Dissertation
submitted to the
Combined Faculties for the Natural Sciences and for Mathematics
of the Ruperto Carola University of Heidelberg, Germany
for the degree of
Doctor of Natural Sciences

presented by
Dipl. Phys. Michael Thesen
born in Trier, Germany
Oral examination: July 9. 2003

Quantum Statistical Physics of a Microscopic Glass Model

Referees: Prof. Dr. Reimer Kühn
Prof. Dr. Heinz Horner

Zusammenfassung

Wir untersuchen die Quantenstatistische Physik eines mikroskopischen Glasmodells in verschiedenen Näherungen und finden Beziehungen zwischen bekannten Arten der Beschreibung glasartigen Verhaltens bei tiefen und hohen Temperaturen. Dabei verwenden wir die Replica-Methode zur Berechnung der freien Energie und implementieren die sich ergebenden Selbstkonsistenzgleichungen in einer Entwicklung nach zweiteilchen-irreduziblen Vakuumgraphen. In der einfachsten variationellen Näherung ergibt sich ein zur quasiklassischen Version des Modells analoges Bild. In dieser Nähreung zeigen wir die Äquivalenz des Problems mit dem eines Ensembles von harmonischen Oszillatoren, die an ein Wärmebad gekoppelt sind. In der nächsten Ordnung der Entwicklung ergibt sich eine Analogie zu einem Spinglasmodell mit 2- und 4-Spin Wechselwirkungen. Der Glasübergang kann durch Quantenfluktuationen zu einem Phasenübergang erster Ordnung werden. Schließlich untersuchen wir eine nichtperturbative Näherung zum gleichen Modell, in der sich die Phänomenologie wieder vereinfacht.

Abstract

We investigate the quantum statistical physics of a microscopic glass model in different kinds of approximation schemes and develop relations between known pictures describing glassy behavior at low and high temperatures. We employ the replica method for the determination of the free energy, and implement the resulting self-consistency equations in an expansion in terms of two particle irreducible vacuum graphs. Within the simple variational approximation we find strong analogies to the quasi-classical version of the model. We show that the problem is equivalent to the problem of an ensemble of harmonic oscillators coupled to a heat bath. We find similarities to a spin-glass model with 2- and 4-spin interactions at the next order of the perturbation expansion. We show that the glass transition can be driven from second to first order by quantum fluctuations. Finally, we investigate a non perturbative approximation to the same model, displaying a much simpler phenomenology again.

Contents

Chapter 1

Introduction

Ever since the first experiments have unveiled the low-temperature anomalies in structural glasses [1] 30 years ago, there was vivid interest in the origin of these rather universal phenomena present in most structurally disordered systems [2, 3]. Almost right from the hour of birth of this field of research it became clear that the low temperature anomalies in glasses have to be in a close relation to the existence of tunneling centers in this type of material. At very low energies, these localized systems give rise an excess density of states as compared to the crystal. Therefore, they dominate the behavior of the probe at temperatures below or of the order of $1K$.

The commonly accepted microscopic picture of these tunneling systems is the one of some *collective* coordinate of a group of atoms, possessing two almost degenerate equilibrium positions separated by an energy barrier. The latter can be penetrated due to quantum tunneling if neither the mass corresponding to the collective coordinate we are looking at is too large nor is the barrier too high nor the energy asymmetry between the minima too large.

In the case of degenerate minima of the energy landscape, the degeneracy is lifted by the process of quantum tunneling – the tunnel splitting. This tunnel splitting gives rise to localized excitations at very low energies accounting for the excess density of states mentioned above.

At very low temperatures, the only states contributing to the dynamical properties of the glass are these pairs of tunneling states. This means that effectively, the relevant Hilbert space becomes two dimensional and the projection of the Hamiltonian can be mapped onto a spin-1/2-system. Now it is an easy task to determine the distribution of 'fields' the ensemble of 'spins' is subject to from the experimentally observed power laws in the temperature dependence of the specific heat and of the various types of susceptibilities.

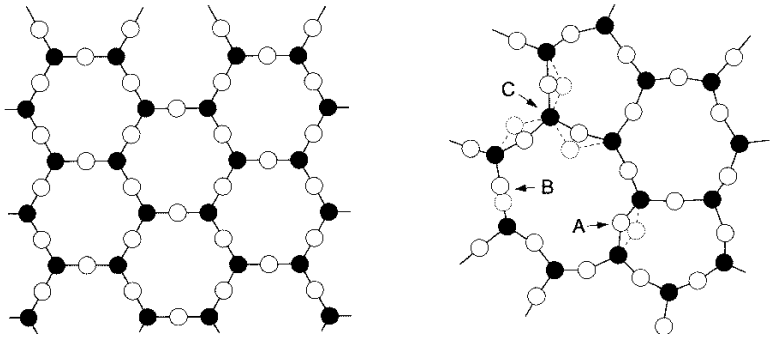


Figure 1.1: *Commonly accepted microscopic picture for tunneling centers in glasses. A group of atoms may penetrate an energy barrier separating two almost degenerate classical equilibrium positions of the system. The tunnel spitting gives rise to localized excitations of very low energy on top of the long-wavelength phonons present in the ordered crystalline counterpart of the system.*

This has been done by Anderson, Halperin and Varma [4] and Phillips [5] and their result has become the 'Standard Tunneling Model' (STM).

In fact, all this would not be very surprising, were the behavior observed in the low-temperature region not very universal – qualitatively and quantitatively. The russian school [6] was able to map the characteristic distribution of 'fields' in the spin-1/2 picture of the STM onto an ensemble of particles in quartic potentials with randomly distributed parameters. The potentials used in this type of approach can be viewed as resulting from a Born-von-Karman expansion around unknown reference positions. This expansion is truncated at quartic order in deviations from these reference positions. This type of model will be referred to as the 'soft potential model' (SPM) throughout this work. However, there is an ambiguity in the choice of the reference positions, such that not all coefficients in the expansion can be independent. For every stable quartic potential one can always find a reference position such that either the prefactor of the linear- or of the cubic term vanishes. It seems sufficient to assume the linear and the quadratic terms of the effective potentials to be widely distributed. The quartic coefficient can be set to 1 by choosing an appropriate *length scale* for every degree of freedom under consideration. At very low temperatures, only those potentials giving rise to an *observable* tunnel splitting are relevant, i.e. the tunneling must take place on a time scale smaller than the experimental one. This requirement projects out a tiny region in the wide space of parameters of the effective potentials. In this region, the probability density of the parameter-distribution can be safely assumed to be constant. It is this fact that is at the origin of a major

part of the universality of the low temperature anomalies in glasses [7].

However, the question of the microscopic nature of the tunneling systems is still unsolved to a large extent. Especially the fact that the observed tunneling systems are *independent* is at least puzzle and sometimes even been called paradox [8]. The argument is that no matter what the precise microscopic picture of the localized tunneling systems may be, they should be interacting with a force proportional to $1/r^3$, where r is the distance between a pair of tunneling systems. The reason is the distortion of the whole lattice due to the change in the local configuration corresponding to the tunneling process. However, such an interaction seems to be absent or at least very weak experimentally.

In recent times, new light was shed on this problem by the works of Horstmann and Kühn (HK) [9]. They were able to show that starting from a model with infinite range interactions and site-independent local potential, the model can be mapped onto an ensemble of *independent* particles moving in effective potentials with parameters distributed similar to the SPM. The mean-field nature of the model allows the authors to describe the effective double-well potentials as being of collective origin. The long-range nature of elastic interactions in real, 3-dimensional glasses gives some confidence, that this mean-field description captures the essentials of the collective origin of tunneling systems in glasses.

Nevertheless, there are severe doubts, concerning the procedure to include quantum tunneling applied by HK: the authors apply classical statistics in order to calculate the *energy landscape*. Only then they quantize the motion of particles within this classical effective energy landscape. If taken into account from the onset, quantum fluctuations could not only modify the ensemble of effective potentials, they could even render the description in *terms* of potentials impossible due to the emergence of memory-terms in the effective action.

These doubts became even more serious when Hunklinger, Strehlow [10, 11] and coworkers experimentally found evidence for a phase transition at a temperature as low as 5.84mK by observing a slight kink in the dielectric constant vs. temperature curve. The mere smallness of the transition temperature made the authors speculate on having found a transition to some kind of coherent quantum state. Moreover, magnetic field effects have been observed in a variety of experiments [12]. Perhaps the most striking ones have been seen in experiments probing the influence of magnetic fields on dielectric echoes of the tunneling systems in glasses [13]. As these phenomena appear on the same temperature scale as the phase transition, there are good reasons to guess that both phenomena share a common ground. Therefore,

it was deemed necessary to carry out a fully quantum statistical version of the HK-model in order not to lose informations on collective quantum excitations and to search for an eventual collective quantum state in glasses at low temperatures. The preliminary results of this project are presented in this work.

In a first part, we will introduce the microscopic mean-field model to be investigated in this work. The derivation presented here is very qualitative. The focus is put on convincing the reader that there are good reasons to believe that the model should capture qualitative features of real glasses rather than rigorously deriving the model as an approximation to some exact microscopic theory – which is not at hand anyway.

The second part is dedicated to the derivations of the mean-field equations for the thermal correlation functions using the replica trick. Furthermore, we will argue that the imaginary time dependence of correlations between different copies is bound to be trivial due to the symmetries of the system. This will be at the origin of the weak influence of quantum fluctuations on the *ultra-metric structure* of the system's phase space.

Afterwards, we investigate a variational or Hartree approximation to the model. Despite its simplicity, the variational approximation presents many interesting features, such as the transition to a glassy state and a low-temperature behavior that approaches the one observed in HK as $T \to 0$ in the sense that the physics can be described in terms of a distribution of *local* potentials. The variational equations can be solved analytically to a large extent. This allows us to study the analytical continuation of the imaginary-time correlation function to real times and to get information on dynamic quantities by this means. Furthermore, we will show that the effective action found in the variational approach is precisely the one of a quite interesting system plus bath Hamiltonian.

In order to go beyond the variational approximation, we will apply a self-consistent perturbation expansion scheme in terms of two-particle irreducible (2PI) vacuum graphs. This approximation scheme results in calculating an effective action obtained by a double Legendre transform of the free energy and is equivalent to expanding the self-energy in terms of skeleton graphs. The application of this method for self-consistency problems as the ones we will encounter in this work is the main methodological point of this work and results in a major simplification of the perturbative expansion for microscopic mean-filed glass models. It is this method that will allow us to obtain trustworthy non perturbative results.

The glassy phase observed in the variational approximation is not really *glassy* in the complexity sense, the solution being symmetric in the replica

indices. This symmetry will be spontaneously broken when we include higher order terms in the loop expansion of the 2PI effective action of the model. Already at 3-loop, we will find an enormous richness of the model: we will see first order and second order phase transitions, a crossover between the latter and a transition from a phase characterized by one order parameter (1-RSB) to one characterized by an order-parameter function (C-RSB). Even though the 3-loop approximation is not stable all over the parameter space, it is of considerable interest by its own because it can be almost identically mapped onto a spherical spin glass model 2-spin and 4-spin interactions. The latter model is considered a good one for glassy behavior by the glassy-dynamics community and its derivation presented here will shed new light on the relations between p-spin models and structural glasses.

Finally, we will present a non perturbative approach to the model by summing a series of diagrams. Even though it is hard to prove systematically that we are doing better than 4-loop, the equations resulting from this approximation have the enormous advantage of possessing solutions throughout the parameter space of our original model. Surprisingly, we recover the replica symmetry in this non perturbative approach.

The first two appendices are dedicated to deriving the effective action formalism applied in this work. They are followed by appendices on technical details.

Chapter 2

The Model

2.1 General Picture

In this chapter we will develop the microscopic model we put forward for glasses and formulate the Hamiltonian of the simple model we want to investigate throughout the major part of this work. We argue that the model presented in this chapter should capture the essential features of glasses in the high- as well as in the low-temerature regime.

As already mentioned in the introduction, we think of the degrees of freedom in amorphous solids as of continouous changes in the local configuration in the amorphous network. These changes in local configuration mainly take place along a line of minimal action in the a priori high dimensional configuration space. The actual position on this line will be labeled x_i . There is one ambiguous value of x_i being set to zero and called the reference position. In general, the reference position will be chosen such that it corresponds to a minimum of the configuration energy or will be at least very close to one such minimum. In this case, x_i would be the projection onto the lowest eigenvector of the Hessian matrix corresponding to minimum number i. In more complicated cases where there are two close minima, x_i would correspond to some point on the path with least action connecting the two minima in configuration space. In order to find a good description of the low-temperature properties of an amorphous material, we concentrate only on the *softest modes* of changes in configuration space and among these especially on those giving rise to tunneling excitations.

As can be concluded from experiments and can be seen from computer Simulations of binary Lennard-Jones mixtures [14, 15], these soft modes are localized objects in a sense that most of the weight of the soft eigenvectors

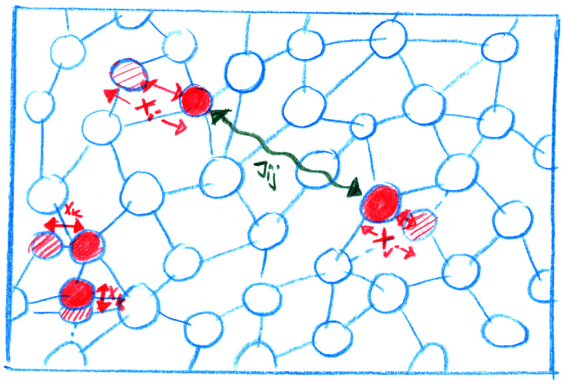


Figure 2.1: *Simplified picture of the degrees of freedom in an amorphous solid. Typically, we deal with changes in local configurations leading to long range distortions of the host network. These distortions give rise to interactions.*

of the Hessian is concentrated on a small number (of order 10) of atomic coordinates. These coordinates will be subsequently called *relevant*. The feature of localization will be one of the essential starting points for this work.

Consider the localized group of atoms whose coordinates have most of the weight of the 'soft mode' i, the *relevant* atoms. The projection of the movement corresponding to mode i onto the space spanned by the relevant coordinates will describe a change in configuration which is *not* an eigenmode of the system as a whole, but approximates such a mode quite well. The important point is that these projections – we will call them x_i – are *independent* degrees of freedom because there are rarely any atoms participating in more than one mode as a consequence of the localization discussed above. We will denote the configuration energy corresponding to the value x_i of the projection of the mode i on its relevant coordinates as $V_i(x_i)$. Of course, these potentials are not known in general.

