k}_1-\vec{h}\right)^2}\right)^2\right) + \left(\frac{\vec{k}_1\cdot\vec{h}}{h^2}\right)\left(\frac{\vec{k}_1\cdot\left(\vec{k}_1-\vec{h}\right)}{\left(\vec{k}_1-\vec{h}\right)^2}\right)\right\}\,. \end{aligned} \tag{8.25}$$

From this we see that apart from the initial deviation due to the Δ_1 and Δ_2 functions this contribution to the power spectrum evolves purely with the square of the density-velocity propagator of SPT. This is not to surprising, since in contrast to the $\mathcal{T}^{2,1}_{1|1}$ contribution there are no terms containing only density correlations in $\mathcal{T}^{2,2}_{1|1}$. In fact, from (6.37) we see that in SPT one must take into account contributions from both the density-density and the density-velocity component of the linear propagator in order to achieve the linear growth behaviour we found in (8.16). The result in (8.25) may thus be understood as an instantaneous mode coupling of momentum correlations at the initial time which are amplified by the linear streaming processes of interacting particles encoded in the field propagator $G^{(1)}_{\rho_1 B_2}$. We again compare our analytic result (8.25) against the numerical one with all damping factors present in Fig. 8 and find very good agreement up to $k = 5 - 7\,h/\mathrm{Mpc}$. The numerical results are obtained from solving the integral equations (8.17) with $G^{(0,2),\mathrm{lin}}_{\rho_1\rho_2} \to G^{(0,2),\mathrm{quad}}_{\rho_1\rho_2}$ exchanged. In Fig. 9, we also compare the analytic result (8.16) corresponding to SPT against the solution of the integral equations with only linear as well as linear and quadratic initial correlations taken into account. We see that the contribution from quadratic initial correlations do not contribute to any non-linear growth of the power spectrum compared to the linear SPT result. Rather, it reduces the damping effect due to the

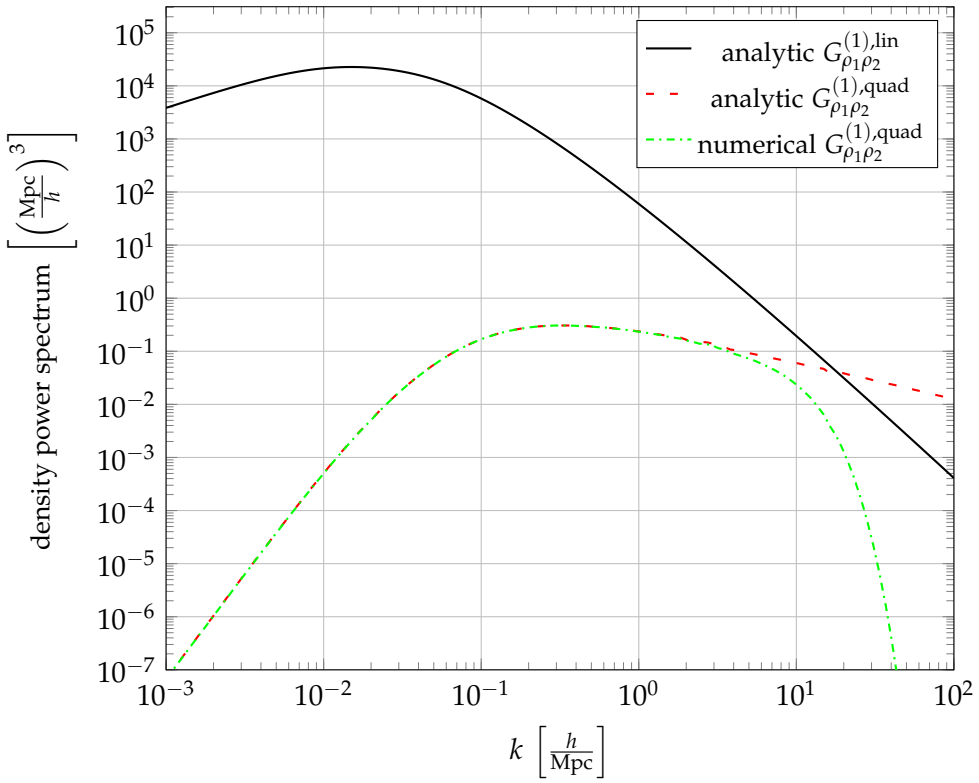


Figure 8: First-order evolution of the power spectrum contributions quadratic in P_δ up to redshift $z = 0$. The undamped first order evolution of the power spectrum (black solid line) is shown for comparison. The analytic result (8.25) (red dashed line) agrees perfectly with the numerical result (green dashed line) as long as the no-damping approximation is valid.

random motion of the particles by a very small amount. In consequence, it slightly extends the range of scales where the analytic result (8.16) is a good approximation to the actual result for the power spectrum. It is an interesting question for future work whether the same holds for contributions of cubic and higher order in the initial correlations and if taking into account arbitrarily high orders of them would in effect restore the linear growth of SPT. This would then justify using (8.16) for calculating loop corrections like those shown in (4.142), which we expect to contain the first non-linear corrections relative to the linear growth of SPT.

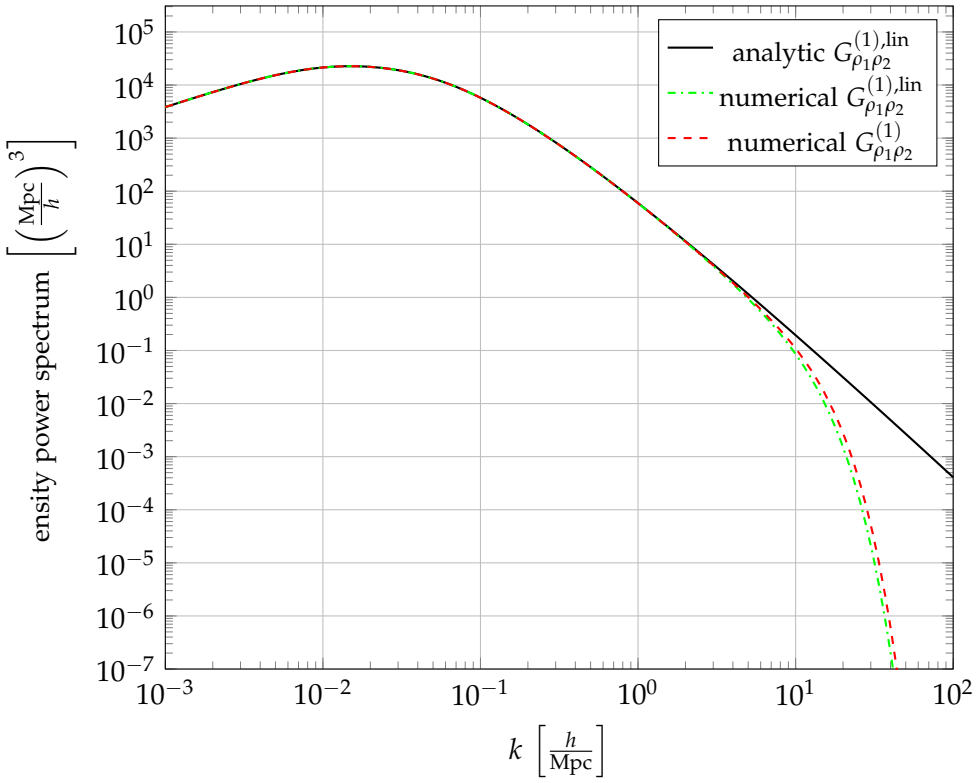


Figure 9: First-order evolution of the power spectrum up to redshift $z = 0$. The undamped first order evolution (8.16) of the power spectrum (black solid line) is shown for comparison. The numerical first order solution including only linear initial correlations (green dashdotted line) and additionally including quadratic initial correlations (red dashed line) only differ slightly.

9

CONCLUSIONS ON PART II AND OUTLOOK

In the second part of this work we briefly introduced the standard ΛCDM-model of cosmology based on the assumption of statistical homogeneity and isotropy on large scales. We discussed why the initial conditions for the formation of structure might have their origin in the quantum fluctuations of some primordial field and in which sense a statistical approach to the study of structure formation is admissible. We then continued by introducing the Standard Perturbation Theory (SPT) of structure formation and pointed out the various drawbacks of this approach compared to SFTCP. Some of these drawbacks arise from approximations to the equations of motion necessary for obtaining an analytic solution which can serve as the starting point of perturbation theory, others are rooted in an unfortunate choice of dynamical variables. We then finally applied SFTCP in its grand canonical version to the problem of structure formation.

- We first calculated the first order solution for the statistical field propagator $G_{\rho B}$ and found that in the regime where the damping due to initial velocity dispersion can be neglected we obtain the same result as found for the density-velocity component $g_{\delta\theta}$ of the linear propagator (6.34) in SPT.
- Using this result we calculated the first order solution for the power spectrum $G_{\rho\rho}$ and found that if we consider only initial correlations which are linear in the initial power spectrum P_δ we obtain the same linear growth behaviour (6.37) as in SPT.
- Contributions coming from those terms in the non-interacting power spectrum $G^{(0,2)}_{\rho\rho}$ which are quadratic in the initial correlations will evolve with $g_{\delta\theta}$ (6.34) and at the present state of investigation seem to have no counterpart in SPT. While their contribution to the evolved power spectrum is negligible once all damping terms are considered, it was shown in Bartelmann et al. [7] that they become a lot more important if one uses unbounded free particle propagators like those of the Zel'dovich approximation. This suggests that these kinds of terms warrant further investigation to exactly see which approximation is responsible for the fact that they do not appear in SPT.

