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How Many Higgs Bosons Does it Take

Consistency of Scalar Field Theories at High Energies

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Abstract

Computations of multiparticle scattering amplitudes in scalar field theories at high multiplicities hint at a rapid growth with the number of final state particles, rendering the theory in conflict with unitarity at high energies. This questions the validity of the perturbative approach or even the interpretation of the underlying quantum field theory. We study the quantum mechanical equivalent of high multiplicity amplitudes in $\lambda \phi^4$ -theory, namely transition amplitudes from the vacuum to highly excited states in the anharmonic oscillator with a quartic potential. Using recursive relations, we compute these amplitudes to high order in perturbation theory and provide evidence that they can be written in exponential form. By resummation techniques, we then construct its exponent beyond leading order and investigate the behaviour of the amplitudes in the region where tree-level perturbation theory violates unitarity constraints. We find that for both the single- and the double-well potential the resummed amplitudes are in agreement with unitarity bounds. We then extend our results to anharmonic oscillators with general monomial potentials and point out possible problems of perturbative expansions even in potentials with a single minimum. Finally, we comment on the relevance of our results for the field theoretical problem.

Zusammenfassung

Berechnungen von Mehrteilchen-Streuamplituden in skalaren Feldtheorien bei hohen Multiplizitäten deuten auf deren rapides Wachstum mit der Anzahl an Teilchen im Endzustand hin. Ein solches Verhalten steht im Widerspruch zur Unitarität der Theorie bei hohen Energien und stellt die Richtigkeit eines perturbativen Ansatzes oder sogar die Interpretation der zugrunde liegenden Quantenfeldtheorie infrage. Wir untersuchen das quantenmechanische Äquivalent der Amplituden bei hohen Multiplizitäten in $\lambda \phi^4$ -Theorie. Dies entspricht Übergangsamplituden vom Vakuum zu hochenergetischen Zuständen im quantenmechanischen anharmonischen Oszillator mit quartischem Potential. Mithilfe von Rekursionsrelationen berechnen wir die Amplituden bis zu hohen Ordnungen in Störungstheorie und liefern Hinweise, dass sie als Exponentialfunktion darstellbar sind. Mit Resummationstechniken konstruieren wir den Exponenten jenseits der führenden Ordnung und untersuchen das Verhalten der Amplituden in jener Region, in der Störungstheorie in führender Ordnung Unitarität verletzt. Wir finden heraus, dass für Potentiale sowohl mit einem als auch mit zwei entarteten Minima die resummierten Amplituden die Unitaritätseinschränkungen erfüllen. Schließlich erweitern wir unsere Resultate auf anharmonische Oszillatoren mit verallgemeinerten monomiellen Potentialen weisen auf potentielle Probleme von störungstheoretische Reihenentwicklungen sogar für Potentiale mit einem einzigen Minimum hin. Abschließend kommentieren wir die Relevanz unserer Resultate im Hinblick auf das feldtheoretische Problem.

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Preface

The research presented in this thesis was conducted at the Institute for Theoretical Physics at Heidelberg University from April 2016 to August 2019. The content of Chapter 3 is based on work in collaboration with Joerg Jaeckel (Heidelberg U.) and has been previously published in

- [1] J. Jaeckel and S. Schenk, "Exploring High Multiplicity Amplitudes in Quantum Mechanics," Phys. Rev. D **98** (2018) no.9, 096007, arXiv:1806.01857 [hep-ph]
- [2] J. Jaeckel and S. Schenk, "Exploring high multiplicity amplitudes: The quantum mechanics analogue of the spontaneously broken case," Phys. Rev. D **99** (2019) no.5, 056010, arXiv:1811.12116 [hep-ph].

In addition, some parts of Chapter 3 are based on work in progress in collaboration with Florent Baume (Madrid, Autonoma U., IFT) and Joerg Jaeckel (Heidelberg U.).

Furthermore, the author is endorser of the following paper not discussed in this thesis,

[3] G. Alonso-Álvarez, J. Gehrlein, J. Jaeckel and S. Schenk, "Very Light Asymmetric Dark Matter," to appear in JCAP, arXiv:1906.00969 [hep-ph].

1 Introduction

Current experimental measurements have lead high energy physics from the high energy frontier into an era of precision tests. The most recent milestones are the confirmation of the well established Standard Model of particle physics (SM) [5–7] by the Higgs boson discovery at the LHC experiments [8,9] as well as the observation of gravitational wave signals by advanced LIGO [10]. Apart from that, the lack of astonishing discoveries challenges our current research efforts and makes us reconsider our current understanding of the field.

In high energy theory, the situation before the Higgs discovery was different from today. It was expected that the LHC would almost certainly find something new, because otherwise the perturbative cross section for weak gauge boson scattering would violate unitarity bounds. Based on this observation, it was argued that either there is a Higgs boson with a mass below the TeV-scale, new degrees of freedom beyond the SM appear, or scattering processes of electroweak gauge bosons enter a non-perturbative regime [11,12]. A posteriori, this problem has been settled by the observation of a Higgs boson with a mass of 125 GeV.

The situation today is vastly different. So far, except for the Planck scale, where quantum gravity effects are expected to become important [13–15], there is no profound theoretical prediction for a fundamental energy scale at which new physics phenomena beyond the SM have to appear. Therefore, one might indeed wonder if the electroweak sector of the SM is valid up to arbitrarily high energies. Fortunately, the Higgs boson might be key in addressing this question. As it marks the ultimate test bed for the underlying framework of spontaneous symmetry breaking [16–21] in perturbative quantum field theory, it can give us insights towards where new physics phenomena beyond the SM might be hiding.

As a major example, to date it is not clear if the SM vacuum is stable or if it is subject to decay via tunneling [22–28]. Given the measured Higgs mass, the renormalization group flow of its self-coupling exhibits an energy scale below the Planck scale, where it may become negative. This would imply that the electroweak vacuum is not the global minimum of the action, as there can either be vacua of lower energy, or the scalar potential is not even bounded from below. Therefore, the SM vacuum may be unstable unless new physics phenomena appear that change the behaviour of the β -function. However the corresponding energy scale, where the vacuum becomes meta-stable, is expected to be around $\Lambda \sim 10^{10}\,\text{GeV}$ or even higher (see, e.g., [28]), which is far beyond the reach of any experiment in the near future.

In fact, analogously to the prediction of a new physics scale by unitarity constraints on scattering processes of weak gauge bosons before the Higgs discovery, the electroweak sector of the SM may indicate an energy scale where the theory behaves inconsistently. Due to the Adler-Bell-Jackiw anomaly [29, 30], electroweak interactions do not conserve the sum of baryon and lepton number, B + L, in the SM [31]. Processes inducing (B + L)-violation are given by transitions between vacua classified by their weak topological charge, while the amount of violation is determined by the change of that charge. Different paths in field space that interpolate between different vacuum configurations can minimize the height of the energy barriers between the vacua. The field configurations at the top of these barriers are called sphalerons [32, 33]. They have an associated energy given by the height of the barrier, which is of the order of 9 TeV in the SM [33]. If the energy available in a given process is much less than the sphaleron energy, B+L can only be violated by quantum tunneling, that can be described by well known instanton solutions [34, 35]. Their transition rate will typically be exponentially suppressed, $\exp(-2\pi/\alpha_w) \sim 10^{-80}$, practically rendering such a process unobservable. However, it was suggested that (B+L)-violating scattering processes induced by instantons may be enhanced in the electroweak theory at high energies [36–38]. This enhancement is associated to the production of a large number n_w of electroweak gauge and Higgs bosons, as the leading S-matrix elements are of order $n_w! \exp(-2\pi/\alpha_w)$. The factorial growth might eventually overcome the instanton suppression factor such that the cross section is drastically enhanced. Therefore, it is expected that the cross section reaches its unitarity limit at energies in the multi-TeV range, such that perturbation theory breaks down in the electroweak instanton sector.

Soon it has been realized that similar growth for multiparticle production at high energies is also present in topologically trivial theories without baryon- and lepton-number violation [39,40]. In fact, the problem appears in most weakly coupled theories, the most simple example being scalar $\lambda \phi^4$ -theory. At sufficiently high energies, the production of many particles in the final state becomes possible. Qualitatively, at leading order in perturbation theory, the production of n scalar particles by a few initial states will be proportional to $n! \lambda^{n/2}$. This is because for each additional pair of particles in the final state an additional power of the coupling is needed. At the same time, due to the lack of destructive interference between different Feynman diagrams, the number of tree graphs grows factorially (see also, e.g., [41,42]). Therefore, even at weak coupling, for a large number of bosons, $n \geq 1/\lambda$, the factorial factor eventually overcomes the power suppression of the small coupling, such that the tree-level amplitudes grow rapidly for large n.

Evidence for factorial growth of scattering amplitudes, corresponding to processes of the form $\phi^* \to \phi^n$ or $\phi\phi \to \phi^n$, is provided by perturbative [39, 40, 43–47] as well as semiclassical [48–51] calculations, rendering the theory in conflict with unitarity as $n \to \infty$. This raises questions about the consistency of the computational techniques or possibly even about the interpretation of the underlying quantum field theory itself. In particular, it has been conjectured that in the double scaling limit, $n \to \infty$ and $\lambda \to 0$ while keeping λn fixed, the amplitudes take on an exponential

form [52–56], $\mathcal{A} \sim \exp(F/\lambda)$, where the exponent F is a function of the combination λn only. Analogously to instanton suppression factors, this form signals an intrinsic non-perturbative nature of the corresponding amplitudes. Intriguingly, similar exponential structures have been recently discovered for scattering amplitudes in $\mathcal{N}=8$ supergravity [57–60].

From a theoretical point of view, as we will later confirm the exponential form in explicit perturbative computations in a quantum mechanical setting, there appears to be a very deep relation between (suitably resummed) perturbation theory and non-perturbative phenomena. Apparently, the perturbative ansatz intrinsically captures its non-perturbative counterpart. Naively, to some extent, this observation is in line with the theory of resurgence [61] and transseries expansions, which formalizes the idea that the asymptotic nature of perturbative series encode deep and valuable information about the exact answer. For instance, the formalism has already been successfully applied to quantum mechanics [62–73], (supersymmetric) quantum field theory [74–83] and topological string theory [84–88]. These results suggest that perturbation theory and non-perturbative physics are closely intertwined: an observation that we, to some extent, recover in our analysis of multiparticle production in scalar field theory. For a pedagogical introduction to resurgence theory see, e.g., [89, 90].

From a phenomenological point of view, in contrast to scalar field theory, in Yang-Mills theory gauge symmetry and on-shell conditions lead to diagrammatic cancellations in the calculation of scattering amplitudes (see, e.g., [91]) such that gluons do not violate unitarity. Still, it turns out that the corresponding amplitudes in a spontaneously broken gauge theory, e.g. a gauge-Higgs theory, exhibit factorial growth in the number of both particle species, i.e. in the number of scalars as well as of gauge bosons [92, 93].

These considerations can of course be applied to the Higgs sector of the SM. Here, the rapidly growing cross sections for multiparticle production give indications for an explicit energy scale $\Lambda \lesssim 1600\,\text{TeV}$ at tree level [94,95], beyond which unitarity constraints are violated. More refined (and more optimistic) computations indicate that this scale could also be much lower, possible even within reach of next generation colliders [95]. That is, remarkably, the Higgs boson essentially reveals an energy scale where *something* has to happen, if we do not want to give up on unitary quantum field theory¹. Therefore, in order to restore unitarity at high energies, either novel non-perturbative behaviour or possibly even new physics phenomena have to appear.

For example, a new physics phenomenon could come in form of a *Higgsplosion* and *Higgspersion* effect, recently proposed in [97]. It describes novel non-perturbative behaviour of a scalar field theory by suppressing the propagator at an energy scale where the scattering amplitudes become large, thereby effectively cutting off loop-integrals. If this energy scale is low, it was argued that this mechanism can potentially even address the hierarchy problem, while at the same time allowing for interesting particle phenomenology [98–100]. In addition, applied to

¹Even though it is a very natural assumption of a quantum theory, it may, of course, also be questioned [96].

the electroweak sector of the SM, the suppression of the scalar field propagator at a potentially low energy scale drastically changes the β -function of the theory. Therefore, provided that the SM is a *higgsplosive* theory, this can have severe consequences for the stability of the electroweak vacuum.

In fact, high multiplicity Higgs production can even be used to probe the Higgs potential beyond its vacuum. The above arguments can be reversed to obtain a classical scalar potential with a unitarity preserving behaviour at high energies. In particular, unitarity bounds on tree-level scattering imply that, asymptotically, the potential should at most grow as $V(\phi) \sim m^2 \phi^2 \log^2{(\phi/m)}$ for large field values [101]. That is, leading-order consistency conditions predict a behaviour for a scalar potential at large field values, that is drastically different from a prototypical quartic polynomial, such as in the electroweak sector of the SM.

In this thesis, we want to follow a different, slightly more conservative approach. The calculations of the scattering amplitudes associated to multiparticle production in scalar field theory that initially established unitarity violation for a large number of bosons in the final state mostly relied on perturbative or semiclassical techniques at leading order, or at most they included the first quantum correction [47, 52, 102]. Beyond that, conventional methods become intractable at higher loop-orders such that the perturbative results might question the validity of the approach at high energies or, equivalently, at high multiplicities. Indeed, there is the possibility that the rapid growth of the scattering amplitudes is merely an artefact of this approximation. Our approach is based on the assumption that the problem could be resolved by refined calculational techniques, i.e. by obtaining the *exact* amplitude without relying on perturbation theory to finite order.

In Chapter 3 we take some initial steps towards this idea. Here, we aim at shedding light on what are the relevant features giving rise to factorial growth of scattering amplitudes at high multiplicities. Furthermore, we address the question if this growth can be cured by improved computational techniques. Although, in the end, we are interested in quantum field theory, we consider a simplified, yet instructive toy model. That is, we study the quantum mechanical analogue of massive ϕ^4 -theory, i.e. the anharmonic oscillator with quartic coupling λ . Here, the scattering amplitudes for multiparticle production correspond to quantum mechanical transition amplitudes from the vacuum to highly excited states. Quantum mechanics has already been a rich testbed for investigations of the asymptotic behaviour of perturbation theory (see, e.g., [68, 103–108]). Most considerations, however, focussed on energy levels and wave functions in the ground state, with only a few notable exceptions [43, 109–114].

The quantum mechanical setting, in fact, enables us to explicitly perform computations to very high orders in perturbation theory. Powerful resummation techniques, such as exact perturbation theory [108, 115], then allow us to access to the large n regime of the perturbative expansion of the high multiplicity scattering amplitudes beyond the point where tree-level perturbation theory violates unitarity constraints.

Compared to our quantum mechanical toy system, we should, however, be aware

that, due to its higher-dimensional nature, quantum field theory is subject to additional complications, such as a nontrivial phase space or the presence of weakly coupled, asymptotic states. Nevertheless, our work can give important insights into possible features responsible for the rapid growth of the high multiplicity amplitudes. In particular, as we find that refined computational techniques restore unitarity at high energies, we are in turn lead to focus efforts of establishing new physics phenomena on those aspects of quantum field theory, that are genuinely different from quantum mechanics.

The structure of this work is as follows. In Chapter 2 we review the theoretical foundations of scattering processes in interacting quantum field theories. In particular, we demonstrate how to obtain S-matrix elements from a classical Lagrangian via the LSZ reduction. Then we introduce the basic notation and framework for the computation of multiparticle production in scalar field theories and derive the factorial growth of tree-level perturbation theory and beyond. Chapter 3 is devoted to a discussion of the quantum mechanical analogue of high multiplicity amplitudes in scalar field theories both with and without spontaneous symmetry breaking. In this setting, we use recursive relations to compute quantum mechanical transition amplitudes from the vacuum to highly excited states to high orders in perturbation theory. By doing so, we provide evidence that the transition amplitude is of exponential form. Using advanced resummation techniques, such as exact perturbation theory, we then construct the corresponding exponent beyond leading order and investigate the behaviour of the amplitude in the region where tree-level perturbation theory violates unitarity bounds. In particular, we show that the exponent remains negative at high energies, such that it avoids problems with unitarity. We finally extend our results in two ways. First, we generalize our methods to compute amplitudes involving more general local operators. Second, we consider potentials involving higher self-interaction terms, such as, e.g., the sextic oscillator and postulate a conjecture on the form of the transition amplitudes in these potentials. Finally, we briefly summarize and conclude in Chapter 4.

2 Quantum Fields and Particle Interactions

An important method for our studies of the fundamental building blocks of nature at the smallest length scales, or equivalently at the high energy frontier, are scattering experiments. The Standard Model of particle physics was originally built from the bottom-up by means of scattering experiments, including the discovery of the weak gauge bosons, quarks and gluons or, most recently, the Higgs boson.

A modern interpretation of measurements in particle scattering experiments relies on quantum field theory (QFT), which has proven extremely successful in the description of elementary particles and the interactions between them. Here, the key observable in the scattering of particles, that is measured in experiments, is the scattering cross section. Roughly speaking, it describes the probability of a certain particle interaction to take place as a function of the energies and momenta of the particles that are involved in the scattering process. A more refined quantity is the differential cross section, which, in addition, takes the angular distribution of the scattered particles into account. In any quantum theory the differential cross section is proportional to the norm squared of the quantum scattering amplitude, $d\sigma/d\Omega \propto |\mathcal{A}|^2$. Naively, this is, to some extent, analogous to the fact that the probability density (in position space) of a quantum particle is given by the norm squared of its wave function, $\rho = |\psi|^2$.

Therefore, scattering amplitudes determine physical observables and can, in the above sense, be understood as the fundamental ingredients of an interacting quantum theory. Even more importantly, they immediately bridge the gap between fundamental theory and experimental measurements. Over the years it has been realized that amplitudes themselves exhibit a rich mathematical structure and physical insights. In the following sections, we therefore want to discuss and explore several theoretical and phenomenological aspects of scattering amplitudes and scattering processes in quantum theories.

In our basic review of scattering processes in quantum field theory, we closely follow the standard textbook [116]. For a more modern interpretation of scattering amplitudes, we refer the reader to [117].

2.1 Scattering processes in quantum field theory

In a quantum theory, a scattering process can be considered as a transition from an initial state $|i\rangle$ to a final state $|f\rangle$, each being a particle state that is characterized by particle species and corresponding momenta. Formally, this can be achieved by the scattering operator S, also called the S-matrix, which maps the initial states to the final states, $\langle f|S|i\rangle$. That is, the probability of scattering from the initial state $|i\rangle$ to a given final state $|f\rangle$ is given by $|\langle f|S|i\rangle|^2$. We can also separate the trivial part from the S-matrix, i.e. the part of the interaction process where no scattering occurs, by writing

$$S = 1 + iT. (2.1)$$

The scattering amplitude that determines the differential cross section of the scattering process $|i\rangle \rightarrow |f\rangle$ is then given by the corresponding T-matrix element, $\mathcal{A} = \langle f|T|i\rangle$.

Almost by definition, a nontrivial scattering process in any quantum theory requires interactions between the particles that are involved. In quantum field theories with a Lagrangian description, interactions are described by potentials, that can be understood as formal power series in the fields beyond quadratic order. To preserve causality in the interacting quantum theory, the particle interactions have to be localized in spacetime. That is, the terms of the potential may only involve fields evaluated at the same spacetime point, e.g. terms of the form $\phi(x)\phi(y)$ are not allowed.

In high energy physics, one of the major aims is to find an exact solution of any interacting quantum field theory, i.e. to determine the spectrum and compute all interactions *exactly*. So far, this has only been possible for theories with a lot of symmetry, such as certain conformal field theories in two dimensions or four-dimensional QFTs with enough supersymmetry. In practice, however, one often has to treat the interaction terms of the potential as a perturbation of the free theory and apply perturbation theory. One then requires that the perturbation is small enough to obtain a reasonable approximation of the exact answer.

Perturbative expansions of scattering amplitudes have a remarkably simple structure. In fact, they can be computed and visualized to arbitrary order by means of Feynman diagrams. Let us briefly recall this diagrammatic way of computing scattering amplitudes in the following section.

2.1.1 The LSZ reduction

So far, our discussion of scattering processes in quantum theories has been rather conceptual. In this and also the following section, we want to discuss how to obtain scattering amplitudes and cross sections in an interacting quantum field theory in practice. That is, we want to obtain an expression for the S-matrix element $\langle f|S|i\rangle$, for some initial and final states of definite momenta. This is commonly done by means of perturbation theory in terms of Feynman diagrams. For concreteness, let us consider a massive scalar field theory in the following.

When treating the interaction terms as a perturbation of the free theory, the S-matrix elements can be formulated by asymptotic in- and outgoing states. In the asymptotic past, $t \to -\infty$, the ingoing states can be described by free wave packets, that correspond to well separated single-particle states. This is an immediate consequence of the locality of the interaction. Therefore, as these wave packets approach each other, they eventually start to interact and finally scatter into the final state particles. In the asymptotic future, $t \to \infty$, these final state particles are again described by asymptotically free single-particle states¹.

In quantum field theory the concept of asymptotic states can be formalized in terms of in- and outgoing fields². This is necessary, since, in crucial contrast to the free theory, an interacting field ϕ cannot be written as a linear superposition of its Fourier modes, because it does not obey the free equation of motion. Instead it satisfies

$$\left(\Box + m^2\right)\phi = j\,,\tag{2.2}$$

for a suitable current j, which vanishes only in a non-interacting theory. Therefore, ϕ acting on the vacuum of the interacting theory, $|\Omega\rangle$, does not generate a simple single-particle state as it does in the free theory. In turn, the asymptotic in- and outgoing fields ϕ_i and ϕ_f , respectively, are defined such that they do obey the free mode equation,

$$\left(\Box + m^2\right)\phi_{i,f} = 0. \tag{2.3}$$

Since asymptotically, $t \to \pm \infty$, all interactions between these fields cease to exist, we can therefore think of them as free fields with single-particle states, $E_p^2 = p^2 + m^2$. However, the self-interaction of the field is still present. Therefore, the single-particle states have a mass m of the full *interacting* theory instead of its free counterpart. In addition, the self-interaction of the field also leads to a nontrivial wave function renormalization.

Having established the concept of asymptotic in- and outgoing fields, we can proceed to compute scattering amplitudes in an interacting quantum field theory explicitly. As a particular example, we want to consider the scattering of r incoming particles with momenta q_l into n particles in the final state with momenta p_k , i.e. we are interested in the S-matrix element $\langle p_1 \dots p_n | S | q_1 \dots q_r \rangle$.

The asymptotic in- and outgoing fields are essential ingredients of the so-called *Lehmann-Symanzik-Zimmermann* (*LSZ*) reduction formula [118]. It connects the *S*-matrix to the time-ordered correlation functions, i.e. vacuum expectation values

¹The Hilbert spaces of asymptotic in- and outgoing states are isomorphic Fock spaces. Mathematically, this is the reason why there exists a scattering operator S that maps the outgoing states onto the ingoing states.