From a kinetic point of view, there will be an effective mass m_i associated with the degree of freedom concerned, such that the total Hamiltonian of the system will be approximately given by a sum of 'single-site' Hamiltonians corresponding to the different relevant degrees of freedom

$$H = \sum_i \left[\frac{p_i^2}{2m_i} + V_i(x_i) \right] \quad . \tag{2.1}$$

While projecting onto the relevant coordinates, we have neglected the long-range distortions of the host network caused by the localized changes in configuration. Alternatively, these interactions can be seen as the consequence of the overlap of the soft modes. Microscopically, they are mediated by atomic coordinates participating in more than one of the quasi-localized excitations. From a macroscopic point of view they correspond to strain fields. Due to their long-range nature, these interactions can be described in terms of elasticity theory. Typically, there will be an elastic long-range interaction with a force proportional to $1/r^3$ due to distortions of the host network. Accounting for these interactions to leading order in the deviations from reference positions x_i, we would find an interaction of type

$$V_{\text{int}} = \sum_{i<j} J_{ij} x_i x_j \tag{2.2}$$

where the J_{ij} are determined by the distances and elastic momenta of the modes. As we do not know anything about the positions of the modes, nor of their microscopic structure, we do not know the distances nor the elastic momenta. Nevertheless, we know that the interaction is long-range, such that every mode interacts with every other mode and that there is a lot of randomness in the distances as well as in the elastic momenta.

We end up with a kind of 'Theory of Everything' for amorphous solids, determined by the Hamiltonian

$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m_i} + V_i(x_i) \right] + \sum_{i<j}^{N} J_{i,j} x_i x_j + \cdots \tag{2.3}$$

where the dots at the end denote higher order terms in the interaction.

Until now we have stated almost nothing except that the problem is very complex. Of course there is no general way of solving (2.3) for an arbitrary choice of parameters $\{m_i, V_i, J_{ij}\}$ such that we necessarily have to do approximations.

2.2 Approximations

In order to simplify (2.3), we have to consult our phenomenological understanding. First of all, we do not know the distribution of the coupling constants J_{ij}, but we know that there are different sources of randomness and their effects sum up to the final distribution of the J_{ij}. The best (and perhaps only) thing we can do is to assume the coupling strength to be uncorrelated Gaussian random variables with $J_{ij} = J_{ji}$, where the assumption

that the variables are uncorrelated is perhaps more crucial and less realist than the assumption of a Gaussian distribution.

When coming to the point of approximating the on-site-parameters V_i and m_i, we have even less physical insights. However, there is experimental [16] and theoretical [7] evidence that the precise choice of the microscopic single-site parameters might be irrelevant - at least for the low-temperature properties. The universality of the latter indicates, that the 'effective theory' at low temperatures is strongly renormalized due to collective effects, largely removing the influence of the microscopic parameters. To put it another way: we expect the distribution of single-site parameters to be strongly material (and probe ?) dependent. The low temperature properties are not. Therefore we hope to capture the essential features of the low-temperature universality in glasses when taking the most simple assumptions for the single-site potentials $V_i(x_i)$ and masses m_i.

Having this in mind, we propose to assume V_i and m_i to be site-independent $V_i(x_i) = V(x_i)$, $m_i = m$, and symmetric $V(-x) = V(x)$ and truncate its Taylor expansion at quartic order. We want $x_i = 0$ to be an equilibrium position in absence of interactions and the whole Hamiltonian to be stable for all choices of J_{ij}.

Finally, we end up with the Hamiltonian

$$H = \sum_i \left[\frac{p_i^2}{2m} + \frac{1}{2} m\omega^2 x_i^2 + \frac{g}{4!} x_i^4 \right] + \sum_{i<j} J_{ij} x_i x_j . \tag{2.4}$$

We stress that we do not explicitly exclude starting with double-well potentials corresponding to $\omega^2 < 0$. This means that we take ω^2 rather than ω to be a real-number input parameter.

This model is closely related to the quantum spherical p-spin glass for p=2, the only difference being, that the stability is enforced through the quartic term instead of a spherical constraint. The interaction strengths J_{ij} are taken from a Gaussian distribution with zero mean and variance

$$\overline{(J_{ij})^2} = \frac{J^2}{N} . \tag{2.5}$$

Here and everywhere in the subsequent text, N is the number of relevant coordinates considered. The scaling of the variance of the Interaction constants J_{ij} with N is necessary in order to obtain a non trivial thermodynamic limit.

2.3 Possible Extensions of the Model

The most obvious extension of (2.4) is immediate from the analogy with spherical p-spin glasses – it consists in accounting for interactions between 3 and more modes using terms like

$$H_{\text{int}} = \sum_{i<j<k} J_{ijk} x_i x_j x_k \ . \tag{2.6}$$

For spherical p-spin glasses such 3-spin interactions bring in some interesting new features. For example the ergodicity is broken at low temperatures and the transition to the glass phase becomes first order in some restricted sense. This will be discussed in a later chapter. However, we will see, that effective interactions just like (2.6) are *generated collectively* in course of the perturbative expansion of (2.4).

A more sophisticated extension was proposed by Reimer Kühn [14]. If we think of it, the separation between the amorphous network and the localized 'defects' described by the relevant coordinates is somewhat ambiguous. We will show in this work how the soft modes we are considering are dynamically *created* by the collective properties of the material such that we could think of the Hamiltonian (2.4) as an effective Hamiltonian at some intermediate level of renormalization, the original 'bare' Hamiltonian describing a system of single particles or molecules with a two-body interaction. However, there is a common feature in all possible types of 'bare' models that should be conserved under the flow of renormalization: the *translational invariance*. The translation of the *whole* system should evidently cost no energy. This would mean that everything should depend only on *translationally invariant quantities* such as $(x_i - x_j)$. Taking this into account we arrive at a modified version of (2.4):

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{N} \sum_{i<j} G(x_i - x_j) + \sum_{i<j} J_{ij} (x_i - x_j)^2 \tag{2.7}$$

where the effective two-point potential $G(x)$ is assumed to be symmetric and the Taylor expansion is truncated at quartic order. This translationally invariant version of the model is known to produce much more 'glassy' results than (2.4) when doing a quasiclassical approximation to it. However, the translational invariance does not lend itself to the parturbative approach pursued in this work.

Chapter 3

Replica Calculation

As we want to study the thermodynamics of this model, we compute the free energy per particle, f, by using the replica identity [17]

$$\beta f = -\frac{1}{N}\overline{\ln Z} = -\frac{1}{N}\lim_{n\to 0}\frac{\overline{Z^n}-1}{n} \ . \tag{3.1}$$

The partition function of the model is given by

$$Z = \mathrm{Tr} e^{-\beta H} \tag{3.2}$$

and H is the Hamiltonian (2.4).

Concerning the details of the replica trick, we refer to the extensive literature [17] on this topic. At this point, only some calming words are indicated. Even if the quantity $\overline{Z^n}$ can be calculated only for integer n and even if the limit $n \to 0$ is far from being unique [18], the spin glass community has developed a catalog of prescriptions to render the replica limit unique and - even more important - make the results coincide with experimental and numerical results and with alternative ways to calculate dynamic and thermodynamic quantities such as the super-symmetric method or the Thouless-Anderson-Palmer (TAP) [19] approach.

The replicated partition function, Z^n, can be written as a functional integral over periodic functions using the Trotter formula, a procedure which is also called the Matsurbara formalism and can be found in every standard textbook on quantum statistical mechanics (see e.g. [20, 21, 22]). As the n replica of the partition function are identical, the quantity Z^n becomes the product of n path integrals over periodic paths $x_a(\tau_a)$ and the origins of the n imaginary time arguments τ_a can be chosen *independently*. This symmetry will have important consequences for the general structure of the self-consistency equations derived below.

The explicit formulation of the replicated partition function in terms of path integrals reads

$$\begin{aligned}
\overline{Z^n} &= \int \prod_{i<j} \frac{dJ_{ij}}{\sqrt{2\pi}} e^{-\frac{NJ_{ij}^2}{2J^2}} \int \mathcal{D}\{x_{a,i}\} \exp\left[-S[\{x_i\},\{J_{ij}\}]\right] \\
S[\{x_i\},\{J_{ij}\}] &= \sum_{a=1}^{n}\sum_{i=1}^{N} \frac{1}{\hbar}\int_0^{\beta\hbar} d\tau_a \left[\frac{m(\dot{x}_{a,i}(\tau_a)^2)}{2} + \frac{1}{2}m\omega^2 x_{a,i}^2(\tau_a) + \frac{g}{4!}x_{a,i}^4(\tau_a)\right] \\
&+ \sum_{i=i}^{N}\sum_{j=1}^{i-1} J_{ij}\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau_a x_{a,i}(\tau_a)x_{a,j}(\tau_a) \qquad (3.3)
\end{aligned}$$

Now the integral over the disorder J_{ij} can be calculated and we find

$$\begin{aligned}
\overline{Z^n} &= \int \mathcal{D}\{x_{a,i}\} \exp\left[-S[\{x_i\}]\right] \\
S[\{x_i\}] &= \sum_{a=1}^{n}\sum_{i=1}^{N} \frac{1}{\hbar}\int_0^{\beta\hbar} d\tau_a \left[\frac{m(\dot{x}_{a,i}(\tau_a)^2)}{2} + \frac{1}{2}m\omega^2 x_{a,i}^2(\tau_a) + \frac{g}{4!}x_{a,i}^4(\tau_a)\right] \\
&- \frac{J^2}{2\hbar^2}\sum_{i<j}^{N}\int_0^{\beta\hbar} d\tau_b \int_0^{\beta\hbar} d\tau_a x_{a,i}(\tau_a)x_{a,j}(\tau_a)x_{b,i}(\tau_b)x_{b,j}(\tau_b) \qquad (3.4)
\end{aligned}$$

Admitting an error of the relative order $\frac{1}{N}$, we can replace the sum $\sum_{i<j}$ by $\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}$.

As the classical analogs of the above model, it will turn out that the mean-field approximation is to this model is exact. Indeed, the last term in (3.4) can be expressed in terms of the fields $Q_{ab}(\tau_a,\tau_b) = \frac{1}{N}\sum_{j=1}^{N} x_{a,j}(\tau_a)x_{b,j}(\tau_b)$. In order to decouple the sites and to express the action in terms of these fields, we follow the procedure analog to the mean mean-field decoupling in classical models and introduce in $\overline{Z^n}$ the identity

$$\begin{aligned}
1 &\sim \int \mathcal{D}Q\,\delta(N\mathcal{Q}_{ab}(\tau,\tau') - \vec{x}_a(\tau)\cdot\vec{x}_b(\tau')) \\
&\sim \int \mathcal{D}Q \int \mathcal{D}\lambda \exp[\frac{1}{2\hbar}\sum_{ab}\int d\tau \int d\tau' \lambda_{ab}(\tau,\tau')(NQ_{ab}(\tau,\tau') - \vec{x}_a(\tau)\cdot\vec{x}_b(\tau'))]
\end{aligned}$$

where $\vec{x}_a$ is the N-vector with the components $x_{a,i}$, $i = 1..N$. The above expression can be understood by thinking of λ as of a purely imaginary matrix and of $\int \mathcal{D}\lambda$ as of a path integral over the space of matrices of this

type. The averaged replicated partition function can now be recast as

$$\overline{Z^n} = \int \mathcal{D}\vec{x}\mathcal{D}Q\mathcal{D}\lambda \exp(-\frac{1}{\hbar}S[Q,\lambda,x] \tag{3.5}$$

where $S[Q,\lambda,x]$ evaluates to

$$\begin{aligned} -\frac{1}{\hbar}S[Q,\lambda,x] &= -\sum_{a,i}\frac{1}{\hbar}\int d\tau \left[\frac{m}{2}\dot{x}_{a,i}(\tau)^2 + \frac{1}{2}m\omega^2 x_{a,i}(\tau^2) + \frac{g}{4!}x_{a,i}(\tau)^4\right] \\ &- \frac{1}{2\hbar}\sum_{ab}\int d\tau \int d\tau' \vec{x}_a(\tau)\lambda_{ab}(\tau,\tau')\vec{x}_b(\tau') \\ &+ \frac{N}{2\hbar}\sum_{ab}\int d\tau \int d\tau' Q_{ab}(\tau,\tau')\lambda_{ab}(\tau,\tau') \\ &+ \frac{J^2N}{4\hbar^2}\sum_{ab}\int d\tau \int d\tau' Q^{*2}_{ab}(\tau,\tau') \ . \end{aligned} \tag{3.6}$$

The function $Q^{*2}_{ab}(\tau,\tau')$ is the square of the *matrix element* rather than the matrix power. It is important to note that this effective action is manifestly *nonlocal* in imaginary time and can *not* be mapped onto an effective ensemble of single-site potentials as in the non-quantum version of the same model [9]. Moreover, the average over disorder generates interactions between different replica of the system just as in the non-quantum version of the model.

3.1 Saddle point equations

Taking the saddle point of (3.6) with respect to $\lambda_{ab}(\tau,\tau')$ yields the *self-consistency condition*

$$Q_{ab}(\tau,\tau') = < x_a(\tau)x_b(\tau') >_{S_{\rm eff}} \tag{3.7}$$

where we have used step that the expectation values are identical for each site i. The angular brackets in the last expression denote the average taken with respect to the effective single-site action

$$\begin{aligned} -\frac{1}{\hbar}S_{\rm eff}[\lambda] &= -\frac{1}{\hbar}\sum_{a}\int d\tau \frac{m}{2}\dot{x}_a(\tau)^2 + \frac{1}{2}m\omega^2 x_a(\tau^2) + \frac{g}{4!}x_a(\tau)^4 \\ &- \frac{1}{2\hbar}\sum_{ab}\int d\tau \int d\tau' x_a(\tau)\lambda_{ab}(\tau,\tau')x_b(\tau') \ . \end{aligned} \tag{3.8}$$

The saddle point with respect to $Q_{ab}(\tau,\tau')$ is

$$\lambda_{ab}(\tau,\tau') = -\frac{J^2}{\hbar}Q_{ab}(\tau,\tau') \tag{3.9}$$

such that we can eliminate $\lambda_{ab}(\tau,\tau')$ from the action, provided we are interested only in the saddle point only and that we keep the self-consistency condition (3.7) as a constraint. Using (3.9), we can write the self-consistent effective single-site action as

$$\begin{aligned} -\frac{1}{\hbar}S[Q] &= -\frac{1}{\hbar}\sum_a \int d\tau \frac{m}{2}\dot{x}_a(\tau)^2 + \frac{1}{2}m\omega^2 x_a(\tau^2) + \frac{g}{4!}x_a(\tau)^4 \\ &+ \frac{J^2}{2\hbar^2}\sum_{ab}\int d\tau \int d\tau' x_a(\tau) Qab(\tau,\tau') x_b(\tau') \ . \end{aligned} \tag{3.10}$$

However, we will take a slightly different route throughout this work. Using the fact that the N degrees of freedom are subject to identical single-site actions we will decompose the effective action (3.6) in three parts: we write

$$\begin{aligned} &\int \mathcal{D}Q\mathcal{D}\lambda\mathcal{D}x \exp\left\{-\frac{1}{\hbar}S[Q,\lambda,x]\right\} = \\ &\qquad \int \mathcal{D}Q\mathcal{D}\lambda \exp\left\{-N[S_1[Q] + S_2[Q,\lambda] + S_3[\lambda]]\right\} \ . \end{aligned} \tag{3.11}$$

The three parts of the single-site action are given by

$$S_1[Q] = -\frac{J^2}{4\hbar^2}\sum_{ab}\int d\tau \int d\tau' Q^*_{ab}(\tau,\tau') \tag{3.12}$$

$$S_2[Q,\lambda] = -\frac{i}{\hbar}\sum_{ab}\int d\tau \int d\tau' Q_{ab}(\tau,\tau')\lambda_{ab}(\tau,\tau') \tag{3.13}$$

$$\tag{3.14}$$

and finally

$$S_3[\lambda] = \ln\left[\int \mathcal{D}x \exp\left(-S_{\text{eff}}[\lambda]\right)\right] \tag{3.15}$$

with the effective action $S_{\text{eff}}[\lambda]$ taken from (3.8).