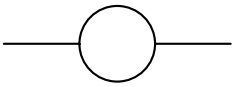
For all three of these quantities the analytic results were checked against the numeric solution of the respective linear integral equations and were found to be in excellent agreement in the specified ranges of validity where the damping factors

can be approximated by unity. Based on these results we can establish an interesting correspondence between SFTCP and SPT.

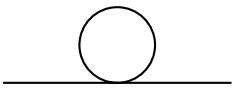
- On the level of two-point cumulants the first order solution of SFTCP appears to be the equivalent of the the tree-level (6.38) of the path integral formulation of SPT.
- As we already mentioned in part i, the structure of SFTCP perturbation theory as investigated in section 4.3.5 points to a reformulation of the generating functional in such a way that the first order solution becomes the tree-level with the non-interacting cumulants acting as vertices.
- It should thus be possible to directly compare the diagrammatic structure of the two theories. In this case we see that SFTCP contains much more information about the system since even at tree-level there are infinitely many non-interacting cumulants and thus vertices of arbitrary n-point order as opposed to only one three-point vertex in SPT. In this way one would be able to connect the truncation of the BBGKY-hierarchy at the core of SPT and the subsequent loss of phase-space information to the structure of perturbation theory.

This again gives credit to our claim that SFTCP should be a valid tool for the investigation of the non-linear statistics of density perturbations in the universe. Once the reformulation of the theory has been achieved a multitude of avenues are open for future pursuit:

- The most obvious task is to calculate the one-loop corrections to the density power spectrum and compare them with SPT. It will be interesting to see if the contributions from loop diagrams of the general form



  built from the respective theories three-point vertices are the same or whether SFTCP can already improve non-linear growth at this level. We however expect an improvement over SPT once loop diagrams of the general form



  are included since four-point vertices are unique to SFTCP at tree-level. In Bartelmann et al. [8] it was already shown that a combination of early linear evolution due to the Zel'dovich approximation and a subsequent one-loop calculation involving the free particle propagators and the interaction to first order leads to impressive results that mimick the power spectrum behaviour found in N-body simulations deep into the non-linear regime even at reshift $z = 0$. Since the reformulated perturbation theory would include the linear growth behaviour we are hopeful to achieve similar results with a one-loop calculation that describes the time evolution with a bare propagator valid at all times.

- Since the reformulated perturbation theory of SFTCP should have the same structure as standard QFT it should be possible to perform Dyson resummation with the amputated one-loop diagrams as the lowest order contributions to the 1PI-self-energy.
- Going further, the application of Renormalisation Group techniques presents itself as a natural next step in order to probe the non-linear regime. This is especially true for the application of SFTCP to the evolution of self-gravitating dark matter haloes where the investigation of scaling laws and meta-stable configurations due to virilisation is of utmost interest. This could lead to insight into how one can explain the appearance of universal density profiles like for example the Navarro-Frenk-White profile (Navarro et al. [43]) on a large range of scales in numerical N-body simulations.
- The diagrammatic approach to the initial conditions described in chapter 3 should allow a generalisation to non-Gaussian random fields and thus for investigations into the effects of primordial non-Gaussianity on the present day statistics of the matter distribution in the universe.

All in all this work can only be the seen as laying the necessary foundations. We feel that having a theory at hand that practically needs no approximations to the underlying dynamical equations of motion will lead to new findings that can improve our understanding of structure formation in cosmology.

Part III

APPENDIX

A

VANISHING OF PURE RESPONSE FIELD CUMULANTS

We will show that correlators containing only the collective response field Φ_B vanish even if all interactions are considered. We will do this in the canonical ensemble. Since pure Φ_B cumulants are defined in terms of pure Φ_B correlators, the vanishing of the latter automatically implies the vanishing of the former. Since the grand canonical generating functional is defined in terms of the canonical one, the vanishing of the canonical cumulants implies that the grand canonical ones vanish as well. We will proceed in an inductive way and start with the one-point correlator. Using (4.20), its basic definition in Fourier space is given by

$$\begin{aligned}\langle \Phi_{B_1} \rangle &= \int \mathrm{d}\Gamma_\mathrm{i} \int_\mathrm{i} \mathcal{D}\mathbf{x} \int \mathcal{D}\boldsymbol{\chi} \left(\sum_{j=1}^{N} \mathrm{i}\vec{\chi}_{p_j}(t_1) \cdot \vec{k}_1 \, \mathrm{e}^{-\mathrm{i}\vec{k}_1 \cdot \vec{q}_j(t_1)} \right) \times \\ &\quad \exp\left\{ \mathrm{i}\boldsymbol{\chi} \cdot \boldsymbol{\mathcal{E}}[\mathbf{x}] + \mathrm{i}\mathbf{J} \cdot \mathbf{x} + \mathrm{i}\mathbf{K} \cdot \boldsymbol{\chi} \right\} \big|_{\mathbf{J}=\mathbf{K}=0} \\ &= \int \mathrm{d}\Gamma_\mathrm{i} \int_\mathrm{i} \mathcal{D}\mathbf{x} \left(\mathrm{i} \sum_{j=1}^{N} \frac{\delta}{\mathrm{i}\delta \vec{K}_{p_j}(t_1)} \cdot \vec{k}_1 \, \mathrm{e}^{-\mathrm{i}\vec{k}_1 \cdot \vec{q}_j(t_1)} \right) \delta_\mathrm{D}[\boldsymbol{\mathcal{E}}[\mathbf{x}] + \mathbf{K}]\big|_{\mathbf{K}=0} \end{aligned} \tag{A.1}$$

We used the notation defined in (2.65) for the integral over initial conditions. In the second line we have replaced the auxiliary 'fields' $\vec{\chi}_{p_j}$ by functional derivatives and then executed the path integral over them. The term in the Dirac delta distribution now defines new equations of motion augmented by the source term $\mathbf{K}$

$$\partial_t \mathbf{x} - \boldsymbol{\mathcal{J}} \boldsymbol{\nabla} \mathcal{H} + \mathbf{K} = 0 \, . \tag{A.2}$$

We can absorb the source term into the Hamiltonian by defining

$$\mathcal{H}' = \mathcal{H} - \mathbf{K}^\mathrm{T} \boldsymbol{\mathcal{J}} \mathbf{x} \, . \tag{A.3}$$

This shows that the augmented equations of motion can still be derived entirely from an Hamiltonian and we may thus rewrite the Dirac delta distribution according to the arguments given in section 2.3.2 as

$$\delta_\mathrm{D}[\partial_t \mathbf{x} - \boldsymbol{\mathcal{J}} \boldsymbol{\nabla} \mathcal{H} + \mathbf{K}] = \delta_\mathrm{D}[\mathbf{x} - \bar{\mathbf{x}}(t, \mathbf{K})] \, , \tag{A.4}$$

where $\bar{\mathbf{x}}(t, \mathbf{K})$ is the solution to (A.2). If we assume that we can split the Hamiltonian as in (2.29), with the interaction part given by a potential, then the equation of motion can be written as

$$\boldsymbol{\mathcal{E}}_0[\mathbf{x}] = \boldsymbol{\mathcal{J}} \boldsymbol{\nabla} V(\vec{q}, t) - \mathbf{K} \, . \tag{A.5}$$

Given the linear propagator that solves this equation without the inhomogeneities on the RHS we can write the formal solution to the full equation as

$$\begin{aligned}\bar{\mathbf{x}}(t,\mathbf{K}) &= \boldsymbol{\mathcal{G}}(t,t_\mathrm{i})\,\mathbf{x}^{(\mathrm{i})} + \int_{t_\mathrm{i}}^{t} \mathrm{d}t'\,\boldsymbol{\mathcal{G}}(t,t')\left(\boldsymbol{\mathcal{J}}\boldsymbol{\nabla}V(\vec{q},t') - \mathbf{K}(t')\right) \\ &= \bar{\mathbf{x}}(t) - \int_{t_\mathrm{i}}^{t} \mathrm{d}t'\,\boldsymbol{\mathcal{G}}(t,t')\,\mathbf{K}(t')\,. \end{aligned} \tag{A.6}$$