 $^{^{2}}$ Note that this is, in fact, not possible for conformal field theories. Due to scale invariance, there is no meaningful notion of asymptotically separated states and hence the S-matrix cannot be defined properly.

of time-ordered products of field operators, of the interacting quantum theory,

$$\prod_{k=1}^{n} \frac{i\sqrt{Z}}{p_k^2 - m^2} \prod_{l=1}^{r} \frac{i\sqrt{Z}}{q_l^2 - m^2} \langle p_1 \dots p_n | S | q_1 \dots q_r \rangle \Big|_{\text{connected}}$$

$$= \prod_{k=1}^{n} \int d^4 y_k e^{ip_k y_k} \prod_{l=1}^{r} \int d^4 x_l e^{-iq_l x_l} \langle \Omega | T \prod_{k=1}^{n} \phi(y_k) \prod_{l=1}^{r} \phi(x_l) | \Omega \rangle . \tag{2.4}$$

Note that, here, only the *connected* part of the S-matrix plays a role. This means that *all* particles do participate in the scattering process, i.e. no initial and final state particles are trivially the same.

By means of (2.4) the computation of S-matrix elements can be reduced to the computation of time-ordered correlation functions. Therefore, the LSZ reduction formula is a step towards computing scattering processes, that are measurable in experiment, from the abstract Lagrangian of a quantum field theory. Note that all momenta appearing in the reduction are on-shell, because they correspond to the physical momenta of the incoming and outgoing single-particle states, i.e. $p_k^2 - m^2 = 0 = q_l^2 - m^2$. As the S-matrix is a quantum probability amplitude, it has to be nonsingular. Therefore, the time-ordered correlation function has to exhibit a suitable pole structure to compensate each kinematic factor $(p_k^2 - m^2)^{-1}$ and $(q_l^2 - m^2)^{-1}$. For instance, terms with fewer poles would at best contribute to disconnected pieces of the scattering amplitude.

Using the LSZ reduction, we have arrived at a prescription to compute the connected S-matrix elements of an interacting quantum field theory by time-ordered correlation functions. We are now left with is the evaluation of the latter. As we will see, this is commonly done in perturbation theory by means of Feynman diagrams.

2.1.2 Perturbation theory and Feynman diagrams

The LSZ reduction formula (2.4) connects the S-matrix elements to the time-ordered correlation functions of an interacting quantum field theory.

The correlation functions are the fundamental building blocks that encode the dynamics of the interacting quantum field theory. For instance, the insertion of two fields, $\langle \Omega | T \phi(x) \phi(y) | \Omega \rangle$, describes the amplitude for the propagation of a particle between the two space time points. In the free theory, it would correspond to the Feynman propagator. Essentially, there are two approaches for the determination of correlation functions.

In the modern path integral approach to quantum theory they are defined by functional derivatives of the *generating functional*

$$Z[J] = \int \mathcal{D}\phi \, \exp\left(iS[\phi] + i \int d^4x \, J\phi\right) \,, \tag{2.5}$$

where J is an auxiliary source-term. As the name already suggests, it generates all correlation functions of the quantum theory, in the sense that

$$\langle \Omega | T \prod_{i=1}^{n} \phi(x_i) | \Omega \rangle = \frac{1}{Z[0]} \left. \frac{\delta}{i \delta J(x_1)} \dots \frac{\delta}{i \delta J(x_n)} Z[J] \right|_{J=0}. \tag{2.6}$$

That is, formally, if one can compute the generating functional as a function of the source analytically, i.e. in closed form, one has essentially solved the dynamics of the quantum field theory.

In the sequel, however, we want to consider the second, probably more pedestrian and intuitive approach. That is, we aim to reduce the computation of the correlation functions, such that it only involves quantities which are tractable more easily. In particular, this means, that it should only contain the vacuum and field operators of the free theory. It is hence suggestive to separate the dynamics of the interactions from the free theory, i.e. in terms of the Hamiltonian $H = H_0 + H_{\text{int}}$.

Commonly, this is done by considering field operators in the *Dirac picture*, ϕ_I , which by construction satisfy a free mode equation. Therefore, such formalism allows us to rewrite the correlation function in terms of the free vacuum, $|0\rangle$, and free field operators only,

$$\langle \Omega | T \prod_{i=1}^{n} \phi(x_i) | \Omega \rangle = \lim_{t \to \infty(1-i\epsilon)} \frac{\langle 0 | T \left\{ \prod_{i=1}^{n} \phi_I(x_i) e^{-i \int_{-t}^{t} dt' H_I(t')} \right\} | 0 \rangle}{\langle 0 | T \left\{ e^{-i \int_{-t}^{t} dt' H_I(t')} \right\} | 0 \rangle}.$$
 (2.7)

Here, H_I denotes the interaction Hamiltonian in the Dirac picture.

Up to this point, (2.7) is an exact relation. However, in practice, it is well suited for a perturbative approach, since the exponential function can easily be expanded in a power series of the coupling of the theory. For instance, in scalar ϕ^4 -theory with coupling λ , the exponential would read,

$$\exp\left(-i\int d^{4}z \,\frac{\lambda}{4}\phi_{I}^{4}(z)\right) = 1 - i\frac{\lambda}{4} \int d^{4}z \,\phi_{I}^{4}(z) + \frac{1}{2} \left(-i\frac{\lambda}{4}\right)^{2} \int d^{4}z_{1} d^{4}z_{2} \,\phi_{I}^{4}(z_{1})\phi_{I}^{4}(z_{2}) + \mathcal{O}\left(\lambda^{3}\right).$$
(2.8)

This expansion is one of the key points of perturbative quantum field theory, as it reduces the time-ordered correlation functions of the interacting theory to an infinite sum of correlation functions involving only the free vacuum and free field operators, $\langle 0|T \{\phi_I(x_1)...\phi_I(x_n)\} |0\rangle$.

By Wick's theorem, these correlation functions vanish for an odd number of field operator insertions. For an even number of field insertions, they reduce to a sum over all possible contractions between two fields. Each contraction then corresponds to the free Feynman propagator between the two spacetime points that the field operators are evaluated at. That is, in summary, Wick's theorem turns the above correlator into a sum of products of Feynman propagators.

This procedure suggests that we can replace the evaluation of time-ordered correlation functions in the interacting theory by the intuitive evaluation of Feynman diagrams. In fact, the denominator of (2.7) is the partition function of the theory and hence cancels all vacuum contributions to the correlator, i.e. vacuum bubbles or disconnected pieces of the diagram. Therefore, we conclude that the time-ordered correlation function $\langle \Omega | T \{\phi(x_1) \dots \phi(x_n)\} | \Omega \rangle$ can be written as the sum over all (at least partially) connected Feynman diagrams with n external points.

The language of evaluating correlation functions by Feynman diagrams together with the LSZ reduction formula allows us to write down S-matrix elements, or, more precisely, scattering amplitudes, in a particularly elegant way. Recall that in the LSZ reduction (2.4), the connected S-matrix elements, $\langle p_1 \dots p_n | S | q_1 \dots q_r \rangle$, by themselves cannot be proportional to the kinematic factors $p_k^2 - m^2$ or $q_l^2 - m^2$, because otherwise it would vanish on-shell, i.e. no scattering would occur. Similarly, it cannot contain powers of the inverse of the kinematic factors, as it would be divergent on-shell and hence singular. Therefore, the only Feynman diagrams that are relevant are the ones with exactly (n+r) poles at the physical single-particle mass m^2 . In fact, these are precisely the ones that contribute to the fully connected correlation function. Here, each external line exhibits a factor of $(p^2 - m^2)^{-1}$ near the pole mass such that all external lines yield the correct singularity structure. For example, partially connected diagrams come with fewer kinematic factors and consequently do not contribute to the connected S-matrix element.

In summary, we conclude that the S-matrix elements are given by

$$\langle p_1 \dots p_n | S | q_1 \dots q_r \rangle \Big|_{\text{connected}} = \left(\sqrt{Z}\right)^{n+r} \times \left(\prod_{k=1}^n \int d^4 y_k \, e^{ip_k y_k} \prod_{l=1}^r \int d^4 x_l \, e^{-iq_l x_l} \, \langle \Omega | T \prod_{k=1}^n \phi(y_k) \prod_{l=1}^r \phi(x_l) | \Omega \rangle \Big|_{\text{fc}} \right) \Big|_{\text{amp}}.$$
(2.9)

Here, by the fully connected, amputated correlation function we denote the corresponding Feynman diagram after removing all external lines, that come with a kinematic factor of the fully resummed propagator. We will later make use of the LSZ reduction formula in the above form to derive multiparticle scattering amplitudes in a diagrammatical approach.

Finally, we have arrived at an elegant prescription for the computation of physical scattering amplitudes by considering a perturbative expansion of the latter in terms of Feynman diagrams that have to be evaluated. In the following, we want to consider a particular set of scattering amplitudes associated to multiparticle production in scalar field theories, which have been attracting some renewed attention recently.

2.2 Unitarity violation by multiparticle production in scalar field theory

In general, in any particle scattering at sufficiently high energies the production of many particles becomes kinematically possible. As we will see momentarily, in a scalar field theory, the mathematical and physical structure of the scattering amplitudes corresponding to the production of a large number of bosons by a few initial particles is remarkably rich and rises some intriguing physical questions. Most critically, the scattering cross section for multiparticle production seems to rise at high energies, or, more precisely, at high multiplicities. This ultimately renders the

theory in conflict with the fundamental principle of unitarity in quantum field theory. Let us hence outline the basic considerations leading to this alarming conclusion in the following.

From the rather general discussion of the previous section, we therefore want to move to a massive scalar field with a quartic self-interaction,

$$\mathcal{L} = \frac{1}{2} \partial_{\mu} \phi \partial^{\mu} \phi - \frac{m^2}{2} \phi^2 - \frac{\lambda}{4} \phi^4. \tag{2.10}$$

In this theory we aim to study the behaviour of multiparticle scattering processes at high energies.

At weak coupling such a scattering process can be expressed by means of Feynman diagrams (cf. our discussion in Section 2.1.2). Qualitatively, at leading order in the perturbative expansion, the production of n scalar particles by a few initial ones will be proportional to $n! \lambda^{n/2}$. Essentially, this is because, in the diagrammatical approach, for each pair of particles that is produced in addition an additional power of the coupling constant is necessary, while at the same time the number of tree graphs grows factorially due to the lack of destructive interference between different diagrams. Therefore, even in a weakly coupled theory, for occupation numbers $n \gtrsim 1/\lambda$ the factorial factor compensates the power suppression due to the small coupling, such that the tree-level amplitudes grow rapidly for large n. Naively, this means that, independently of the small coupling, it becomes more and more likely to produce a large rather than small number of particles in the final state.

This qualitative estimate appears to be in deep conflict with the fundamental requirement of unitarity in quantum field theory. Unitarity ensures that probabilities are conserved in scattering processes³ and is therefore a very natural assumption in interacting quantum theories. Formally, it is imposed by requiring that the S-matrix is unitary. At the level of scattering amplitudes, the optical theorem is an immediate consequence of this property. It relates the imaginary part of a forward-scattering amplitude to the total cross section of a process. As the norm squared of partial amplitudes contributing to a process cannot exceed the total cross section, it in turn implies (see, e.g., [95])

$$\sum_{n \neq i} \left| \mathcal{A} \left(\phi^i \to \phi^n \right) \right|^2 \le 1, \tag{2.11}$$

where \mathcal{A} denotes the scattering amplitude corresponding to the process $\phi^i \to \phi^n$. That is, loosely speaking, the probability of *something* happening should not exceed a hundred percent. This situation is even more dire than the problem of divergences of perturbation theory at large orders [119–122]. While the latter typically reflects the asymptotic nature of perturbative series expansions in quantum field theory (as, e.g., Dyson argues for quantum electrodynamics [119]), here we encounter an unphysical breakdown of perturbation theory already at leading order of the expansion.

³From a different perspective, the time evolution operator of quantum theory is required to be unitary, such that is preserves the norm of a state during time evolution. In other words, the probability to find a normalized state $|\psi\rangle$ in the state $|\psi\rangle$ is required to be one over all times.

In other words, such processes are only accessible at a high order in the perturbative expansion. This either indicates an end of perturbative behaviour, or possibly even a breakdown of the theory itself.

In order to make this assertion precise let us consider processes, where a large number of massive scalars are produced by a few initial particles, $|i\rangle \rightarrow |n\rangle$. Here, $|i\rangle$ denotes the initial state with small particle number and $|n\rangle$ is a multiparticle state of multiplicity n. In particular, we restrict $|i\rangle$ to be a one- or two-particle state. Hence, strictly speaking, we are considering two different physical situations. If $|i\rangle$ is a single-particle state, this process describes a decay of an off-shell scalar into n on-shell particles, $\phi^* \rightarrow \phi^n$, while for a two-particle initial state, we are dealing with physical scattering of two on-shell states, $\phi\phi \rightarrow \phi^n$. Nevertheless, our qualitative estimate from above still applies to both cases. More precisely, the single-particle initial state has to be understood as a highly virtual particle that is subject to decay. As such it has to be produced, e.g., in a particle collision at high energies. For instance, in a physical high energy scattering process, $X \rightarrow \phi^n$, the virtual one-particle state would correspond to the s-channel resonance which then subsequently decays into n on-shell particles. In this example, the amplitude $\mathcal{A}(\phi^* \rightarrow \phi^n)$ then corresponds to the decay of the resonance in the scattering process.

In the following, we want to work out the physical as well as mathematical details of these scattering processes. For concreteness, we will focus on the amplitudes corresponding to the decay of a virtual boson state, $\phi^* \to \phi^n$. We will, however, comment on the physical scattering processes involving only on-shell external states, $\phi\phi \to \phi^n$, whenever it is qualitatively different from the former.

2.2.1 Tree-level processes at the kinematic threshold

Our previous estimate of rapidly growing multiboson amplitudes, $\mathcal{A} \propto n! \lambda^{n/2}$, was entirely based on simple counting of tree-level Feynman diagrams. We now want to move to precise expressions for the corresponding scattering amplitudes. In order to simplify and clarify our discussion, let us first consider topologically trivial ϕ^4 -theory in the symmetric phase, i.e. we choose $m^2 > 0$ in (2.10).

Evidence for factorial growth of multiboson amplitudes was first provided by perturbative arguments [39, 40, 43–47]. Similar to our intuitive counting arguments, these rely on the diagrammatical approach to particle scattering. As we are dealing with a large number of diagrams that can be grouped into several subdiagrams, recursive relations turn out to be extremely useful for the computation of the corresponding amplitudes. That is, we can recursively generate any tree-level diagram by connecting all sets of subdiagrams (at tree level) to the original vertex of the incoming particle. More precisely, the scattering amplitude $\mathcal{A}(n)$ corresponding to the process $\phi^* \to \phi^n$ can be written as a sum over all possible combinations of subtrees that originate from this root vertex [44,45],

$$\mathcal{A}(n) = \lambda \sum_{\substack{n_1, n_2, n_3 \text{odd}}} \delta_{n, n_1 + n_2 + n_3} \frac{n!}{n_1! \, n_2! \, n_3!} \mathcal{D}(n_1) \mathcal{A}(n_1) \mathcal{D}(n_2) \mathcal{A}(n_2) \mathcal{D}(n_3) \mathcal{A}(n_3) . \quad (2.12)$$

Here, $\mathcal{D}(n_i)$ denotes the propagator connecting the subtree with n_i particles to the root vertex. In addition, the combinatorial factor $n!/(n_1! n_2! n_3!)$ counts the number of possibilities of how n particles can be grouped into three subsets of n_1, n_2 and n_3 final states. In fact, as the theory exhibits a \mathbb{Z}_2 symmetry at the Lagrangian level, the occupation number of all final states has to be odd. Therefore, the sum over all subsets only involves odd integers n_i .

Note carefully, that the propagators appearing in (2.12) arise because of the definition of the objects $\mathcal{A}(n)$. In fact, as they are defined as scattering amplitudes, the propagators of all external states are amputated (cf. Section 2.1.2). In contrast, the corresponding n-point Green's function would be obtained by multiplying with the external propagators accordingly.

So far, the recursive relation (2.12) is an exact equation that generates all treelevel Feynman diagrams contributing to the process $\phi^* \to \phi^n$. Unfortunately, it can only be solved in closed form in certain kinematic regions. A specific region of phase space, where such a solution can be found, is the kinematic threshold, at which all final state particles have vanishing momentum. That is, we consider a highly virtual initial boson of energy nm decaying into n bosons of mass m at rest. In this kinematic setting, the tree-level amplitude takes the form [44]

$$\mathcal{A}_{\text{tree}}(n) = m^2(n^2 - 1)n! \left(\frac{\lambda}{8m^2}\right)^{\frac{n-1}{2}},$$
 (2.13)

where n is necessarily odd. As pointed out earlier, the factor $m^2(n^2 - 1)$ now corresponds to the inverse propagator of the off-shell initial state with energy nm.

Note that, so far, we have only considered ϕ^4 -theory in the symmetric phase, for which (2.13) is the exact result for the tree-level amplitude. In a theory featuring spontaneous symmetry breaking, $m^2 < 0$, the recursive relations (2.12) are modified by the appearance of additional cubic interactions (see, e.g., [45]). Nevertheless, the modified equations still allow for an exact, closed form solution at the kinematic threshold. It reads [45]

$$\mathcal{A}_{\text{tree}}(n) = m^2(n^2 - 1)n! \left(\frac{1}{2v}\right)^{n-1},$$
 (2.14)

where v denotes the vacuum expectation value of the field, given by $v = \sqrt{-m^2/\lambda}$. Here, the scattering amplitude now refers to the field excitations around the minimum, i.e. around $\langle \phi \rangle = v$. In addition, because of the broken symmetry, n does not necessarily need to be odd anymore. Thus, modulo numerical factors, the tree-level amplitudes in theories both with and without spontaneous symmetry breaking are equal.

We conclude that our naive arguments based on simple counting of Feynman diagrams are indeed correct and we find rapid factorial growth of the scattering amplitudes $\mathcal{A}(\phi^* \to \phi^n)$ at leading order in perturbation theory. This growth appears in ϕ^4 -theory both with and without spontaneous symmetry breaking. Therefore,

the amplitudes are in conflict with the unitarity principle of quantum field theory, rephrased in (2.11). A different way to see this involves the non-amputated amplitudes, i.e. Green's functions. By the LSZ reduction formula (2.9), the matrix element of the process, $\langle p_1 \dots p_n | \phi(0) | 0 \rangle$, will be proportional to the propagator times the Fourier transform of the time-ordered correlation function with n+1 field insertions. In this setting, the corresponding Green's function can be understood as the probability amplitude of the field operator $\phi(x)$ to create n particles of fixed energy from the vacuum at x = 0, $\langle n | \phi(0) | 0 \rangle$ (see also (2.17)). In summary, we obtain the relation between the scattering amplitude and the corresponding Green's function,

$$\langle n|\phi(0)|0\rangle = \mathcal{D}(n)\mathcal{A}(n)$$
. (2.15)

As can be seen from this relation, these amplitudes are part of the definition of the Källén-Lehmann spectral density, $\rho(s) = \sum_n 2\pi \delta \left(s - m_n^2\right) |\langle n|\phi(0)|0\rangle|^2$, where the sum has to be understood as a summation over a continuum of states. Hence, they are integral part of the *definition* of an interacting quantum field theory. Explicitly evaluating the vacuum expectation value of the commutator of the canonical field variables, $\langle 0|\left[\phi(x),\Pi(y)\right]|0\rangle$, at equal times yields (see also the discussion on the spectral decomposition in [123])

$$\sum_{n} |\langle n|\phi(0)|0\rangle|^2 = 1.$$
 (2.16)

This condition and the unitarity constraint (2.11), are clearly violated by the treelevel amplitudes (2.13) and (2.14) as $n \to \infty$, independently of the coupling of the theory.

However, one might indeed argue that our conclusions should not worry us too much for two reasons. First, the kinematic setting of the amplitudes we are considering lies outside the physical phase space region. More precisely, the kinematic threshold just describes the very edge, or, mathematically, it is a null set, of the physical phase space. Therefore, strictly speaking, the corresponding cross section vanishes. Reliable estimates of the cross section should hence use bounds which lie inside physical phase space regions (see, e.g., [45]). Second, it is a perturbative computation at leading order of a scattering amplitude, which, in addition, is only part of a physical scattering process. For instance, in contrast, it is known that multiparticle tree-level amplitudes corresponding to physical processes $\phi\phi \to \phi^n$ are exactly vanishing at the kinematic threshold [47, 52, 124–126]. Moreover, there are hints that this even holds when quantum corrections are taken into account [125]. Therefore, the physical relevance of unitarity violating $\phi^* \to \phi^n$ processes at tree level is questionable to some extent. However, as we will see, the problem still persists in a more physically relevant setting. Note, for instance, that pure ϕ^4 -theory is very special in this regard. For example, in the Standard Model nullification of tree-level amplitudes at threshold only occurs for certain values of the particle masses [124, 127, 128].

We are going to address these aspects in the following section, where we aim to go beyond tree-level perturbation theory as well as to comment on the corresponding amplitudes beyond the kinematic threshold.

2.2.2 Going beyond tree-level perturbation theory

In this section, we want to consider the results of the previous section from a slightly different point of view by going beyond leading order perturbation theory at the kinematic threshold.

The original approach to include the first quantum correction beyond tree level, however, did not rely on the recursive methods of (2.12). Instead it makes use of the generating field technique by Brown [43], which is based on evaluating the matrix element of the initial state, $\langle 0_{\text{out}}|\phi(x)|0_{\text{in}}\rangle_{\rho}$, in the presence of a source term, $\rho\phi$, and then applying the LSZ reduction,

$$\langle n|\phi(x)|0\rangle = \prod_{a=1}^{n} \lim_{p_a^2 \to m^2} \int d^4x_a \, e^{ip_a x_a} (m^2 - p_a^2) \frac{\delta}{\delta\rho(x_a)} \, \langle 0_{\text{out}}|\phi(x)|0_{\text{in}}\rangle_{\rho} \bigg|_{\rho=0} \, .$$
 (2.17)

As the tree-level amplitudes themselves can be understood as classical objects, they are then obtained by replacing the initial state matrix element by a solution to the classical field equation in the presence of ρ . That is, the classical field is now a functional of the source, $\phi_0[\rho]$. At the kinematic threshold, where all final state particles are at rest, $\vec{p}_a = 0$, the source can be taken to be spatially constant. Differentiating the matrix element with respect to the source and sending it to zero afterwards, one indeed obtains an exact expression for all tree-level amplitudes at threshold. Schematically, this relation can be written as [43]

$$\mathcal{A}_{\text{tree}}(n) = m^2(n^2 - 1) \left(\frac{\partial}{\partial z} \right)^n \phi_0 \Big|_{z=0} , \qquad (2.18)$$

where z is now a change of variable involving the original source ρ .