We note that $S_3[\lambda]$ is formally the same as the generating functional for two-point functions for a single particle in the original bare potential $V(x) = \frac{1}{2}m\omega^2x^2 + \frac{g}{4!}x^4$, and $\lambda_{ab}(\tau,\tau')$ plays the role of a source field. In this work we will mainly treat approximations for the last term, $S_3[\lambda]$. Using the analogy of this part of the effective action with generating functionals we will dispose of a variety of tools imported form quantum field theory in order to construct such approximations. Nevertheless, there is an important difference: in order to obtain the physical two-point function $Q_{ab}(\tau,\tau')$, we do not have to set the source term λ_{ab} to zero at the end of the calculation but have to set lambda to its self-consistent value (3.9).

3.2 Fixing of Notations and Orders of Magnitude

In this section we will discuss the convenient choice of the relevant scales of the problem. This will be an important feature for the comparison of the different degrees of approximation with the results for the so-called spherical p-spin models well-known in the field of spin-glasses. Furthermore, we will fix notations and Conventions for the Fourier transforms in the imaginary time domain. Finally, we will give estimations for the orders of magnitude of the parameters in the model.

Consider the action

$$\begin{aligned} S_{\text{eff}} &= \frac{1}{\hbar}\sum_a \int_0^{\beta\hbar} d\tau \Big(\frac{m}{2}\Big[\Big(\frac{dx_a(\tau)}{d\tau}\Big)^2 + \omega^2 x_a^2(\tau)\Big] + \frac{g}{4!}x_a^4(\tau) \\ &- \frac{J^2}{4\hbar^2}\sum_{ab}\int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau' x_a(\tau) Q_{ab}(\tau,\tau') x_b(\tau') \end{aligned} \tag{3.16}$$

as it has been derived in the previous section [1].

Given an elementary length scale l_0, we would like to measure the energy in terms of the disorder energy scale $E_J = J l_0^2$ and the time in units of $t_0 = \hbar/E_J$. Introducing $\tilde{x}(\tilde{\tau}) = x(\tau)/l_0$ and $\tilde{Q}_{ab}(\tilde{\tau},\tilde{\tau}') = \frac{1}{l_0^2} Q_{ab}(\tau,\tau')$ and finally $\tilde{\tau} = \tau/t_0$ the effective action can be expressed as

$$\begin{aligned} S_{\text{eff}} &= \frac{1}{2J}\sum_a \int_0^{\beta E_J} d\tilde{\tau} \Big(m\Big[\Big(\frac{d\tilde{x}_a(\tilde{\tau})}{t_0 d\tilde{\tau}}\Big)^2 + \omega^2 \tilde{x}_a^2(\tilde{\tau})\Big] + \frac{g E_J}{4! J}\tilde{x}_a^4(\tilde{\tau}) \\ &- \frac{1}{4}\sum_{ab}\int_0^{\beta E_J} d\tilde{\tau} \int_0^{\beta E_J} d\tilde{\tau}' \tilde{x}_a(\tilde{\tau}) \tilde{Q}_{ab}(\tilde{\tau},\tilde{\tau}') \tilde{x}_b(\tilde{\tau}') \ . \end{aligned} \tag{3.17}$$

We can still choose the length scale l_0 at our convenience. This is most conveniently done by setting the disorder energy to one, $E_J = 1$, i.e $l_0^2 = 1/J$. We want to define the quantum parameter

$$\Gamma = \hbar^2 \frac{J}{m} \tag{3.18}$$

and the parameters $\tilde{\omega}^2 = \frac{m\omega^2}{J}$ and $\tilde{g} = \frac{g}{J^2}$ and end up with the effective action in its final form:

$$-S_{\text{eff}} = \frac{1}{2}\sum_a \int_0^{\beta} d\tilde{\tau} \Big(\Big[\frac{1}{\Gamma}\Big(\frac{d\tilde{x}_a(\tilde{\tau})}{d\tilde{\tau}}\Big)^2 + \tilde{\omega}^2 \tilde{x}_a^2(\tilde{\tau})\Big] + \frac{\tilde{g}}{4!}\tilde{x}_a^4(\tilde{\tau})$$

[1] We have inserted the self-consistent value of (3.9) λ for simplicity.

$$- \quad \frac{1}{4}\sum_{ab}\int_0^\beta d\tilde{\tau}\int_0^\beta d\tilde{\tau}'\tilde{x}_a(\tilde{\tau})\tilde{Q}_{ab}(\tilde{\tau},\tilde{\tau}')\tilde{x}_b(\tilde{\tau}') \ . \tag{3.19}$$

The previous considerations allow us to always set $J = 1$, $m = 1$ and $\hbar = 1$ for numerical purposes by an appropriate choice of the energy-, length- and time-scale. Furthermore, we will frequently encounter the dimensionless quantities $\gamma \equiv \frac{qT}{J^2}$ and $\mu = \frac{T}{\Gamma}$, defining different temperature scales. At high temperatures we have $\gamma \gg 1$ and the particle is subject to large thermal fluctuations such that the energy is essentially determined by the quartic part of the local potentials. In the opposite limit, the influence of the quartic part is small as compared to the disorder- and harmonic contributions. The parameter μ will determine the strength of quantum effects. For small values of μ, the thermal energy is much smaller than the quantum energy scale Γ and we expect quantum fluctuations to be stronger than thermal fluctuations. In the following chapters we will freely switch between the original and dimensionless versions of the quantities. Whenever there is no danger of confusion we will suppress the tildes for the sake of simplicity.

Even if we will always choose the energy scale such that $J = 1$ we will make the J-dependence explicit in order to keep track of the influence of disorder. Powers of m and $\hbar$ can be always reconstructed by dimensional considerations.

Conventions for the Fourier Transforms

In accordance with the literature on spherical quantum p-spin models [23, 24], we have decided to use the following conventions for Fourier transforms with respect to imaginary time.

For single-time quantities $x_a(\tau)$ we define

$$x_a(\omega_k) = \frac{1}{\sqrt{\beta}}\int_0^\beta x_a(\tau)e^{-i\omega_k\tau}d\tau \tag{3.20}$$

$$x(\tau) = \frac{1}{\sqrt{\beta}}\sum_k x(\omega_k)e^{i\omega_k} \tag{3.21}$$

whereas for two-time quantities $Q_{ab}(\tau,\tau')$ we will always assume time-translational invariance $Q_{ab}(\tau,\tau') \equiv Q_{ab}(\tau-\tau')$ and define

$$Q_{ab}(\omega_k) = \int_0^\beta Q_{ab}(\tau)e^{-i\omega_k\tau}d\tau \tag{3.22}$$

$$Q_{ab}(\tau) = T\sum_k Q_{ab}(\omega_k)e^{i\omega_k} \tag{3.23}$$

This convention may seem somewhat strange but has its advantages because when dealing with correlation functions $Q_{ab}(\tau - \tau') =< x_a(\tau)x_b(\tau') >$ we have $Q_{ab}(\omega_k) =< x(\omega_k)\sum_l x(-\omega_l) >=< |x(\omega_k)|^2$ with no additional factors β. The obvious drawback is that in the classical limit, where the correlation functions do not depend on imaginary time, we have $Q_{ab}(\tau) = Q_{ab} = TQ_{ab}(\omega_0)$ – the matrices differ by a factor T. Whenever there is no danger of confusion we will skip the tildes.

We note that combining the definition of the Fourier transform with the scaling discussed in the previous subsection we find for the kinetic part of the effective action

$$m\frac{\partial^2}{\partial\tau^2} \to \frac{1}{\Gamma}\tilde{\omega}_k^2 \qquad \text{where} \qquad \tilde{\omega}_k = \frac{2\pi k}{\beta} \ .$$

Effectively we are setting $\hbar \to 1$ and introduce an effective inverse mass Γ.

Orders of Magnitude

We assume the motions of the relevant degrees of freedom to take place on atomic length scales of about 10Å and the energies to be of the order of typical weak binding energies $\sim 10^{-2}eV$. This translates into

$$J \times (10\text{Å})^2 \sim m\omega^2 \times (10\text{Å})^2 \sim g \times (10\text{Å})^4 \sim 0.1\text{eV} \tag{3.24}$$

It will turn out that the glass transition temperature is approximately

$$T_g \approx \frac{2J}{g}\mathrm{k_B}(2J - \omega^2) \sim 10^4 K \tag{3.25}$$

which is not too bad as an estimate of the order of magnitude.

We find $J \sim 18^{18}\mathrm{eV/m^2}$ and assume the clusters of atoms under consideration to consist of some ten atoms weighing some ten times the weight of a nucleon. This gives $m \sim 10^3\mathrm{GeV/c^2}$ and we find for the quantum energy scale

$$\sqrt{\Gamma} = \hbar\sqrt{\frac{J}{m}} \sim 10\mathrm{k_B K}. \tag{3.26}$$

Therefore we expect quantum fluctuations to play a decisive role below 10K and to be almost irrelevant above. This coincides with the experimental findings and with their interpretation in terms of the STM, were quantum tunneling dominates the behavior at temperatures below this scale.

Chapter 4

Variational or Hartree Approximation

4.1 Derivation of the Saddle Point Equations

The first and most simple thing to do is to treat our microscopic glass-model in a variational approximation. We will show in appendix B that the Gaussian variational theory is equivalent to the 2-loop result from the 2PI effective action. The variational approach will lead to equations formally equivalent to a spherical p-spin model with 2-spin interactions that is known not to display a genuine glass transition at low temperatures [25]. The phase transition occurring in this model is of the type ferromagnetic-paramagnetic in the sense that there are two (disordered) ground states being transformed into one another under operation of inverting every 'spin' degree of freedom.

We start with a rather general effective action with general generating field for two-point functions $\lambda_{ab}(\tau,\tau')$. The identification, $\lambda_{ab} = \frac{J^2}{\hbar^2} Q_{ab}$ has to be done in the end, as discussed in the previous chapter.

The replicated action reads

$$\begin{aligned} \frac{1}{\hbar} S_{\text{eff}} &= \sum_a \int d\tau \left(\frac{1}{2} \dot{x}_a^2(\tau) + \frac{1}{2} \sum_{ab} \omega^2 x^2(\tau) + \frac{g}{4!} x_a^4(\tau) \right) \\ &- \frac{1}{2} \sum_{ab} \int d\tau \int d\tau' x_a(\tau) \lambda_{ab}(\tau,\tau') x_b(\tau) \ . \end{aligned} \tag{4.1}$$

For the test action we choose the *ansatz*

$$\frac{1}{\hbar} S_\sigma = \sum_a \int d\tau \left(\frac{1}{2} \dot{x}_a^2(\tau) + \frac{1}{2} \omega^2 x^2(\tau) \right)$$

$$- \quad \frac{1}{2}\sum_{ab}\int d\tau \int d\tau' x_a(\tau)\sigma_{ab}(\tau,\tau')x_b(\tau) \ . \tag{4.2}$$

We restrict ourselves to the space of time-translational invariant correlation functions $Q_{ab}(\tau_a,\tau_b) = Q_{ab}(\tau_a - \tau_b)$ and do the same for σ_{ab}. The exact propagator for the test action can then be given in Fourier space:

$$Q^{\sigma}_{ab}(\omega_l) = \left((\omega_l^2+\omega^2)\mathbb{1} - \hat{\sigma}\right)^{-1}_{ab} \tag{4.3}$$

which is equivalent to $\hat{\sigma}(\omega_l) = (\omega_l^2+\omega^2)\mathbb{1} - (\hat{Q}^{\sigma})^{-1}$.

We note that in most of the works on quantum spin glasses (e.g. [26, 23]) the *independent* time translational invariance of the imaginary times of different replications is taken for granted. This has the consequence, that the off-diagonal elements $Q_{ab}(\tau_a,\tau_b)$ for $a \neq b$ *must* be independent of their time arguments. Sometimes [23], this *ansatz* has even been called a *theorem*. Of course we admit that this symmetry holds for every integer number of replicas and any given realization of disorder. Therefore it is plausible to assume that it holds in the limit $n \to 0$ as well. However, there is another symmetry that is exact for integer n and is spontaneously broken in the $n \to 0$ limit: the permutational symmetry of the replicas. It is well established [27], that the breaking of this symmetry, the 'replica symmetry breaking' is related to the breaking of ergodicity which is at the very heart of glassy low-temperature physics. Therefore we will allow for a restricted time dependence of the off-diagonal elements of the correlation function. We only requre invariance under uniform translations of *all* times and show that the *ansatz* $Q_{ab}(\tau,\tau') = Q_{ab}$ for $a \neq b$ is exact at least in the variational approximation (where, however, the replica symmetry turns out to be exact as well).