We can thus execute the path integral over the phase-space coordinates to find

$$\begin{aligned}\langle \Phi_{B_1}\rangle &= \mathrm{i}\int \mathrm{d}\Gamma_\mathrm{i} \sum_{j=1}^{N} \vec{k}_1 \cdot \frac{\delta}{\mathrm{i}\delta \vec{K}_{p_j}(t_1)} \times \\ &\qquad \exp\left\{-\mathrm{i}\vec{k}_1 \cdot \left(\bar{\vec{q}}_j(t_1) - \mathcal{P}_q^{\mathrm{T}} \int_{t_\mathrm{i}}^{t_1} \mathrm{d}t'\,\mathcal{G}(t_1,t')\,\vec{K}_j(t')\right)\right\}\Big|_{\mathbf{K}=0} \\ &= -\mathrm{i}\int \mathrm{d}\Gamma_\mathrm{i} \sum_{j=1}^{N} \vec{k}_1 \cdot \left(\mathrm{g}_{qp}(t_1,t_1)\,\vec{k}_1\right) \exp\left\{-\mathrm{i}\vec{k}_1 \cdot \bar{\vec{q}}_j(t_1)\right\} = 0\,, \end{aligned} \tag{A.7}$$

where $\mathcal{P}_q$ is the projection operator defined in (3.54). We see that the correlator vanishes due to $g_{qp}(t_1,t_1) = 0$, which is a purely causal argument. We move on to the two-point correlator. We can repeat the calculation from the one-point case to find

$$\begin{aligned}\langle \Phi_{B_1}\Phi_{B_2}\rangle &= \mathrm{i}^2\int \mathrm{d}\Gamma_\mathrm{i} \sum_{i=1}^{N}\sum_{j=1}^{N} \left(\vec{k}_1 \cdot \frac{\delta}{\mathrm{i}\delta \vec{K}_{p_i}(t_1)}\right)\left(\vec{k}_2 \cdot \frac{\delta}{\mathrm{i}\delta \vec{K}_{p_j}(t_2)}\right) \times \\ &\qquad \exp\left\{-\mathrm{i}\vec{k}_1 \cdot \left(\bar{\vec{q}}_i(t_1) - \mathcal{P}_q^{\mathrm{T}} \int_{t_\mathrm{i}}^{t_1} \mathrm{d}t'\,\mathcal{G}(t_1,t')\,\vec{K}_i(t')\right)\right\} \times \\ &\qquad \exp\left\{-\mathrm{i}\vec{k}_2 \cdot \left(\bar{\vec{q}}_j(t_2) - \mathcal{P}_q^{\mathrm{T}} \int_{t_\mathrm{i}}^{t_2} \mathrm{d}t'\,\mathcal{G}(t_2,t')\,\vec{K}_j(t')\right)\right\}\Big|_{\mathbf{K}=0} \\ &= (-\mathrm{i})^2 \sum_{i=1}^{N}\sum_{j=1}^{N} \exp\left\{-\mathrm{i}\left(\vec{k}_1 \cdot \bar{\vec{q}}_i(t_1) + \vec{k}_2 \cdot \bar{\vec{q}}_j(t_2)\right)\right\} \times \\ &\qquad \left(\vec{k}_1 \cdot \left(\vec{k}_1\,\mathrm{g}_{qp}(t_1,t_1) + \delta_{ij}\,\vec{k}_2\,\Theta(t_2-t_1)\,\mathrm{g}_{qp}(t_2,t_1)\right)\right) \times \\ &\qquad \left(\vec{k}_2 \cdot \left(\delta_{ij}\,\vec{k}_1\,\Theta(t_1-t_2)\,\mathrm{g}_{qp}(t_1,t_2) + \vec{k}_2\,\mathrm{g}_{qp}(t_2,t_2)\right)\right) \\ &= -\sum_{i=1}^{N} \exp\left\{-\mathrm{i}\left(\vec{k}_1 \cdot \bar{\vec{q}}_i(t_1) + \vec{k}_2 \cdot \bar{\vec{q}}_i(t_2)\right)\right\} \times \\ &\qquad (\vec{k}_1 \cdot \vec{k}_2)^2\,\Theta(t_1-t_2)\,\Theta(t_2-t_1)\,\mathrm{g}_{qp}(t_1,t_2)\,\mathrm{g}_{qp}(t_2,t_1) = 0\,. \end{aligned} \tag{A.8}$$

We again see that the correlator vanishes due to a causality argument which is exactly the same as the one employed in the proof of Theorem 1. This will also hold for all higher n-point cases, so that we can finally state

$$\langle \Phi_{B_1}\ldots\Phi_{B_n}\rangle = 0 \quad \Rightarrow \quad G_{\Phi_{B_1}\ldots\Phi_{B_n}} = 0\,. \tag{A.9}$$

B

CUMULANT PERTURBATION EXPANSION IN THE CANONICAL ENSEMBLE

Working in the canonical ensemble, our goal is to find the cumulant analogue of the correlator perturbation expansion (2.58) in the one and two-point case up to second order in the interaction potential. Our starting point is the general definition (2.46) of the cumulants. We use the various shorthand notations employed throughout section 4.3. We can define non-interacting cumulants by

$$G^{(0)}_{\alpha_1\dots\alpha_n} := \hat{H}_{\alpha_1}\dots\hat{H}_{\alpha_n} W^{(0)}[H,\mathbf{J},\mathbf{K}]\big|_0 \,, \tag{B.1}$$

where we have the relation

$$W^{(0)}[H,\mathbf{J},\mathbf{K}] = \ln Z_{\mathrm{C},0}[H,\mathbf{J},\mathbf{K}] \quad \Rightarrow \quad Z_{\mathrm{C},0}[H,\mathbf{J},\mathbf{K}] = \mathrm{e}^{W^{(0)}[H,\mathbf{J},\mathbf{K}]} \,. \tag{B.2}$$

Note that it also holds that $Z_{\mathrm{C},0}[H,\mathbf{J},\mathbf{K}]\big|_0 = 1$ as long as the initial phase-space probability density $\mathcal{P}(\mathbf{x}^{(\mathrm{i})})$ is normalised properly. In the following calculations we will encounter many functional derivatives of $W^{(0)}$. For the sake of easier notation we break with our custom of using greek letters for field labels and use latin characters instead, but still understand all other notational principles described in section 1.2.2 to apply. Derivatives will be denoted as

$$\hat{H}_{a_1}\dots\hat{H}_{a_n} W^{(0)}[H,\mathbf{J},\mathbf{K}] = W^{(0)}_{a_1\dots a_n} \quad \Rightarrow \quad W^{(0)}_{a_1\dots a_n}\big|_0 = G^{(0)}_{a_1\dots a_n} \,. \tag{B.3}$$

We start with the one-point cumulant. Combining (2.46) with (B.1) we have

$$\begin{aligned} G_a &= \hat{H}_a \ln Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}]\big|_0 = \frac{1}{Z_{\mathrm{C}}[0]}\hat{H}_a\left(\mathrm{e}^{\mathrm{i}\hat{S}_I} Z_{\mathrm{C},0}[H,\mathbf{J},\mathbf{K}]\right)\big|_0 \\ &= \mathrm{e}^{\mathrm{i}\hat{S}_I}\hat{H}_a\,\mathrm{e}^{W^{(0)}}\big|_0 = \mathrm{e}^{\mathrm{i}\hat{S}_I}\left(W^{(0)}_a\,\mathrm{e}^{W^{(0)}}\right)\big|_0 \\ &= \left(1+\frac{1}{2}\left(\mathrm{i}\sigma_{bc}\hat{H}_b\hat{H}_c\right)+\frac{1}{8}\left(\mathrm{i}\sigma_{bc}\hat{H}_b\hat{H}_c\right)\left(\mathrm{i}\sigma_{de}\hat{H}_d\hat{H}_e\right)+\dots\right)\left(W^{(0)}_a\,\mathrm{e}^{W^{(0)}}\right)\big|_0 \,. \end{aligned} \tag{B.4}$$

We also note at this point that in the second line one could in principle apply the same reasoning that leads to the self-consistent perturbation theory of the grand-canonical ensemble, i. e. one would try to commute the interaction operator with $W^{(0)}_a$ in order to reobtain the full generating functional on the RHS. While this must lead to the same result, it would however be a somewhat more complicated affair to

do this calculation explicitly since in the canonical ensemble we do not have a simple expression for $W^{(0)}$ like its grand canonical counterpart (4.15). We thus have chosen to take the route employed in (2.58) and expand the interaction operator in orders of the potential σ_{bc}. As they always occur together we absorb the imaginary units into the potential $\mathrm{i}\sigma_{bc} \to \sigma_{bc}$. The first term just gives the non-interacting one-point cumulant

$$\left(W_a^{(0)}\,\mathrm{e}^{W^{(0)}}\right)\big|_0 = G_a^{(0)}\,. \tag{B.5}$$

The second term is already more involved and gives

$$\begin{aligned}
&\frac{1}{2}\left(\sigma_{bc}\hat{H}_b\hat{H}_c\right)\left(W_a^{(0)}\,\mathrm{e}^{W^{(0)}}\right)\big|_0 = \frac{1}{2}\sigma_{bc}\hat{H}_c\left(\left(W_{ab}^{(0)} + W_a^{(0)}W_b^{(0)}\right)\mathrm{e}^{W^{(0)}}\right)\big|_0 \\
&= \frac{1}{2}\sigma_{bc}\left(W_{abc}^{(0)} + W_a^{(0)}W_{bc}^{(0)} + W_{ac}^{(0)}W_b^{(0)} + W_{ab}^{(0)}W_c^{(0)} + W_a^{(0)}W_b^{(0)}W_c^{(0)}\right)\mathrm{e}^{W^{(0)}}\big|_0 \\
&= \frac{1}{2}G_{abc}^{(0)}\sigma_{bc} + \frac{1}{2}G_a^{(0)}G_{bc}^{(0)}\sigma_{bc} + G_{ab}^{(0)}\sigma_{bc}G_c^{(0)} + \frac{1}{2}G_a^{(0)}G_b^{(0)}\sigma_{bc}G_c^{(0)} \\
&= \frac{1}{2}G_{abc}^{(0)}\sigma_{bc} + G_{ab}^{(0)}\sigma_{bc}G_c^{(0)}\,.
\end{aligned} \tag{B.6}$$