The first quantum correction to the threshold amplitudes can then be obtained by linearizing the field around the generating function for the tree-level amplitudes, i.e. around the classical background, and keeping track of the quantum correction throughout the procedure [47,52]. Later, the recursive methods (2.12) have been extended to also include the one-loop correction [102]. It turns out that the first quantum correction is of order λn^2 compared to the tree-level result. Naively, this is because there are order n^2 possible ways to introduce an internal propagator into the tree-level amplitude with n external legs. Due to this scaling, in the large n regime, in particular for $n \gtrsim 1/\lambda$, the unitarity violating behaviour of the amplitudes still persists.

Analogously, we expect the kth loop contribution to be of order $(\lambda n^2)^k$ compared to tree level [102]. Therefore, when probing the regime $n \gtrsim 1/\lambda$ beyond tree-level perturbation theory, a robust calculation of the scattering amplitude requires the resummation of all terms of the perturbative expansion, which, obviously,

becomes more and more complicated at higher loop-orders. However, if one is interested the leading-n contribution at each loop-order, one can drastically simplify the computation. They key point is that the contribution from the kth loop-order, ϕ_k , is completely determined by the leading singularity structure of the classical background, $\phi_0 \sim \cosh^{-1}(\tau)$, in Euclidean time τ [53]. Taking only the leading singularity into account, one then tries to determine the loop contribution, $\langle 0|\phi_k|0\rangle$, to the matrix element in the classical background ϕ_0 by means of Feynman diagrams. That is, naively, one only considers tadpole graphs at each loop-order and represents them by their leading singularity structure by cutting all internal lines to obtain a connected tree graph. Finally, these tree graphs can be evaluated by Feynman rules that are modified by the classical background [53].

This sophisticated technique is, in fact, well suited to probe the regime $n \gtrsim 1/\lambda$ beyond tree-level perturbation theory, as it in principle gives access to the leading-n behaviour of arbitrary loop-orders. A useful limit in this regime is the double scaling limit $\lambda \to 0$ and $n \to \infty$ while keeping λn fixed. In this limit, the loop contributions exhibit a remarkable structure. It is conjectured that the scattering processes for multiboson production in ϕ^4 -theory take on exponential form [52–56],

$$\mathcal{A}(n) = \mathcal{A}_{\text{tree}}(n) \exp\left(\frac{1}{\lambda}F\right),$$
 (2.19)

where F is sometimes called *holy grail function* and depends on the particular scalar field model in question. At the kinematic threshold F is a function of the combination λn only [53],

$$F(\lambda n) = B\lambda^2 n^2 + \mathcal{O}\left(\lambda^3 n^3\right), \qquad (2.20)$$

with coefficients $B = -\left(\ln\left(7 + 4\sqrt{3}\right) - i\pi\right)/(64\pi^2)$ for the symmetric theory, and $B = \sqrt{3}/(8\pi)$ for a theory with spontaneously broken symmetry [47, 52, 102].

The exponentiation of the amplitudes for multiparticle production (2.19) is quite remarkable. Naively, similar to exponential suppression factors in theories with instanton solutions, this form signals an intrinsic non-perturbative nature of the corresponding scattering amplitudes in the weakly coupled theory, $\lambda \to 0$. Intriguingly, the exponentiation even appears to be independent of the precise nature of the initial state, as long as it is still of comparably small occupation number, i.e. one would expect that $\langle n|\phi^2|0\rangle \sim \langle n|\phi|0\rangle$ up to subleading, non-exponential prefactors [54]. In practice, as we will see later, the leading-n exponentiation is highly nontrivial and allows to study the corresponding scattering amplitudes in a regime, where tree-level perturbation theory is in clash with unitarity.

So far, the precise, analytic form of the exponent F is unknown. Still, for the consistency of the field theory at high energies the sign of F is crucial. If F is positive for some positive value of λn , one always finds unitarity violation in the limit where λn is kept fixed at that value while the coupling is sent to zero, $\lambda \to 0$. In light of the above results, the case for ϕ^4 -theory both with and without spontaneous symmetry breaking is unclear. Both theories, however, appear to be very different, as the quantum corrections to the holy grail function, $B\lambda^2 n^2$, are of opposite sign. While the correction in the symmetric phase is negative, providing some hope for

convergence, the correction in the broken phase is positive, leaving the situation even more unclear.

The observation of rapidly growing tree-level amplitudes and the exponentation of quantum corrections is further supported by computations based on semiclassical techniques [48–51]. The exponential form (2.19) is inherent to the semiclassical approach to multiboson production in scalar field theories, which, in fact, only attempts to compute the exponent F. This approach is modeled after the Landau-WKB method known from quantum mechanics [129] and makes use of functional integrals in the coherent state representation. One of the main assumptions used in the Landau-WKB method is that, to exponential accuracy, the amplitude in question is independent of the precise form of the local operator, $\langle n|\phi^2|0\rangle \sim \langle n|\phi|0\rangle$, which we will support with explicit computations in Section 3.4. The initial and final states are specified as boundary conditions for the functional integral, which can be evaluated using Morse theory and steepest descent methods (or in the language of complex variables, Picard-Lefschetz theory). The integration will then be dominated by certain (classical) field configurations, which, in the path integral language, correspond to saddle-points of the action. For a recent review of the technical details of these semiclassical techniques see [130].

Let us close our discussion of the exponentiation of scattering amplitudes for multiparticle production with a few words on their kinematics. Up to this point, we have been dealing with multiboson production at the kinematic threshold, i.e. all final state particles are at rest. Both the perturbative as well as the semiclassical approach allow to move away from the threshold by going into a regime where the final state particles are non-relativistic, i.e. their momenta are small compared to their mass. The non-relativistic regime can be characterized by the kinetic energy of the final state particles in their center-of-mass frame, T. In fact, non-relativistically, one can treat the kinetic energy as a small perturbation to the kinematic threshold, which in turn corresponds to T=0. Due to the permutation symmetry of the particle momenta and Galilean invariance, the leading order correction to the threshold amplitude is proportional to the kinetic energy itself [53],

$$\mathcal{A}(p_1,\ldots,p_n) = \mathcal{A}_{\varepsilon=0}(n) + \mathcal{M}(n)n\varepsilon + \ldots \qquad (2.21)$$

Here, ε denotes the kinetic energy per particle per mass, $\varepsilon = T/(nm)$. The non-relativistic limit is then equivalent to the condition $\varepsilon \ll 1$.

Even when going beyond the kinematic threshold by (2.21), the modified recursion relation can still be solved for the tree-level amplitude (see, e.g., [93]). In the regime $n \to \infty$ and $\varepsilon \to 0$ with $n\varepsilon$ fixed, the perturbative solution reproduces the observation first made in [53],

$$\mathcal{A}(p_1, \dots, p_n) = \mathcal{A}_{\text{tree}}^{\varepsilon=0}(n) e^{An\varepsilon}.$$
 (2.22)

Here, $\mathcal{A}_{\text{tree}}^{\varepsilon=0}(n)$ denotes the tree-level amplitude at the kinematic threshold, previously given in (2.13) and (2.14). The prefactor of the exponent is given by A = -5/6

for the symmetric theory and A = -7/6 for the theory with spontaneously broken symmetry.

Finally, we have arrived at an expression for the kinematic dependence of the tree-level amplitudes in the non-relativistic regime. However, importantly, the characteristic factorial growth inherent to the tree-level amplitudes at the kinematic threshold still persists. That is, even inside the physical regions of phase space, we encounter unitarity violating behaviour of multiparticle production in ϕ^4 -theory.

In summary, we have gone beyond tree-level perturbation theory in multiparticle production in scalar field theory away from the kinematic threshold, where we find a remarkable exponentiation of the quantum corrections. Still, we find rapid growth of the corresponding amplitudes, rendering the theory in conflict with unitarity constraints. In the following section we want to discuss physical consequences of this, both from a theoretical as well from a phenomenological perspective. In addition, we comment on possible ways how unitarity might be restored in multiparticle processes.

2.3 Towards the restoration of unitarity in multiparticle processes

In ϕ^4 -theory both with and without spontaneous symmetry breaking, one finds strong indications that unitarity is violated by multiboson production in scattering processes at the kinematic threshold and even in the non-relativistic regime of the final state particles. The rapid growth of these amplitudes is caused by the factorially growing number of diagrams at large n, as there is no destructive interference between different Feynman diagrams in a scalar field theory.

The factorial growth of high multiplicity amplitudes in the scalar theory can be compared to its equivalent in gauge theory. In Yang-Mills theory gauge symmetry and on-shell conditions lead to diagrammatic cancellations in the computation of scattering amplitudes. This can, for instance, be seen by the application of maximal helicity violating (MHV) rules [131] or Britto-Cachazo-Feng-Witten (BCFW) recursion relations [132]. As a particular example, for any n, the amplitude⁴ for n-gluon scattering is given by the famous Parke-Taylor expression [91], which does not yield rising cross sections for large n. That is, in contrast to scalars, gluons do not seem to violate unitarity. It is therefore natural to investigate the behaviour of a scalar field charged under a gauge symmetry at high energies. The case of a spontaneously broken gauge theory, i.e. a gauge-Higgs theory, has been studied in [92, 93]. In particular, all tree-level amplitudes involving n scalar fields and m longitudinal vector bosons in the final state have been calculated. Similar to the pure scalar field case, they again exhibit factorial growth in both species, $A \propto n!m!$, which is also expected to be true when quantum corrections are included at fixed order perturbation theory.

⁴For introductions to the spinor helicity formalism see, e.g., [117,133,134].

From a phenomenological point of view, although spontaneously broken gauge theory only resembles a toy system, these results indicate a breakdown of perturbative behaviour in the electroweak sector of the Standard Model. Hence, the discovery of a scalar Higgs boson [8,9] has turned this problem into an issue of the electroweak theory. In such a scenario, the rapidly growing cross sections provide us with an explicit upper scale $\Lambda \lesssim 1600\,\text{TeV}$ [94,95], beyond which conventional field theory techniques cease to be meaningful. Higher order quantum corrections indicate that this scale could even be lower, possibly within the range of the next generation of colliders [95].

In order to restore unitarity at high energies, either non-perturbative behaviour or new physics must set in. A possible form of novel non-perturbative behaviour, that was recently proposed, could be a Higgsplosion and Higgspersion effect [97]. The idea is that the increase in the $\phi^* \to \phi^n$ amplitudes leads to an increase of the decay width of the particle. This large width suppresses the propagator, such that loop-integrals are effectively cut off at the energy scale where the amplitudes become large. As this scale can potentially be low, in the Standard Model, this mechanism can possibly even address the hierarchy problem. At the same time, a low scale allows for a rich particle phenomenology [98–100]. For a discussion on the nature of the underlying quantum field theory, in particular, on aspects of localizability in a theory featuring Higgsplosion see [135–137].

For the remainder of this work, we, however, want to pursue a different approach. The exponentiation of the multiparticle amplitudes at high multiplicities, $\mathcal{A} \sim \exp{(F/\lambda)}$, intrinsically inherits some form of non-perturbative nature in the limit $\lambda \to 0$, demanding for a deeper investigation. So far, the calculations of multiparticle production in scalar field theory mostly relied on perturbative or semiclassical methods at leading order, or possibly including the first quantum correction. Beyond that, conventional Feynman diagrams to higher loop-orders become intractable and the perturbative answer might not be reliable at high energies. For instance, taking the exponentiation of the amplitude into account, we observe that, at tree-level, the exponent F turns positive beyond some critical value of λn , signaling an instability of the perturbative expansion. In fact, it is possible that the rapid growth is merely an artefact of an "incomplete" calculation and could possibly be lifted by writing down the full scattering amplitude without relying on perturbation theory to finite order. Here, we are particularly interested in establishing the sign of the holy grail function F.

In order to shed light on this problem, we want to make use of advanced computational techniques. Although we are ultimately interested in quantum field theory, we will consider a much simpler quantum mechanical system. That is, we will study the quantum mechanical analogue of ϕ^4 -theory, which corresponds to the anharmonic oscillator with a quartic potential. The quantum mechanical setting will allow us to do explicit calculations to very high order in perturbation theory, that, by resummation theory, later enable us to investigate the large λn regime of scattering amplitudes at high multiplicities.

3 High Multiplicity Amplitudes in Quantum Mechanics

In Chapter 2 we have argued that scattering amplitudes, corresponding to the process $\phi^* \to \phi^n$ in scalar ϕ^4 -theory, are in conflict with fundamental unitarity constraints of quantum field theory for large n. This indicates the end of the perturbative regime or even the need for new physics phenomena. In this chapter, our aim is somewhat conservative, as we want to focus on the former possibility. That is, we want to shed some light on the question what are the relevant features of the theory to exhibit rapidly growing amplitudes at a large number of particles. Furthermore, we aim to determine whether this flaw of the theory can be cured by improved computational techniques.

We will do so by considering a simplified toy model of scalar quantum field theory: quantum mechanics with a quartic potential, both with and without spontaneous symmetry breaking. We study the quantum mechanical equivalent of high multiplicity amplitudes in ϕ^4 -theory, which correspond to transition amplitudes from the vacuum to highly excited states in the anharmonic oscillator with a quartic potential. Using recursive relations, we compute these amplitudes to high order in perturbation theory and provide evidence that they can be written in exponential form. We then construct the exponent beyond leading order and investigate the behaviour of the amplitudes in the region where tree-level perturbation theory violates unitarity constraints. Furthermore, we generalize our results and study the asymptotic behaviour of perturbation theory in potentials with self-interactions of arbitrary power. Finally, we comment on the similarities and differences of our results on quantum mechanics and quantum field theory.

The contents of this chapter presented in Sections 3.2, 3.3, 3.4 and the related Appendices A, B and C are based on work in collaboration with Joerg Jaeckel (Heidelberg U.) that has been previously published in [1,2]. Almost all the results presented in these sections, including the Figures as well as significant part of the text are identical to the published works. The contents of Section 3.5 are based on work in progress together with Florent Baume (Madrid, Autonoma U., IFT) and Joerg Jaeckel (Heidelberg U.) to appear in [4]. All results presented there are preliminary and subject to change.

3.1 Introduction

As pointed out at the beginning of this chapter, quantum mechanics will serve as an instructive toy system for our investigation of multiparticle production in scalar field theories at high energies. That is, we want to consider the quantum mechanical analogue of massive ϕ^4 -theory, corresponding to the anharmonic oscillator with quartic coupling λ ,

$$V(x) = m^2 x^2 + \lambda x^4. \tag{3.1}$$

At the level of scattering amplitudes, we reduce the complexity of the problem by making the identification¹ (cf. Section 2.2.1)

$$\langle n|\phi|0\rangle \hookrightarrow \langle n|\hat{x}|0\rangle$$
 (3.2)

That is, after a dimensional reduction, we aim at computing vacuum transition amplitudes $\langle n|\hat{x}|0\rangle$ in the quartic anharmonic oscillator. Therefore, we essentially reduce the problem to determining the spectrum of the Schroedinger operator associated to the above potential.

Such a quantum mechanical setting allows us to explicitly perform computations to high orders in perturbation theory. A resummation of the perturbative series then enables us to investigate the large λn behaviour of the scattering amplitude. We will consider the case of a symmetric theory, $m^2 > 0$, and a theory exhibiting spontaneous symmetry breaking, $m^2 < 0$, separately.

Ever since, quantum mechanics has been providing an instructive testbed for investigations of high order perturbation theory and non-perturbative effects (see, e.g., [68, 103–108]). Most works, however, focussed on energy levels and wave functions in the ground state (for a few exceptions see [43, 109–114]). Here, in contrast, we are interested in computing transition amplitudes to highly excited states.

3.2 The symmetric anharmonic oscillator

In order to introduce notation and computational techniques let us consider the anharmonic oscillator with a single minimum first,

$$V(x) = x^2 + \lambda x^4, \tag{3.3}$$

where $\lambda > 0$ and we normalize everything to the mass term, $m^2 = 1$. If necessary, the mass can be easily reintroduced on dimensional grounds.

In this potential we want to compute the quantum mechanical amplitudes $\langle n|\hat{x}|0\rangle$. In practice, this requires the determination of the exact spectrum of the Schroedinger operator,

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + \lambda x^4 - E\right)\psi = 0, \qquad (3.4)$$

 $^{^{1}}$ Note that, here, we naively identify quantum mechanics with a (0+1)-dimensional quantum field theory. In Section 3.6 we will comment on the similarities and differences between both theories with respect to particle scattering.

where we stick to the quantum field theory conventions, $\hbar = 1$. In the following, we will reconstruct the spectrum perturbatively.

3.2.1 The wave functions of the anharmonic oscillator

As they are integral part of the vacuum transition amplitudes, we want to find solutions of the Schroedinger equation (3.4). An efficient way to organize perturbative calculations to high orders are recursion relations. For the anharmonic oscillator such relations were first introduced by Bender and Wu [103, 104]. Let us briefly recall their methods.

In order to find the spectrum we start by making a perturbative ansatz for both the *n*-th energy level E_n and its corresponding wave function ψ_n ,

$$E_n(\lambda) = 2n + 1 + \sum_{m=1}^{\infty} \lambda^m a_m^n, \qquad (3.5)$$

$$\psi_n(x,\lambda) = c_n e^{-\frac{x^2}{2}} \sum_{m=0}^{\infty} \lambda^m B_m^n(x).$$
 (3.6)

Here, c_n is a normalization constant and the $B_k^n(x)$ are polynomials of the form,

$$B_m^n(x) = \sum_k B_{m,k}^n x^k \,. \tag{3.7}$$

To simplify the notation we will drop the eigenstate label n from now and keep it implicit instead.

Plugging this ansatz into the Schroedinger equation (3.4) and solving it order by order in the coupling, we can derive a recursive set of differential equations for the polynomials $B_m(x)$. At order $\mathcal{O}(\lambda^m)$ one finds

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}B_m + 2x\frac{\mathrm{d}}{\mathrm{d}x}B_m + x^4B_{m-1} = 2nB_m + \sum_{k=0}^{m-1} a_{m-k}B_k.$$
 (3.8)

For instance, at leading order m=0 we obtain the well-known differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}B_0 - 2x\frac{\mathrm{d}}{\mathrm{d}x}B_0 + 2nB_0 = 0, \qquad (3.9)$$

which is solved by the Hermite polynomials of order n, i.e. $B_0^n(x) = H_n(x)$.

We now want to go beyond leading order. As we make a polynomial ansatz for the functions $B_m(x)$, the differential equation (3.8) can in turn be translated into a recursive relation for the polynomial coefficients $B_{m,k}$, which reads

$$(k+1)(k+2)B_{m,k+2} = 2(k-n)B_{m,k} + B_{m-1,k-4} - \sum_{p=0}^{m-1} a_{m-p}B_{p,k}.$$
 (3.10)

Solutions to the above recursion relation, with $m \geq 1$, can be distinguished by two physical cases. Because the theory is symmetric under parity, we can either consider even or odd wave functions, i.e. even or odd n, respectively.

(i) For even n the odd coefficients of the polynomial expansion of $B_m(x)$ have to vanish, i.e. $B_{m,k} = 0$ for all odd k. In addition, if (3.10) is evaluated for k = 0, we obtain

$$2B_{m,2} + 2nB_{m,0} = -\sum_{p=0}^{m-1} a_{m-p}B_{p,0}.$$
 (3.11)

If we set² $B_{m,0} = 0$ for $m \ge 1$, we obtain the values of the energy expansion coefficients,

$$a_m = -2\frac{B_{m,2}}{B_{0,0}}. (3.12)$$

(ii) Similarly, for odd n the even coefficients of the polynomial expansion of $B_m(x)$ have to vanish, i.e. $B_{m,k} = 0$ for all even k. Similar to the case considered before, evaluating (3.10) for k = 1 yields

$$6B_{m,3} - 2(1-n)B_{m,1} = -\sum_{p=0}^{m-1} a_{m-p}B_{p,1}.$$
 (3.13)

Fixing $B_{m,1} = 0$ for $m \ge 1$ finally gives the energy expansion coefficients

$$a_m = -2\frac{B_{m,3}}{B_{0,1}}. (3.14)$$

Both cases can be summarized in the relation

$$(k+1)(k+2)B_{m,k+2} - 2(k-n)B_{m,k} - B_{m-1,k-4} = \begin{cases} \frac{2}{B_{0,0}} \sum_{p=0}^{m-1} B_{m-p,2}B_{p,k} & n \text{ even} \\ \frac{6}{B_{0,1}} \sum_{p=0}^{m-1} B_{m-p,3}B_{p,k} & n \text{ odd} \end{cases}$$
(3.15)

Together with the initial condition $B_0^n(x) = H_n(x)$, the above recursion relation in k can easily be solved for all coefficients $B_{m,k}$ at each order in m.

Note that for each order m the recursion relation becomes vacuous for sufficiently large values of k. That is, the polynomial coefficients become proportional to each other $B_{m,k+2} \propto B_{m,k}$ for $k \geq k_{\text{max}}$, which, by an explicit computation, can be shown to happen at $k_{\text{max}} = n + 4m + 2$. From a physical point of view, we expect this behaviour, since the wave function has to be square-integrable. This can be achieved by truncating the polynomial expansion at order k_{max} , i.e. by setting $B_{m,k} = 0$ for $k \geq n + 4m + 2$. Due to the proportionality between the coefficients at high orders the polynomial will then be finite.