Using the convexity of the exponential function we can apply Jensen's inequality in order to find an upper bound for the free energy. The result is the variational expression for the free energy:

$$F[\sigma] = \frac{1}{\hbar} < S_{\text{eff}} - S_\sigma > -T \ln\left(\int \mathcal{D}x e^{-\frac{1}{\hbar}S_\sigma}\right) \ . \tag{4.4}$$

Using (4.3) we can express the expectation value above as

$$\begin{aligned}\frac{1}{\hbar} < S_{\text{eff}} - S_\sigma > \quad &= \quad -\frac{1}{2} < \sum_{ab}\int d\tau \int d\tau' x_a(\tau)\left[\lambda_{ab}(\tau,\tau') - \sigma_{ab}(\tau,\tau')\right] x_b(\tau') > \\ &+ \quad \frac{g}{4!} < \sum_a \int d\tau x_a(\tau)^4 >_{S_\sigma}\end{aligned}$$

$$
\begin{aligned}
&= -\frac{1}{2}T\sum_k\sum_{ab} Q^\sigma_{ab}(\omega_k)[\lambda_{ab}(\omega_k) - \delta_{ab}(\omega_k^2+\omega^2) - 1] \\
&+ \frac{3g}{4!}T^2\sum_{k,k'}\sum_a Q^\sigma_{aa}(\omega_k)Q^\sigma_{aa}(-\omega_k') \; . \qquad (4.5)
\end{aligned}
$$

The subscript at the angular brackets means that the latter denote the expectation value with respect to S_σ.

Using the Gaussian nature of the variational test action, the last term in the variational free energy (4.4) can be written as

$$
\ln\left(\int \mathcal{D}x e^{-\frac{1}{\hbar}S_\sigma}\right) = -\frac{1}{2}\mathrm{Tr}\ln(\hat{Q}^\sigma) \; . \qquad (4.6)
$$

Variation with respect to Q yields:

$$
\begin{aligned}
2\beta\frac{\delta F^\sigma}{\delta Q^\sigma_{ab}(\omega_k)} &= -Q^{(\sigma)+1}_{ab}(\omega_k) - \lambda_{ab}(\omega_k) \\
&+ \delta_{ab}(\omega_k^2+\omega^2) + \delta_{ab}\frac{gT}{2}\sum_{k'} Q^\sigma_{aa}(\omega_k') = 0 \; . \qquad (4.7)
\end{aligned}
$$

In the case of our mean-field equations we have to use $\lambda_{ab}(\tau,\tau') = J^2 Q_{ab}(\tau,\tau')$ where $Q = Q^{(\sigma)}$ by virtue of (3.7). Furthermore, we find that $Q_{ab} \equiv G_{ab} + \Phi_a\Phi_b = G_{ab}$ where G_{ab} is the *connected* two point function because the mean values $\Phi_a =< x_a >$ vanish. A non vanishing value of Φ_a would correspond to a ferromagnetic order which we do not expect for our model because of the immanent disorder of the system.

Using $z = T\sum_k Q_{aa}(\omega_k) \equiv Q_{aa}(\tau=0)$ eqn. (4.7) reads

$$
Q^{(\sigma)-1}(\omega_k) = -J^2 Q(\omega_k) + (\omega_k^2 + \omega^2 + \frac{gz}{2})\mathbb{1} \; . \qquad (4.8)
$$

Eqn. (4.8) represents a complete set of equations for the components of Q and will be solved in the next section.

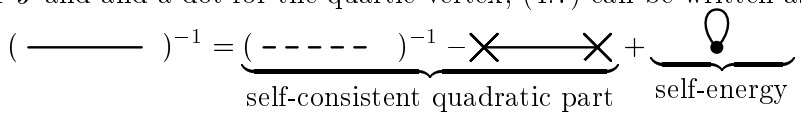
For completeness we state the minimal σ which can be read off easily by comparing eqn. (4.8) and (4.3):

$$
\sigma^{\min}_{ab}(\tau_a,\tau_b) = J^2 Q_{ab}(\tau_a,\tau_b) - \delta_{ab}\delta(\tau_a-\tau_a')\frac{g}{2}Q^{\sigma^{\min}}_{aa}(\tau_a,\tau_a) \qquad (4.9)
$$

and in Fourier space

$$
\sigma^{\min}(\omega_k)_{ab} = J^2 Q_{ab}(\omega_k) - \frac{gz}{2}\delta_{ab} \; . \qquad (4.10)
$$

From eqn.(4.3) we can read off that σ is related to the self-energy in the variational approximation. This allows a diagrammatical discussion of (4.9). The first term in (4.9) represents scattering with the 'spin-bath' due to the interaction J and is nonlocal in the replica indices and in imaginary time. Thinking of the propagator as a transfer rate of excitation energy we find that the energy may be transferred from one replica of the system to another with a rate J independent of the time-arguments. The system a does not know about the proper time of system b. Using dashes for the quadratic part of the *bare* propagator $Q_0^{-1}(\omega_k) = (\omega^2 + \omega_k^2)\delta_{ab}$, a plain line for the full propagator $Q_{ab}(\omega_k)$, crosses for elastic disorder scattering associated with a factor J and and a dot for the quartic vertex, (4.7) can be written as



For $a = b$, the equations have to be read differently: the process described by the first term in (4.9) is the transfer of the excitation to some other replication of the system and the return to the original system at a later time. This gives rise to an effective 'dressed' propagator $\mathcal{G}_0^{-1} = G_0^{-1} - J^2 Q$ described by the first two terms of the rhs. of the diagrammatic equation above. The last term in (4.9) can be read as the self-consistent Hartree correction to this propagator, summing up all tadpole contributions.

When evaluating the free energy, we have to keep in mind that the variational expression (4.4) is only the contribution corresponding to the single-site part $S_3[\lambda]$ (3.15) of the free energy. The terms $S_1[Q]$ and $S_2[Q, \lambda]$ contribute an additional term

$$\lim_{n\to 0} \frac{J^2}{4} \sum_{ab} \sum_k Q^*_{ab}(\omega_k)$$

to the free energy per particle. The total free energy per particle at its minimum value reads

$$\begin{aligned} \beta f[\sigma_{\min}] &= \lim_{n\to 0} \frac{1}{n} \left\{ \frac{1}{4} J^2 \sum_k \sum_{ab} Q^{*2}_{ab}(\omega_k) + \frac{1}{2} \mathrm{Tr} \ln(Q^{-1}) \right. \\ &+ \left. \frac{1}{2} \sum_k \sum_a \Big[(\omega^2 + \omega_k^2) Q_{aa}(\omega_k) - 1 \Big] - \frac{J^2}{2} \sum_k \sum_{ab} Q^{*2}_{ab}(\omega_k) + \frac{n\beta g z^2}{8} \right\} . \end{aligned} \tag{4.11}$$

Introducing the renormalized frequency $\Omega^2 = \omega^2 + \frac{gz}{2}$, and using the partial cancellation in expression (4.11) we have

$$\beta f[\sigma_{\min}] = \lim_{n\to 0} \frac{1}{n} \left\{ -\frac{1}{4} J^2 \sum_k \sum_{ab} Q^{*2}_{ab}(\omega_k) + \frac{1}{2} \mathrm{Tr} \ln(Q^{-1}) \right.$$

$$+ \quad \frac{1}{2}\sum_k \sum_a \Big[(\Omega^2 + \omega_k^2) Q_{aa}(\omega_k) - 1\Big] - \frac{n\beta g z^2}{8} \Bigg\} \quad . \quad (4.12)$$

where again Q_{ab}^{*2} is the square of the matrix *element* rather than the matrix power. This expression will be of use for calculating the thermodynamic quantities such as the Entropy and specific heat of the model. But let us first solve equations (4.8).

4.2 High-Temperature Solution

In this section we want to solve the above equations in the high temperature phase. In this regime, the correlation function is expected to be of diagonal form in the replica indices: $Q_{ab}(\omega_k) = q_d(\omega_k)\delta_{ab}$. This enables us to write 4.8 as

$$q_d(\omega_k)\left[(\omega_l^2 + \omega^2 + \frac{gz}{2})\mathbb{1} - J^2 q_d(\omega_k)\right] = 1 \tag{4.13}$$

where we have introduced $z = T\sum_k q_d(\omega_k)$. Given z, there is a simple quadratic equation to solve for each mode k. The solutions are

$$q_d(\omega_l) = \frac{(\omega_l^2 + \omega^2 + \frac{gz}{2})}{2J^2} \pm \frac{1}{2J^2}\sqrt{(\omega_l^2 + \omega^2 + \frac{gz}{2})^2 - 4J^2}\ . \tag{4.14}$$

We always have to choose the negative sign corresponding to the minimum of the free energy. This solution ceases to be real if $\omega^2 + \frac{gz}{2} \leq 2J$. It exists for all temperatures if $\omega^2 \geq 2J$. For $\omega^2 \leq 2J$, there is a temperature below which the paramagnetic solution does not exist anymore.

The parameter z has to be determined self-consistently by virtue of the equation

$$z = f(z) \equiv T\sum_k q_d(\omega_k) \tag{4.15}$$

where the $q_d(\omega_k)$ are given by 4.14 and depend on z. It turns out that $f(z)$ is a decreasing function of z having its maximum value at the minimum value of z. In the interesting regime $\omega^2 \leq 2J$ the minimal value z_c of z, below which the zero - mode becomes unstable is given by

$$z_c = \frac{2}{g}(2J - \omega^2)\ . \tag{4.16}$$

For this value of z we have

$$q_d(\omega_0) = \frac{1}{J} \tag{4.17}$$

and

$$q_d^{z_c}(\omega_k) = \frac{\omega_k^2}{2J^2} + \frac{1}{J} - \frac{\omega_k}{2J^2}\sqrt{\omega_k^2 + 4J} \tag{4.18}$$

note that at this point the dependence on ω^2 and g has vanished. It will turn out that the criterion $z = z_c$ determines the phase transition of the model in the variational approximation.

Now we may solve (4.15) for $z = z_c$ numerically and thereby determine the transition temperature. In this section we will discuss two limiting cases

analytically. First of all, we consider the case of vanishing quantum fluctuations $\Gamma \to 0$. In this limit, the function $f(z)$ is dominated by the first term in (4.15) and we have

$$\frac{2}{g}(2J - \omega^2) = \frac{T_c}{J} \Longrightarrow T_c = \frac{2J}{g}(2J - \omega^2) \ . \tag{4.19}$$

It is worthwhile to note that result coincides with the result obtained by HK [9].

The critical Temperature T_c becomes negative when $\omega^2 > 2J$ and no phase transition will ever occur. The physical interpretation of this is easily given in terms of random matrix theory. The interaction matrix J_{ij} can be diagonalized and one will find a semicircular density of states, the so-called Wigner semi-circle, with the radius $2J$. If $\omega^2 > 2J$, the Hessian of the potential at the origin will have positive eigenvalues only and no saddle points or maxima may occur in the energy landscape. However, the requirement for a symmetry breaking is the existence of configurations of double - well type with an unstable equilibrium position at the origin. This happens if $\omega^2 < 2J$, when the Wigner semicircle, with a center shifted by J, overlaps with the negative real axis.

The opposite limit, where quantum fluctuations dominate the behavior of the system, (4.15) can be approximately solved as follows: as $\gamma \equiv \frac{\hbar^2}{m(2\pi T)^2} \to \infty$, the sum in (4.15) can be approximated by an integral. Using $\omega_k^2 = k^2/\gamma$ we find

$$\begin{aligned} f(z_c) &\approx \frac{T}{2\gamma J^2} \int_0^\infty dk \left[(k^2 + 2\gamma J - k\sqrt{k^2 + 4\gamma J} \right] \\ &= \frac{4T}{3}\sqrt{\frac{\gamma}{J}} = \frac{2\hbar}{3\pi\sqrt{mJ}} = \frac{2}{3\pi}\frac{\sqrt{\Gamma}}{J} \end{aligned} \tag{4.20}$$

with the quantum energy scale $\sqrt{\Gamma} = \hbar\sqrt{\frac{J}{m}}$ defined in section (3.2). This expression must be equal to z_c at the phase transition and hence, the $T = 0$ phase - diagram is determined by

$$\omega_c^2 = 2J - \frac{g\hbar\sqrt{\Gamma}}{3\pi J} \ . \tag{4.21}$$

The second term on the rhs. can be interpreted as an additional stabilization of the symmetric equilibrium position due to quantum fluctuations probing the quartic contribution to the potential.

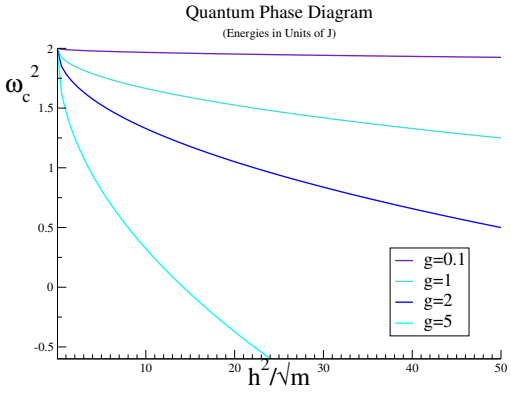


Figure 4.1: *$T = 0$ - phase diagram of the model in the variational approximation. For ω^2 smaller than ω_c^2 we have a RS ground state, else a paramagnetic one.*

4.3 Replica Symmetric (RS) Spin Glass Solution

In the case $\omega^2 < 2J$, the paramagnetic solution ceases to exist below a certain critical Temperature. At this point we have to be very careful when taking the $n \to 0$ - limit of the equations 4.7. Using a replica symmetric (RS) ansatz $Q_{ab}(\omega_0) = q + (q_d - q)\delta_{ab}$ and $Q_{ab}(\omega_k) = q_d(\omega_k)\delta_{ab}$ for $k \neq 0$, we find for the zero - mode

$$\begin{aligned} \frac{1}{q_d - q} - \frac{q}{(q_d - q)^2} &= \omega^2 + \frac{gz}{2} - J^2 q_d \\ \frac{q}{(q_d - q)^2} &= J^2 q \ . \end{aligned} \tag{4.22}$$

The second equation allows for the solution $q = 0$ discussed above. For $q \neq 0$ we may divide by q and find an additional solution $q_d = \frac{1}{J} + q$. Eliminating q in the equation for q_d gives

$$J = \omega^2 + \frac{gz}{2} \ . \tag{4.23}$$

This means that in this phase, z becomes independent of temperature and takes the constant value $z = z_c$ throughout the whole low-temperature phase.

The equations for the higher modes $k \neq 0$ remain unchanged due to the constancy of z and we find the solution (4.18) for all $T < T_c$.

It is interesting to note that this function depends only on T/T_0 where $T_0^2 = \frac{J\hbar^2}{m(\pi k_B)^2} = JT\lambda_{dB}^2$ where λ_{dB} is the thermal de-Broglie - wavelength.

Furthermore, all of the explicit dependence on ω and g has vanished. These parameters merely determine the energy scale via the transition temperature (4.19) and the length scale by defining the value of z at its freezing point. This could be taken as an argument in favor of the insensitivity of the low - temperature phase to the parameters of the microscopic on-site potential.