In the third line we have used the symmetry $\sigma_{bc} = \sigma_{cb}$ in order to combine terms. In the last line we have used that $G_b^{(0)}\sigma_{bc}G_c^{(0)} = 2G_{\rho_1}^{(0)}\sigma_{\rho_1 B_2}G_{B_2}^{(0)} = 0$ since $G_{B_1}^{(0)} = 0$ and that $G_{bc}^{(0)}\sigma_{bc} = G_{\rho_1 B_2}^{(0)}\sigma_{\rho_1 B_2} = 0$ due to causality. With the help of the second line of (B.6) the second order term is obtained as

$$\begin{aligned}
&\frac{1}{8}\left(\sigma_{bc}\hat{H}_b\hat{H}_c\right)\left(\sigma_{de}\hat{H}_d\hat{H}_e\right)\left(W_a^{(0)}\,\mathrm{e}^{W^{(0)}}\right)\big|_0 \\
&= \frac{1}{8}\left(\sigma_{de}\hat{H}_d\hat{H}_e\right)\sigma_{bc}\Big[\Big(W_{abc}^{(0)} + W_a^{(0)}W_{bc}^{(0)} + W_{ac}^{(0)}W_b^{(0)} + W_{ab}^{(0)}W_c^{(0)} \\
&\quad + W_a^{(0)}W_b^{(0)}W_c^{(0)}\Big)\mathrm{e}^{W^{(0)}}\Big]\big|_0 \\
&= \frac{1}{8}\sigma_{bc}\sigma_{de}\hat{H}_e\Big[\Big(W_{abcd}^{(0)} + W_a^{(0)}W_{bcd}^{(0)} + W_b^{(0)}W_{acd}^{(0)} + W_c^{(0)}W_{abd}^{(0)} + W_d^{(0)}W_{abc}^{(0)} \\
&\quad + W_{ab}^{(0)}W_{cd}^{(0)} + W_{ac}^{(0)}W_{bd}^{(0)} + W_{ad}^{(0)}W_{bc}^{(0)} + W_{ab}^{(0)}W_c^{(0)}W_d^{(0)} + W_{ac}^{(0)}W_b^{(0)}W_d^{(0)} \\
&\quad + W_{ad}^{(0)}W_b^{(0)}W_c^{(0)} + W_{bc}^{(0)}W_a^{(0)}W_d^{(0)} + W_{bd}^{(0)}W_a^{(0)}W_c^{(0)} + W_{cd}^{(0)}W_a^{(0)}W_b^{(0)} \\
&\quad + W_a^{(0)}W_b^{(0)}W_c^{(0)}W_d^{(0)}\Big)\mathrm{e}^{W^{(0)}}\Big]\big|_0\,.
\end{aligned} \tag{B.7}$$

We stop at this point because executing the last derivative will inflate the entire expression to an enormous extent. On the other hand we can already see a general pattern emerging in the above calculation. At the m-th interaction order we need to consider all ways how we can distribute the $2m$ internal field labels and the one external label a over products of cumulants of all n-point orders between 1 and m. It will thus be easier to just group the various possible 'topologies' of terms and consider representatives for each of them. For example $W_{ab}^{(0)}W_c^{(0)}W_d^{(0)}$ and $W_{bc}^{(0)}W_a^{(0)}W_d^{(0)}$ are topologically equivalent while $W_{ab}^{(0)}W_{cd}^{(0)}$ is topologically distinct from them. One then has to consider all possible ways how one can contract labels of these expres-

sions with the interaction matrix and assign symmetry factors. If we do this for the second order term we finally find

$$\begin{aligned}
&\frac{1}{8}\left(\sigma_{bc}\hat{H}_b\hat{H}_c\right)\left(\sigma_{de}\hat{H}_d\hat{H}_e\right)\left(W_a^{(0)}\,\mathrm{e}^{W^{(0)}}\right)\big|_0 \\
&= \frac{1}{8}\sigma_{bc}\sigma_{de}\Big(G^{(0)}_{abcde} + 4\,G^{(0)}_{abcd}G^{(0)}_{e} + G^{(0)}_{a}G^{(0)}_{bcde} + 4\,G^{(0)}_{abd}G^{(0)}_{ce} + 4\,G^{(0)}_{a}G^{(0)}_{b}G^{(0)}_{cde} \\
&\quad + 4\,G^{(0)}_{abd}G^{(0)}_{c}G^{(0)}_{e} + 2\,G^{(0)}_{a}G^{(0)}_{bd}G^{(0)}_{ce} + 8\,G^{(0)}_{ab}G^{(0)}_{cd}G^{(0)}_{e} + 4\,G^{(0)}_{a}G^{(0)}_{bd}G^{(0)}_{c}G^{(0)}_{e}\Big)
\end{aligned} \tag{B.8}$$

We already dropped terms that contained factors of the same form already dropped in (C.6). We can now drop a few more terms. First off we have

$$G^{(0)}_{bcde}\sigma_{bc}\sigma_{de} = 4\,G^{(0)}_{\rho_1 B_2\rho_3 B_4}\sigma_{\rho_1 B_2}\sigma_{\rho_3 B_4} = 0 \tag{B.9}$$

due to causality. Both B_2 and B_4 need other fields to whose time argument they can direct their time flow contained in their b factors (see (4.31)). But the Dirac delta distributions w. r. t. time in the potentials have reduced all time arguments to either t_2 or t_4. With only B field time arguments remaining we can use the arguments presented in Theorem 1. The same argument also holds for

$$\begin{aligned}
G^{(0)}_{bd}G_{ce}\sigma_{bc}\sigma_{de} &= 2\,G^{(0)}_{\rho_1 B_3}G^{(0)}_{B_2\rho_4}\sigma_{\rho_1 B_2}\sigma_{B_3\rho_4} = 0 \\
G^{(0)}_{b}\sigma_{bc}G_{cde}\sigma_{de} &= 2\,G^{(0)}_{\rho_1}\sigma_{\rho_1 B_2}G^{(0)}_{B_2\rho_3 B_4}\sigma_{\rho_3 B_4} = 0\,,
\end{aligned} \tag{B.10}$$

where we have again used $G^{(0)}_B = 0$ in the second equation. This also leads to

$$G^{(0)}_{bd}G^{(0)}_{c}G^{(0)}_{e}\sigma_{bc}\sigma_{de} = G^{(0)}_{B_1B_3}G^{(0)}_{\rho_2}G^{(0)}_{\rho_4}\sigma_{B_1\rho_2}\sigma_{B_3\rho_4} = 0\,, \tag{B.11}$$

since $G^{(0)}_{BB} = 0$. We can now write down the perturbation expansion of the one-point cumulant up to second order in the interaction as

$$\begin{aligned}
G^{(2)}_a = G^{(0)}_a &+ \frac{1}{2}G^{(0)}_{abc}\sigma_{bc} + \frac{1}{8}G^{(0)}_{abcde}\sigma_{bc}\sigma_{de} \\
&+ G^{(0)}_{ab}\sigma_{bc}\left(G^{(0)}_{c} + \frac{1}{2}G^{(0)}_{cde}\,\sigma_{de} + G^{(0)}_{cd}\sigma_{de}G^{(0)}_{e}\right) \\
&+ \frac{1}{2}G^{(0)}_{abcd}\,\sigma_{bc}\sigma_{de}G^{(0)}_{e} + \frac{1}{2}G^{(0)}_{abd}\,\sigma_{bc}\sigma_{de}G^{(0)}_{c}G^{(0)}_{e} + \frac{1}{2}G^{(0)}_{abd}\,\sigma_{bc}\sigma_{de}G^{(0)}_{ce}\,.
\end{aligned} \tag{B.12}$$

If we would restrict the equation only to first order terms we find

$$G^{(1)}_a = G^{(0)}_a + \frac{1}{2}G^{(0)}_{abc}\,\sigma_{bc} + G^{(0)}_{ab}\sigma_{bc}G^{(0)}_{c} \tag{B.13}$$

and we immediately recognize this as the expression in parentheses in the second line of (B.12). We can furthermore identify its first line with the second order expansion of $G^{(\mathrm{c})}$ which we denote as

$$G^{(\mathrm{c},2)}_a = G^{(0)}_a + \frac{1}{2}G^{(0)}_{abc}\,\sigma_{bc} + \frac{1}{8}G^{(0)}_{abcde}\,\sigma_{bc}\sigma_{de} \tag{B.14}$$

and can then write the second order expansion of G_a as

$$G_a^{(2)} = G_a^{(\mathrm{c},2)} + G_{ab}^{(0)}\sigma_{bc}G_c^{(1)} + \frac{1}{2}G_{abcd}^{(0)}\sigma_{bc}\sigma_{de}G_e^{(0)} + \frac{1}{2}G_{abd}^{(0)}\sigma_{bc}\sigma_{de}G_c^{(0)}G_e^{(0)} + \frac{1}{2}G_{abd}^{(0)}\sigma_{bc}\sigma_{de}G_{ce}^{(0)} \,. \tag{B.15}$$

Let us now promote terms in the following way. On the LHS we replace $G_a^{(2)} \to G_a$. In the second term of the RHS we promote $G_c^{(1)} \to G_c$ and in the third term $G_e^{(0)} \to G_e$. In the same way we promote $G_c^{(0)} \to G_c$ and $G_e^{(0)} \to G_e$ in the fourth term as well as $G_{ce}^{(0)} \to G_{ce}$ in the fifth term. We then find

$$G_a = G_a^{(\mathrm{c},2)} + \left(G_{ab}^{(0)} + G_{acdb}^{(0)}\sigma_{cd}\right)\sigma_{bc}G_c + \frac{1}{2}G_{abd}^{(0)}\sigma_{bc}\sigma_{de}G_cG_e + \frac{1}{2}G_{abd}^{(0)}\sigma_{bc}\sigma_{de}G_{ce} \,. \tag{B.16}$$