The Bender and Wu method yields sufficient information to reconstruct the *n*-th energy level and the corresponding wave function. In particular, both can in principle be determined to arbitrary order in perturbation theory. For instance, the

²Similar to the theory of ordinary differential equations, we are free to fix the boundary conditions of a recursive relation.

lowest states of the spectrum read

$$\psi_0 = c_0 e^{-\frac{x^2}{2}} \left(1 - \frac{\lambda}{8} \left(x^4 + 3x^2 \right) + \frac{\lambda^2}{384} \left(3x^8 + 26x^6 + 93x^4 + 252x^2 \right) + \dots \right),$$

$$(3.16)$$

$$\psi_1 = c_1 e^{-\frac{x^2}{2}} \left(2x - \frac{\lambda}{4} \left(x^5 + 5x^3 \right) + \frac{\lambda^2}{192} \left(3x^9 + 38x^7 + 177x^5 + 660x^3 \right) + \dots \right).$$

$$(3.17)$$

What remains undetermined so far for each state is the wave function normalization constant c_n . It is fixed by the normalization condition

$$\langle n|n\rangle = \int_{\mathbb{R}} \mathrm{d}x \, \psi_n^{\dagger} \psi_n = 1 \,,$$
 (3.18)

which again yields a perturbative series in powers of the coupling of the theory. For example, at leading order we recover the well known harmonic oscillator result,

$$|c_n|_0^2 = \frac{1}{\sqrt{\pi}2^n n!} \,. \tag{3.19}$$

3.2.2 Exponentiation of the amplitude and the holy grail function

Given the efficient way to compute the spectrum of the anharmonic oscillator to high order in perturbation theory, we now want to proceed and consider transitions from the vacuum to highly excited states. In our perturbative approach these are given by the expression

$$\langle n|\hat{x}|0\rangle = \int_{\mathbb{R}} dx \, \psi_n^{\dagger} x \psi_0 = \int_{\mathbb{R}} dx \, x e^{-x^2} \sum_m \lambda^m B_m^n(x) \sum_p \lambda^p B_p^0(x) \,. \tag{3.20}$$

Using the polynomial coefficients derived from (3.15), the amplitude can then be written as³

$$\langle n|\hat{x}|0\rangle = \sum_{m=0}^{\infty} \lambda^m t_m^n \text{ with } t_m^n = \sum_{p=0}^m \sum_{k=0}^{n+4p} \sum_{l=0}^{4(m-p)} B_{p,k}^n B_{m-p,l}^0 \Gamma\left(\frac{k+l+2}{2}\right). \quad (3.21)$$

At this stage, let us point out two immediate yet nontrivial observations. First, we observe that the amplitude vanishes for all even n. This reflects the fact that the theory exhibits a \mathbb{Z}_2 symmetry, i.e. parity in our case, at the Lagrangian level. Furthermore, we can read off that $t_m^n = 0$ for m < (n-1)/2. In fact, this is exactly

³Note carefully that we exchange the order of integration and summation here. This, however, might not be strictly allowed and may indeed give rise to problems of perturbation theory.

what we would expect from a naive tree-level Feynman diagram approach in the scalar field theory given in (2.13),

$$\langle n|\hat{x}|0\rangle_{\text{tree}} \sim \lambda^{\frac{n-1}{2}}$$
. (3.22)

Similar to the computation of the transition amplitude, we can also give the perturbative expression for the wave function normalization,

$$\langle n|n\rangle = \sum_{m=0}^{\infty} \lambda^m \mu_m^n \text{ with } \mu_m^n = \sum_{p=0}^m \sum_{k=0}^{n+4p} \sum_{l=0}^{n+4(m-p)} B_{p,k}^n B_{m-p,l}^n \Gamma\left(\frac{k+l+1}{2}\right).$$
 (3.23)

Since only quantum mechanical amplitudes involving suitably normalized wave functions are physical, we will focus on the normalized amplitude in the following,

$$\mathcal{A}_n = \frac{\langle n|\hat{x}|0\rangle}{\sqrt{\langle n|n\rangle}\sqrt{\langle 0|0\rangle}}.$$
 (3.24)

In principle, the proper wave function normalization could also be ignored without qualitatively changing any of our conclusions.

We now want to find the explicit analytic dependence of \mathcal{A}_n on the quantum number n, which is contained in the numerical expressions (3.21) and (3.23) only implicitly. However, since we are dealing with a finite number of degrees of freedom, we can match the analytic behaviour to the numerical power series by fitting polynomial coefficients. An explicit computation yields

$$\mathcal{A}_{n} = \mathcal{A}_{n}^{\text{tree}} \times \left(1 - \frac{\lambda}{16} \left(17n^{2} + 5n - 12\right) + \frac{\lambda^{2}}{512} \left(289n^{4} + 1170n^{3} + 13n^{2} + 664n - 944\right) + \dots\right),$$
(3.25)

where the tree-level factor is given by

$$\mathcal{A}_n^{\text{tree}} = \sqrt{\frac{n!}{2}} \left(\frac{\lambda}{8}\right)^{\frac{n-1}{2}}.$$
 (3.26)

That is, the amplitude completely factorizes into a tree-level part and higher order contributions, $\mathcal{A}_n = \mathcal{A}_n^{\text{tree}} \mathcal{A}_{\Sigma}$. In particular, we observe that \mathcal{A}_n has the schematic form

$$\mathcal{A}_n = \mathcal{A}_n^{\text{tree}} \sum_{m=0}^{\infty} \lambda^m P_{2m}(n), \qquad (3.27)$$

where $P_{2m}(n)$ denotes a polynomial of degree 2m in n.

In fact, the tree-level result is precisely what we expect from the corresponding field theory counterpart (2.14). Note, however, that the reduced factorial factor $\sqrt{n!}$ instead of n! arises from the normalization condition in quantum mechanics. In quantum field theory this role is played by the phase space integration of the

squared matrix element. Here, the phase space volume element contains a factor of 1/n!, effectively reducing the growth of the matrix element by $\sqrt{n!}$.

Remarkably, the structure of \mathcal{A}_n is much more rich than we mentioned so far. For example, the first few leading terms of \mathcal{A}_{Σ} in λn^2 ,

$$\mathcal{A}_{\Sigma} \sim 1 - \frac{17}{16} \lambda n^2 + \frac{289}{512} \lambda^2 n^4 - \frac{4913}{24576} \lambda^3 n^6 + \mathcal{O}\left(\lambda^4 n^8\right) , \qquad (3.28)$$

resemble the series representation of the exponential function,

$$\mathcal{A}_{\Sigma} \sim \exp\left(-\frac{17}{16}\lambda n^2\right)$$
 (3.29)

This observation strongly supports the conjecture that in the double scaling limit $n \to \infty$ and $\lambda \to 0$ with λn fixed the amplitude is of exponential form [49, 52–56], as we already pointed out in Section 2.2.2,

$$\mathcal{A}_n \sim \exp\left(\frac{1}{\lambda}F(\lambda n)\right)$$
 (3.30)

The exponent F is called *holy grail function*.

This exponentiation of the amplitude can be understood as a powerful (partial) resummation of its perturbative expansion, because a finite number of terms contained in the exponent F will generate an infinite number of terms in the series representation of the amplitude. All physical information, in particular about the large n regime, is then encoded in the holy grail function. In particular, the sign of F is crucial. If F > 0 for some value of λn , there is always rapid growth of the amplitudes in the double scaling limit $n \to \infty$ where we keep λn fixed at this value (cf. Section 2.2.2),

$$A_n \to \infty \quad (n \to \infty) \,. \tag{3.31}$$

In the spirit of (3.30) we now want to investigate the structure of the amplitude A_n beyond leading order. Therefore, we write

$$\mathcal{A}_n = \mathcal{A}_n^{\text{tree}} \mathcal{A}_{\Sigma} \sim \exp\left(\frac{1}{\lambda} \left(F^{\text{tree}} + F_{\Sigma}\right)\right),$$
 (3.32)

i.e. we separate F into a tree-level part and higher order contributions,

$$F(\lambda n) = F^{\text{tree}}(\lambda n) + F_{\Sigma}(\lambda n). \tag{3.33}$$

Here, F^{tree} and F_{Σ} correspond to the factors $\mathcal{A}_{n}^{\text{tree}}$ and \mathcal{A}_{Σ} of the amplitude, respectively. For convenience let us introduce the abbreviation

$$\epsilon = \lambda n. \tag{3.34}$$

Let us consider the tree-level contribution (3.26) first. It can trivially be written in exponential form. We can then use Stirling's formula as $n \to \infty$ to obtain the approximate form of the holy grail function,

$$F^{\text{tree}}(\epsilon) \sim \frac{\epsilon}{2} \left(\ln \frac{\epsilon}{8} - 1 \right) .$$
 (3.35)

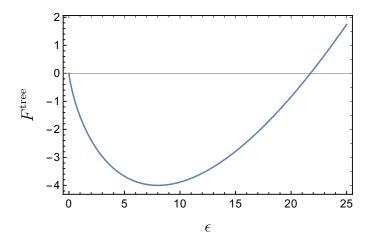


Figure 3.1: Tree-level holy grail function F^{tree} corresponding to the tree-level amplitude in the double scaling limit $n \to \infty$, $\epsilon = \lambda n = const$. Corrections of order 1/n are neglected. It exhibits a minimum at $\epsilon = 8$ and a root at $\epsilon = 8e$.

It is illustrated in Fig. 3.1.

At tree-level, the holy grail function F^{tree} exhibits two phenomenologically relevant points, the global minimum at $\epsilon_{\min} = 8$ and the root at $\epsilon_0 = 8e$. As pointed out earlier, since F^{tree} changes from negative to positive sign at ϵ_0 , i.e. for any $\epsilon > \epsilon_0$ the tree-level amplitude diverges at large n, $\mathcal{A}_n^{\text{tree}} \to \infty$ as $n \to \infty$. Therefore, for highly excited states, unitarity is violated and hence this result cannot be meaningful in a quantum mechanical setup. In particular, it implies $\langle n|\hat{x}|0\rangle > (2E_n)^{-1}$, which is, however, incompatible with the canonical commutation relation $[\hat{x}, \hat{p}] = i$ [43].

This raises the question of how this behaviour is changed, if corrections beyond leading order are included. Phenomenologically, we are most interested in the overall sign of F for any value of ϵ . Therefore, we now want to compute F explicitly in the regime $n \to \infty$ with ϵ fixed. In fact, we will find that the full perturbative expansion of the amplitude can be reproduced by writing⁵

$$\mathcal{A}_n = \mathcal{A}_n^{\text{tree}} \exp\left(\frac{1}{\lambda} F_{\Sigma}(\epsilon, n)\right) ,$$
 (3.36)

with

$$F_{\Sigma}(\epsilon, n) = F_0(\epsilon) + \frac{F_1(\epsilon)}{n} + \frac{F_2(\epsilon)}{n^2} + \dots, \qquad (3.37)$$

where the $F_i(\epsilon)$ are analytic functions in ϵ .

⁴To see this, one can, for example, explicitly compute the vacuum expectation value of the double commutator $[\hat{x}, [H, \hat{x}]]$.

⁵In general, one could be tempted to write $\mathcal{A}_n^{\text{tree}} = \exp\left(\frac{1}{\lambda}F^{\text{tree}}\right)$ with $F^{\text{tree}} = F_0^{\text{tree}}(\epsilon) + \frac{1}{n}F_1^{\text{tree}} + \dots$... However, using Stirling's formula to higher orders we would have to factor out a power of $\lambda^{3/4}$ in order to arrive at this form. Furthermore, one should keep in mind that Stirling's series is only asymptotic, suggesting missing pieces of the type we discuss in the main text.

The polynomial structure of \mathcal{A}_{Σ} given in (3.25) completely determines the possible coefficients and powers of ϵ present in F_{Σ} . Schematically it is given by

$$F_{\Sigma}(\epsilon, n) = \sum_{i,j=0}^{\infty} c_{ij} \frac{\epsilon^{i-j+2}}{n^j} \text{ with } c_{ij} = 0 \text{ for } j > \frac{i+2}{2}.$$
 (3.38)

Then a series expansion yields

$$\exp\left(\frac{1}{\lambda}F_{\Sigma}\right) = \sum_{k=0}^{\infty} \frac{\lambda^{-k}}{k!} \left(c_{ij}\frac{\epsilon^{i-j+2}}{n^{j}}\right)^{k} = e^{c_{01}} \left(1 + \lambda \left(c_{00}n^{2} + c_{11}n + c_{22}\right) + \dots\right),$$
(3.39)

where a sum over i and j is understood. The emerging structure might be described as a triangular expansion of F and can be schematically written as

$$F_{\Sigma}(\epsilon, n) \simeq \begin{cases} c_{00}\epsilon^{2} & c_{01}\frac{1}{n}\epsilon^{1} \\ c_{10}\epsilon^{3} & c_{11}\frac{1}{n}\epsilon^{2} \\ c_{20}\epsilon^{4} & c_{21}\frac{1}{n}\epsilon^{3} & c_{22}\frac{1}{n^{2}}\epsilon^{2} \\ c_{30}\epsilon^{5} & c_{31}\frac{1}{n}\epsilon^{4} & c_{32}\frac{1}{n^{2}}\epsilon^{3} \\ c_{40}\epsilon^{6} & c_{41}\frac{1}{n}\epsilon^{5} & c_{42}\frac{1}{n^{2}}\epsilon^{4} & c_{43}\frac{1}{n^{3}}\epsilon^{3} \\ \vdots & & & \ddots \end{cases}$$
(3.40)

Here, the i-th column corresponds to the terms of the polynomial $F_i(\epsilon)$, e.g.

$$F_0(\epsilon) = c_{00}\epsilon^2 + c_{10}\epsilon^3 + c_{20}\epsilon^4 + c_{30}\epsilon^5 + \dots$$
 (3.41)

The *a priori* unknown coefficients c_{ij} can be determined by expanding the exponential and matching it to the perturbative expansion of the amplitude order by order in the coupling. This way, F can in principle be determined to arbitrary order in ϵ and 1/n. However, in practice, the computational effort increases rapidly. For instance, the first few terms of the holy grail function read

$$F_{\Sigma}(\epsilon, n) = -\frac{17}{16}\epsilon^2 + \frac{125}{64}\epsilon^3 + \dots + \frac{1}{n}\left(-\frac{5}{16}\epsilon^2 + \frac{99}{128}\epsilon^3 + \dots\right) + \mathcal{O}\left(\frac{1}{n^2}\right). \quad (3.42)$$

Remarkably, such a partial resummation of the amplitude allows us to translate a perturbative expansion of \mathcal{A}_n in powers of λn^2 into a series expansion of F in powers of λn . The latter to be small is a much less restrictive requirement. Moreover, the exact correspondence between the amplitude and the holy grail function is very powerful, because a finite number of terms in F will generate infinitely many terms of \mathcal{A}_n .

In fact, it is nontrivial that *all* coefficients of perturbation theory can be recovered exactly by the exponential. Let us briefly describe why this is the case. In principle, we can trivially write any function $B(\lambda, n)$ as an exponential,

$$B(\lambda, n) = \exp(L(\lambda, n)), \qquad (3.43)$$

where $L(\lambda, n) = \log(B(\lambda, n))$. Let us now go to the double scaling limit $n \to \infty$ with λn fixed. Assuming that in this regime L behaves as $L \sim n^{\kappa} + \mathcal{O}(1/n)$, we schematically have

$$L(\lambda, n) = n^{\kappa} \hat{L}(\lambda n) + \mathcal{O}\left(\frac{1}{n}\right) = \frac{1}{\lambda^{\kappa}} (\lambda n)^{\kappa} \hat{L}(\lambda n) + \mathcal{O}\left(\frac{1}{n}\right), \qquad (3.44)$$

where the function \hat{L} now only depends on the combination λn . Defining $f(\lambda n) = (\lambda n)^{\kappa} \hat{L}(\lambda n)$, we arrive at the desired form

$$B(\lambda, n) \sim \exp\left(\frac{1}{\lambda^{\kappa}} f(\lambda n)\right)$$
 (3.45)

Indeed, this result can be generalized to also include 1/n corrections by writing

$$B(\lambda, n) \sim \exp\left(\frac{1}{\lambda^{\kappa}} \left(f_0(\lambda n) + \frac{1}{n} f_1(\lambda n) + \dots \right) \right).$$
 (3.46)

In this section we explicitly computed such 1/n-corrections for the anharmonic oscillator and have found the remarkable property that we have exact exponentiation in the sense that *all* coefficients of perturbation theory, i.e. not only those that are dominant in the limit $n \to \infty$ and λn fixed, can be recovered from the exponent, if it is calculated to sufficiently high order. In particular, we have $\kappa = 1$.

Note that in more general quantum mechanical systems this is not universally true. Instead, the statement has to be modified as we will discuss in Section 3.5.

In order to illustrate that an exact exponentiation is far from trivial let us consider the following example,

$$B(\lambda, n) = 2 \cosh\left(\frac{1}{\lambda}(\lambda n)^2\right) = 2 + \lambda^2 n^4 + \frac{1}{12}\lambda^4 n^8 + \dots$$
 (3.47)

We now identify $f(\lambda n) = (\lambda n)^2$, which remains true to all orders in 1/n. However, the function that we want to reconstruct,

$$\exp\left(\frac{1}{\lambda}f(\lambda n)\right) = 1 + \lambda n^2 + \frac{1}{2}\lambda^2 n^4 + \frac{1}{6}\lambda^3 n^6 + \frac{1}{24}\lambda^4 n^8 + \dots,$$
 (3.48)

contains terms that are not part of the expansion of the original function. Instead, the logarithm of the original function differs from $f(\lambda n)$ by

$$L(\lambda, n) - \frac{f(\lambda n)}{\lambda} = \exp\left(-2(\lambda n)n\right) - \frac{1}{2}\exp\left(-4(\lambda n)n\right) + \dots, \tag{3.49}$$

i.e. the logarithm of the original function contains terms that are exponentially suppressed as $n \to \infty$ with λn fixed. These terms, that are not a function of the combination λn only, encode all the information about the coefficients that are not correctly reproduced by the exponential $\exp(f(\lambda n)/\lambda)$.

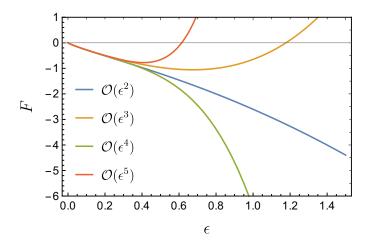


Figure 3.2: Holy grail function F in the double scaling limit $n \to \infty$ with $\epsilon = \lambda n$ fixed, neglecting corrections of order 1/n. The label denotes the highest polynomial order in ϵ that is included. Using a naive summation, the asymptotic behaviour for large ϵ is governed the truncation of the series expansion.

As we have just pointed out, it is nontrivial that a finite number of coefficients of F reproduce infinitely many terms of the amplitude *exactly*. Lacking a rigorous proof, we have nevertheless verified this to very high order in perturbation theory. For instance, we have checked that the first three nontrivial terms of the holy grail function,

$$F_{\Sigma} = -\frac{17}{16}\epsilon^2 + \frac{125}{64}\epsilon^3 - \frac{5}{16}\frac{\epsilon^2}{n} + \dots,$$
 (3.50)

reproduce the subleading corrections $(\lambda n^2)^k/n$ of \mathcal{A}_{Σ} up to order k=15.

In the 1/n-expansion of the holy grail function, all information about the large n asymptotics of \mathcal{A}_n is contained in the leading order contribution,

$$F_0(\epsilon) = -\frac{17}{16}\epsilon^2 + \frac{125}{64}\epsilon^3 - \frac{17815}{3072}\epsilon^4 + \frac{87549}{4096}\epsilon^5 + \dots$$
 (3.51)

The holy grail function F including the above leading order corrections is shown in Fig. 3.2.

We find that the leading order correction F_0 of the holy grail function is given by an alternating sum with monotonically growing coefficients. That is, the large ϵ asymptotics of the expansion will be governed by the truncation of the series. Therefore, naively, we cannot simply read off the value of F for large ϵ . In order to still make sense of it, we have to resum the perturbative series. Since we only know a finite (but still arbitrary) number of terms of F, we make use of Padé approximation. For details of this approximation procedure see Section A.1. The first few Padé approximants of the diagonal sequence P_m^m and P_{m+1}^m are shown in Fig. 3.3. Note that we use a compact notation here. The labels we use here, P_n^m , correspond to the Padé approximants of order [m, n] denoted by $Z_{[m,n]}$ in Section A.1.

The Padé resummation of F drastically enhances the predictivity for large ϵ (note the different scale in ϵ as compared to Fig. 3.2). When going to higher order

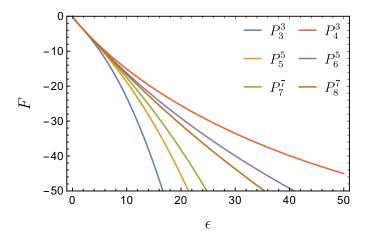


Figure 3.3: Diagonal sequence of Padé approximants of the holy grail function F in the double scaling limit $n \to \infty$, $\epsilon = \lambda n$ fixed. We consider the leading order in 1/n, i.e. $F = F^{\text{tree}} + F_0$.

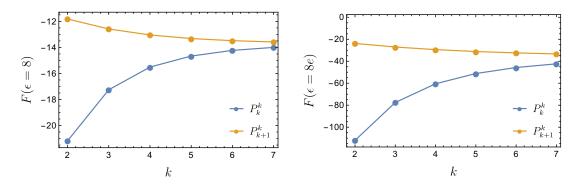


Figure 3.4: Padé approximants of F evaluated at the minimum $\epsilon = 8$ (left) and the root $\epsilon = 8e$ (right) of F^{tree} . We use the limit $n \to \infty$, $\epsilon = \lambda n$ fixed and neglect corrections of order 1/n.

in the approximants P_{m+1}^m the minima and roots are shifted towards large values of ϵ . In addition, the diagonal approximants P_m^m monotonically decrease without exhibiting any minima or roots at all. As we point out in Appendix A, the true value of F for any value of ϵ is then bounded from above and below by the diagonal Padé approximants P_{m+1}^m and P_m^m . All these observations give good evidence that the holy grail function F is negative for any ϵ in the limit $n \to \infty$. That is, the corresponding transition amplitude does not diverge, but remains finite in that regime and, in particular, does not violate unitarity at high energies. This observation is further supported by Fig. 3.4, where we evaluate the diagonal Padé sequence at the minimum, $\epsilon = 8$, and root, $\epsilon = 8e$, of the tree-level holy grail function. We find a good convergence to a value of F, which is still negative at $\epsilon = 8e$.

Furthermore, we find that the holy grail function which we systematically computed in this section is in line with two nontrivial results on the large n behaviour of the amplitudes $\langle n|\hat{x}|0\rangle$. First, in [109] Bachas rigorously derives a nontrivial upper

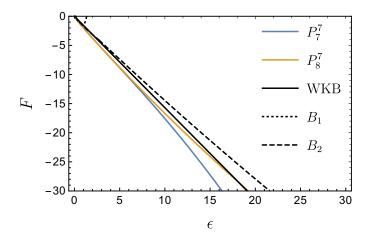


Figure 3.5: Highest Padé approximants of the holy grail function F at leading order in 1/n compared to earlier works. B_1 and B_2 are rigorous bounds corresponding to the regimes $\epsilon \ll 1$ and $\epsilon \gg 1$, respectively [109]. The label WKB corresponds to an explicit result obtained by complex WKB methods [113]. The Padé resummed holy grail function is consistent with both.

bound on $|\langle n|\hat{x}|0\rangle|$. If the exponential form of the amplitude is indeed correct, this also implies that the exponent F is bounded, too, and in particular negative for any value of ϵ as $n \to \infty$. Bachas gives explicit bounds for two regimes, $\epsilon \ll 1$ and $\epsilon \gg 1$, which in Fig. 3.5 we denote by B_1 and B_2 , respectively. Second, in [111–113] the authors use complex WKB methods in order to derive an explicit behaviour for $\langle n|\hat{x}|0\rangle$ for large n. In particular, for $\epsilon \gg 1$, they obtain [113]

$$\langle n|\hat{x}|0\rangle \sim \exp\left(-\frac{\pi}{2}n\right)$$
 (3.52)

We illustrate this result as a solid black line in Fig. 3.5.