4.4 Thermodynamic Quantities

In order to calculate entropy and specific heat in the quantum regime, we need to express the free energy (4.12) in terms of the solutions we found. Using the expressions from appendix C for the term $\mathrm{Tr}\ln(Q^{-1})$ we end up with

$$\begin{aligned}\beta f \equiv \frac{\beta F}{N} &= -\frac{1}{2}\frac{q}{q_d - q} - \frac{1}{2}\ln(q_d - q) - \frac{1}{2}\sum_{k\neq 0}\ln(Q(\omega_k)) \\ &+ \frac{1}{2}\sum_k \Big[(\Omega^2 + \omega_k^2)Q(\omega_k) - 1\Big] - \beta\frac{gz^2}{8} \\ &+ \frac{J^2}{4}\left(q_d^2 - q^2 + \sum_{k\neq 0} Q^2(\omega_k)\right). \end{aligned} \tag{4.24}$$

The most dangerous term is of course the sum over the logarithms because it diverges. However, the divergence is the same as for a usual harmonic oscillator because $Q(\omega_k)$ is proportional to $1/\omega_k^2$ asymptotically. In order to control the divergences we add and subtract the free energy of an harmonic oscillator with frequency $\omega = \sqrt{2J}$ and inverse propagator $Q_0^{-1} = \omega_k^2 + 2J$. The free energy of the latter is given by

$$\beta f_0 \equiv \frac{1}{2}\sum_k \ln(Q_0^{-1}(\omega_k)) = \ln\sinh(2\frac{\beta\sqrt{2\Gamma J}}{2}) \tag{4.25}$$

up to a divergent but temperature independent constant which results from an discretization error in the formulation of the path integral. This error can be cured by taking the Trotter-limit more carefully [28].

We switch to the dimensionless quantities introduced in section 3.2 where $\omega_k^2 = \tilde{\omega}_k^2/\Gamma$, $\Gamma = \hbar^2\frac{J}{m}$ and $\tilde{\omega}_k = 2\pi k/\beta$. Furthermore, we are mainly interested in the spin-glass phase where $\Omega^2 = 2J$. We introduce the variables

$$\tilde{q}_d(\omega_k) = \begin{cases} q_d - q & \text{for} \quad k = 0 \\ q_d(\omega_k) & \text{else} \end{cases}$$

Using $J^2\tilde{q}_d^2(\omega_k) = Q_0^{-1}(\omega_k)\tilde{q}_d(\omega_k) - 1$ and $\tilde{q}_d(\omega_0) = 1/J$, the free energy in the spin-glass phase can now be written after some algebra as

$$\begin{aligned}\beta f &= -\frac{1}{2}\sum_k \left[\ln(\tilde{q}_d(\omega_k)Q_0^{-1}(\omega_k)) - \frac{3}{2}(Q_0^{-1}(\omega_k)\tilde{q}_d(\omega_k) - 1)\right] \\ &- \frac{\beta g z^2}{8} + Jq + \ln(2\sinh(\frac{\beta\sqrt{2\Gamma J}}{2}))\,. \end{aligned} \tag{4.26}$$

For the first term we may write

$$I_1 = \frac{1}{2}\sum_k \ln(\tilde{q}_d(\omega_k)Q_0^{-1}(\omega_k)) = \frac{1}{2}\sum_k \ln\left(2((x_k^2+1)^2-(x_k^2+1)\sqrt{(x_k^2+1)^2-1}\right) \quad (4.27)$$

where $x_k^2 = \omega_k^2/(2\Gamma J) \equiv \alpha^2 k^2$ and $\alpha^2 \equiv \frac{(2\pi)^2}{\beta^2 \Gamma J}$. This is a perfectly convergent series.

The second term can be expressed by the function

$$I_2 = \frac{1}{4}\sum_k (\tilde{q}_d(\omega_k)Q_0^{-1}(\omega_k)-1) = \frac{1}{2}\sum_k ((x_k^2+1)^2-(x_k^2+1)\sqrt{(x_k^2+1)^2-1}-\frac{1}{2}) \, . \quad (4.28)$$

The third relevant parameter determines q and reads

$$z' \equiv T\sum_k \tilde{q}_d(\omega_k) = \frac{T}{J}\sum_k (x_k^2+1-\sqrt{(x_k^2+1)^2-1}) \, . \quad (4.29)$$

In the paramagnetic phase we have $z' = z$, whereas in the spin-glass regime q is determined by

$$Jq = \beta J z - I_3 \quad (4.30)$$

$$I_3 = \sum_k (x_k^2+1-\sqrt{(x_k^2+1)^2-1}) = \frac{Jz'}{T} \quad (4.31)$$

and z is frozen at its critical value $z_c = \frac{2}{g}(2J-\omega^2)$.

Finally we find

$$\beta f = -I_1 + 3I_2 - I_3 + \beta J z - \frac{\beta g z^2}{8} + \ln(2\sinh(\beta\sqrt{\Gamma J}/2)) \, . \quad (4.32)$$

Obviously, the behavior of the system in the spin glass phase depends only on the value of the parameter α. Large α corresponds to $\beta\hbar \to 0$ and we recover the quasi-classical limit. Small values of α correspond to strong quantum fluctuations. We will discuss the two regimes separately.

4.4.1 Quasi-Classical Regime

If $\alpha \gg 1$ we have $x_k \gg 1$ for all $k > 0$ and we find

$$I_1 \approx \frac{1}{2}\ln 2 + \frac{1}{8\alpha^2}\sum_{k>0}\frac{1}{(k^2+1/\alpha^2)^2} = \frac{\ln 2}{2} + \frac{1}{8}f(\alpha) \quad (4.33)$$

$$I_2 \approx \frac{1}{16\alpha^2}\sum_{k>0}\frac{1}{(k^2+1/\alpha^2)^2} = \frac{1}{16}f(\alpha) \quad (4.34)$$

where

$$f(\alpha) = -\frac{\alpha^2}{2} + \frac{\alpha\pi}{4}\mathrm{cotanh}(\pi/\alpha) + \frac{\pi^2}{4}\mathrm{csch}^2(\pi/\alpha) \ . \tag{4.35}$$

As $\alpha \gg 1$ in the quasi-classical regime we may use a Laurent series expansion for the hyperbolic functions and find

$$f(\alpha) \approx \frac{\pi^2}{90\alpha^2} + \mathcal{O}(1/\alpha^4) \ . \tag{4.36}$$

For the parameter z' we find in the same approximation

$$z' = \frac{T}{2J} + \frac{T\pi}{2J\alpha}\mathrm{cotanh}(\frac{\pi}{\alpha}) \approx \frac{T}{J}(1 + \frac{\pi}{6\alpha}) - \mathcal{O}(1/\alpha^4) \ . \tag{4.37}$$

Because $q = \beta(z - z')$ we have

$$q = \beta z_{\mathrm{c}} - \frac{1}{J} - \frac{\pi}{6J\alpha} + \cdots \ . \tag{4.38}$$

As a byproduct, we can determine the first quantum correction to the transition temperature by requiring $q = 0$. The result is

$$T_c = T_c^0 - \frac{\hbar\sqrt{J}}{8\sqrt{m}} \ . \tag{4.39}$$

The free energy reads in the approximations done above

$$\begin{aligned} \beta f &= -I_1 + 3I_2 - \beta\frac{gz^2}{8} + Jq + \ln(2\sinh(\frac{\pi}{\alpha})) \qquad (4.40) \\ &= -\frac{\ln 2}{2} - 1 + \frac{2\beta}{g}(J^2 - \frac{\omega^4}{4}) - \frac{\pi}{6\alpha} + \frac{\pi^2}{16\cdot 90\alpha^2} + \ln(2\sinh(\frac{\pi}{\alpha})) \ . \end{aligned}$$

In the end,we find that for $\alpha \gg 1$ the system behaves just as an harmonic oscillator of frequency $2J$ because the free energy is dominated by the last term in (4.40) in this limit. The reasons for this behavior will be discussed in the next section.

4.4.2 Quantum Regime

At very low temperatures we find $\alpha \ll 1$ and the frequency sums may be approximated by an integral. However, we have to take care of the corrections of order α and α^2 because they will eventually give rise to a linear contribution to the specific heat.

To this end, we reverse the extended Simpson's rule [29]:

$$\begin{aligned}\int_{x_0}^{x_N} f(x) &= \alpha[\frac{5}{12}f(x_0)+\frac{13}{12}f(x_1)+f(x_3)+\cdots \\ &+ f(x_{N-2})+\frac{13}{12}f(x_{N-1})+\frac{5}{12}f(x_N)]+\mathcal{O}(\alpha^3) \quad (4.41)\end{aligned}$$

where $x_i = x_0 + \alpha i$. Inverting this formula gives

$$\sum_{i=1}^{N} f(x_i) = \frac{1}{\alpha}\int_{x_0}^{x_N} f(x)dx+\frac{7}{12}(f(x_0)+f(x_N))-\frac{1}{12}(f(x_1)+f(x_{N-1}))+\mathcal{O}(\alpha^3)\,. \quad (4.42)$$

As we are interested in improper integrals over functions vanishing faster than $1/x^2$, we can neglect the corrections at the endpoints. Furthermore, we write

$$f(x_1) = f(x_0)+\alpha f'(x_0)+\frac{\alpha^2}{2}f''(x_0)+\cdots \quad (4.43)$$

and end up with

$$\sum_{i=1}^{N} f(x_i) = \frac{1}{\alpha}\int_{x_0}^{x_N} f(x)dx+\frac{1}{2}f(x_0)-\frac{\alpha}{12}f'(x_0)-\frac{\alpha^2}{24}f''(x_0)+\mathcal{O}(\alpha^3)\,. \quad (4.44)$$

Using this expression for the functions I_1, I_2 and I_3 we find

$$\begin{aligned}I_1 &= \frac{1}{2\alpha}\int_0^\infty dx \ln\left[2(1+x^2)(1+x^2-\sqrt{(1+x^2)^2-1})\right] \\ &+ \frac{ln2}{4}+\frac{\sqrt{2}\alpha}{24}-\frac{\alpha^2}{24} \\ &= \frac{1}{2\alpha}\left[\pi-2^{3/2}\right]+\frac{ln2}{4}+\frac{\sqrt{2}\alpha}{24}-\frac{\alpha^2}{24} \quad (4.45)\end{aligned}$$

and with the same approximation

$$\begin{aligned}I_2 &= \frac{1}{2\alpha}\int_0^\infty dx\left[(1+x^2)(1+x^2-\sqrt{(1+x^2)^2-1})-1/2\right] \\ &+ \frac{1}{8}+\frac{\alpha}{12\sqrt{2}}-\frac{\alpha^2}{12} \\ &= \frac{1}{2\alpha}\frac{2^{3/2}}{15}+\frac{1}{8}+\frac{\alpha}{12\sqrt{2}}-\frac{\alpha^2}{12}\,. \quad (4.46)\end{aligned}$$

The last function can finally be approximated by

$$I_3 = \frac{2^{3/2}}{3\alpha}+\frac{1}{2}+\frac{\sqrt{2}\alpha}{12}-\frac{\alpha^2}{12}\,. \quad (4.47)$$

Collecting all terms, we find

$$\beta f = -\frac{1}{\alpha}(\frac{\pi}{2} - \frac{16\sqrt{2}}{15}) - \frac{2\ln 2 + 1}{8} - \frac{5}{24}\alpha^2 + \ln(2\sinh(\frac{\pi}{\alpha}) \ . \tag{4.48}$$

For small α, the last term cancels the first one. Note that the terms linear in α cancel. Writing $\alpha = \alpha_0 T$, where $\alpha_0 = \frac{\pi\sqrt{2}}{\sqrt{\Gamma}J}$, we find for the entropy

$$S = \frac{1 + \ln(2)}{4} + \frac{5}{8}\alpha_0^2 T^2 \tag{4.49}$$

and for the specific heat

$$C = T\frac{\partial S}{\partial T} = \frac{5}{4}T^2 \ . \tag{4.50}$$

This is not the result one would have *wished* to find, because *linear* specific heat is one of the hallmark features of structural glasses. However, the absence of linear specific heat is due to the cancellation of the terms linear in α contributing to (4.48). For the comparison with experiments however, one may doubt in the validity of the assumption of thermal equilibrium implicit in the above calculations. In the next section we will show that a non vanishing value of q is related to frozen strain fields in the sample. These will probably not equilibrate on experimental time scales. Therefore one could identify the experimentally observed specific heat with the specific heat being derived from (4.32) for *given* q. If we do so we have to neglect the corresponding term in the free energy we would end up with a linear contribution to the 'experimental' specific heat

$$C_{\rm exp} = \frac{\sqrt{2}\alpha_0}{6} = \frac{2\pi}{6J\sqrt{\Gamma}}T \ . \tag{4.51}$$

This is of course a result derived using hand-waving arguments and has to be confirmed by dynamics calculations for the same model.

Even if one may doubt in the validity of the variational approximation at very low temperatures, we think that it is interesting by itself. The constant contribution to the entropy indicates a degenerate ground state as one might have expected for a glassy system, whereas the linear specific heat is one of the most distinguished features of the low-temperature anomalies in glasses. Furthermore, the variable α depends only very weakly on the parameters J and m and not at all on the parameters g and ω^2 describing the bare potentials. This leads to a qualitative and *almost quantitative* universality of the low-temperature properties of our model.

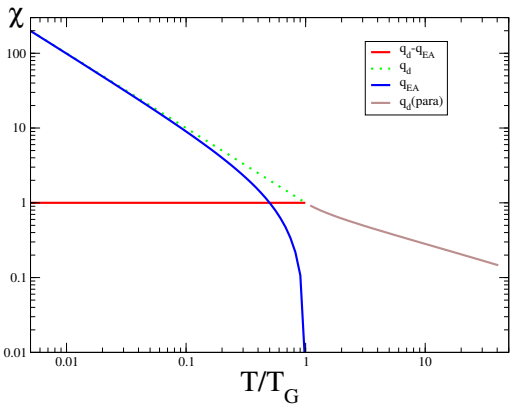


Figure 4.2: *Susceptibility as a function of T/T_g, where T_g is the classical transition temperature. The parameters are $J = 1$, $\omega^2 = J$, $g = 0.01$ and $\Gamma = 0.110$.*

Formally, the 'experimental' linear specific heat has its origin in the terms $\mathcal{O}(\alpha^2)$ we have derived above as 'discretization corrections' in the low-temperature regime. Consequently, it has nothing to do with quantum tunneling because there are no double-well terms in our entirely harmonic variational test action. This has to be confronted with the fact that is well known from the quasi-classical treatment of the model [9], that the linear specific heat has its origin in tunneling excitations. The variational approximation *mimics* the quantum tunneling contribution to the free energy by another process that will be discussed in 4.5.2.