In the second term we can now identify the first order expansion $G_{ab}^{(\mathrm{c},1)}$. If we furthermore identify the remaining non-interacting cumulants as the zeroth order expansion of the respective $G^{(\mathrm{c})}$ functions and then promote all $G^{(\mathrm{c})}$ expansions to the full quantity we finally have

$$G_a = G_a^{(\mathrm{c})} + G_{ab}^{(\mathrm{c})}\sigma_{bc}G_c + \frac{1}{2}G_{abd}^{(\mathrm{c})}\sigma_{bc}\sigma_{de}G_cG_e + \frac{1}{2}G_{abd}^{(\mathrm{c})}\sigma_{bc}\sigma_{de}G_{ce} \,. \tag{B.17}$$

This is precisely the same as the perturbation expansion (4.101) we found in the grand canonical ensemble. The second order expansion (B.12) can also be obtained by solving (4.101) iteratively but only keeping terms which contain no more than two orders of the interaction when one writes them out explicitly. This demonstrates that the perturbative expansion of cumulants contains the same terms in both approaches and that one must thus be able to find the same self-consistent form in the canonical ensemble. The fact that this would nonetheless be more cumbersome in the canonical ensemble due to the reasons given after (B.4) highlights again that the main advantage of the grand canonical approach is the simple form of the free generating functional and the consequent reduction of combinatorial complexity in calculating the free cumulants.

We now also want to calculate the second order expansion of the two-point cumulant. We again start with its definition

$$\begin{aligned} G_{ab} &= \hat{H}_a\hat{H}_b \ln Z_{\mathrm{C}}[H,\mathbf{J},\mathbf{K}]\big|_0 = \hat{H}_a\left(\frac{1}{Z_{\mathrm{C}}}\mathrm{e}^{\mathrm{i}\hat{S}_I}W_b^{(0)}\mathrm{e}^{W^{(0)}}\right)\big|_0 \\ &= \frac{1}{Z_{\mathrm{C}}[0]}\mathrm{e}^{\mathrm{i}\hat{S}_I}\left(W_{ab}^{(0)} + W_a^{(0)}W_b^{(0)}\right)\mathrm{e}^{W^{(0)}}\big|_0 \\ &\quad - \frac{1}{(Z_{\mathrm{C}}[0])^2}\left(\mathrm{e}^{\mathrm{i}\hat{S}_I}W_a^{(0)}\mathrm{e}^{W^{(0)}}\right)\left(\mathrm{e}^{\mathrm{i}\hat{S}_I}W_b^{(0)}\mathrm{e}^{W^{(0)}}\right)\big|_0 \,. \end{aligned} \tag{B.18}$$

We alread know the second term from (B.12). We expand the first term

$$\left(1 + \frac{1}{2}\left(\sigma_{cd}\hat{H}_c\hat{H}_d\right) + \frac{1}{8}\left(\sigma_{cd}\hat{H}_c\hat{H}_d\right)\left(\sigma_{ef}\hat{H}_e\hat{H}_f\right) + \dots\right)\left(\left(W_{ab}^{(0)} + W_a^{(0)}W_b^{(0)}\right)\mathrm{e}^{W^{(0)}}\right)\big|_0$$

(B.19)

The zeroth order contribution from this together with the zeroth order contribution from the second term is

$$\left(W^{(0)}_{ab} + W^{(0)}_{a} W^{(0)}_{b}\right) \mathrm{e}^{W^{(0)}}|_0 - \left(W^{(0)}_{a} \mathrm{e}^{W^{(0)}}\right)\left(W^{(0)}_{b} \mathrm{e}^{W^{(0)}}\right)|_0 = G^{(0)}_{ab} \,. \tag{B.20}$$

The first order contribution from (B.19) is

$$\begin{aligned} &\sigma_{cd} \hat{H}_c \hat{H}_d \left(\left(W^{(0)}_{ab} + W^{(0)}_{a} W^{(0)}_{b}\right) \mathrm{e}^{W^{(0)}}\right)|_0 \\ &= \sigma_{cd} \hat{H}_d \left(W^{(0)}_{abc} + W^{(0)}_{ab} W^{(0)}_{c} + W^{(0)}_{ac} W^{(0)}_{b} + W^{(0)}_{bc} W^{(0)}_{a} + W^{(0)}_{a} W^{(0)}_{b} W^{(0)}_{c}\right) \mathrm{e}^{W^{(0)}}|_0 \,. \end{aligned} \tag{B.21}$$

At this point we can just read off the result from (B.7) and together with the first order contribution from the second term in (B.18) which we can directly take from (B.6) we find

$$\begin{aligned} &\frac{1}{2}\sigma_{cd}\left(G^{(0)}_{abcd} + G^{(0)}_{a} G^{(0)}_{bcd} + G^{(0)}_{b} G^{(0)}_{acd} + 2\, G^{(0)}_{abc} G^{(0)}_{d} + 2\, G^{(0)}_{ac} G^{(0)}_{db}\right. \\ &\left. + 2\, G^{(0)}_{a} G^{(0)}_{bc} G^{(0)}_{d} + 2\, G^{(0)}_{b} G^{(0)}_{ac} G^{(0)}_{d}\right) - G^{(0)}_{a} \sigma_{cd}\left(\frac{1}{2} G^{(0)}_{bcd} + G^{(0)}_{bc} G^{(0)}_{d}\right) \\ &- G^{(0)}_{b} \sigma_{cd}\left(\frac{1}{2} G^{(0)}_{acd} + G^{(0)}_{ac} G^{(0)}_{d}\right) \\ &= \frac{1}{2} G^{(0)}_{abcd}\, \sigma_{cd} + G^{(0)}_{abc}\, \sigma_{cd} G^{(0)}_{d} + G^{(0)}_{ac} \sigma_{cd} G^{(0)}_{cb} \,. \end{aligned} \tag{B.22}$$

The first order expansion thus has the form

$$G^{(1)}_{ab} = G^{(0)}_{ab} + \frac{1}{2} G^{(0)}_{abcd}\, \sigma_{cd} + G^{(0)}_{abc}\, \sigma_{cd} G^{(0)}_{d} + G^{(0)}_{ac} \sigma_{cd} G^{(0)}_{cb} \,. \tag{B.23}$$

The second order contribution can in principle be obtained by applying yet another instance of the interaction operator to (B.21). However, the calculation again becomes cumbersome to such an extent that it will be more sensible to employ the same strategy described for the second order contribution in the one-point case. Substracting the second order contribution from the second term in (B.18) we finally arrvive at

$$\begin{aligned} G^{(2)}_{ab} = G^{(0)}_{ab} &+ \frac{1}{2} G^{(0)}_{abcd}\, \sigma_{cd} + \frac{1}{8} G^{(0)}_{abcdef}\, \sigma_{cd}\sigma_{ef} \\ &+ G^{(0)}_{abc}\, \sigma_{cd}\left(G^{(0)}_{d} + \frac{1}{2} G^{(0)}_{def}\, \sigma_{ef} + G^{(0)}_{de} \sigma_{ef} G^{(0)}_{f}\right) + \frac{1}{2} G^{(0)}_{abcde}\, \sigma_{cd}\sigma_{ef} G^{(0)}_{f} \\ &+ G^{(0)}_{ac} \sigma_{cd}\left(G^{(0)}_{db} + \frac{1}{2} G^{(0)}_{defb}\, \sigma_{ef} + G^{(0)}_{de} \sigma_{ef} G^{(0)}_{fb} + G^{(0)}_{deb}\, \sigma_{ef} G^{(0)}_{f}\right) \\ &+ \frac{1}{2} G^{(0)}_{acde}\, \sigma_{cd}\sigma_{ef} G^{(0)}_{fb} \\ &+ \sigma_{cd}\sigma_{ef}\left(\frac{1}{2} G^{(0)}_{abce}\, G^{(0)}_{df} + \frac{1}{2} G^{(0)}_{abce}\, G^{(0)}_{d} G^{(0)}_{f} + \frac{1}{2} G^{(0)}_{ace}\, G^{(0)}_{dfb} + G^{(0)}_{ace}\, G^{(0)}_{f} G^{(0)}_{db}\right) \,. \end{aligned} \tag{B.24}$$

Just like in the one-point case we can identify first order terms, namely the first order result (B.13) for the one-point function as the parentheses in the second line and the first order two-point function (B.23) as the parentheses in the third line. The first line is the second order expansion $G^{(\mathrm{c},2)}_{ab}$ and we thus find

$$\begin{aligned} G^{(2)}_{ab} = G^{(\mathrm{c},2)}_{ab} &+ G^{(0)}_{abc}\,\sigma_{cd} G^{(1)}_{d} + \frac{1}{2} G^{(0)}_{abcde}\,\sigma_{cd}\sigma_{ef} G^{(0)}_{f} \\ &+ G^{(0)}_{ac}\sigma_{cd} G^{(1)}_{db} + \frac{1}{2} G^{(0)}_{acde}\,\sigma_{cd}\sigma_{ef} G^{(0)}_{fb} \\ &+ \sigma_{cd}\sigma_{ef}\left(\frac{1}{2} G^{(0)}_{abce}\, G^{(0)}_{df} + \frac{1}{2} G^{(0)}_{abce}\, G^{(0)}_{d} G^{(0)}_{f} + \frac{1}{2} G^{(0)}_{ace}\, G^{(0)}_{dfb} + G^{(0)}_{ace}\, G^{(0)}_{f} G^{(0)}_{db}\right) . \end{aligned} \tag{B.25}$$

Let us again do the same promotions as in the one-point case.