In summary, Fig. 3.5 illustrates that our method of systematically computing the holy grail function F is in agreement with (rigorous) results of earlier works. In particular, this indicates that in the double scaling limit the vacuum transition amplitude $\langle n|\hat{x}|0\rangle$ indeed fully resums to an exponential function with a negative exponent F, hence preventing rapid growth for large n.

Finally, we conclude that for the anharmonic oscillator with a quartic coupling in the symmetric phase the vacuum transition amplitudes $\langle n|\hat{x}|0\rangle$ can be recovered exactly from the exponential function

$$\langle n|\hat{x}|0\rangle = \exp\left(\frac{1}{\lambda}F\right).$$
 (3.53)

In particular, we find that in the regime $n \to \infty$ the exponent F is negative for any value of λn , therefore preventing a rapid growth of the vacuum transition amplitudes involving highly excited states.

3.3 The spontaneously broken anharmonic oscillator

Having established powerful techniques to study high order perturbation theory for the anharmonic oscillator with a single minimum, we now want to move to the anharmonic oscillator with a symmetric double-well potential,

$$V(x) = m^2 x^2 + \lambda x^4$$
 with $m^2 < 0$, (3.54)

where, similar to the symmetric case, $\lambda > 0$. In particular, we want to make use of the same perturbative techniques that have proven suitable for the single-well potential.

Yet, this is not a straightforward generalization, as there is a delicate issue when applying perturbative techniques to potentials with degenerate minima, such as the double-well. Indeed, almost by construction, all known methods rely on perturbations around the harmonic oscillator solution. A naive application to the symmetric double-well would imply a perturbation theory in an inverted harmonic oscillator background, including the obvious problems arising from the instability of the potential. Therefore, one has to choose another (locally harmonic) reference point for the perturbative expansion. A suitable point of the symmetric double-well is one of the two minima $x_{\pm} = \pm \sqrt{-m^2/2\lambda}$. Then, expanding around⁶ x_+ , shifting the coordinate $\tilde{x} = x - x_+$ and subtracting the zero-point energy yields the asymmetric double-well potential

$$\tilde{V}(\tilde{x}) = \tilde{m}^2 \tilde{x}^2 + 2\sqrt{\tilde{m}^2} \sqrt{\lambda} \tilde{x}^3 + \lambda \tilde{x}^4$$
(3.55)

with $\tilde{m}^2 = -2m^2$. In the field theoretical picture this expansion corresponds to a spontaneous breaking of the symmetry by a tachyonic scalar field that acquires a vacuum expectation value x_+ .

Note that a constant shift in the ground state energy or in the definition of the position operator does not alter the transition amplitude $\langle n|\hat{x}|0\rangle$. The former does not have any effect, as, even in quantum mechanics, only energy differences are relevant⁷ which do not change by an additional constant in the Hamiltonian. The latter does not have any effect, because $\langle n|\hat{x}|0\rangle$ involves different energy eigenstates, which are orthogonal to each other. Consequently, a constant shift in the position operator does not modify the transition amplitude between those states.

Naively, due to the positive mass term, the potential V is well suited for the perturbative techniques that we established in the previous section. However, computationally this comes at the cost of introducing an additional cubic term $\sqrt{\lambda}\tilde{x}^3$. By the approach of Bender and Wu [103, 104] presented in the previous section, we can then reconstruct the spectrum of the Schroedinger operator associated to the potential \tilde{V} order by order in the coupling λ . However, note some important

⁶Both choices are equivalent, since they are related by parity.

⁷This picture drastically changes for a gravitational theory, where absolute energies have a physical meaning.

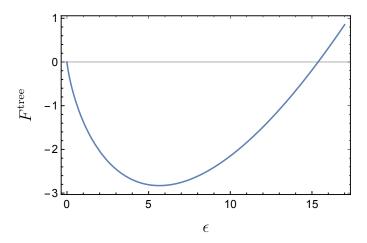


Figure 3.6: Tree-level holy grail function of the symmetric double-well potential in the double scaling limit $n \to \infty$, $\epsilon = \lambda n = const$. It exhibits a minimum at $\epsilon = 4\sqrt{2}$ and a root at $\epsilon = 4\sqrt{2}e$.

technicality here. Since the cubic term $\sqrt{\lambda}x^3$ appears with a fractional power of the coupling, we instead define $\Lambda = \sqrt{\lambda}$ and solve the recursion relations by integer orders in Λ .

Similar to the single-well potential, we find that the (normalized) transition amplitudes can be factorized into a tree-level and higher order part, $\mathcal{A}_n = \mathcal{A}_n^{\text{tree}} \mathcal{A}_{\Sigma}$. Here, the tree-level contribution reads

$$\mathcal{A}_n^{\text{tree}} = \sqrt{\frac{n!}{2\tilde{m}}} \left(\frac{\lambda}{2\tilde{m}^3}\right)^{\frac{n-1}{2}}.$$
 (3.56)

In particular, it again turns out that the perturbative expansion of the amplitude is reproduced *exactly* by an exponential function with a suitable exponent,

$$\mathcal{A}_n = \mathcal{A}_n^{\text{tree}} \exp\left(\frac{1}{\lambda} F_{\Sigma}\right) \,. \tag{3.57}$$

In order to determine the large n asymptotics of the transition amplitude, we therefore rewrite it as

$$\mathcal{A}_n \sim \exp\left(\frac{1}{\lambda}\left(F^{\text{tree}} + F_{\Sigma}\right)\right),$$
 (3.58)

such that, for phenomenological purposes, we can focus on the sign of the exponent. The part of the exponent that corresponds to the tree-level contribution (3.56) reads

$$F^{\text{tree}}(\epsilon) \sim \frac{\epsilon}{2} \left(\ln \frac{\epsilon}{4\sqrt{2}} - 1 \right) \,.$$
 (3.59)

This is illustrated in Fig. 3.6.

Similar to the symmetric case, F^{tree} exhibits a root at $\epsilon = 4\sqrt{2}e$ where it changes from negative to positive sign, ultimately leading to a rapid growth of the amplitude

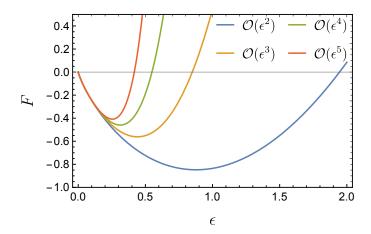


Figure 3.7: Holy grail function F of the symmetric double-well potential in the double scaling limit $n \to \infty$ with $\epsilon = \lambda n$ fixed, neglecting corrections of order 1/n. The label denotes the highest polynomial order in ϵ that is included. The asymptotic behaviour for large ϵ is governed the truncation of the series expansion, indicating that we have to apply resummation techniques.

as $n \to \infty$. For the single-well anharmonic oscillator, we have seen in Section 3.2 that a suitable resummation of F_{Σ} resolves this issue. However, a direct resummation for the double-well potential is problematic. Let us briefly outline why this is the case. In the double scaling limit $n \to \infty$ with ϵ fixed, the only relevant contribution in the 1/n expansion is the leading order correction F_0 , which reads

$$F_0(\epsilon) = \frac{17}{32} \epsilon^2 + \frac{125}{64\sqrt{2}} \epsilon^3 + \frac{17815}{3072} \epsilon^4 + \frac{87549}{2048\sqrt{2}} \epsilon^5 + \mathcal{O}\left(\epsilon^6\right) . \tag{3.60}$$

As can be seen in Fig. 3.7, it is not possible to read off the sign of F directly, as the position of the root strongly depends on the series truncation. In contrast to the single-well, however, the series representation of F_0 only contains positive (and growing) coefficients, indicating problems with an unambiguous Borel resummation. Ambiguities in a Borel resummation can, e.g., arise due to poles in the Borel plane. These can lead to imaginary contributions that are possibly lifted by including non-perturbative effects (see, e.g., [66,68]). Therefore, to this point, the overall sign of the holy grail function F for the symmetric double-well potential remains unclear.

In summary, ordinary perturbation theory – even when naively resummed – does not allow for a clear resolution of the rapid growth of high multiplicity amplitudes. Let us therefore turn to more powerful methods.

3.3.1 Exact perturbation theory

From a perturbative point of view, the crucial difference between the single- and the double-well case is the presence of two degenerate vacua. These can lead, e.g., to instantonic configurations which cannot be captured by a conventional perturbative ansatz. Still, in principle, they have to be included in the quantum mechanical

path integral where they appear as nontrivial saddle points of the action⁸. It is well known that such quantum effects can cause perturbative expansions (of e.g. the vacuum energy) to be non Borel-resummable [139–144].

Non-perturbative effects (and their relation to perturbation theory) in quantum mechanics and quantum field theory have been widely studied in the literature, e.g. in [66, 106, 138, 145–155]. Instead of applying these well known techniques, such as instanton calculus, we want to follow a novel approach put forward by Serone et al. in [108, 115]. As we will see later, this approach makes efficient use of our previous results on the single-well case, making it well suited for our study. Let us briefly outline its basic concepts.

The key idea is to recover non-perturbative contributions from the perturbative expansion by smart deformations thereof. In this sense, it is in line with the notion of resurgence and trans-series expansions in quantum mechanics and quantum field theory, see, e.g., [68,79]. Applied to our example, suitable deformations exploit the nontrivial exponentiation of the amplitude.

Very generally, let us consider a quantum mechanical potential $V(x;\lambda)$ with coupling λ . We require it to admit bound states, or, more precisely, $\lim_{|x|\to\infty} V(x;\lambda) = \infty$. If it, in addition, satisfies $V(x;\lambda) = V(x\sqrt{\lambda};1)/\lambda$, we call the potential classical, because then a perturbative expansion in λ coincides with the expansion in \hbar , i.e. with the quantum loop-expansion.

Now let us consider two such classical potentials, $V_0(x;\lambda)$ and $V_1(x;\lambda)$. Crucially, if $V_0(x;\lambda)$ admits a theory with perturbative expansion that is Borel resummable exactly, the perturbative series of $V(x;\lambda) = V_0(x;\lambda) + \lambda V_1(x;\lambda)$ is also Borel resummable to the exact result, given that V_1 is asymptotically bounded, $\lim_{|x|\to\infty} V_1(x;1)/V_0(x;1) = 0$. That is, we treat the part of the potential that leads to an ambiguous Borel resummation as a perturbation of order λ , thereby rearranging the perturbative expansion. This procedure was coined exact perturbation theory in [108, 115].

Obviously, each of the two potentials can depend on an additional auxiliary parameter λ_0 . Therefore, we can also try to find potentials, suitably depending on λ_0 , such that

$$\hat{V}(x;\lambda,\lambda_0) = V_0(x;\lambda,\lambda_0) + \lambda V_1(x;\lambda,\lambda_0)$$
(3.61)

and

$$\hat{V}(x;\lambda,\lambda) = V(x;\lambda). \tag{3.62}$$

That is, we want to find an auxiliary potential $\hat{V}(x; \lambda, \lambda_0)$ for which we recover the original potential $V(x; \lambda)$, if we set $\lambda_0 = \lambda$. If we have such auxiliary potential at hand, we can extract the full information about $V(x; \lambda)$ by performing a perturbative expansion in λ in $\hat{V}(x; \lambda, \lambda_0)$ and removing the deformation by setting $\lambda_0 = \lambda$ after carrying out the Borel resummation. Serone et al. discuss a variety of quantum mechanical examples in [108, 115].

⁸The quantum mechanical double-well potential is the prime example where instanton solutions play an important role. For instance, they lift the vacuum degeneracy (see, e.g. [106,138]).

Exact perturbation theory can be useful for systems, where standard perturbation theory is not applicable or does not admit an unambiguous Borel resummation. In the following we want to apply it to the double-well potential,

$$V(x;\lambda) = -x^2 + \lambda x^4, \tag{3.63}$$

which we now have normalized to the mass, $m^2 = 1$. As pointed out before, we want to find an auxiliary potential $\hat{V}(x; \lambda, \lambda_0) = V_0(x; \lambda, \lambda_0) + \lambda V_1(x; \lambda, \lambda_0)$ that reproduces $V(x; \lambda)$ at finite coupling. Furthermore, $V_0(x; \lambda)$ has to admit a perturbative expansion that is Borel resummable to the exact result.

Obviously, the choice of \hat{V} is by no means unique. In fact, there is a plethora of different choices of V_0 and V_1 which are more or less suited depending on what quantity we are interested in. In general, neglecting constant and linear terms of the potential, the requirement on V_0 and V_1 to be classical gives the most general form of \hat{V} ,

$$\hat{V}(x;\lambda,\lambda_0) = (v_2 + \lambda w_2) x^2 + (v_3 + \lambda w_3) \sqrt{\lambda} x^3 + v_4 \lambda x^4.$$
 (3.64)

Here, the coefficients v_i and w_i belong to V_0 and V_1 , respectively. In particular, they are functions of λ_0 only, $v_i = v_i(\lambda_0)$ and $w_i = w_i(\lambda_0)$. Furthermore, in order to reproduce the symmetric double-well potential at the coupling $\lambda = \lambda_0$, the coefficients have to satisfy the conditions

$$v_2(\lambda) + \lambda w_2(\lambda) = -1, \qquad (3.65)$$

$$v_3(\lambda) + \lambda w_3(\lambda) = 0, \qquad (3.66)$$

as well as the trivial normalization

$$v_4 = 1$$
. (3.67)

Up to terms in v_i and w_i that exactly cancel at $\lambda_0 = \lambda$, this implies that the properties of the perturbative ansatz are entirely controlled by the functions $v_i(\lambda_0)$ which we can choose suitably. In the end, the only requirement is then that V_0 has to admit a perturbative expansion that is Borel summable.

While the above conditions yield the most general choice of the auxiliary potential \hat{V} , we will discuss a specific example with a simple but nontrivial v_2 ,

$$V_0(x;\lambda,\lambda_0) = x^2 + \lambda x^4, \qquad (3.68)$$

$$V_1(x;\lambda,\lambda_0) = -\frac{2}{\lambda_0}x^2, \qquad (3.69)$$

where the single-well anharmonic oscillator V_0 is known to be Borel resummable [105, 156]. The associated auxiliary potential is then

$$\hat{V}(x;\lambda,\lambda_0) = \left(1 - 2\frac{\lambda}{\lambda_0}\right)x^2 + \lambda x^4. \tag{3.70}$$

It reproduces the symmetric double-well potential when setting $\lambda_0 = \lambda$,

$$\hat{V}(x;\lambda,\lambda) = -x^2 + \lambda x^4. \tag{3.71}$$

Note that this simple example is just a particular case, $v_2 = 1$, of a more general parametrization, $v_2(\lambda_0) = const$. In Appendix B we discuss the convergence properties of the associated perturbation theory as a function of v_2 .

According to the idea of exact perturbation theory we can now consider the potential $\hat{V}(x; \lambda, \lambda_0)$ instead of the double-well potential $V(x; \lambda)$. In this potential we can then compute any quantity of interest by a perturbative expansion in λ (while keeping λ_0 fixed), perform the Borel resummation and finally remove the deformation of the perturbative expansion, $\lambda_0 = \lambda$.

3.3.2 Reconstructing the holy grail function

Let us now make use of the powerful idea of exact perturbation theory. Accordingly, in order to obtain $\langle n|\hat{x}|0\rangle$ in the double-well potential, we could in principle repeat the original computation of the wave functions and transition amplitudes of Section 3.2.1 in the auxiliary potential $\hat{V}(x;\lambda,\lambda_0)$. However, we observe that the deformation V_1 of the single-well potential effectively introduces a mass term that depends on the coupling, $m^2(\lambda) = 1 - 2\lambda/\lambda_0$. Therefore, as an alternative approach, we can use our previous results on $\langle n|\hat{x}|0\rangle$ obtained for the symmetric case in Section 3.2.2 by simply plugging in the λ -dependent mass term.

For convenience, let us briefly recall our previous results for the single-well potential. Reintroducing the positive mass term $m^2 > 0$, we found

$$\langle n|\hat{x}|0\rangle = \langle n|\hat{x}|0\rangle_{\text{tree}} \exp\left(\frac{1}{\lambda}F_{\Sigma}\right)$$
 (3.72)

where

$$\langle n|\hat{x}|0\rangle_{\text{tree}} = \sqrt{\frac{n!}{2m}} \left(\frac{\lambda}{8m^3}\right)^{\frac{n-1}{2}}.$$
 (3.73)

The leading order correction in the 1/n-expansion of the holy grail function reads

$$F_0(\epsilon) = -\frac{17}{16} \frac{\epsilon^2}{m^3} + \frac{125}{64} \frac{\epsilon^3}{m^6} - \frac{17815}{3072} \frac{\epsilon^4}{m^9} + \frac{87549}{4096} \frac{\epsilon^5}{m^{12}} + \mathcal{O}\left(\epsilon^6\right) . \tag{3.74}$$

Note that, in general, a mass term that depends on the coupling of the theory might introduce additional factors in the 1/n-expansion of F_{Σ} which are not subdominant anymore. However, this does not happen for our choice of deformation, which, in fact, partially motivates this particular choice.

Plugging in the mass term $m^2 = 1 - 2\lambda/\lambda_0$, performing a perturbative expansion in λ and thereby rearranging the result in the corresponding 1/n-expansion then yields

$$\hat{F}_{0}(\epsilon, \epsilon_{0}) = -\frac{17}{16}\epsilon^{2} + \frac{125}{64}\epsilon^{3} - \frac{17815}{3072}\epsilon^{4} + \dots + \frac{1}{\epsilon_{0}}\left(\frac{3}{2}\epsilon^{2} - \frac{51}{16}\epsilon^{3} + \dots\right) + \mathcal{O}\left(\frac{\epsilon^{3}}{\epsilon_{0}^{2}}\right), \tag{3.75}$$

where we defined the abbreviation $\epsilon_0 = \lambda_0 n$, which will be useful for the double scaling limit that we consider later. We can now obtain the holy grail function F associated to the double-well potential by resumming \hat{F}_0 as a series in ϵ before the deformation is finally lifted by evaluating it at $\epsilon_0 = \epsilon$.

Note that the order of resummation and removing the deformation is important here. For example, performing a Borel summation requires a computation of the Laplace transformation $F(\epsilon, \epsilon_0) = \int_0^\infty dt \exp(-t) \mathcal{B}F(\epsilon t, \epsilon_0)$, where $\mathcal{B}F(\epsilon t, \epsilon_0)$ is the Borel sum of the power series in ϵt while ϵ_0 is still treated as an auxiliary parameter. In particular, the argument in the integral is ϵt while the external parameter ϵ_0 is not multiplied by the integration variable t. Only after performing the Laplace transformation correctly we can finally evaluate $F(\epsilon, \epsilon)$.

Similar to the symmetric case, in order to resum the series expansion of the holy grail function we make use of Padé approximation. However, here a crucial difference is that we have to perform a separate Padé resummation for every value of ϵ_0 that we want to probe.

We find that, while the different Padé approximants converge well to negative values for large values of ϵ , the approximation seems to be spoiled by spurious poles in the region of small ϵ . Such spurious poles can also occur in the Padé approximation for a number of well-behaved functions and might question the validity of the approximation beyond the pole⁹. In fact, looking more closely at the series expansion for $\epsilon_0 < 1$, we find that the series seems to forfeit oscillating signs of the coefficients that typically indicate stability in a resummation with a finite number of known terms. We discuss the technical details of such instability in Appendix B where the relevant sign structure is illustrated in Fig. B.1.

In order to avoid these problems we have tried several different approximation schemes, for which the Borel-Padé approximation scheme turns out to provide good results. The first few diagonal approximants of F in that scheme are shown in Fig. 3.8.

Using Borel-Padé approximation, we observe that F is negative for a wide range of values of ϵ . In particular, this is even more pronounced when going to higher orders in the approximation. Therefore, similar to the single-well, we find strong hints that suitably resummed perturbation theory is sufficient to resolve the rapid growth of $\langle n|\hat{x}|0\rangle$ as $n\to\infty$.

However, we also remark that some potential problems of the approximation still remain. For small values of ϵ the Padé approximant of the Borel sum inherits the problem of spurious poles. However, these poles do not contribute significantly in the Laplace transformation when taking the principal value for the integral. At large values of ϵ the effect of spurious poles is subdominant, because the integrand of the Laplace transform is exponentially suppressed in the region containing the poles. Overall, this gives the smooth estimate of F illustrated in Fig. 3.8. We

⁹For instance, the third diagonal Padé approximant of the exponential function, $P_3^3(x) = \left(1 + \frac{x}{2} + \frac{x^2}{10} + \frac{x^3}{120}\right) / \left(1 - \frac{x}{2} + \frac{x^2}{10} - \frac{x^3}{120}\right)$, features a pole on the real axis, at $x \approx 4.64$, which is not present in the original function.

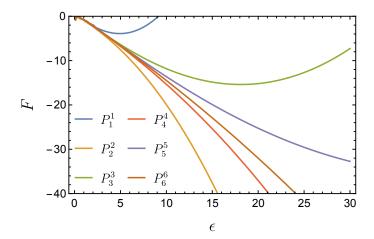


Figure 3.8: Diagonal Borel-Padé approximants of the holy grail function F associated to the symmetric double-well potential in the double scaling limit $n \to \infty$, $\epsilon = \lambda n = const$. Higher order corrections in the 1/n-expansion are neglected. F is obtained with the ansatz of exact perturbation theory using the auxiliary potential (3.70).

further note that liftable poles are a common feature of Borel-Padé approximation, as Padé approximants sometimes suffer from poles along the real axis. Hence, in order to verify the results obtained by Borel-Padé approximation, we have tried a number of other resummation schemes, which are briefly presented in Appendix A. A particularly promising resummation scheme, that makes use of the large order Borel asymptotics, we point out in Section 3.3.3. All of them consistently feature negative values of F for large ϵ but also some instability to a certain degree. For example, in Fig. 3.9 we illustrate their behaviour at the minimum and the root of the tree-level contribution to the holy grail function (3.59). We observe that, while convergence is not completely monotonous everywhere, the different approximations generally agree well with each other. For instance, at the tree-level root the spread between the different results is smaller than the distance to zero, strongly indicating that the sign of the holy grail function is indeed negative at this point.

Furthermore, in Fig. 3.10 we compare the different approximations of the holy grail function to earlier results from WKB estimates [113] and a rigorous bound by Bachas [109]. We find that F obtained within exact perturbation theory is in line with both results, providing even further evidence that our ansatz is indeed valid.

Finally, we conclude that, similar to the single-well potential, suitably resummed (exact) perturbation theory resolves the rapid growth of the vacuum transition amplitudes $\langle n|\hat{x}|0\rangle$ in the symmetric double-well potential for large n.