4.5 Interpretation of the Results

4.5.1 Analytic Continuation

In order to calculate the linear response quantities of the system, we have to do the analytical continuation [30, 20] of (4.18) to imaginary frequencies. As we are mainly interested in the thermodynamics of this model we will only briefly outline this continuation because it will help us in the interpretation of the physics contained in the variational approximation. Let

$$q_d(\omega_k) \equiv \Delta(i\omega_k) = \frac{1}{2\Gamma J^2}\left[2\Gamma J - (i\omega_k)^2 \pm \sqrt{(i\omega_k)^2}\sqrt{4\Gamma J - (i\omega_k)^2}\right] . \tag{4.52}$$

$$\Delta(z) = \frac{1}{2\Gamma J^2}\left[2\Gamma J - z^2 \pm \sqrt{z^2}\sqrt{4\Gamma J - z^2}\right] . \tag{4.53}$$

There are several possibilities for analytical continuations differing in the choices of the $\sqrt{\ }$-function. However, the continuation is unique [31] if one requires that

- $\Delta(z)$ is analytic off the real axis
- $\Delta(z)$ goes to zero as z approaches infinity along any straight line in the upper or lower half -plane.

We will choose the $\sqrt{\ }$-function with $\sqrt{z^2} = z$ in the upper half plane. This function has a cut along the *positive real axis*. Whenever we write a $\sqrt{\ }^+$ in this section, we refer to this definition. Close to the real axis we have

$$\begin{aligned} \sqrt{x \pm i\epsilon}^+ &= \pm\sqrt{|x|} \quad \text{for} \quad x > 0 \\ \sqrt{x \pm i\epsilon}^+ &= i\sqrt{|x|} \quad \text{for} \quad x < 0 \ . \end{aligned}$$

In order to get the right values at the points $z = i\omega_k$, we have to define

$$\Delta(z) = \frac{1}{2\Gamma J^2}\left[2\Gamma J - z^2 + i\sqrt{z^2}^+\sqrt{4\Gamma J - z^2}^+\right] \quad \text{for} \quad \mathrm{Im}(z) > 0 \ .$$

The Fourier modes of the retarded and advanced Green's functions are given by

$$D_R(\omega) = -i\Delta(\omega + i\eta) \qquad D_A(\omega) = i\Delta(\omega - i\eta) \tag{4.54}$$

$$D_R(\omega) = \frac{1}{2\Gamma J^2}\left[|\omega|\sqrt{2 - \frac{\omega^2}{4J}} - i(\omega^2 - 1)\right] \tag{4.55}$$

$$D_A(\omega) = D_R(\omega)^* \ . \tag{4.56}$$

The spectral function $\rho(\omega)$ is given by

$$\rho(\omega) = -i(D_R(\omega) - D_A(\omega)) = \frac{1}{2\Gamma J^2}\theta(4\Gamma J - \omega^2)|\omega|\sqrt{4\Gamma J - \omega^2} \ . \tag{4.57}$$

We recognize a 'deformed' Wigner semi-circle law.

From the spectral function, we immediately get the Fourier transform of the retarded correlator at finite temperature

$$G_<(\omega) = i\frac{\rho(\omega)}{1 - e^{\beta\omega}} \ . \tag{4.58}$$

From this, the time-dependent correlation function at finite temperature follows as

$$G_<(t) = i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \frac{\rho(\omega)}{1 - e^{\beta\omega}} \ . \tag{4.59}$$

Due to the branch cut in the correlation function we obtain an algebraic long-time decay. Indeed, for $t \gg 1/\omega$ only the lowest modes contribute to the integral and we can approximate $\rho(\omega) \sim |\omega|$ and extend the integration to infinity.

For $T = 0$, the real-time correlation function (4.59) can be expressed in a closed form and one finds in a combination of Bessel- and Digamma-functions. As we are mainly concerned with thermodynamics we refer to [33, 34] for details.

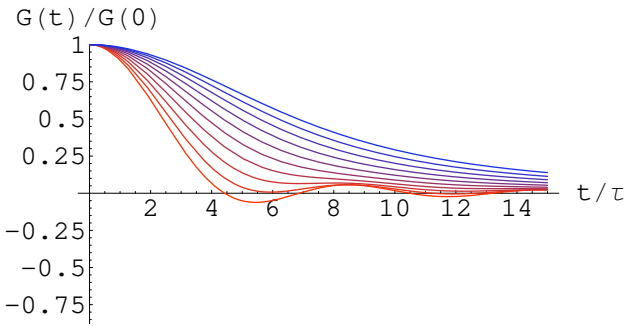


Figure 4.3: *Correlation in time as a function to t/τ where $\tau = \frac{\hbar}{2J}$ for different temperatures. At high temperatures (red curves) the correlation shows damped oscillations. for lower temperatures (bluer curves) we find an algebraic long-time behavior.*

4.5.2 Physical Content of the Variational Solution

In this section we will show that the variational effective action we found is equivalent to an ensemble of harmonic oscillators, each coupled to a super-ohmic heat bath. The variational effective action in its minimized form reads

$$\begin{aligned} S_{\rm var} &= \frac{1}{2} \sum_k \sum_a \left[\omega_k^2/\Gamma + \omega^2 + \frac{gz}{2} - J^2(q_d(\omega_k) - q\delta(\omega_k) \right] |x_a(\omega_k)|^2 \\ &- \frac{1}{2} q J^2 (\sum_a x_a(0))^2 \ . \end{aligned} \tag{4.60}$$

We insert the solutions for z and $q_d(\omega_k)$ the spin-glass phase and find

$$\begin{aligned} S_{\rm var,SG} &= \frac{1}{2}\sum_k\sum_a\left[\omega_k^2/\Gamma+2J\right] \\ &- \frac{1}{4}\sum_k\sum_a\left[\omega_k^2/\Gamma+2J-\sqrt{(\omega_k^2/\Gamma+2J)^2-4J^2}\right)\right]x_a(\omega_k)^2 \\ &- \frac{1}{2}qJ^2(\sum_a x_a(\omega_0))^2\ . \end{aligned} \tag{4.61}$$

The first part of the effective action is just the one of an harmonic oscillator with frequency $\sqrt{2J}$. For the second term we write

$$\frac{1}{2}\left[\omega_k^2/\Gamma+2J-\sqrt{(\omega_k^2/\Gamma+2J)^2-4J^2}\right]=\frac{1}{\pi}\int_0^{2\sqrt{J}}\frac{\omega^2\sqrt{4J-\omega^2}}{\omega^2+\omega_k^2/\Gamma}\ . \tag{4.62}$$

However, this is just the the form self energy contribution we would have if the oscillator was coupled to a bath of harmonic oscillators with spectral function

$$J(\omega)=\frac{\omega^3\sqrt{4J-\omega^2}}{\pi}\ . \tag{4.63}$$

This is a super-ohmic bath [32]. For an exact solution of this model see [33].

The last term in (4.61) can be decoupled with a Gauss-Hubbard transformation using

$$e^{\frac{1}{2}qJ^2(\sum_a x_a(0))^2}=\int\frac{d\xi}{\sqrt{2\pi}}\exp{}^{-\xi^2/2+\xi J\sqrt{q}\sum_a\int d\tau x_a(\tau)}\ . \tag{4.64}$$

The integration over the ξ can be taken out of the replica limit such that we finally end up with the ensemble free energy

$$\beta F=\int\frac{d\xi}{\sqrt{2\pi}}e^{-\xi^2/2}\ln\left[\int\mathcal{D}x\mathcal{D}\{y_i\}\exp\left(-S(x,\{y_i\};\xi)\right)\right]\ . \tag{4.65}$$

The integration over ξ can be interpreted as an average over non interacting degrees of freedom with an action

$$\begin{aligned} S(x,\{y_i\};\xi) &= S_{\rm System}+S_{\rm Interaction}+S_{\rm Bath} \\ &= \frac{1}{2}\int d\tau\left[\frac{1}{2}\dot{x}^2(\tau)+Jx^2(\tau)+J\sqrt{q}\xi x(\tau)\right] \\ &+ \frac{1}{2}\sum_i\int d\tau x(\tau)y_i(\tau) \\ &+ \frac{1}{2}\sum_i\int d\tau\left[\dot{y}_i(\tau)+\omega_i y_i^2(\tau)\right]\ . \end{aligned} \tag{4.66}$$

The y_i are the bath oscillators and assumed to be distributed such that the spectral function is given by (4.63). We find that the action (4.66) is just the action of an harmonic oscillator in a field $\xi J\sqrt{q}$ coupled to a bath of harmonic oscillators. The Gaussian distributed external fields can be interpreted as frozen strain fields and because q and thereby their strength depends on temperature. As we have shown above, assuming them not to take part in the dynamics on experimental time scales immediately leads to a linear specific heat.

4.5.3 Zero Temperature Limit

Because we started with an harmonic test action, we will never be able to encounter double well potential types of configurations within the variational approach. Nevertheless, there is another way to obtain a physical interpretation of the results of this chapter. One may simply use the solution found here to approximate the nonlocal term in (3.10). We note that the solution for the modes $q_d(\omega_k)$ is such that $q_d(\omega_k) \approx \frac{1}{J}$ for $\omega_k^2 \ll J$ and $q_d(\omega_k) \sim \frac{1}{\omega_k^2+2J}$ for $\omega_k^2 \gg J$. As $\omega_k^2 \sim T^2$ we conclude that $\lim_{T\to 0} q_d(\omega_k) = 1/J$ and therefore $Q_{ab}(\tau) \to \frac{1}{J}\delta(\tau)\delta_{ab} + q$. Inserting this into the time dependent version of (3.10) we find

$$S_{\text{eff}}(T \to 0) = \frac{1}{2}\sum_a \int \tau \left[m(\dot{x}_a(\tau))^2 + (m\omega^2 - J)x_a^2(\tau)\right] - \frac{qJ^2}{2}(\sum_a \int d\tau x_a(\tau))^2 \ . \tag{4.67}$$

The last term can be decoupled using a Gauss transformation just as in the previous section. We will end up with an ensemble average over particles with a completely *local* action corresponding to particles moving in potentials

$$V(x;\xi) = J\xi\sqrt{q}x + \frac{1}{2}(m\omega^2 - J)x^2 + \frac{g}{4!}x^4 \tag{4.68}$$

where again ξ is a Gaussian random variable with unit variance and zero mean. Note that this is formally the ensemble of potentials found by Kühn and Horstmann [9] in the quasi-classical approach. However, the quantity q does *not* coincide with the quasi-classical approach as it is renormalized due to quantum fluctuations. The interpretation in the light of the results of the previous subsection would be that at low temperatures all the 'bath' harmonic oscillators are in the ground state and cannot give rise to memory terms anymore. Therefore the effective single-site action must become local.

The parameter J^2q describes the variance of the random field and therefore of the asymmetry distribution. The 'experimental' specific heat would

therefore be the specific heat measured for a fixed distribution of the microscopic soft potentials.

4.6 Stability of The RS Solution

In this section we will study the stability of the solution presented above with respect to breaking of the replica symmetry and with respect to *replica synchronization*, i.e. an imaginary time dependence of the Edwards -Anderson order parameter q. In order to do so, we will solve the equations with a 1-step replica symmetry breaking (1-RSB) ansatz and with an ansatz allowing for an RS structure in the matrix $Q_{ab}(\omega_k)$ for $k \neq 0$.

4.6.1 1-RSB solution

The 1RSB *ansatz* consists in assuming

$$Q_{ab}(\omega_0) = (q_d - q)\delta_{ab} + q\epsilon^m_{ab} \tag{4.69}$$

where

$$\epsilon^m_{ab} = \begin{cases} 1 & \text{when} \quad \lfloor \frac{a}{m} \rfloor = \lfloor \frac{b}{m} \rfloor \\ 0 & \text{else} \end{cases} . \tag{4.70}$$

The Gauss brackets $\lfloor \cdot \rfloor$ denote the largest integer smaller than the argument in the brackets. The correlators $Q_{ab}(\omega_k)$ for $k \neq 0$ are assumed to be diagonal in the replica indices.

The algebra of matrices of this type is well known in the field of spin-glass physics [27, 17] and the derivations are relegated to appendix C.

The resulting saddle-point equations for the variational approximation come from requiring the variational free energy to be stationary with respect to the parameters q_d, q and m and read

$$\frac{1}{q_d - q} - \frac{q}{(q_d - q)(q_d + (m-1)q)} = \omega^2 \quad + \quad \frac{gz}{2} - J^2 q_d \tag{4.71}$$

$$\frac{q}{(q_d - q)(q_d + (m-1)q)} \quad = \quad J^2 q \tag{4.72}$$

$$\frac{q}{m(q_d + (m-1)q)} + \frac{1}{m^2} \ln\left(\frac{q_d - q}{q_d + (m-1)q}\right) \quad = \quad -\frac{J^2}{2} q^2 . \tag{4.73}$$

Equation (4.72) has the solution $q = 0$ corresponding to the paramagnetic phase. We add twice (4.73) to q times (4.72) in order to eliminate the

J-dependence and introduce $y = \frac{q}{q_d}$ and $x = \frac{my}{1-y}$ and find an equation depending on x alone:

$$\frac{x^2}{1+x} + \frac{2x}{(1+x)} - 2\ln(1+x) = 0 \; . \tag{4.74}$$

This equation has the unique solution $x = 0$. In the SG phase, where q is different from zero, this necessitates $m = 0$ and we are back at the RS solution.

However, the situation is not as clear as one might think from the above statement. This is because the system is *marginally stable* with respect to higher order breaking of the replica symmetry. As we will derive in chapter 5, the stability of the 1RSB solution with respect to higher order breaking is determined by the sign of the so-called *replicon eigenvalue* $\Lambda = \frac{1}{(q_d-q)^2} - J^2$ [35] which is identically zero within the variational solution as stated by (4.72) together with $m = 0$. This means that the structure of the off-diagonal part of the matrix Q_{ab} is in reality *undetermined* within the above solution and that we have to go beyond the variational ansatz in order find the manifestations of real glassiness in the RSB structure of the correlator.

4.6.2 Replica Synchronization

As we have already discussed in the first section of this chapter, there is a very fundamental symmetry of the quantum-statistical description of the model, the time-translational invariance of the partition function. Especially, the effective action is invariant under *independent* time translations of the replicated times τ_a. However, we have seen that averaging out the disorder generates interactions not only between different replications of the system but also between different *times*. In this section we will allow for a spontaneous breaking of this symmetry, just as we have done for a breaking of the permutational symmetry between replicas in the previous section. Nevertheless we will keep the *global* time translational invariance $\tau_a \to \tau_a + h$ simultaneously for all $a \in \{1 \cdots n\}$.