- On the LHS we promote $G^{(2)}_{ab} \to G_{ab}$.
- In the first line, we promote $G^{(1)}_{d} \to G_d$ and $G^{(0)}_{f} \to G_f$.
- In the second line, we analogously promote $G^{(1)}_{db} \to G_{db}$ and $G^{(0)}_{fb} \to G_{fb}$.
- In the last line we then promote every first cumulant in a term as $G^{(0)}_{abce} \to G^{(\mathrm{c},0)}_{abce}$ and all other cumulants in a term to its full counterpart as e. g. $G^{(0)}_{df} \to G_{df}$ in the first term.

With these promotions we arrive at

$$\begin{aligned} G_{ab} = G^{(\mathrm{c},2)}_{ab} &+ G^{(\mathrm{c},1)}_{abc}\sigma_{cd} G_d + G^{(\mathrm{c},1)}_{ac}\sigma_{cd} G_{db} \\ &+ \frac{1}{2}\sigma_{cd}\sigma_{ef}\left(G^{(\mathrm{c},0)}_{abce} G_{df} + G^{(\mathrm{c},0)}_{abce} G_d G_f + \frac{1}{2} G^{(\mathrm{c},0)}_{ace} G_{dfb} + G^{(\mathrm{c},0)}_{ace} G_f G_{db}\right) . \end{aligned} \tag{B.26}$$

If we then promote all $G^{(\mathrm{c},n)}$ to their full counterpart we finally find

$$\begin{aligned} G_{ab} = G^{(\mathrm{c})}_{ab} &+ G^{(\mathrm{c})}_{abc}\,\sigma_{cd} G_d + G^{(\mathrm{c})}_{ac}\,\sigma_{cd} G_{db} \\ &+ \frac{1}{2} G^{(\mathrm{c})}_{abce}\,\sigma_{cd}\sigma_{ef}\left(G_{df} + G_d G_f\right) + \frac{1}{2} G^{(\mathrm{c})}_{ace}\,\sigma_{cd}\sigma_{ef}\left(G_{dfb} + 2\, G_f G_{db}\right) , \end{aligned} \tag{B.27}$$

which we recognize as the second order self-consistent equation (4.103). Just like in the one-point case we could go the other way by solving (4.103) iteratively and then only keeping terms which are explicitly second order in σ_{cd}.

C

ON THE MEAN DENSITY

We want to show that in our case of a statistically homogeneous and isotropic system the mean particle number density $\bar{\rho}$ is not affected by interactions, i. e. $G_\rho = G_\rho^{(0)}$. A general proof is complicated in the self-consistent form of the perturbation theory because we need to make assumptions about the full cumulants. It seems more promising to find the reformulation of perturbation theory alluded to in section 4.3.5. There, both the basic propagator and vertices in form of non-interacting cumulants should be known exactly and one can then hope to find a general argument why diagrams of arbitrary loop order with only one external leg must vanish. Nonetheless we will show that any contribution to G_ρ in the self-consistent perturbation expansion up to second order vanishes, showing that our claim is at least justified. We start with the full second order equation with all tadpole terms set to zero

$$G_{\rho_1} = G^{(\mathrm{c})}_{\rho_1} + \frac{\mathrm{i}^2}{2} G^{(\mathrm{c})}_{\rho_1\mu\nu}\, \sigma_{\mu\alpha}\sigma_{\nu\beta} G_{\alpha\beta}\ . \tag{C.1}$$

Expanding the first term up to second order we find with the help of Corollary 4

$$\begin{aligned} G^{(\mathrm{c})}_{\rho_1} &= G^{(0,1)}_{\rho_1} + \mathrm{i}\left(G^{(0,1)}_{\rho_1\rho_2 B_3} + G^{(0,2)}_{\rho_1\rho_2 B_3}\right)\sigma_{\rho_2 B_3} \\ &\quad + \frac{\mathrm{i}^2}{2}\left(G^{(0,1)}_{\rho_1\rho_2 B_3\rho_4 B_5} + G^{(0,2)}_{\rho_1\rho_2 B_3\rho_4 B_5} + G^{(0,3)}_{\rho_1\rho_2 B_3\rho_4 B_5}\right)\sigma_{\rho_2 B_3}\sigma_{\rho_4 B_5} \\ &= G^{(0,1)}_{\rho_1} + \mathrm{i} G^{(0,2)}_{\rho_1\rho_2 B_3}\sigma_{\rho_2 B_3} + \frac{\mathrm{i}^2}{2}\left(G^{(0,2)}_{\rho_1\rho_2 B_3\rho_4 B_5} + G^{(0,3)}_{\rho_1\rho_2 B_3\rho_4 B_5}\right)\sigma_{\rho_2 B_3}\sigma_{\rho_4 B_5}\ . \end{aligned} \tag{C.2}$$

In the second step we used that all contractions of one-particle cumulants will lead to self-interactions in the sense of (4.123) and must thus vanish. Let us look at the second term in the above last line. In the language of section 4.2.4 there are only two non-vanishing label groupings here. The first is $(1;2,3)$ which leads to self-interaction of the particle carrying labels 2 and 3 and thus vanishes in the sense of (4.123). The second grouping is $(2;1,3)$ which has the overall prefactor

$$b(2;1,3) = \vec{k}_3 \cdot \vec{k}_1\, \mathrm{g}_{13} \tag{C.3}$$

due to the label 3 coming from a Φ_B field. But we also have

$$\begin{aligned} G^{(0,2)}_{\rho_1\rho_2 B_3}\sigma_{\rho_2 B_3} &\propto \int \mathrm{d}2 \int \mathrm{d}3\, (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_2 + \vec{k}_3)\, (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_2 + \vec{k}_3)\, v(k_2) \times \\ &\qquad \delta_{\mathrm{D}}(t_2 - t_3)\, \bar{G}^{(0,2)}_{\rho_1\rho_2 B_3} \\ &= \int \mathrm{d}2\, (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_1)\, v(k_2)\, \bar{G}^{(0,2)}_{\rho_1\rho_2 B_{-2}} \end{aligned}$$

$$
\begin{aligned}
&= \bar{\rho}^2 \int \mathrm{d}2\, (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_1)\, v(k_2) \left(-\vec{k}_2 \cdot \vec{k}_1\, \mathrm{g}_{12}\right) \mathcal{T}^{(2)}_{1|2}(2;1,3) \\
&= 0\,, \qquad \text{(C.4)}
\end{aligned}
$$

where $\bar{G}^{(0,\ell)}_{\alpha_1\ldots\alpha_n}$ is to be understood in the sense of (4.119). By analoguous calculations we also find that the two remaining terms in (C.2) have an overall prefactor $\delta_{\mathrm{D}}(\vec{k}_1)$. Consequently we only have to investigate the structure of the b factors of the individual groupings to show that they vanish. For the $G^{(0,2)}_{\rho_1\rho_2 B_3\rho_4 B_5}$ term there are again only two groupings that do not vanish due to self-interaction or causality in the sense of Theorem 1. For these two we find

$$
\begin{aligned}
\delta_{\mathrm{D}}(\vec{k}_1)\, b(1,3,4;2,5) &= \delta_{\mathrm{D}}(\vec{k}_1) \left(\vec{k}_3 \cdot \left(\vec{k}_1\, \mathrm{g}_{13} + \vec{k}_4\, \mathrm{g}_{43}\right)\right) \left(\vec{k}_5 \cdot \vec{k}_2\, \mathrm{g}_{25}\right) \\
&= \delta_{\mathrm{D}}(\vec{k}_1) \left(\vec{k}_3 \cdot \vec{k}_4\, \mathrm{g}_{43}\right) \left(\vec{k}_5 \cdot \vec{k}_2\, \mathrm{g}_{25}\right) \overset{\substack{3=-2\\5=-4}}{\to} \left(\vec{k}_2 \cdot \vec{k}_4\right)^2 \mathrm{g}_{42}\, \mathrm{g}_{24} = 0 \qquad \text{(C.5)}
\end{aligned}
$$

due to causality and similarly

$$
\begin{aligned}
\delta_{\mathrm{D}}(\vec{k}_1)\, b(1,2,5;3,4) &= \delta_{\mathrm{D}}(\vec{k}_1) \left(\vec{k}_5 \cdot \left(\vec{k}_1\, \mathrm{g}_{15} + \vec{k}_2\, \mathrm{g}_{25}\right)\right) \left(\vec{k}_3 \cdot \vec{k}_4\, \mathrm{g}_{43}\right) \\
&= \delta_{\mathrm{D}}(\vec{k}_1) \left(\vec{k}_5 \cdot \vec{k}_2\, \mathrm{g}_{25}\right) \left(\vec{k}_3 \cdot \vec{k}_4\, \mathrm{g}_{43}\right) \overset{\substack{3=-2\\5=-4}}{\to} \left(\vec{k}_2 \cdot \vec{k}_4\right)^2 \mathrm{g}_{42}\, \mathrm{g}_{24} \\
&= 0\,. \qquad \text{(C.6)}
\end{aligned}
$$