3.3.3 Resummation by guessing the Borel asymptotics

We have just seen that, due to possible instabilities, different resummation schemes are more or less suitable in the framework of exact perturbation theory. In conven-

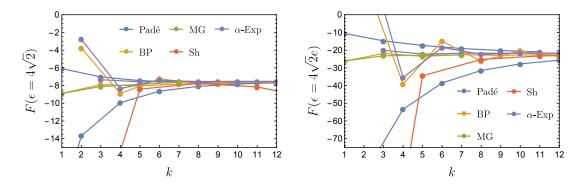


Figure 3.9: Value of the different approximants of the holy grail function F associated to the symmetric double-well potential in the double scaling limit $n \to \infty$, $\epsilon = \lambda n$ fixed at the minimum, $\epsilon = 4\sqrt{2}$, (left panel) and at the root, $\epsilon = 4\sqrt{2}e$, (right panel) of the tree-level holy grail function. The k denotes the number of coefficients of the power series of F taken into account in the corresponding approximation scheme. The approximation schemes shown are Padé, Borel-Padé (BP), Meijer G (MG), Shafer (Sh) and an α -exponential scheme (α -Exp), all of which are discussed in Appendix A and Section 3.3.3.

tional resummation schemes, including the large order behaviour in an approximation scheme seems promising, as is, for instance, done by the Meijer G approximation scheme discussed in Section A.4. Yet, in the Meijer G scheme, it might happen that the successive ratios of coefficients in the Borel sum are not well approximated by a constant. For instance, in our scenario of exact perturbation theory for the double-well anharmonic oscillator, we find that they behave approximately as

$$\frac{b_{n+1}}{b_n} \sim f(\epsilon_0) n^{\alpha} \tag{3.76}$$

with α in the range $\frac{1}{2}$...1 and the function f depending on the precise value of α . The large order Borel asymptotics can then be accounted for with a so called α -exponential,

$$\exp_{\alpha}\left(f(\epsilon_0)\epsilon\right) = \sum_{k=0}^{\infty} \frac{f(\epsilon_0)^k}{k!^{\alpha}} \epsilon^k \quad \text{with} \quad 0 < \alpha \le 1.$$
 (3.77)

The function f can be expressed as an expansion in $1/\epsilon_0$ by fitting to the known coefficients of the Borel sum.

As expected, this function does not very well represent the low order behaviour of the series. Therefore, we can correct the Borel transform by explicitly including the known coefficients (up to n = 14),

$$\mathcal{B}F(\epsilon, \epsilon_0) = \sum_{k=0}^{\infty} \frac{f(\epsilon_0)^k}{k!^{\alpha}} \epsilon^k + \sum_{k=0}^{14} \left(\frac{F_{0,k}(\epsilon_0)}{k!} - \frac{f(\epsilon_0)^k}{k!^{\alpha}} \right) \epsilon^k.$$
 (3.78)

In principle, we could now proceed by Laplace transforming $\mathcal{B}F$ with respect to ϵ while keeping ϵ_0 fixed. However, the behaviour can be significantly improved by

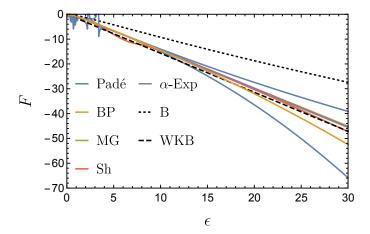


Figure 3.10: Different approximants (to highest available order) of the holy grail function F of the symmetric double-well potential in the double scaling limit $n \to \infty$, $\epsilon = \lambda n = const$ (as in Fig. 3.8) compared to WKB estimates [113] and a rigorous bound derived by Bachas [109], labelled WKB and B, respectively. The other labels are as in Fig. 3.9.

applying a Padé approximation to the remainder function given by the second term on the right hand side of (3.78). In practice, we apply a Padé approximation of the same order to the remainder function as well as the α -exponential.

Let us now apply this resummation procedure to our problem of exact perturbation theory in the symmetric double-well potential. Fitting the known coefficients for the remainder function we find,

$$f(\epsilon_0) \approx -1.476 + 0.66/\epsilon_0 + 0.064/\epsilon_0^2 \quad \text{for} \quad \alpha = \frac{1}{2}.$$
 (3.79)

The results are illustrated in Fig. 3.11. We remark that this approximation is only good for $\epsilon_0 \gtrsim 2$. Therefore, the spread in the different Padé orders possibly underestimates the true uncertainty.

Finally, let us finish this discussion with some technical remarks. In principle, by estimating the large order behavior of the Borel sum $\mathcal{B}F$ from the coefficients at low order, we gain access to the Borel-Padé approximants of higher order. However, a subtle issue arises when naively summing $\mathcal{B}F$. Although the α -exponential has an infinite radius of convergence, $\mathcal{B}F$ cannot be summed term by term as it still contains the exact coefficients at low order. That is, the remainder function is a polynomial that will dominate over the quickly falling α -exponential above a certain critical value of ϵ , most likely yielding the wrong asymptotics of the Borel sum. Consequently, the Laplace transform of $\mathcal{B}F$ does not give a good approximation of the function F. Therefore, we think that a Padé approximation of both sums yields a better estimate of the asymptotics for large ϵ . In fact, we have checked that it indeed does not exceed the α -exponential term for a large range of values $\epsilon \gtrsim 2$, but still gives a significant contribution to the Laplace transform.

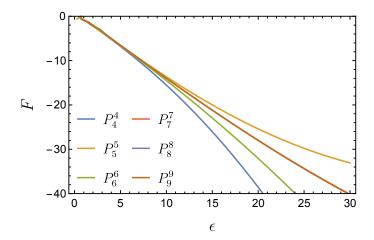


Figure 3.11: Diagonal Borel-Padé approximants of the holy grail function F with an estimated large order behaviour using (3.78). The higher order approximants are already nicely converged. Note, however, that this does not represent the full error. There is an additional systematic uncertainty at small ϵ due to the use of the approximate formula (3.79), as well as a general uncertainty due to our guessing of the large order behaviour.

3.4 Transition amplitudes involving general local operators

So far we have only considered transition amplitudes from the vacuum to highly excited states, $\langle n|\hat{x}|0\rangle$. In this section we want to go beyond that and use our techniques to compute transitions between arbitrary states involving arbitrary local operators, $\langle n|\hat{x}^q|m\rangle$, where, for simplicity, q is integer. In particular, we will argue that, in the double scaling limit $n\to\infty$ with λn and m fixed, the transition amplitudes are, to exponential accuracy, independent of the power of the local operator. More precisely, we want to show that

$$\langle n|\hat{x}^q|m\rangle \sim R_q(n,m) \frac{\langle n|\hat{x}|0\rangle}{\langle m|\hat{x}|0\rangle},$$
 (3.80)

where R_q follows at most a power law of the quantum numbers n and m.

In fact, by this computation, we will support a crucial assumption of the semiclassical approach to multiparticle production (cf. Section 2.2), where, to exponential accuracy, the amplitude is supposed to be independent of the local operator, $\langle n|\phi^2|0\rangle \sim \langle n|\phi|0\rangle$.

Our general idea is to compute $\langle n|\hat{x}^q|m\rangle$ and compare it to the right hand side of (3.80). In principle, this can be done recursively by reducing the power of the local operator with suitable insertions of the identity,

$$\langle n|\hat{x}^q|m\rangle = \sum_{l} \langle n|\hat{x}^{q-1}|l\rangle \langle l|\hat{x}|m\rangle .$$
 (3.81)

Therefore, the basic building blocks are indeed the transition amplitudes involving only a linear local operator, q=1. In terms of the perturbative ansatz (cf. Section 3.2) they read

$$\langle n|\hat{x}|m\rangle = \sum_{i=0}^{\infty} \lambda^{i} t_{i}^{n,m} \text{ with } t_{i}^{n,m} = \sum_{p=0}^{i} \sum_{k=0}^{n+4p} \sum_{l=0}^{m+4(i-p)} B_{p,k}^{n} B_{i-p,l}^{m} \Gamma\left(\frac{k+l+2}{2}\right).$$
(3.82)

Using properly normalized states, we can again extract the tree-level amplitude,

$$\langle n|\hat{x}|m\rangle_{\text{tree}} = \sqrt{\binom{n}{m} + \binom{m}{n}} \sqrt{\frac{|n-m|!}{2}} \left(\frac{\lambda}{8}\right)^{\frac{|n-m|-1}{2}}.$$
 (3.83)

Note that here some care has to be taken when establishing a correspondence between $\langle n|\hat{x}|m\rangle$ and its field theory analogue. In fact, the interpretation in terms of a quantum field theory is not at all obvious. For instance, increasing m in the above expression effectively decreases the number of couplings, i.e. vertices, for a given transition from m to n. However, naively, in the Feynman language of perturbative quantum field theory we would expect the opposite, as the number of couplings corresponds to the number of vertices in a connected diagram. Indeed, $\langle n|\hat{x}|m\rangle_{\rm tree}$ not only contains information about the fully connected amplitude, but also about all disconnected pieces.

Nevertheless, the transition amplitude between arbitrary states exhibits a rich and interesting structure. Let us point out a few features in the following. For example, the tree-level part shows a certain form of crossing symmetry,

$$\langle n|\hat{x}|m\rangle_{\text{tree}} = \sqrt{\binom{n}{m} + \binom{m}{n}} \langle |n-m| |\hat{x}|0\rangle_{\text{tree}}$$
 (3.84)

Furthermore, it completely factorizes into distinct amplitudes. For example, taking n > m to write (3.83) as

$$\langle n|\hat{x}|m\rangle_{\text{tree}} = \frac{\sqrt{n!}}{\sqrt{m!}} \frac{2^{-n/2}}{2^{-m/2}} \left(\frac{\lambda}{4}\right)^{\frac{n-m-1}{2}},$$
 (3.85)

we observe that the tree-level contribution is in fact a quotient of two distinct tree-level amplitudes,

$$\langle n|\hat{x}|m\rangle_{\text{tree}} = \sqrt{\frac{m+1}{2}} \frac{\langle n|\hat{x}|k\rangle_{\text{tree}}}{\langle m+1|\hat{x}|k\rangle_{\text{tree}}}.$$
 (3.86)

Here, $|k\rangle$ denotes an arbitrary state with $k \leq m$ and n+k odd. For odd n we could for example choose k=0 or k=1 for n even.

Below we will show that these properties are not limited to the tree-level contribution, but indeed also hold for the full amplitude to all orders in perturbation theory.

The higher order corrections of the amplitude can be computed using the methods of Section 3.2. They are given by

$$\langle n|\hat{x}|m\rangle = \langle n|\hat{x}|m\rangle_{\text{tree}} \left(1 + \frac{\lambda}{16} \left(-17n^2 - 5n + 17m^2 + 29m + 12\right) + \frac{\lambda^2}{512} \left(289n^4 + 289m^4 + \dots\right) + \dots\right).$$
(3.87)

Remarkably, the states n and m completely decouple, i.e. the first mixed terms of the form $n^x m^y$ appear only at quadratic order in the coupling, $\mathcal{O}(\lambda^2 n^2 m^2)$. Therefore, it is straightforward to again rewrite the amplitude in exponential form, satisfying

$$\langle n|\hat{x}|m\rangle = \langle n|\hat{x}|m\rangle_{\text{tree}} \exp\left(\frac{1}{\lambda}\mathcal{F}_{\Sigma}(\lambda, n, m)\right),$$
 (3.88)

where the exponent is given by

$$\mathcal{F}_{\Sigma}(\lambda, n, m) = \lambda^2 \left(-\frac{17}{16}n^2 - \frac{5}{16}n + \frac{17}{16}m^2 + \frac{29}{16}m + \frac{3}{4} \right) + \mathcal{O}\left(\lambda^3\right). \tag{3.89}$$

The decoupling of n and m then implies that the holy grail function can be written as a sum of two independent components,

$$\mathcal{F}_{\Sigma}(\lambda, n, m) = F_{\Sigma}(\lambda, n) + \hat{F}_{\Sigma}(\lambda, m), \qquad (3.90)$$

where F_{Σ} is determined by the vacuum amplitude $\langle n|\hat{x}|0\rangle$ given in (3.25) and \hat{F}_{Σ} denotes the additional contribution from the initial state $|m\rangle$. Intriguingly, it can be fully recovered from the vacuum amplitude by observing

$$\hat{F}_{\Sigma}(\lambda, m) = -F_{\Sigma}(-\lambda, -(m+1)). \tag{3.91}$$

Therefore, $\langle n|\hat{x}|m\rangle$ for arbitrary m is in principle fully determined by the vacuum amplitude $\langle n|\hat{x}|0\rangle$. This has remarkable consequences, as it allows us to extend the tree-level result (3.86) to the full amplitude to all orders,

$$\langle n|\hat{x}|m\rangle \sim \sqrt{\frac{m+1}{2}} \frac{\langle n|\hat{x}|k\rangle}{\langle m+1|\hat{x}|k\rangle}.$$
 (3.92)

Note that here we neglect terms of the order 1/n in the exponent, i.e. we drop terms of the form $\exp(1/n)$. It is therefore valid to exponential accuracy.

The above observation is key for the computation of transition amplitudes between arbitrary states for polynomials of local operators,

$$\langle n|P(\hat{x})|m\rangle = \sum_{q} a_q \langle n|\hat{x}^q|m\rangle$$
 (3.93)

Hence, we now want to generalize the above results to the transition amplitudes $\langle n|\hat{x}^q|m\rangle$. At leading order in the 1/n expansion of the holy grail function, our general claim for an arbitrary power of local operators is

$$\langle n|\hat{x}^{q}|m\rangle \sim c_{q} \left((n+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}} \right)^{q-1} \frac{\langle n|\hat{x}|k_{n}\rangle}{\langle m+1|\hat{x}|k_{m}\rangle},$$
 (3.94)

where c_q is a positive constant and we take n > m with n + m + q and $m + k_m$ even while $n + k_n$ is odd. For example, it is convenient to choose $k_{n,m} = 0, 1$ depending on the parity of the states $|n\rangle$ and $|m\rangle$.

By induction in q, we now want to argue that (3.94) holds in general. Because of parity even and odd q have to be considered separately.

Let us consider the case with n, m and q even explicitly. In this case the claim reads

$$\langle n|\hat{x}^{2p}|m\rangle \sim c_{2p} \left((n+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}} \right)^{2p-1} \frac{\langle n|\hat{x}|1\rangle}{\langle m+1|\hat{x}|0\rangle},$$
 (3.95)

where q = 2p. The first nontrivial case p = 1, for which the full derivation be found in Appendix C, can be shown to be

$$\langle n|\hat{x}^2|m\rangle \sim \frac{(n+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}}}{3\sqrt{2}} \sqrt{\frac{m+1}{2}} \frac{\langle n|\hat{x}|1\rangle}{\langle m+1|\hat{x}|0\rangle}.$$
 (3.96)

Having established the first nontrivial case, we can now proceed with the induction step $p \to p+1$ and insert the identity operator,

$$\langle n|\hat{x}^{2(p+1)}|m\rangle = \sum_{l=0}^{\infty} \langle n|\hat{x}^{2p}|l\rangle \langle l|\hat{x}^{2}|m\rangle . \tag{3.97}$$

Depending on the state $|l\rangle$, the sum can be split into three different contributions

$$\langle n|\hat{x}^{2(p+1)}|m\rangle \sim c_{2p}\left(S_1 + S_2 + S_3\right)$$
 (3.98)

where we defined

$$S_{1} = \langle n|\hat{x}|1\rangle \langle m|\hat{x}|1\rangle \times \sum_{l=0}^{m} \frac{l+1}{2} \left((n+1)^{\frac{3}{2}} - (l+1)^{\frac{3}{2}} \right)^{2p-1} \frac{(m+1)^{\frac{3}{2}} - (l+1)^{\frac{3}{2}}}{3\sqrt{2}} \frac{1}{\langle l+1|\hat{x}|0\rangle^{2}},$$

$$S_{2} = \sqrt{\frac{m+1}{2}} \frac{\langle n|\hat{x}|1\rangle}{\langle m+1|\hat{x}|0\rangle}$$

$$\times \sum_{l=m}^{n} \sqrt{\frac{l+1}{2}} \left((n+1)^{\frac{3}{2}} - (l+1)^{\frac{3}{2}} \right)^{2p-1} \frac{(l+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}}}{3\sqrt{2}} \frac{\langle l|\hat{x}|1\rangle}{\langle l+1|\hat{x}|0\rangle},$$

$$S_{3} = \sqrt{\frac{(n+1)(m+1)}{2}} \frac{1}{\langle n+1|\hat{x}|0\rangle \langle m+1|\hat{x}|0\rangle}$$

$$\times \sum_{l=m}^{\infty} \left((l+1)^{\frac{3}{2}} - (n+1)^{\frac{3}{2}} \right)^{2p-1} \frac{(l+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}}}{3\sqrt{2}} \langle l|\hat{x}|1\rangle^{2}.$$

$$(3.101)$$

Here, we already applied the induction hypothesis (3.94) together with the initial result (3.96). That is, there are three different contributions to the leading n behaviour of the transition amplitude, which can be analysed independently with respect to their large n asymptotics.

(i) The sum contained in the first contribution S_1 does not exhibit any explicit dependence on n. Therefore, the term with the highest power of n will be the dominant contribution. That is, we can write

$$S_1 \sim (n+1)^{\frac{3}{2}(2p-1)} \langle n|\hat{x}|1\rangle$$
 (3.102)

(ii) The second contribution S_2 , however, depends on n both explicitly and implicitly, as it involves a sum where n appears as a boundary term. However, because of the relation $\langle l|\hat{x}|1\rangle / \langle l+1|\hat{x}|0\rangle \sim \mathcal{O}(1)$, we can evaluate this sum explicitly by rewriting it as an integral. Taking into account that the only non-vanishing contributions come from even l, we conclude

$$S_2 \sim \frac{\left((n+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}}\right)^{2p+1}}{(3\sqrt{2})^2 2p(2p+1)} \langle n|\hat{x}|1\rangle \ .$$
 (3.103)

(iii) In contrast to the first two contributions, S_3 cannot be evaluated exactly, because the sum not only involves n as a boundary term but also depends on the explicit form of $\langle l|\hat{x}|1\rangle$. In order to recover the parametric dependence on n, we make use of our earlier observation that the amplitudes are of exponential form,

$$\langle n|\hat{x}|0,1\rangle \sim e^{-cn}$$
, (3.104)

with c being a positive constant. Such parametric ansatz allows us to establish an upper bound for the sum contained in S_3 by writing

$$\sum_{l=n}^{\infty} \left((l+1)^{\frac{3}{2}} \right)^{3p} \langle l | \hat{x} | 1 \rangle^2 \sim \int_{n/2}^{\infty} dl \, (2l+1)^{3p} e^{-4cl}$$

$$= \frac{1}{2} e^{2c} (n+1)^{3p+1} E_{-3p} \left(2c(n+1) \right) ,$$
(3.105)

where $E_m(z)$ denotes the exponential integral function. Note that the integration takes into account that the only non-trivial contributions to the sum come from even l. Using the large z asymptotics of $E_m(z)$,

$$E_m(z) \sim \frac{e^{-z}}{z} \left(1 - \frac{m}{z} + \mathcal{O}\left(\frac{m^2}{z^2}\right) \right) \quad (z \to \infty),$$
 (3.106)

we conclude that the dominant terms of S_3 are at most of order

$$S_3 \lesssim (n+1)^{\frac{3}{2}(2p+\frac{1}{3})} \sqrt{\frac{m+1}{2}} \frac{\langle n+1|\hat{x}|0\rangle}{\langle m+1|\hat{x}|0\rangle}.$$
 (3.107)

Comparing all the asymptotic expressions for large n from above, we find that the dominant contribution is given by S_2 . Therefore, finally, we conclude

dominant contribution is given by
$$S_2$$
. Therefore, finally, we conclude
$$\langle n|\hat{x}^{2(p+1)}|m\rangle \sim c_{2(p+1)} \left((n+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}}\right)^{2(p+1)-1} \sqrt{\frac{m+1}{2}} \frac{\langle n|\hat{x}|1\rangle}{\langle m+1|\hat{x}|0\rangle},$$
(3.108)

which is exactly the induction hypothesis for $p \to p+1$.

A similar computation can be carried out for odd n and m also for odd q (with n and m of different parity) without changing the general conclusions. For simplicity, however, we will skip this straightforward proof here.

In summary, we find that the transition amplitude between arbitrary states for any power of a local operator is equivalent to the linear one to exponential accuracy,

$$\langle n|\hat{x}^{q}|m\rangle \sim c_{q} \left((n+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}} \right)^{q-1} \frac{\langle n|\hat{x}|k_{n}\rangle}{\langle m+1|\hat{x}|k_{m}\rangle},$$
 (3.109)

where c_q is a positive constant and the parities of $|n\rangle$, $|m\rangle$ and $|k_{n,m}\rangle$ are chosen suitably. In particular, this implies that

$$\langle n|\hat{x}^q|0\rangle \sim c_q(n+1)^{\frac{3}{2}(q-1)} \langle n|\hat{x}|0\rangle ,$$
 (3.110)

suggesting that, for large n and to exponential accuracy, the linear vacuum transition amplitude $\langle n|\hat{x}|0\rangle$ contains all the information about amplitudes of the form $\langle n|\hat{x}^q|0\rangle$. Therefore, if $\langle n|\hat{x}|0\rangle$ is exponentially suppressed for large n, $\langle n|\hat{x}^q|0\rangle$ will also be suppressed and hence remain finite as $n \to \infty$.

Finally, our result supports a key assumption of semiclassical calculations already pointed out in Section 2.2.2. That is, to exponential accuracy, the scattering amplitude in question is independent of the precise form of the local operator, for example [54]

$$\langle n|\phi^2|0\rangle \sim \langle n|\phi|0\rangle$$
 . (3.111)

However, note that, as the semiclassical methods of [49–51] make use of the local operator $j^{-1} \exp(j\phi)$, some caution is needed. For finite j, (3.110) is not sufficient to guarantee that there are no exponential prefactors, such that the limit $j \to 0$ has to be taken with care.

3.5 Generalization to higher monomial potentials

The suitable resummation of perturbation theory appears to play an important role in the restoration of unitarity in scalar field scattering amplitudes at high multiplicities. In particular, for theories with spontaneous symmetry breaking, the inclusion of non-perturbative effects in the perturbative ansatz seems to be crucial. Among the two quantum mechanical examples that we studied, however, this might be a very special feature of the quartic anharmonic oscillator as we will see in this section.

Let us consider the vacuum transition amplitudes $\langle n|\hat{x}|0\rangle$ in massive anharmonic oscillators with potential,

$$V(x) = x^2 + \lambda x^{2M} \,, \tag{3.112}$$

where $M \geq 2$ is integer, λ is positive and we have normalized everything to the mass, $m^2 = 1$. That is, we explicitly consider potentials that are not subject to spontaneous symmetry breaking. Due to the lack of instantonic configurations, we therefore naively expect perturbation theory to work well.