This translates into $Q_{ab}(\tau, \tau') = [q_d(\tau - \tau') - q(\tau - \tau')]\,\delta_{ab} + q(\tau - \tau')$. The saddle-point equations can be translated into Fourier space and we find

$$\begin{aligned} \frac{1}{(q_d(\omega_k) - q(\omega_k))} - \frac{q(\omega_k)}{(q_d(\omega_k) - q(\omega_k)^2} &= \omega^2 + \omega_k^2 + \frac{gz}{2} - J^2 q_d(\omega_k) \\ \frac{q(\omega_k)}{(q_d(\omega_k) - q(\omega_k))^2} &= J^2 q(\omega_k) \end{aligned} \tag{4.75}$$

where z is still given by $z = T\sum_k q_d(\omega_k)$. For every mode k, equation 4.75 has the solutions $q(\omega_k) = 0$ and $q(\omega_k) = q_d(\omega_k) - \frac{1}{J}$. If we choose the second solution for some k, we can put it into the first of the above equations and find

$$\frac{gz}{2} = 2J - \omega^2 - \omega_k^2. \tag{4.76}$$

This equation can obviously hold for one value of k at most. Assume 4.76 to hold for some $k_0 \neq 0$. Then the equation for the zero mode would read

$$\frac{1}{q_d(\omega_0)} = 2J - \omega_{k_0}^2 - J^2 q_d(\omega_0)\ . \tag{4.77}$$

This equation has real and negative solutions only if $\omega_\omega^2 > 4J$ and no positive solution at all! This is a contradiction because $q_d(\omega_0) =< \int d\tau x^2(\tau) >$ must be positive by virtue of the self-consistency condition.

We conclude that within the variational approximation, neither the permutational symmetry nor the invariance under independent translations of the time-arguments is broken.

Chapter 5

The Model at its 3-Loop Approximation

In this chapter we want to go one step further in the loop expansion of the generating functional $S_3[\lambda]$ (3.15). However, the simplest way of doing this is not obvious. A standard loop expansion would be in terms of vacuum diagrams with lines corresponding to the quadratic part of (3.8) with $\lambda_{ab}(\tau, \tau')$ set to its self-consistent value (3.9). This quadratic part would correspond to the 'bare' inverse propagator $Q_0(\omega_k) = (\omega^2 + \omega_k^2 - J^2 Q(\omega_k))^{-1}$, sometimes called the 'Weiss field' in the framework of the dynamical mean-field theory [40, 41]. Because this propagator *depends* already on the fully renormalized propagator $Q_{ab}(\tau, \tau')$ in a non trivial way, the resulting equations e.g. for the self-energy would become functional self-consistency equations of a rather involved structure. Therefore we face a problem where the loop expansion in terms of the bare propagator is very complicated and a considerable simplification arises when we formulate the self-energy in terms of the *full* propagator immediately. Such expansion schemes are well known as expansions of the self-energy in terms of *skeleton graphs* [43, 44] or on the level of the generating functional as the expansion in terms of two-particle irreducible (2PI) vacuum graphs [45].

For the sake of compactness, we have relegated the derivation of the formalism to appendix B. As we will see, the replica symmetric ansatz is no longer stable at this level of approximation and we will encounter a close relationship of our model to a spherical spin glass with 2-spin and 4-spin interaction. Just as the latter, our model undergoes a phase transition from 1-RSB to an C-RSB solution at very low temperatures. We will argue that this phase transition could eventually be what has been found in the

experiments on the low-temperature dielectric constant in structural glasses by Strehlow, Hunklinger and Enss [10]. It will turn out that the 3-loop approximation suffers from spurious instabilities. Therefore we will propose a 'toy' approximation consisting in keeping only those terms giving rise to corrections to the replicon eigenvalue. This approximation can be motivated by adding an additional stabilizing term to the full action.

5.1 The Equations of Motion

The 3-loop approximation consists in taking the first two 2PI graphs for the self energy into account. We find the 2PI effective action

$$\Gamma = \frac{1}{2}\mathrm{Tr}\ln Q^{-1} + \frac{1}{2}\mathrm{Tr}(Q_0^{-1}Q) + \frac{g}{8}\sum_a \int d\tau Q_{aa}^2(\tau,\tau) - \frac{g^2}{48}\sum_{ab}\int d\tau \int d\tau' Q_{ab}^4(\tau,\tau') \tag{5.1}$$

where

$$(Q_0^{-1}(\tau-\tau'))_{ab} = \omega^2 + \frac{\partial^2}{\partial\tau^2}\delta_{ab}\delta(\tau-\tau') - J^2 Q_{ab}(\tau-\tau') \tag{5.2}$$

is the self-consistent quadratic part of the effective potential if time-translational invariance is assumed.

When looking for the saddle points we have to assume *fixed* Q_0 and do not account for the implicit dependence of Q_0 on Q because the identification (5.2) has to be done *in the end*. The extrema of the effective action obey

$$\left[Q^{-1}(\tau-\tau')\right]_{ab} = (Q_0^{-1})_{ab}(\tau-\tau') + \frac{g}{2}Q_{aa}(0)\delta_{ab}\delta(\tau-\tau') - \frac{g^2}{6}Q_{ab}^3(\tau-\tau') \tag{5.3}$$

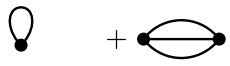
which, transformed into Fourier space, reads

$$\left[Q^{-1}(\omega_k)\right]_{ab} = \omega^2 + \omega_k^2 - J^2 Q_{ab}(-\omega_k) + \frac{gT}{2}\sum_k Q_{aa}(\omega_k)\delta_{ab} - \Sigma_{ab}^{(2)}(\omega_k)\ . \tag{5.4}$$

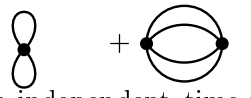
The function $\Sigma^{(2)}(\omega_k)$ is the 2-loop contribution to the self-energy. The latter is given by

$$\Sigma^{(2)}(\omega_k)_{ab} = \frac{g^2}{6}\int d\tau e^{-i\omega_k\tau} Q_{ab}^3(\tau)\ . \tag{5.5}$$

The full self energy is given by $\Sigma = \Sigma^{(1)} + \Sigma^{(2)}$ where $\Sigma^{(1)}$ sums up all tadpole contributions and $\Sigma^{(2)}$ finds its field-theoretic analog in pair production. Diagramatically we can write for the self energy

$\mathbf{\Sigma} =$  .

We remind that the full lines represent the full propagator. The two terms are derived from the two- and three-loop vacuum diagrams contributing to the 2PI part Γ_2 of the effective action. These can be written as

$\mathbf{\Gamma_2} =$  .

Due to the invariance under independent time-translations in different replicas, it is natural to assume again that the off-diagonal elements of the correlator are independent of time : $Q_{ab}(\tau) = Q_{ab}$ for $a \neq b$. This means that $Q_{ab}(\omega_k)$ is *diagonal* for $\omega_k \neq 0$ as in the variational approximation.

Furthermore, we will assume a 1-RSB structure for the ω_0-components of the correlation function, such that $Q_{ab}(\omega_k) = q_d(\omega_k)\delta_{ab}$ for $k \neq 0$ and $Q_{ab}(\omega_0) = \epsilon^m_{a,b} q_{\rm EA} + (q_d - q_{\rm EA})\delta_{ab}$ where $\epsilon^m_{ab} = 1$ when $\lfloor \frac{a}{m} \rfloor = \lfloor \frac{a}{m} \rfloor$. We note that this is not a full 1-RSB ansatz because in principle one could allow for $Q_{ab} = q_0$ for $\epsilon^m_{ab} = 0$. However, due to the strong analogies with the p-spin model investigated in the next section, we will always find $q_0 = 0$ in absence of external fields and we will suppress this additional parameter for the sake of simplicity.

With this structure, the Schwinger-Dyson equations for $a = b$ and for ω_0 read

$$\frac{1}{q_d - q_{\rm EA}} - \frac{q_{\rm EA}}{(q_d - q_{\rm EA})(q_d + (m-1)q_{\rm EA})} = \Omega^2 - J^2 q_d - \Sigma^{(2)}(\omega_0)_{aa} \quad (5.6)$$

where $\Omega^2 = \omega^2 + \frac{gT}{2}\sum_k q_d(\omega_k)$.

For a and b different but in the same block we find

$$\frac{q_{\rm EA}}{(q_d - q_{\rm EA})(q_d + (m-1)q_{\rm EA})} = J^2 q_{\rm EA} + \frac{g^2 T^2}{6} q^3_{\rm EA} \ . \quad (5.7)$$

This equation allows for the solution $q_{\rm EA} = 0$ corresponding to the paramagnetic phase and for solutions $q_{\rm EA} \neq 0$ obeying

$$\frac{1}{\tilde{J}^2(q_{\rm EA})} = (q_d - q_{\rm EA})(q_d + (m-1)q_{\rm EA}) \quad (5.8)$$

with $\tilde{J}^2(q_{\rm EA}) \equiv J^2 + \frac{g^2T^2}{6} q^2_{\rm EA}$. Using this, we can express q_d as a function of $q_{\rm EA}$:

$$q_d(q_{\rm EA}) = q_{\rm EA} - \frac{m q_{\rm EA}}{2} \pm \sqrt{\frac{1}{\tilde{J}^2(q_{\rm EA})} + \frac{m^2 q^2_{\rm EA}}{4}} \quad (5.9)$$

where we have to choose the upper sign in order to have a stable solution (non negative eigenvalues of Q) with $q_d > q_{\rm EA}$.

Inserting (5.7) and (5.9) into (5.6) gives

$$\frac{1}{q_d - q_{\mathrm{EA}}} = \Omega^2 - J^2(q_d - q_{\mathrm{EA}}) - (\Sigma(0)_{aa} - \frac{g^2T^2}{6}q_{\mathrm{EA}}^3) \ . \tag{5.10}$$

Unfortunately, it turns out that (5.10) has no paramagnetic solution with $q_{\mathrm{EA}} = 0$ in a large and interesting region of the parameter space. The reason is that the effective action has a contribution scaling as $-q_d^4$, coming from the 3-loop term. Therefore, the minimum we find is at most metastable and it turns out that there is no minimum at all in a large region of the parameter space. This is clearly unphysical: the quartic term in the bare single-site potentials of our model should always confine the degrees of freedom x_i and therefore q_d should remain finite. The problem could be cured by going to 4-loop in the effective action or by adding a term proportional to $g^3q_d^6$ to it. This would formally not make any difference because we would still be exact to order g^2.

Concerning the break point m, there are two different approaches. First one could try minimizing the effective action with respect to m. This leads to the so-called equilibrium solution. Second, one could require the replicon eigenvalue to vanish. This is called the *marginally stable* solution[35, 36, 23]. It is well known in the field that the phase diagram of the marginally stable solution reproduces the dynamical phase diagram and the breakpoint m then corresponds to the factor X describing the violation of the fluctuation dissipation theorem (FDT).

But let us state state the equations for the non-zero modes $q_d(\omega_k)$:

$$\frac{1}{q_d(\omega_k)} = \Omega^2 - J^2 q_d(-\omega_k) + \Sigma^2(\omega_k) \tag{5.11}$$

where we have assumed $q_d(-\omega_k) = q_d(\omega_k)$ because of time inversion invariance. It turns out that these equations depend on q_d alone and do *not* explicitly depend on the parameters q and m describing the off- diagonal structure of the correlation matrix. In the same vein, the equations for the off-diagonal elements do not depend on $q_d(\omega_k)$ for $k \neq 0$ explicitly. *Given* $q_d(\omega_0)$, all other parameters could be found.

In order to elucidate the relations between our model in a 3-loop approximation and an equivalent quantum spherical p-spin model, we will undertake a short excursion in the next section. We will newly meet (5.11) and (5.7) together with one of the two possible conditions for the breakpoint parameter m. These equations have to be solved *given* q_d in the context of a spherical model.

5.2 Excursion: The Equivalent P-Spin Model

In this section we want to undertake a brief excursion to the field of spherical p-spin models and emphasize the striking similarity between our model in its 3-loop approximation and an equivalent p-spin model. We will find indeed that the equations for the correlation matrix are exactly identical to ours, except that the equation obtained from deriving the free energy with respect to q_d has to be interpreted as an equation that determines z for p-spin models whereas it determines q_d for our model.

Consider an spin-glass Hamiltonian with 2-spin and 4-spin interaction as follows:

$$H = \sum_i \frac{p_i^2}{2} + \sum_{i<j} J_{ij} x_i x_j + \sum_{i<j<k<l} J^4_{ijkl} x_i x_j x_k x_l \ . \tag{5.12}$$

The variables x_i are assumed to be continuous and subject to the spherical constraint $\sum_i x_i^2 = l_0^2 N$, where l_0 is the length of the spin. The couplings are Gaussian distributed random variables with zero mean and variance

$$\overline{J_{ij}^2} = \frac{J^2}{N} \tag{5.13}$$

and

$$\overline{(J^4_{ijkl})^2} = \frac{6 J_4^2}{N^3} \tag{5.14}$$

where $J_{ij} = J_{ji}$ and J^4_{ijkl} is symmetric under permutations of the indices. The variance of general p-spin interaction constants is given by

$$\overline{(J^p_{i_1 \cdots i_p})^2} = \frac{(p-1)! J_p^2}{N^{p-1}} \tag{5.15}$$

for the conventions used here. This type of model has been investigated by numerous authors. We will follow the notations and conventions of [37].

The partition function can easily be calculated using the replica trick. The spherical constraint will be implemented in the different replicas using Lagrange parameters z_a and the saddle - point may be taken. Once the saddle point has been taken in the quantum partition function, the direct translation of the spherical constraint reads $< \int \tau x_a(\tau) x_a(\tau) >= l_0^2$ and one will be facing a completely harmonic effective action. Introducing

$$f(q) = \frac{1}{2} J^2 q^2 + \frac{1}{4} J_4^2 q^4 \tag{5.16}$$

we find for the effective action of the corresponding single-site problem

$$\begin{aligned}\Gamma[Q] &= \frac{1}{2}\mathrm{Tr}\ln Q^{-1} + \frac{1}{2}\mathrm{Tr}_n \sum_k (\omega_k^2 + z_a)\delta_{ab} Q(\omega_k) \\ &- \sum_{ab}\int d\tau \int d\tau' f(Q_{ab}(\tau,\tau'))\ . \end{aligned} \tag{5.17}$$

This leads to the Schwinger - Dyson - equation

$$Q_{ab}^{-1}(\tau-\tau') = (\frac{\partial}{\partial\tau^2}+z_a)\delta_{ab}\delta(\tau-\tau') - J^2 Q_{ab}(\tau-\tau') - \frac{J_4^2}{6}Q_{ab}^3(\tau-\tau')\ . \tag{5.18}$$

Note that this equation exactly coincides with the equations for our model in its 3 - loop approximation if only we replace

$$z_a \to \Omega^2 \equiv \omega^2 + \frac{g}{2}Q(\tau=0) \tag{5.19}$$

and

$$J_4^2 \to g^2/6\ . \tag{5.20}$$

This means that the at the 3-loop level the *local* anharmonicity in our model is indistinguishable from terms generated by a random 4-spin interaction.