For the $G^{(0,3)}_{\rho_1\rho_2 B_3\rho_4 B_5}$ term things become even easier. We now have only three groupings that do not vanish after taking into account self-interaction and Theorem 1. The first of them vanishes purely due to causality as

$$
b(1;2,5;3,4) = \left(\vec{k}_5 \cdot \vec{k}_2\, \mathrm{g}_{25}\right) \left(\vec{k}_3 \cdot \vec{k}_4\, \mathrm{g}_{43}\right) \overset{\substack{3=-2\\5=-4}}{\to} \left(\vec{k}_2 \cdot \vec{k}_4\right)^2 \mathrm{g}_{24}\, \mathrm{g}_{42} = 0\,, \qquad \text{(C.7)}
$$

the second due to homogeneity as

$$
\delta_{\mathrm{D}}(\vec{k}_1)\, b(2;1,5;3,4) = \delta_{\mathrm{D}}(\vec{k}_1) \left(\vec{k}_5 \cdot \vec{k}_1\, \mathrm{g}_{15}\right) \left(\vec{k}_3 \cdot \vec{k}_4\, \mathrm{g}_{43}\right) = 0\,. \qquad \text{(C.8)}
$$

The third grouping is $(4;2,5;1,3)$ and vanishes analogously to (C.8). We thus have shown that $G^{(\mathrm{c})}_{\rho} = G^{(0,1)}_{\rho}$ up to second order in the interaction. The second term in (C.1) can be written out as

$$
G^{(\mathrm{c})}_{\rho_1\mu\nu}\sigma_{\mu\alpha}\sigma_{\nu\beta}G_{\alpha\beta} = G^{(0)}_{\rho_1 B_2 B_3}\sigma_{B_2\rho_4}\sigma_{B_3\rho_5}G_{\rho_3\rho_5} + 2\, G^{(0)}_{\rho_1\rho_2 B_3}\sigma_{\rho_2 B_4}\sigma_{B_3\rho_5}G_{B_4\rho_5}\,, \qquad \text{(C.9)}
$$

where we have used $G_{BB} = 0$ (see Appendix A) and since we only consider terms up to second order in $\sigma_{\mu\nu}$ we have set $G^{(\mathrm{c})}_{\rho_1\mu\nu} \to G^{(0)}_{\rho_1\mu\nu}$. Corollary 4 leads to $G^{(0)}_{\rho_1 B_2 B_3} = G^{(0,1)}_{\rho_1 B_2 B_3}$ and using (4.119) we find for the first term

$$
\begin{aligned}
G^{(0,1)}_{\rho_1 B_2 B_3}\sigma_{B_3\rho_5}G_{\rho_3\rho_5} &= \int \mathrm{d}2 \int \mathrm{d}t_3\, (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_1)\, \bar{G}^{(0,1)}_{\rho_1 B_2 B_3}\, v(k_2)^2\, \bar{G}_{\rho_{-2}\rho_{-3}} \\
&= \bar{\rho} \int \mathrm{d}2 \int \mathrm{d}t_3\, (2\pi)^d\, \delta_{\mathrm{D}}(\vec{k}_1) \left(\vec{k}_2 \cdot \left(\vec{k}_1\, \mathrm{g}_{12} + \vec{k}_3\, \mathrm{g}_{32}\right)\right) \times \\
&\quad \left(\vec{k}_3 \cdot \left(\vec{k}_1\, \mathrm{g}_{13} + \vec{k}_2\, \mathrm{g}_{23}\right)\right) v(k_2)^2\, \bar{G}_{\rho_{-2}\rho_{-3}}
\end{aligned}
$$

$$
\begin{aligned}
&= \bar{\rho} \int \mathrm{d}2 \int \mathrm{d}t_3 \, (2\pi)^d \, \delta_{\mathrm{D}}(\vec{k}_1) \left(\vec{k}_2 \cdot \vec{k}_3 \, \mathrm{g}_{32}\right) \left(\vec{k}_3 \cdot \vec{k}_2 \, \mathrm{g}_{23}\right) \times \\
&\quad v(k_2)^2 \, \bar{G}_{\rho_{-2}\rho_{-3}} \\
&= 0
\end{aligned} \tag{C.10}
$$

due to causality. For the second term we infer from Corollary 4 that $G^{(0)}_{\rho_1\rho_2 B_3} = G^{(0,1)}_{\rho_1\rho_2 B_3} + G^{(0,2)}_{\rho_1\rho_2 B_3}$. Causality also dictates that at every order in the interaction $G_{B_1\rho_2} \propto \Theta(t_2 - t_1)$. The principal structure of the term is the same as in (C.10) and as such we only look at the combination of the surviving Dirac delta distribution, the Heaviside function coming from the full $G_{B\rho}$ and the b factors. For the one-particle contribution we have

$$
\delta_{\mathrm{D}}(\vec{k}_1) \, \Theta(t_3 - t_2) \, b(1,2,3) = \delta_{\mathrm{D}}(\vec{k}_1) \, \Theta(t_3 - t_2) \, \vec{k}_3 \cdot \left(\vec{k}_1 \, \mathrm{g}_{13} + \vec{k}_2 \, \mathrm{g}_{23}\right) = 0 \,, \tag{C.11}
$$

where the first term vanishes because of to the Dirac delta distribution and thus due to homogeneity and the second because of the Heaviside function and thus due to causality. For the two-particle function we have two groupings that do not already vanish according to Theorem 1 and for those we find

$$
\begin{aligned}
\delta_{\mathrm{D}}(\vec{k}_1) \, \Theta(t_3 - t_2) \, b(1;2,3) &= \delta_{\mathrm{D}}(\vec{k}_1) \, \Theta(t_3 - t_2) \, \vec{k}_3 \cdot \vec{k}_2 \, \mathrm{g}_{23} = 0 \\
\delta_{\mathrm{D}}(\vec{k}_1) \, \Theta(t_3 - t_2) \, b(2;1,3) &= \delta_{\mathrm{D}}(\vec{k}_1) \, \Theta(t_3 - t_2) \, \vec{k}_3 \cdot \vec{k}_1 \, \mathrm{g}_{13} = 0 \,.
\end{aligned} \tag{C.12}
$$

Up to second order in the interaction we thus see that the one-loop term vanishes and we have in total

$$
G_{\rho_1} = G^{(0)}_{\rho_1} = \bar{\rho} \, (2\pi)^d \, \delta_{\mathrm{D}}(\vec{k}_1) \tag{C.13}
$$

as one would expect for a statistically homogeneous and isotropic system.

We now want to comment on why Das and Mazenko find a first order correction to the mean density. In [22], they also considered a statistically homogeneous and isotropic system which however explicitly obeys Newtonian mechanics and which is in equilibrium at the initial time t_{i}, i. e. the initial phase-space probability density is given by

$$
\mathcal{P}(\mathbf{x}^{(\mathrm{i})}) \propto \exp\left\{-\beta \mathcal{H}(\mathbf{x}^{(\mathrm{i})})\right\} = \exp\left\{-\beta \sum_{j=1}^{N} \left(\frac{\vec{p}^{\,(\mathrm{i})^2}}{2m} + V(\vec{q}_j^{\,(\mathrm{i})}, t)\right)\right\} \,, \tag{C.14}
$$

where $\beta = \frac{1}{k_{\mathrm{B}} T}$. There are no initial correlations. One can move the potential part of the above initial condition into the interaction matrix which then obtains the element

$$
\sigma_{\rho_1\rho_2} = (2\pi)^d \, \delta_{\mathrm{D}}(\vec{k}_1 + \vec{k}_2) \, \delta_{\mathrm{D}}(t_1 - t_{\mathrm{i}}) \, \delta_{\mathrm{D}}(t_2 - t_{\mathrm{i}}) \, v(k_1) \,. \tag{C.15}
$$

In this form of the theory one finds that the free cumulants obey time translation invariance (TTI), i. e. at the two-point level they only depend on $(t_1 - t_2)$. This invariance of the statistics is broken once corrections with the interaction matrix $\sigma_{\mu\nu}$ are computed due to the initial time t_{i} appearing in (C.15). In order to retain both

TTI and equilibrium Das and Mazenko [22] adopt what they call the 'field theory' protocol in [39]. They require a fluctuation-dissipation theorem (FDT) to hold for the two-point cumulants and push the initial time $t_\mathrm{i} \to -\infty$ wherever it appears as an integral boundary. To correct for this they introduce counterterms and with the help of the FDT they can then show that at first order in the self-consistent perturbation theory these exactly cancel against those terms coming from the initial condition $\sigma_{\rho\rho}$. One thus can describe a system in equilibrium by requiring the FDT to hold and using the initial time $t_\mathrm{i} \to -\infty$ whilst ignoring $\sigma_{\rho\rho}$. This however has consequences for the first order correction to the mean density. It is given by

$$G_{\rho_1} = G^{(0)}_{\rho_1} + G^{(0)}_{\rho_1 B_2} \sigma_{B_2\rho_3} G_{\rho_3} \,. \tag{C.16}$$

We assume the system to be in a static situation where G_{ρ_1} does not depend on time and we thus have

$$G_{\rho_1} = (2\pi)^d \, \delta_\mathrm{D}(\vec{k}_1) \, \bar{G}_\rho \tag{C.17}$$

with some constant $\bar{G}_\rho$. The non-interacting $G^{(0)}_{\rho B}$ cumulant is given in [22] as

$$G^{(0)}_{\rho_1 B_2} = \bar{\rho} \, (2\pi)^d \, \delta_\mathrm{D}(\vec{k}_1 + \vec{k}_2) \, \Theta(t_1 - t_2) \left(-\frac{k_1^2}{m} \right) (t_1 - t_2) \exp\left\{ -\frac{k_1^2}{2\beta m} (t_1 - t_2)^2 \right\} . \tag{C.18}$$