Note carefully, that for $M \geq 3$, there is no obvious uplift to a quantum field theory that is (perturbatively) renormalizable. For instance, scalar field theories with potentials such as $V(\phi) = m^2 \phi^2 + \lambda \phi^6$ in more than two dimensions suffer from divergences that cannot be regularized consistently. Nevertheless, these toy models exhibit some very instructive features of perturbation theory and its relation to non-perturbative phenomena.

3.5.1 The sextic anharmonic oscillator

As the first nontrivial example we want to consider the sextic oscillator, M=3,

$$V(x) = x^2 + \lambda x^6 \,. \tag{3.113}$$

In this potential, similar to the quartic anharmonic oscillator, we are interested in finding the analytic form of the vacuum transition amplitudes $\langle n|\hat{x}|0\rangle$. In practice, for this computation we make use of the perturbative techniques developed in Section 3.2.1, which can be applied to the present example in a straightforward way.

By our field theory intuition, we can already note some important differences to the quartic case. For instance, in addition to the restrictions imposed by the \mathbb{Z}_2 symmetry of the Hamiltonian, we expect that there is only a subset of states that can be excited at tree level, i.e. truly without loop corrections. Indeed, these states are given by the condition n = 4k + 1 for natural numbers k. For simplicity, in the following we will focus on these states only.

Using the perturbative techniques of Section 3.2.1, we find that, similar to the quartic case, the amplitudes factorize into a tree-level and higher order part, $\mathcal{A}_n = \mathcal{A}_n^{\text{tree}} \mathcal{A}_{\Sigma}$, where the tree-level amplitude is now given by

$$\mathcal{A}_{n}^{\text{tree}} = \sqrt{\frac{n!}{2^{n}}} \binom{(n-3)/4}{(n-1)/4} \left(\frac{\lambda}{4}\right)^{\frac{n-1}{4}}.$$
 (3.114)

By an explicit computation we find that the higher order contribution can in turn be written as a perturbative expansion in the coupling where the coefficients are polynomials in n. For instance, the first few terms read

$$\mathcal{A}_{\Sigma} = 1 + \lambda \left(\frac{1}{8} n^4 - \frac{7}{6} n^3 - \frac{3}{4} n^2 - \frac{233}{96} n + \frac{45}{32} \right) + \lambda^2 \left(\frac{1}{384} n^8 - \frac{1}{6} n^7 + \dots \right) + \dots$$
(3.115)

Recall that for the quartic anharmonic oscillator we have observed an exact exponentiation of the perturbative expansion. Intriguingly, in the sextic case we find a more complicated structure. In fact, the leading terms of the higher order

contributions in λn^4 , compared to tree-level perturbation theory,

$$\mathcal{A}_{\Sigma} \sim 1 + \frac{1}{8}\lambda n^4 + \frac{1}{384}\lambda^2 n^8 + \frac{1}{46080}\lambda^3 n^{12} + \mathcal{O}\left(\lambda^4 n^{16}\right), \tag{3.116}$$

represent the Taylor series expansion of the hyperbolic cosine function,

$$\mathcal{A}_{\Sigma} \sim \cosh\left(\sqrt{\frac{\lambda n^4}{4}}\right)$$
 (3.117)

This observation, together with the exponentiation for the quartic oscillator, inspires us to conjecture that the above results is indeed true for the *full* amplitude to all orders in perturbation theory. That is, in case of the sextic oscillator we expect

$$\mathcal{A}_n = \mathcal{A}_n^{\text{tree}} \cosh\left(\sqrt{\frac{F}{\lambda}}\right) \,, \tag{3.118}$$

where F is analogous to the holy grail function we have found for the quartic case. Note, however, that the precise form of F is different here.

Indeed, the first subleading corrections $\mathcal{O}(\lambda^k n^{4k-1})$ at each order k of the perturbative expansion are reproduced by a combination of hyperbolic cosine functions. Each of these comes with a different argument,

$$\mathcal{A}_{\Sigma} = \frac{1}{4} \sum_{i,j=\pm} \cosh\left(\sqrt{\frac{F_{ij}}{\lambda}}\right). \tag{3.119}$$

The different arguments read

$$F_{\pm\pm}(\epsilon, n) = \frac{1}{4}\epsilon^4 \pm \frac{17}{6\sqrt{6}}\epsilon^5 - \frac{17}{216}\epsilon^6 + \dots + \frac{1}{\sqrt{n}}\left(\pm i\sqrt{\frac{17}{6}}\epsilon^4 + \dots\right) + \frac{1}{n}\left(-\frac{7}{3}\epsilon^4 + \dots\right) + \frac{1}{n^{\frac{3}{2}}}\left(\pm i\frac{283}{8\sqrt{102}}\epsilon^4 + \dots\right) + \dots,$$
(3.120)

where, for convenience, we defined the abbreviation $\epsilon = \sqrt{\lambda}n$. The indices of F denote the signs of the first and second coefficient in order, i.e. the coefficients of the terms ϵ^5 and ϵ^4/\sqrt{n} , which can be chosen independently of each other. The last sign in order, i.e. the coefficient of $\epsilon^4/n^{3/2}$ is, however, not independent but is instead equal to the first one, ϵ^5 , in any combination. We have verified this relation up to order k=8.

As the sextic anharmonic oscillator now involves hyperbolic cosine functions instead of simple exponentials of the quartic case, the resummation of the perturbative expansion of the amplitude appears to be much more complicated. In contrast to the quartic case, where we determined the holy grail function in an 1/n-expansion, we observe that for the sextic oscillator we need additional terms of the form $1/\sqrt{n}$ to systematically reconstruct the entire function of F. We furthermore need a summation over contributions that come with different signs of certain coefficients

In addition, this structure has phenomenologically important consequences. However, before discussing these in detail, we want to generalize the above results and postulate a conjecture on the general form of vacuum transition amplitudes in arbitrary potentials. In the general case, the physical implications are even more severe, as we will discuss in the following section.

3.5.2 Resummation beyond tree-level

All the results we obtained for the sextic oscillator in Section 3.5.1 can be straightforwardly generalized to an arbitrary power of the self-interaction term of potential,

$$V(x) = x^2 + \lambda x^{2M} \,. \tag{3.121}$$

Defining q = 2(M - 1), we can again use the diagrammatical approach of perturbative quantum field theory to argue that there is only a certain subset of final states that can be reached at tree-level. In general, this set is given by n = qk + 1 for natural numbers k. As we did before, we will only focus on those states in the following.

Even for the general case, we find a complete factorization of the amplitudes,

$$\mathcal{A}_n = \mathcal{A}_n^{\text{tree}} \sum_k \lambda^k P_{qk}(n) , \qquad (3.122)$$

where $P_{qk}(n)$ denotes a polynomial of degree qk in n. In this case, the tree-level contribution is given by

$$\mathcal{A}_n^{\text{tree}} = \sqrt{\frac{n!}{2^n}} \binom{(n+1)/q - 1}{(n-1)/q} \left(\frac{\lambda}{4}\right)^{\frac{n-1}{q}}.$$
 (3.123)

In principle, using the recursive techniques of Section 3.2.1, the perturbative series representation of the amplitude can be computed to arbitrary order in the coupling. Doing this to very high order, in line with our results on the quartic and sextic anharmonic oscillator, where we found the series representations of exponential and hyperbolic cosine functions, respectively, we observe an even more interesting pattern in the general case. Noting that the hyperbolic cosine is a linear combination of two exponential functions, we find indications that for any M the amplitude is given by

$$\mathcal{A}_n = \mathcal{A}_n^{\text{tree}} \frac{1}{M-1} \sum_{M-1 \text{ roots}} \exp\left(\frac{1}{\Lambda} \sqrt[M-1]{F}\right), \qquad (3.124)$$

where we define $\Lambda = \lambda^{1/(M-1)}$. That is, the vacuum transition amplitude can be written as a tree-level factor times a sum of exponentials over all complex roots of an analytic function F, that we similarly call holy grail function. Note carefully that this is not a rigorous result, but we have checked it for different theories, M = 3, 4, 5, 6, each to leading order in λn^q . In this sense (3.124) is only a conjecture.

In summary, we find that the vacuum transition amplitudes in a general anharmonic oscillator are represented by a linear combination of exponential functions. This appears to be an immediate extension of the quartic anharmonic oscillator, where the amplitudes can be written as a single exponential (2.19). We remark, however, that, even beyond our discussion in Section 3.2.2, the exact exponentiation seems to be a peculiar feature of the quartic case with a single- or symmetric double-well potential. For instance, in the case of a general, asymmetric double-well potential, $V(x) = x^2 + \mu \sqrt{\lambda} x^3 + \lambda x^4$, we find indications that an exact exponentiation only occurs for $\mu = 0$ and $\mu = 2$, i.e. for the single-well or the symmetric double-well discussed in Section 3.2 and Section 3.3. For arbitrary μ , however, the resummation seems to involve more complicated linear combinations of exponentials.

Speculatively, the exponentiation, or more precisely the combination of exponential functions, might be ultimately related to the classical energy-momentum relation, $p^2(x) = 2(E - V(x))$. Geometrically, this relation can be understood as an algebraic curve that defines surfaces of constant energy in (complex) phase space. The shape of the potential then determines the topology of this curve, in particular its genus. Remarkably, it was recently shown that if the algebraic curve is of genus one, i.e. an elliptic curve, perturbation theory captures all non-perturbative effects and vice versa, to all orders in the WKB approach [72]. This is a very explicit realization of the resurgence idea. In fact, the quartic single-well and the symmetric double-well potential exactly fall into this class of quantum spectral problems of genus one, while the general asymmetric double-well potential does not. For example, there is a class of sextic and higher monomial potentials, the so-called Chebyshev potentials, which define elliptic curves of genus one. It would be interesting to see, if these potentials feature an exact exponentiation that we found for the symmetric quartic case. We will discuss this in future work [4].

The general form of (3.124) also has some important physical consequences. In contrast to the quartic anharmonic oscillator, for $M \geq 3$ it does not allow for a decrease of the amplitudes $\langle n|\hat{x}|0\rangle$ at high energies, or equivalently, at large n. This is because, in the complex plane, the M-1 complex roots of the function F will generally arrange in a regular polygon with M-1 vertices. Then, as long as $M \geq 3$, there will always be at least one root with a positive real part, thereby dominating the sum of exponentials (3.124). Note that this is completely independent of the precise form of the holy grail function F. Therefore, any combination of exponents or roots will generically lead to exponential growth of the amplitudes for large n. This will then ultimately lead to a violation of unitarity as $n \to \infty$.

In summary, we conclude that, in contrast to the quartic anharmonic oscillator, a suitable resummation of perturbation theory in higher monomial potentials does not seem to be sufficient to guarantee the restoration of unitarity in the quantum mechanical transition amplitudes $\langle n|\hat{x}|0\rangle$ as $n\to\infty$. In this sense, the quartic case that we discussed in Section 3.2 and Section 3.3, is special, because the resummation involves only a single exponential whose exponent can be and indeed *is* negative, thereby restoring unitarity at high energies.

Nevertheless, as we are dealing with potentials with a unique minimum, we

would naively expect standard perturbation theory to work well. That is, a suitable resummation of the perturbative expansion should be able to reconstruct all physical observables of the theory, because non-perturbative effects, such as, e.g., instantons in double-well potentials, should be absent. By our observation, this, however, does not seem to be the case for theories with $M \geq 3$. Let us therefore comment on possible reasons as well as resolutions to this puzzling problem. However, we should be keenly aware that the result (3.124) is by no means rigorous, but merely a conjecture based on the leading-n correction at each order in perturbation theory. It is well possible that this structure is no longer valid, once subleading corrections are included, as is, for example, suggested by the sextic case (3.119). Therefore, our conclusions have to treated with some care.

On the speculative side of things, the apparent breakdown of perturbation theory in these quantum mechanical examples might be related to the increasing number of vacua and possible (non-)perturbative trajectories connecting them.

In the path integral formulation of a quantum theory, any correlation function or transition amplitude will be dominated by the classical trajectories, which, by definition, minimize the action. When we argued that we do not expect any non-perturbative configurations to play a role in our quantum mechanical example, we only considered real trajectories. These trajectories can be associated to the perturbative vacuum of the theory. In principle, however, there might also be complex trajectories that contribute to the path integral (see, e.g., [108]). These, in turn, can be related to the non-perturbative saddle points of the action, which connect the different complex vacua (or rather extrema) of the theory. That is, to some extent, we still seem to be missing non-perturbative contributions in the perturbative expansion in the theory. This is in line with recent discussions on resurgence and transseries expansions, which relate perturbation theory and non-perturbative phenomena in a very intricate way (see also our discussion in Chapter 1). For an overview on these aspects see, e.g., [68, 79].

For the general case, the number of the complex vacua is 2M-1, which again describe a polygon with 2(M-1) vertices¹⁰ in the complex plane. Speculatively, this is also why the quartic case, M=2, might be special. Here, the polygon is degenerate, such that the complex trajectories might contribute with opposite sign, thereby canceling each other¹¹. Such cancellation does not seem to happen for $M \geq 3$. Therefore, to obtain physical results from a perturbative expansion in these theories, a naive resummation of perturbation theory is not sufficient. Instead, all classical trajectories, i.e. real and complex ones, might have to be taken into account consistently. There might be some accidental cancellations between the complex trajectories for the case of the quartic anharmonic oscillator. This possibility certainly merits some further investigation. A promising approach might involve

¹⁰Note that we subtracted the perturbative vacuum at the origin here.

¹¹This is also reflected by the fact that the quartic oscillator with a single minimum can be transformed into the double-well potential by the rotation $x \to ix$. The vacua are all aligned on a single axis. In this sense, both theories are similar, but, importantly, the latter admits additional non-perturbative configurations compared to the single minimum case.

resurgent transseries expansions [68] or path integral methods of exact perturbation theory [108]. We will discuss this in detail in future work [4].

3.6 Quantum mechanics versus quantum field theory

Let us close our discussion on high multiplicity amplitudes in quantum mechanics with a few remarks on the relation between our results and higher-dimensional quantum field theory. Here, we closely follow the arguments given in [130].

The quantum mechanical example allowed us to do explicit calculations to high order in perturbation theory, which gave important insights into the amplitudes corresponding to processes $\phi^* \to \phi^n$ at high energies. Nevertheless, we should be aware that quantum field theory in higher dimensions is subject to additional features and complications.

In the beginning of this chapter we have made the naive identification of quantum mechanics with quantum field theory in (0+1) dimensions. In general, the canonical field theory is then defined by the Hamiltonian [103]

$$H = \frac{1}{2}\dot{\phi}^2 + \frac{m^2}{2}\phi^2 + \frac{\lambda}{4}\phi^4, \qquad (3.125)$$

together with the commutation relation

$$\left[\phi, \dot{\phi}\right] = i. \tag{3.126}$$

That is, implicitly, we imposed the correspondence of fields $\phi(\vec{x},t) \sim x(t)$ in (0+1) dimensions. This field theory describes a single degree of freedom which is the coherently oscillating field without any spatial dependence. Therefore, in a particle interaction there is no phase space to integrate over, such that we are left with the computation of the squared matrix element only. In fact, this is one of the reasons why the calculation in this toy model is tractable.

Furthermore, as there are no spatial degrees of freedom, there are no weakly coupled, asymptotic states in the quantum theory and, strictly speaking, hence no particle scattering. In particle interactions in higher-dimensional quantum field theory, the fields become solutions of the free field equations at early and late times, $t \to \pm \infty$, as they are spatially separated from each other (cf. Section 2.1). This, however, is not possible in quantum mechanics. Energy eigenstates of the theory are trapped in the potential of the anharmonic oscillator and hence cannot be asymptotically free.

In addition, in quantum mechanics it is impossible to distinguish between energy E and occupation number n. Both are instead related,

$$E = nm(1 + \epsilon). \tag{3.127}$$

Here, the parameter ϵ depends on the energy level n and is determined by the specific quantum mechanical model that we consider. That is, unlike in quantum

field theory, it is not a free parameter in quantum mechanics. In particular, ϵ is negative valued, because the energy levels of an anharmonic oscillator with non-vanishing self-interaction are spaced more densely compared to the harmonic one. Consequently, transitions $E \to nm$ are kinematically not allowed in quantum mechanics. In quantum field theory such decays are only disfavored because of the vanishing phase space at the kinematic threshold. However, they become possible for arbitrarily small particle momenta in the final state corresponding to a small positive ϵ .

In practice, semiclassical techniques for the computation of high multiplicity amplitudes do not work in quantum mechanics either, as it lacks a meaningful boundary value problem in (0+1) dimensions. These computations rely on the nontrivial extremization of singularity surfaces, for which there is no meaningful zero-dimensional analogue in quantum mechanics. For a detailed discussion of this issue we refer the reader to the review article [130].

In summary, quantum field theory in higher dimensions provides for much more structure and complications compared to quantum mechanics. Amongst others, the most important differences include the nontrivial phase space and the existence of weakly coupled, asymptotic states in the quantum theory. Nevertheless, our findings on the quantum mechanical anharmonic oscillator can give important insights into the features that are shared between both theories, such as the quartic potential or the presence of a single or multiple degenerate vacua. In particular, as we argue that advanced computational techniques restore unitarity at high energies, we are in turn lead to focus efforts to establish the onset of new, most likely non-perturbative, phenomena on those aspects of quantum field theory, that are different from quantum mechanics.

4 Conclusion

Scattering experiments have proven extremely useful for our study of the fundamental building blocks of nature at the smallest length scales, or, equivalently, at the high energy frontier. Being physical observables, scattering cross sections immediately bridge the gap between theory and experiment. On the theory side, the corresponding scattering amplitudes encode the dynamics of all particle interactions and thus are crucial ingredients of the interacting quantum theory. A very natural and fundamental assumption of this quantum theory is the conservation of probabilities in scattering processes. Formally, this is imposed by the unitarity of the scattering matrix. Loosely speaking, this means, that the probability of something happening in a scattering process should not exceed one. However, there are indications that scalar quantum field theory in the high energy regime is in conflict with this fundamental principle.

In this thesis, we studied the consistency of scalar field theories at high energies. In particular, we considered scattering processes in massive ϕ^4 -theory associated to the production of a large number of bosons by a few initial state particles, i.e. processes of the form $\phi^* \to \phi^n$ or $\phi\phi \to \phi^n$ for large n. Due to the lack of destructive interference between different Feynman diagrams, these processes exhibit rapid growth, $n! \lambda^{n/2}$, with the number of particles in the final state, rendering the theory in clash with unitarity constraints as $n \to \infty$, independently of the coupling λ . Evidence for factorial growth of these amplitudes is given by perturbative [39,40,43–47] as well as semiclassical calculations [48–51]. This raises questions about the consistency of the computational techniques, or possibly even about the interpretation of the underlying quantum field theory.

Applied to the Higgs sector of the Standard Model, the rapidly growing cross sections provide us with an explicit upper energy scale, possibly within the reach of future particle colliders, beyond which conventional field theory interpretations cease to be meaningful [94,95]. That means, in order to restore unitarity at high energies, either novel non-perturbative behaviour or new physics phenomena have to appear. For instance, possible phenomena in the electroweak sector of the Standard Model might allow for entirely different phenomenology such as a *Higgsplosion* mechanism [97].

In this work, we follow a more conservative approach. The calculations of multiparticle production in scalar field theory that established unitarity violation for a large number of bosons mostly relied on perturbative or semiclassical techniques at leading order. Beyond that, conventional methods become intractable at higher loop-orders such that the perturbative answer might not be reliable at high energies. It is possible that the rapid growth of the scattering amplitudes is merely an artefact of this "incomplete" calculation and could possibly be resolved by obtaining the *exact* amplitude without relying on perturbation theory to finite order.

In Chapter 3 we take some initial steps towards this direction. As a simplified, yet instructive, toy model of scalar ϕ^4 -theory we study its quantum mechanical equivalent, the anharmonic oscillator with quartic coupling λ , both with and without spontaneous symmetry breaking, respectively. That is, we identify the high multiplicity scattering amplitudes of the scalar field theory with quantum mechanical transition amplitudes from the vacuum to highly excited states, $\langle n|\phi|0\rangle \hookrightarrow \langle n|\hat{x}|0\rangle$. This identification reduces the problem to determining the spectrum of the Schroedinger operator of the quartic anharmonic oscillator. By means of recursive relations due to Bender and Wu [103, 104], we construct the wave functions and energy levels to very high orders in perturbation theory. These are then used to derive perturbative expressions for the corresponding transition amplitudes.

We find that they take on an exponential form, $\langle n|\hat{x}|0\rangle \sim \exp{(F/\lambda)}$, where the exponent F depends on the combination λn only. That is, we provide crucial evidence for this form conjectured in the field theory counterpart [52–56]. In fact, it is nontrivial that the perturbative expansion of the amplitude is reproduced by the exponential function exactly. In order to study the asymptotic behaviour of perturbation theory in the large n regime, we systematically construct the exponent F in a 1/n-expansion beyond leading order.

From a phenomenological point of view, the sign of F is crucial. For instance, we observe that, at tree level, F turns positive beyond some critical value of λn , indicating an instability of the perturbative expansion. We are therefore interested in establishing the sign of the exponent in the double scaling limit $n \to \infty$ and $\lambda \to 0$ while keeping λn fixed. In this regime the large-n behaviour of the amplitude is governed by the tree-level and leading order contribution of the 1/n-expansion of the exponent F.

For the anharmonic oscillator with a single minimum discussed in Section 3.2, we observe that a Padé resummation of the series representation of F significantly improves its predictivity for large values of λn . Importantly, we find strong indications that the holy grail function is negative, F < 0, for any value of λn , thereby avoiding problems with unitarity and rigorous as well as semiclassical bounds [109, 113].

For the anharmonic oscillator with a symmetric double-well potential as presented in Section 3.3, the situation is more complicated. Indeed, in the standard perturbative approach we find that F has a series representation with only positive, growing coefficients, such that a Borel resummation may suffer from ambiguities. Therefore, we turn to more powerful methods and make use of exact perturbation theory (EPT) [108, 115]. This technique was recently put forward for the perturbative study of quantum mechanical and field theoretical models that are governed by non-perturbative effects. In this approach, we are able to obtain the holy grail

function associated to vacuum transitions in the symmetric double-well potential. Using different schemes to resum the exact perturbative series (in the sense of EPT), we confirm that, similar to the quartic case with a single minimum, F is negative everywhere in the double scaling limit. Therefore, also in the double-well case, the vacuum transition amplitudes are in line with fundamental unitarity constraints.

We conclude that suitably resummed perturbation theory seems to prevent a rapid growth of quantum mechanical amplitudes $\langle n|\hat{x}|0\rangle$ in the anharmonic oscillator both in the symmetric and in the broken phase.