The second term of (C.16) then reads

$$\begin{aligned} G^{(0)}_{\rho_1 B_2} \sigma_{B_2\rho_3} G^{(0)}_{\rho_3} = \int \mathrm{d}2 \, \bar{\rho} \, (2\pi)^d \, \delta_\mathrm{D}(\vec{k}_1 + \vec{k}_2) \, \Theta(t_1 - t_2) \left(-\frac{k_1^2}{m} \right) (t_1 - t_2) \times \\ \mathrm{e}^{-\frac{k_1^2}{2\beta m}(t_1 - t_2)^2} \int \mathrm{d}3 \, (2\pi)^d \, \delta_\mathrm{D}(\vec{k}_2 + \vec{k}_3) \, \delta_\mathrm{D}(t_2 - t_3) \, (-v(k_2)) \times \\ (2\pi)^d \, \delta_\mathrm{D}(\vec{k}_3) \, \bar{G}_\rho \\ = -\bar{\rho} \, (2\pi)^d \, \delta_\mathrm{D}(\vec{k}_1) \, v(k_1) \, \beta \, \bar{G}_\rho \int_{t_\mathrm{i}}^{t_1} \mathrm{d}t_2 \left(-\frac{k_1^2}{\beta m} \right) (t_1 - t_2) \, \mathrm{e}^{-\frac{k_1^2}{2\beta m}(t_1 - t_2)^2} \end{aligned} \tag{C.19}$$

We focus on the remaining time integral and define $f(k_1) = -\frac{k_1^2}{\beta m}$ and $t = t_1 - t_2$. With $\mathrm{d}t = -\mathrm{d}t_2$ the integral can be solved exactly as

$$\int_0^{t_1 - t_\mathrm{i}} \mathrm{d}t \, f(k_1) \, t \, \mathrm{e}^{\frac{1}{2} f(k_1) \, t^2} = \int_0^{t_1 - t_\mathrm{i}} \mathrm{d}t \, \frac{\partial}{\partial t} \, \mathrm{e}^{\frac{1}{2} f(k_1) \, t^2} = \mathrm{e}^{\frac{1}{2} f(k_1)(t_1 - t_\mathrm{i})^2} - 1 \,. \tag{C.20}$$

Since $f(k) \leq 0$, the above exponential will tend to zero as $t_\mathrm{i} \to -\infty$. The complete first order equation in this limit is then

$$\begin{aligned} G_{\rho_1} = G^{(0)}_{\rho_1} + \bar{\rho} \, \beta \, v(k_1) \left((2\pi)^d \, \delta_\mathrm{D}(\vec{k}_1) \, \bar{G}_\rho \right) = G^{(0)}_{\rho_1} + \bar{\rho} \, \beta \, v(k_1) \, G_{\rho_1} \\ \Rightarrow G_{\rho_1} = \frac{G^{(0)}_{\rho_1}}{1 - \bar{\rho} \, \beta \, v(k_1)} \,. \end{aligned} \tag{C.21}$$

One can understand this entire scheme such that the system is in some state out of equilibrium at $t_\mathrm{i} \to -\infty$ and is then driven into equilibrium by the 'noise' that comes from the particle interactions over an infinite amount of time. Since the mean particle number density $\bar{\rho}$ now pertains to the non-interacting system out of equilibrium it may receive corrections in order to fullfill an equation of state for the equilibrium the system relaxes into.

We want to point out that the appearance of this correction strongly depends on the TTI of the statistics and taking limits in the appropriate order. If we do not have the $t_\mathrm{i} \to -\infty$ limit in (C.20) we see that taking the $\vec{k}_1 \to 0$ limit due to the leading Dirac delta distribution from (C.19) will put the integral to zero and we do not find a correction to the mean density. For the kind of systems we describe in this work these conditions are no longer met. Since we explicitly force the system to have a specific correlation structure at some initial time t_i with a fixed $\bar{\rho}$, the statistics cannot obey TTI. This can for example be seen in the time dependence of the two-particle contributions to the non-interacting two-point cumulant shown in (4.67) and (4.68). These are not invariant under time translation no matter the actual form of the particle propagator g_{qp} since they do not depend solely on the difference $g_1 - g_2$. If we consider our application to cosmology we even do not have TTI for the free dynamics since the Hubble expansion drains away the initial momentum of particles and we thus *do not* have $g_1 - g_2 \propto \tau_1 - \tau_2$. It is thus not surprising that for our system the mean density is unaffected by interactions.

D

TRANSFER FUNCTION FOR THE INITIAL POWER SPECTRUM

The initial power spectrum P_δ that serves as the input parameter for the calculation of general n-point density cumulants in any theory of structure formation must be obtained by following the linear evolution of density perturbations seeded by inflation through the radiation dominated epoch of the universe and the decoupling of matter from radiation thereafter. Since relativistic effects are important in this case one needs to employ numerical Boltzmann codes (cf. Bernardeau et al. [13] for references). The principal form one finds is

$$P_\delta(k) = A * k^{n_s}\, T^2(k)\,, \tag{D.1}$$

where n_s is the *primordial spectral index*, $T(k)$ is the transfer function and A is the amplitude. A primordial spectral index of unity corresponds to scale-independent fluctuations in the gravitational potential as predicted by inflationary models. Recent observations of the CMB by the Planck mission [49] have lead to $n_s \approx 0.96$, and we thus adopt $n_s = 1$ for simplicity. The transfer function is the actual result of the numerical Boltzmann codes. A collection of transfer function fits for different dark matter models can be found in Bardeen et al. [2], from which we take the following fitting formula valid for the case where there is much more dark matter than baryonic matter:

$$T(k) = \frac{\ln(1+2.34q)}{2.34q}\left(1+3.89q+(16.1q)^2+(5.46q)^3+(6.71q)^4\right)^{-1/4} \tag{D.2}$$

where the the dependence on k is contained in

$$q = \frac{k}{\Omega_{m_0} h^2 \left(\frac{h}{\mathrm{Mpc}}\right)}\,. \tag{D.3}$$

The mode k is understood to have dimensions h/Mpc in the above formula. Finally, the amplitude A is fixed by requiring that when one evolves the initial powerspectrum to the present day with the linear growth factor $D(t)$ its variance filtered on a scale of $\ell = 8\,\mathrm{Mpc}/h$ is given by

$$\sigma_8 \stackrel{!}{=} \left(\frac{D(z=0)}{D(z_\mathrm{i})}\right)^2 (4\pi) \int \frac{\mathrm{d}k}{(2\pi)^3}\, k^2\, P_\delta(k)\, W_L^2(k) \tag{D.4}$$

for which the Planck mission [49] found values around $\sigma_8 \approx 0.83$. We use $\sigma_8 = 0.8$ for simplicity. In the above formula $W_L^2(k)$ is the Fourier transform of some window

function with typical length scale L. We use a top-hat filter $W_L(\vec{q}) = \Theta(L - |\vec{q}|)$ in real space which leads to the Fourier transform

$$W_L(k) = \frac{3\left(\sin(kL) - (kL)\cos(kL)\right)}{(kL)^3} \,. \tag{D.5}$$

E

VELOCITY DISPERSION FROM INITIAL POWERSPECTRUM

We start with (4.49) and set $\vec{q}_i^{\,(\mathrm{i})} = \vec{q}_j^{\,(\mathrm{i})}$ to find

$$\begin{aligned} C_{p_i p_i} &= \int \frac{\mathrm{d}\vec{h}}{(2\pi)^3} \frac{\vec{h}\otimes\vec{h}}{h^2} P_\delta(h) \\ &= \int_0^\infty \mathrm{d}h \frac{h^2}{(2\pi)^3} \int_0^{2\pi} \mathrm{d}\varphi \int_{-1}^{1} \mathrm{d}\cos\theta \frac{P_\delta(h)}{h^2} \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix} \otimes \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix} \\ &= \int_0^\infty \mathrm{d}h \frac{P_\delta(h)}{(2\pi)^3} \int_0^{2\pi} \mathrm{d}\varphi \int_{-1}^{1} \mathrm{d}\cos\theta \begin{pmatrix} \sin^2\theta\cos^2\varphi & 0 & 0 \\ 0 & \sin^2\theta\sin^2\varphi & 0 \\ 0 & 0 & \cos^2\theta \end{pmatrix} . \end{aligned} \tag{E.1}$$

We can now use

$$\begin{aligned} \int_0^{2\pi} \mathrm{d}\varphi \, \sin^2\varphi &= \int_0^{2\pi} \mathrm{d}\varphi \, \cos^2\varphi = \pi \,, \\ \int_{-1}^{1} \mathrm{d}\cos\theta \, \sin^2\theta &= \int_{-1}^{1} \mathrm{d}\cos\theta \, (1-\cos^2\theta) = \frac{4}{3} \,, \\ \int_{-1}^{1} \mathrm{d}\cos\theta \, \cos^2\theta &= \frac{2}{3} \end{aligned} \tag{E.2}$$

to find that

$$C_{p_i p_i} = \int_0^\infty \mathrm{d}h \frac{P_\delta(h)}{(2\pi)^3} \frac{4\pi}{3} \mathcal{I}_3 = \frac{1}{3} \int \frac{\mathrm{d}\vec{h}}{(2\pi)^3} \frac{P_\delta(h)}{h^2} \mathcal{I}_3 = \sigma_p^2 \mathcal{I}_3 \,. \tag{E.3}$$

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