Although our results are obtained for its quantum mechanical equivalent, they still suggest a guideline for resolving the factorial growth of multiparticle amplitudes in scalar field theory, including the case of the Standard Model Higgs. However, note carefully that ϕ^4 -theory, being a higher-dimensional quantum field theory, is subject to additional complications. Most importantly, these include a nontrivial phase space and the presence of weakly coupled, asymptotic states. Both do not exist in our quantum mechanical setup.

From a theoretical point of view, as our calculational techniques appear to restore unitarity in the quantum mechanical amplitudes, it would be very interesting to go beyond this simplified toy model. It is tempting to apply similar methods to systems that are closer to quantum field theory in higher dimensions, for instance, by incorporating more of the distinguishing features of a quantum field theory into our approach. For instance, in contrast to the discrete spectrum of the quantum mechanical anharmonic oscillator, quantum field theory exhibits a continuous spectrum. Furthermore, since the exponentiation of the multiparticle amplitudes, $\mathcal{A} \sim \exp(F/\lambda)$, intrinsically inherits a form of non-perturbative nature in the limit $\lambda \to 0$, there appears to be a very deep relation between the resummation of perturbation theory and non-perturbative phenomena. Supported by the application of exact perturbation theory to the symmetric double-well potential, apparently, the perturbative ansatz intrinsically captures its non-perturbative counterpart. This suggests that both cannot rigorously be distinguished but are essentially the same instead. Moreover, as we find hints for unitarity violation in the resummation of perturbation theory, our results presented in Section 3.5 indicate that perturbative expansions can be unphysical even in potentials with a single minimum. However, in these potentials, one would naively expect perturbation theory to work well due to the lack of instantonic configurations associated to degenerate vacua. This hints at missing non-perturbative contributions, which, however, might be recovered in resurgence theory and transseries expansions, see, e.g., [68, 79].

Perhaps, as a next step, a promising testbed for the combination of both ideas would be the quantum mechanical Mathieu system, $V(x) \sim \cos^2(x)$, which also exhibits a continuous spectrum, see, e.g., [157]. Due to its band structure and the infinite number of classically degenerate vacua, important results on the connection between perturbation theory and the different instanton sectors of this theory could already be obtained by means of resurgence theory [69, 70].

One could then proceed by investigating low-dimensional quantum field theories, where dualities and integrable structures might be beneficial, see, e.g., [158, 159]. If

a restoration of unitarity occurs, it would be very interesting to determine its phenomenological consequences. These could include, e.g., deviations from perturbative behaviour in analogue systems or the appearance of instantonic field configurations, that could be observed at collider experiments, see, e.g., [36,37,160–165]. Perhaps, it might even be possible that high energy scattering amplitudes might self-unitarize by the production of extended, classical objects. These so-called *classicalons* play the analogous role of black holes in non-gravitational theories [166]. The above aspects go beyond the scope of high multiplicity amplitudes and would have important implications on our general knowledge on quantum mechanics and quantum field theory. For example, they could deepen our understanding of non-perturbative effects in the path integral of a generic quantum theory or even provide a non-perturbative definition of quantum field theory in the continuum, which is computationally tractable at the same time.

From a phenomenological point of view, unitarity might also be restored by additional, possibly new, physics phenomena. For instance, in Yang-Mills theory gauge symmetry and on-shell conditions lead to diagrammatic cancellations in the computation of scattering amplitudes (see, e.g., [91]), such that, in contrast to scalars, gluons do not seem to violate unitarity. Following this result, one might well ask, what are the distinct features of a quantum field theory in order to exhibit scattering amplitudes that violate unitarity at high energies, i.e. how is the problem manifest in the landscape of quantum field theories. In this bottom-up approach, highly symmetric quantum field theories, where *exact* computations are possible, could potentially serve as a laboratory.

On the more speculative side, one possible new physics phenomenon could come in form of the recently proposed *Higgsplosion* mechanism [97]. If realized in nature, this mechanism would have remarkable consequences and gives access to yet unexplored territory of physics beyond the SM. However, so far it is unclear if Hig*qsplosion* can be consistently realized in a scalar quantum field theory. Currently, there is an active discussion on the nature of the underlying quantum field theory, in particular, on aspects of localizability [135–137]. In fact, a theory featuring Higgsplosion requires a Källén-Lehmann spectral density that grows exponentially with energy. Naively, this seems to be in conflict with the common requirement of a quantum field theory to be local, which would only allow the spectral density to grow polynomially. However, due to works by Jaffe [167], there is a weaker notion of locality in (constructive) quantum field theory. In fact, one can rigorously distinguish between strictly localizable, quasi-localizable and non-localizable field theories, all of which can exhibit exponentially growing spectral densities at high energies. The different classes are determined by the power scaling of its exponent with energy [168]. As the *Higgsplosion* mechanism does not make a prediction for the exponent of the sprectral density, it would be interesting to address the question to which of the above classes a quantum field theory featuring Higgsplosion belongs, i.e. if Higgsplosion still renders a scalar field theory local and hence in line with conventional quantum field theories or if such a theory is non-localizable and hence exhibits non-localities. The possible phenomenological consequences of these

theories would be remarkable. For instance, if a higgsplosive theory turns out to be non-localizable, it might cease to respect CPT symmetry [169, 170]. Consequently, a theory that features Higgsplosion consistently would give access to intriguing observable consequences that can possibly be tested in experiment.

In summary, calculations of scattering amplitudes associated to multiparticle production in scalar field theories seem to reveal an inherent energy scale beyond which non-perturbative behaviour or even new physics phenomena have to set in. We shed light on the high energy behaviour by studying the high multiplicity scattering amplitudes in the quantum mechanical analogue of ϕ^4 -theory. Using advanced perturbative resummation techniques, we provide evidence for their non-perturbative behaviour at high energies, $A_n \sim \exp(F/\lambda)$. The exponential form is nontrivial and at least in quantum mechanics we show that the exponent is negative, thereby demonstrating a nontrivial restoration of unitarity at high energies by suitably resummed perturbation theory. There are many promising research possibilities and directions to explore in view of and even beyond the approach described in this thesis. Possible implications include the interplay between perturbation theory and non-perturbative phenomena or observable consequences of a restoration of unitarity that is either non-perturbative or that is due to the localizability properties of the underlying quantum field theory. These go far beyond the scope of the calculation of scattering amplitudes at high multiplicities and will likely deepen our current understanding of the high energy behaviour of scalar quantum field theories.

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A Resummation of Power Series

A key ingredient in order to make sense of perturbation theory is the resummation of divergent power series expansions. In this chapter we want to give a brief overview of different resummation techniques.

In practice, often only a finite number of terms of a power series expansion is known. This is why we sometimes have to deal with approximations of a (divergent) series rather than the formal analytic continuation. In the following, let us consider the formal power series

$$Z(g) = \sum_{k=0}^{\infty} z_k g^k. \tag{A.1}$$

A.1 Padé approximation

One of the most widely used techniques to resum divergent series expansions where only a finite number of terms is available is $Pad\acute{e}$ approximation [171]. It tries to approximate Z(g) by a rational function of two polynomials $P_M(g)$ and $Q_N(g)$ of degree M and N, respectively, such that this rational function reproduces the first few coefficients of Z,

$$P_M + Q_N Z(g) = \mathcal{O}\left(g^{M+N+1}\right). \tag{A.2}$$

That is, the Padé approximant $Z_{[M,N]}(g)$ of order [M,N] is defined by the condition

$$P_M + Q_N Z_{[M,N]}(g) = 0.$$
 (A.3)

Typically the diagonal sequence of approximants, $Z_{[N,N]}$, features the best convergence properties to reconstruct Z,

$$Z_{[N,N]}(g) \to Z(g) \quad (N \to \infty).$$
 (A.4)

In particular, if the coefficients of Z(g) have an oscillating sign, the true value of Z(g) will normally lie in between neighbouring Padé approximants, $Z_{[N,N]}$ and $Z_{[N,N+1]}$.

¹Mathematically, a sufficient condition is that the approximated function Z(g) is a Stieltjes function (see, e.g., [172]). However, this cannot be rigorously deduced from a finite number of series coefficients.

A.2 Borel resummation

A common resummation technique if the large order asymptotics of the series coefficients are known is *Borel resummation* [173]. The idea is to cancel any (possibly factorial) growth of the coefficients z_k that can cause the series to be divergent by considering the Borel transform of Z(g),

$$\mathcal{B}Z(g) = \sum_{k=0}^{\infty} \frac{z_k}{k!} g^k, \qquad (A.5)$$

therefore providing much better chances for convergence of $\mathcal{B}Z(g)$ compared to Z(g). Inspired by the integral formula for the factorial function,

$$n! = \int_0^\infty \mathrm{d}t \, t^n \mathrm{e}^{-t} \,, \tag{A.6}$$

the factorial factor can be recovered by a Laplace transform,

$$Z(g) = \int_0^\infty dt \, e^{-t} \mathcal{B} Z(gt) \,. \tag{A.7}$$

However, in practice, the large order asymptotics of the coefficients z_k might not be known analytically. Therefore, for all practical purposes, Borel-Padé approximation is typically used to make sense of Z(g). Instead of explicitly computing the Borel sum $\mathcal{B}Z(g)$, it tries to approximate it using Padé approximation (cf. previous section). The corresponding Padé approximants $\mathcal{B}Z_{[M,N]}(g)$ can then be Laplace transformed. In particular, the diagonal Padé sequence will then converge to the exact result,

$$\int_0^\infty dt \, e^{-t} \mathcal{B} Z_{[N,N]}(gt) \to Z(g) \quad (N \to \infty).$$
 (A.8)

In this sense, Borel-Padé approximation is literally the combination of Padé approximation and Borel resummation.

A.3 Shafer approximation

Naively, the Shafer approximation [174] can be viewed as the quadratic extension of Padé approximation. That is, it tries to approximate Z(g) by means of three polynomials $P_L(g)$, $Q_M(g)$ and $R_N(g)$ of degree L, M and N, respectively, such that

$$P_L + Q_M Z(g) + R_N Z^2(g) = \mathcal{O}\left(x^{L+M+N+2}\right)$$
 (A.9)

The Shafer approximant $Z_{[L,M,N]}$ of order [L,M,N] is then defined by the quadratic equation

$$P_L + Q_M Z_{[L,M,N]}(g) + R_N Z_{[L,M,N]}^2(g) = 0.$$
 (A.10)

Similar to the Padé approximants, the diagonal Shafer approximants $Z_{[N,N,N]}$ typically features the best convergence properties to Z,

$$Z_{[N,N,N]}(g) \to Z(g) \quad (N \to \infty).$$
 (A.11)

A.4 Meijer G approximation

The recently proposed Meijer~G~approximation scheme [175] is closely related to the idea of Borel-Padé approximation. While the latter reconstructs the Borel sum $\mathcal{B}Z(g)$ by means of Padé approximation, the Meijer G approximation tries to estimate the large order asymptotics of the Borel transform by representing it through generalized hypergeometric functions,

$$\mathcal{B}Z(g) \sim_{N+1} F_N(\mathbf{x}, \mathbf{y}; g)$$
 (A.12)

Here, the argument vectors \mathbf{x} and \mathbf{y} are defined by singular points of the Padé approximants of successive coefficient ratios of $\mathcal{B}Z(g)$. Then the Laplace transform of the Borel sum can be performed analytically and yields a Meijer G function. For further details we refer the reader to the original work [175].

B Exact Perturbation Theory and Choice of Auxiliary Potentials

In general, the auxiliary potential,

$$\hat{V}(x;\lambda,\lambda_0) = V_0(x;\lambda,\lambda_0) + \lambda V_1(x;\lambda,\lambda_0), \qquad (B.1)$$

used in exact perturbation theory has to satisfy only very requirements. These are, apart from recovering the original potential $V(x; \lambda)$ when the deformation is lifted, $\lambda_0 = \lambda$,

$$\hat{V}(x;\lambda,\lambda) = V(x;\lambda), \tag{B.2}$$

that the potential V_0 has to admit bound states and both V_i have to be classical, i.e. their perturbative expansion in λ coincides with the expansion in \hbar .

In particular, this means that the choice of \hat{V} is not unique and we are left with a plethora of possibilities to construct the auxiliary potential. It is obvious that the physical result after removing the potential deformation must be independent of the choice of V_0 and V_1 . Still, the particular choice of deformation can affect the convergence properties of the perturbative expansion. In fact, different choices might be more or less useful for different computational tasks. In the following we aim to discuss different choices of the potentials V_0 and V_1 .

In line with the example we presented in Section 3.3 we focus on the auxiliary mass term v_2 . Let us discuss the most simple case of a constant mass, $v_2(\lambda_0) = v_2$, corresponding to the potentials

$$V_0(x;\lambda,\lambda_0) = v_2 x^2 + \lambda x^4 \tag{B.3}$$

and

$$V_1(x; \lambda, \lambda_0) = -\frac{v_2 + 1}{\lambda_0} x^2$$
. (B.4)

In addition, the potential V_0 has to admit a perturbation theory that is Borel resummable to the exact result. Therefore, we require $v_2 > 0$. Altogether, we deal with the auxiliary potential

$$\hat{V}(x;\lambda,\lambda_0) = \left(v_2 - \frac{\lambda}{\lambda_0}(v_2 + 1)\right)x^2 + \lambda x^4.$$
 (B.5)

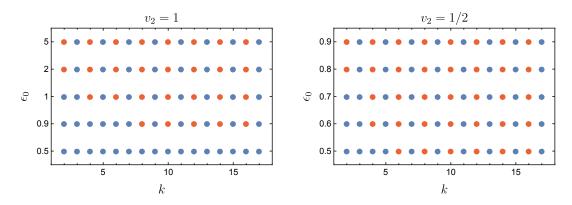


Figure B.1: Sign of each coefficient of $\hat{F}_0(\epsilon, \epsilon_0) = \sum_k \hat{F}_{0,k}(\epsilon_0) \epsilon^k$ for different values of ϵ_0 shown on the vertical axes. Blue dots denote a positive while red dots denote a negative sign, respectively. The left panel corresponds to $v_2 = 1$ whereas the right panel is for $v_2 = 1/2$. All input parameters are normalized to the mass, $m^2 = 1$. Note the different scales for ϵ_0 .

The effective dimensionless¹ coupling of the theory with potential V_0 is $\lambda/v_2^{3/2}$. This is why different choices of v_2 can affect the converge properties of perturbative expansions in that theory. Note that the choice $v_2 = 1$ corresponds to the simple example discussed in Section 3.3. We now want to move away from this point and consider the two regimes $v_2 \ll 1$ and $v_2 \gg 1$.

In the first case, $v_2 \ll 1$, already the theory given by V_0 is strongly coupled, as the effective coupling of this theory is $\lambda/v_2^{3/2}$. That is, even at small λ we are trying to do a perturbative expansion that is not well-defined to begin with.

In the second case, $v_2 \gg 1$, perturbation theory for V_0 naively should work well, because the effective coupling is small. However, at the same time V_1 is large in this case, indicating potential issues. We will see momentarily that this is indeed the case.

In general, according to exact perturbation theory, the perturbative expansion of F has to be Borel summable at fixed values of both v_2 and λ_0 . An alternating sign at high orders (i.e. up to a finite number of exceptions) typically indicates well-behaved Borel summability. In our example, this criterion is problematic, as by construction we only know a finite number of terms of the perturbative series of F.

In Fig. B.1 we illustrate the sign of the k-th coefficient of $\hat{F}_0(\epsilon, \epsilon_0) = \sum_k \hat{F}_{0,k}(\epsilon_0) \epsilon^k$ for various values of ϵ_0 and two values of v_2 . We can see that, for $v_2 = 1$, the series is only fully alternating for $\epsilon_0 > 1$, indicating a good convergence with the first few approximants for $\epsilon > 1$ after removing the deformation $\epsilon_0 = \epsilon$. In addition, this alternating sign pattern is preserved for smaller values of ϵ_0 when lowering the value of v_2 . However, as argued above, in this case the effective coupling is larger, such that we need more terms of the series for good convergence (despite the alternating signs).

¹Note, again, that we use the common quantum field theoretical conventions.

Unfortunately, increasing v_2 can turn out problematic, too. In this case the alternating sign pattern only appears for large values of ϵ_0 . Even though the alternating series is eventually restored at high orders in perturbation theory, approximations based on the low order coefficients clearly cannot capture this and behave as if the theory were not Borel summable. In this sense such choice of v_2 is expected to exhibit worse convergence properties.

In summary, we note that the choice $v_2 \ll 1$ is problematic because we try to do perturbation theory in a strongly coupled theory, while $v_2 \gg 1$ suffers from an apparent absence of Borel summability. Therefore, for a reasonable range of ϵ the choice $v_2 \simeq \mathcal{O}(1)$ seems suitable. An optimal choice of v_2 in turn will depend on the desired range of ϵ .

C Transition Amplitudes Involving Quadratic Position Operators

The simplest example of transitions amplitudes involving local operators of higher powers is the quadratic one, $\langle n|\hat{x}^2|m\rangle$. Because of the \mathbb{Z}_2 symmetry of the theory, the states $|n\rangle$ and $|m\rangle$ have to be of the same parity in order to obtain a non-vanishing result. Therefore, we can distinguish between the two cases of even and odd parity. First, let us consider the case of n and m odd.

As already pointed out in the main text, we want to reduce the power of the local operator by insertion of the identity operator,

$$\langle n|\hat{x}^2|m\rangle = \sum_{l=0}^{\infty} \langle n|\hat{x}|l\rangle \langle l|\hat{x}|m\rangle ,$$
 (C.1)

where we only have non-vanishing contributions for even l. That is, we have traded one power of the operator for an infinite sum. The latter can then be split into three different contributions (depending on l). Using the nontrivial result (3.92), we can therefore write

$$\langle n|\hat{x}^{2}|m\rangle \sim \langle n|\hat{x}|0\rangle \langle m|\hat{x}|0\rangle \sum_{l=0}^{m} \frac{m+1}{2} \frac{1}{\langle l+1|\hat{x}|0\rangle^{2}} + \sqrt{\frac{m+1}{2}} \frac{\langle n|\hat{x}|0\rangle}{\langle m+1|\hat{x}|1\rangle} \sum_{l=m}^{n} \sqrt{\frac{l+1}{2}} \frac{\langle l|\hat{x}|1\rangle}{\langle l+1|\hat{x}|0\rangle} + \sqrt{\frac{n+1}{2}} \sqrt{\frac{m+1}{2}} \frac{1}{\langle n+1|\hat{x}|1\rangle} \frac{1}{\langle m+1|\hat{x}^{2}|1\rangle} \sum_{l=n}^{\infty} \langle l|\hat{x}|1\rangle^{2} ,$$
(C.2)

where each sum only takes even l into account.

We are only interested in the large n asymptotics of the amplitude $\langle n|\hat{x}^2|m\rangle$. Hence, it is sufficient to determine the dominant of the three contributions for large n. Let us discuss them separately.

(i) The large n behavior of the first contribution,

$$S_1 = \langle n|\hat{x}|0\rangle \langle m|\hat{x}|0\rangle \sum_{l=0}^{m} \frac{m+1}{2} \frac{1}{\langle l+1|\hat{x}|0\rangle^2},$$
 (C.3)

is straightforward to determine, as the sum does not involve any terms that depend on n. That is, the leading terms of S_1 behave as

$$S_1 \sim \langle n|\hat{x}|0\rangle$$
 (C.4)

(ii) In contrast to (i) the second contribution.

$$S_2 = \sqrt{\frac{m+1}{2}} \frac{\langle n|\hat{x}|0\rangle}{\langle m+1|\hat{x}|1\rangle} \sum_{l=m}^n \sqrt{\frac{l+1}{2}} \frac{\langle l|\hat{x}|1\rangle}{\langle l+1|\hat{x}|0\rangle}, \qquad (C.5)$$

involves n both explicitly and implicitly as a boundary term of the summation. However, using $\langle l|\hat{x}|1\rangle / \langle l+1|\hat{x}|0\rangle \sim \mathcal{O}(1)$, we can estimate the parametric dependence of the sum on n. By going to the continuum limit we therefore evaluate

$$\sum_{l=m}^{n} \sqrt{\frac{l+1}{2}} = \int_{\frac{m}{2}}^{\frac{n}{2}} dl \sqrt{l+\frac{1}{2}} = \frac{(n+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}}}{3\sqrt{2}}, \quad (C.6)$$

where we used that the summation contains only terms with even l. That is, for large n, S_2 parametrically behaves as

$$S_2 \sim \left((n+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}} \right) \langle n | \hat{x} | 0 \rangle .$$
 (C.7)

(iii) The remaining contribution,

$$S_3 = \sqrt{\frac{n+1}{2}} \sqrt{\frac{m+1}{2}} \frac{1}{\langle n+1|\hat{x}|1\rangle} \frac{1}{\langle m+1|\hat{x}^2|1\rangle} \sum_{l=n}^{\infty} \langle l|\hat{x}|1\rangle^2 , \qquad (C.8)$$

can be evaluated in a similar way like S_2 . This time the summation in addition involves the *a priori* unknown amplitudes $\langle l|\hat{x}|1\rangle$. However, in Section 3.2.2 we found that these should parametrically be of exponential form,

$$\langle l|\hat{x}|0,1\rangle \sim e^{-cl}$$
, (C.9)

with c > 0. With this ansatz the sum can again be rewritten as an integral, such that we obtain

$$\sum_{l=n}^{\infty} \langle l | \hat{x} | 1 \rangle^2 \sim e^{-2cl} \sim \langle n | \hat{x} | 0 \rangle^2 . \tag{C.10}$$

Thus, we conclude that for large n the third contribution behaves as

$$S_3 \sim \sqrt{\frac{n+1}{2}} \langle n+1|\hat{x}|1\rangle$$
 (C.11)

In summary, comparing all three different contributions, we find that, for large n, the dominant contribution to the amplitude $\langle n|\hat{x}^2|m\rangle$ is given by S_2 . Therefore, we conclude

$$\langle n|\hat{x}^2|m\rangle \sim \frac{(n+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}}}{3\sqrt{2}} \sqrt{\frac{m+1}{2}} \frac{\langle n|\hat{x}|0\rangle}{\langle m+1|x|1\rangle},$$
 (C.12)

for n and m odd and n > m. Similarly, the same computation can be carried out for n and m even. Here, the low lying states are exchanged because of parity symmetry, such that the final result reads

$$\langle n|\hat{x}^2|m\rangle \sim \frac{(n+1)^{\frac{3}{2}} - (m+1)^{\frac{3}{2}}}{3\sqrt{2}} \sqrt{\frac{m+1}{2}} \frac{\langle n|\hat{x}|1\rangle}{\langle m+1|\hat{x}|0\rangle}.$$
 (C.13)

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