However, in the spherical J_2 - J_4 - p- spin model, the Lagrange - parameter is determined such that the spherical constraint is fulfilled whereas in our model it is fixed by the mere minimization of the free - energy functional. However, if we *had* defined our model such that ω^2 was *temperature - dependent*, and determined such that the spherical constraint is fulfilled, the two models would be completely equivalent. Discussing the phase - diagram of our model in terms of ω^2 would correspond to the unnatural way of discussing the equivalent p-spin model in terms of the actual value the Lagrange multiplier takes. However, as long as there is a unique relation between the Lagrange parameter and one other order parameter, there exists a mapping between the two models.

5.2.1 The Classical Limit

The p-spin model with $p = 2$ and $p = 4$ interaction has already been studied by Th. M. Nieuwenhizen [37], whom we will follow in this subsection, in the classical case and for bosonic spherical quantum spins in a coherent - state - path-integral formulation. In this section we will briefly describe the results presented in that letter. In the classical limit the time - dependence of all quantities will vanish and we find for the replicated free energy

$$2\beta F_n = -\beta^2 \sum_{ab} f(q_{ab}) - \mathrm{Tr}_n \ln Q - n\ . \tag{5.21}$$

Expanding in the off - diagonal elements q_{ab} one obtains

$$\begin{aligned} 2\beta F_n &= -n\left\{1+\ln q_d+\beta^2 f(q_d)\right\} \\ &- \frac{1}{2}(\beta^2 J_2^2-\frac{1}{q_d^2})\sum_{a\neq b} q_{ab}^2-\frac{1}{3}\sum_{a\neq b\neq c} q_{ab}q_{bc}q_{ca}-\frac{\beta^2 J_4^2}{4}\sum_{a\neq b} q_{ab}^4+\cdots . \end{aligned} \tag{5.22}$$

It is worthwhile to note that this is exactly the relevant part of the free energy of the SK - model. Our model will thus belong to the same universality class and display full RSB for an appropriate choice of J and J_4.

5.2.2 The 1-RSB Solution

If $J_2 < J^*(J_4)$ the system will have a low-temperature phase characterized by one-step replica symmetry breaking (1-RSB) which we want to discuss in zero external field $H = 0$. This approximation consists in assuming $Q_{ab} = (q_d - q_{\rm EA})\delta_{ab} + q_{\rm EA}\epsilon_{ab}^m$. The free energy functional can be written as

$$\begin{aligned} \lim_{n\to 0}\frac{2}{n}\Gamma[q_d, q_{\rm EA}, m] &= -\frac{1}{m}\log(q_d+(m-1)q_{\rm EA})-\frac{m-1}{m}\log(q_d-q_{\rm EA}) \\ &- \beta^2 f(q_d)-(m-1)\beta^2 f(q_{\rm EA})+z(q_d-l_0^2)\ . \end{aligned} \tag{5.23}$$

The saddle point equations with respect to the parameters $z, q_d, q_{\rm EA}$ and m read

$$q_d = l_0^2 \tag{5.24}$$

$$\frac{q_d+(m-2)q_{\rm EA}}{(q_d-q_{\rm EA})(q_d+(m-1)q_{\rm EA})} = z-\beta^2 f'(q_d) \tag{5.25}$$

$$\frac{q_{\rm EA}}{(q_d-q_{\rm EA})(q_d+(m-1)q_{\rm EA})} = \beta^2 f'(q_{\rm EA}) \tag{5.26}$$

$$\frac{1}{m^2}\ln(1+\frac{mq_{\rm EA}}{q_d-q_{\rm EA}})-\frac{q_{\rm EA}}{m(q_d+(m-1)q_{\rm EA})} = \beta^2 f(q_{\rm EA}) \tag{5.27}$$

where equation (5.25) merely defines z for the spherical model. In our original model however, z is a function of q_d and of the higher quantum modes $q_d(\omega_k)$ and equation (5.25) *determines* q_d. The important point to note is that *given* q_d, equations (5.26) and (5.27) are identical to the ones we find for our model in its 3-loop approximation. This has the consequence that the *structure of the correlations in replica space is identical in both models.* As one could always work with a length scale where $q_d = 1$ we could equally well say that both models are identical up to some temperature dependent scale transformation.

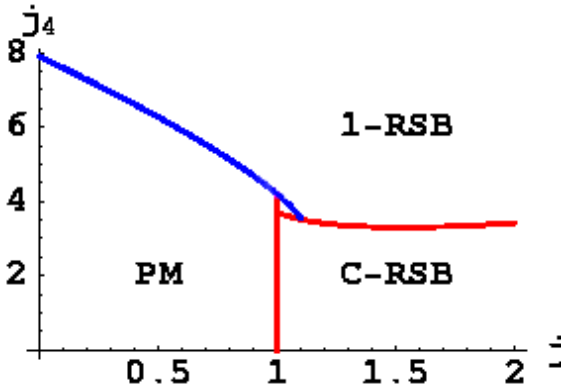


Figure 5.1: *The equilibrium phase - diagram of the j - j_4 - spin glass in the static approximation. The phases are labeled PM for paramagnetic, C-RSB for continuous breaking of the replica symmetry and 1-RSB for one - step breaking.*

In the case of a pure spherical model, f is a monomial and it is possible to multiply (5.27) by pq_{EA}, subtract it form (5.26) and find an equation that is independent of the disorder and the temperature. It turns out that the ratio $x_p = \frac{my}{1-y}$ with $y = q_{\mathrm{EA}}/q_d$ depends on p alone and takes e.g for $p = 3$ the value $x_3 = 1.81696$ [23].

This is not possible in our case, when two nonzero couplings are present. Nevertheless we can use a similar strategy in order to obtain equations independent of J and J_4. We define $x = \frac{mq_{\mathrm{EA}}}{q_d - q_{\mathrm{EA}}}$, multiply (5.27) with 2 and 4 respectively, and subtract from q_{EA} times (5.26) from these. We find

$$4\ln(1+x) - \frac{4x}{(1+x)} - \frac{2x^2}{(1+x)} = -m^2 \frac{j_4 x^4}{(m+x)^4} \tag{5.28}$$

$$4\ln(1+x) - \frac{4x}{(1+x)} - \frac{x^2}{(1+x)} = m^2 \frac{j x^2}{(m+x)^2} \tag{5.29}$$

which have to be solved for m and x. We have introduced the dimensionless parameters $j_4 = \beta^2 J_4^2 q_d^4$ and $j = \beta^2 J^2 q_d^2$.

We find an 1-RSB solution to the above equations if the disorder is strong enough. There is one solution if $j > 1$ and $j_4 < j_4^c(j) \approx 4$. If the four point interaction is strong, $j_4 > j_4^c(j)$ we have to choose between two solutions for $j < 1$ and three solutions for $j > 1$ but smaller than some other critical

value. We always choose the solution with the largest absolute value as it *maximizes* the free energy. When crossing the critical line at a value $j < 1$, the Edwards-Anderson order parameter jumps from zero to some value $< q_d$ and the breakpoint m is equal to one at the phase transition. Because of the jump of q, this transition is often referred to as first order, even if it is not first order in a thermodynamical sense because only the product $(m-1)q$ enters thermodynamic quantities. This product varies continuously. Crossing the critical line at $j = 1$, q increases continuously and does not jump. Therefore this transition is of second order in any sense. However, we will see in that the 1-RSB solution is not stable in this region of parameter space.

5.2.3 Stability of the 1-RSB - Solution

In order to study the stability of the 1-RSB - phase, we have to calculate the second derivative of the free energy functional with respect to the off - diagonal elements q_{ab} and evaluate the resulting Hessian at the 1RSB - solution. The variation is required to be orthogonal to any 1-RSB - matrix because we are looking for the transverse, 'replicon' - eigenvalue [38], i.e.

$$(\epsilon_m \cdot \delta Q)_{ab} = 0 \tag{5.30}$$

and

$$(1 - \epsilon_{ab})\delta Q_{ab} = 0 \ . \tag{5.31}$$

We find for the second variation

$$2\beta\delta^2 F_n = \mathrm{Tr}(Q^{-1}\delta Q)^2 - \beta^2 \sum_{ab} f''(q_{ab})\delta Q_{ab}\delta Q_{ab} \ . \tag{5.32}$$

The inverse of Q can be written as

$$Q^{-1} = \frac{1}{q_d - q_{\mathrm{EA}}}\mathbb{1} - \frac{q_{\mathrm{EA}}}{(q_d - q_{\mathrm{EA}})(q_d + (m-1)q_{\mathrm{EA}})}\epsilon \equiv A\mathbb{1} - B\epsilon \ . \tag{5.33}$$

This means that we are looking for an eigenvalue Λ_T determined by the equation

$$\begin{aligned} A^2\delta Q_{ab} + AB\left[(\delta Q \cdot \epsilon)_{ab} + (\epsilon \cdot \delta Q)_a b)\right] \\ +B^2(\epsilon \cdot \delta Q \cdot \epsilon)_{ab} - \beta^2 f''(q_{\mathrm{EA}})\epsilon_{ab}\delta Q_{ab} = \Lambda_T \delta Q_{ab} \ . \end{aligned} \tag{5.34}$$

This gives the result

$$\Lambda_T = A^2 - \beta^2 f''(q_{\mathrm{EA}}) \equiv \frac{1}{(q_d - q_{\mathrm{EA}})^2} - \beta^2(J^2 + 3J_4^2 q_{\mathrm{EA}}^2) \ . \tag{5.35}$$

In terms of our dimensionless parameters one may write

$$q_{\mathrm{EA}}^2 \Lambda_T = \frac{x^2}{m^2} - \frac{jx^2}{(x+m)^2} - \frac{3j_4 x^4}{(x+m)^4} \ . \tag{5.36}$$

In order to find the critical line in the j, j_4 - plane, we have to solve $\Lambda_T = 0$ in (5.36) together with (5.28) and (5.29).

5.2.4 The Marginally Stable Spin-Glass Solution

It has become clear in the studies of the dynamics of p-spin models [38], that the system gets trapped within configurations corresponding to saddle points of the Energy landscape in coordination space rather than ever reaching its equilibrium state in finite time. This situation can be mimicked within our thermodynamical formalism by requiring the replicon eigenvalue discussed above to always be zero [23, 36]. The breakpoint m will be determined by this requirement and we do *not* extremalize the free energy with respect to m. The new set of equations to solve is

$$\frac{1}{(q_d - q_{\mathrm{EA}})^2} = \beta^2 (J^2 + 3J_4^2 q_{\mathrm{EA}}^2) \tag{5.37}$$

$$\frac{1}{(q_d - q_{\mathrm{EA}})(q_d + (m-1)q_{\mathrm{EA}})} = \beta^2 (J^2 + J_4^2 q_{\mathrm{EA}}^2) \ . \tag{5.38}$$

We note that these equations are *identical* to the ones that can be derived from a dynamics calculation [42]. The breakpoint parameter m is replaced by the Factor X describing the violation of the fluctuation dissipation theorem [36].

Subtracting (5.37) form (5.38) gives

$$\frac{m}{q_d + (m-1)q_{\mathrm{EA}}} = 2\beta^2 J_4^2 q_{\mathrm{EA}} (q_d - q_{\mathrm{EA}})^2 \tag{5.39}$$

and subtracting 3 times (5.38) from (5.37) gives

$$\frac{m q_{\mathrm{EA}} - 2(q_d - q_{\mathrm{EA}})}{(q_d + (m-1)q_{\mathrm{EA}})} = 2\beta^2 J^2 (q_d - q_{\mathrm{EA}})^2 \ . \tag{5.40}$$

Dividing the last two equations gives

$$m = \frac{2q_{\mathrm{EA}}(q_d - q_{\mathrm{EA}})}{q_{\mathrm{EA}}^2 - J^2/J_4^2} \ . \tag{5.41}$$

As (5.37) is independent of the breakpoint m, it can be solved for $q_{\rm EA}$ and (5.41) would then give us m. Moreover, this equation determines a lower bound q_c for $q_{\rm EA}$ because m may not be larger than 1. We find

$$q_c = \frac{q_d}{3} + \sqrt{\frac{J^2}{3J_4^2} + \frac{q_d^2}{9}} \ . \tag{5.42}$$

The upper bound for $q_{\rm EA}$ is given by q_d. The bounds meet when

$$q_d^2 = \frac{J^2}{J_4^2} \ . \tag{5.43}$$

Next, we discuss(5.37). It has no solution for $q_{\rm EA}$ in the interval $[0, q_d]$ if $j_4 < j_4^*(J) \approx 4$ and has two such solutions if $j_4 > j_4^*$. One of these solutions can always be discarded because it violates the lower bound derived above. The line $j_4 = j_4^*(j)$ marks the dynamical phase transition for transitions from the paramagnetic to the 1-RSB spin-glass phase. The transitions may be first or second order just as in the equilibrium calculation. However, the dynamical first order transition occurs at a smaller value of j_4, and therefore at a higher temperature, than the corresponding equilibrium transition. This means that already at a temperature above the thermodynamical phase transition, the dynamics freezes and the system will not be able to reach the equilibrium state in any finite time. It gets trapped on the saddle points we have picked out of the phase space by requiring the replicon eigenvalue to vanish.

5.2.5 The C-RSB Solution

When J is smaller than some threshold value $J^*(J_4)$, the physics will be dominated by the J_4 - interaction and the system will display one - step RSB. The more interesting case is $J > J^*(J_4)$ where the system will be characterized by a full Parisi RSB-scheme displaying continuous replica symmetry breaking (C-RSB). We will assume this to be the case. Again we will follow [37].

We express q_{ab} in terms of the Parisi function $q(x)$ and use well known expressions from 'replica - algebra' (see e.g. the appendix of [38]). It takes a plateau value $q_{\rm EA}$ for $x_1 < x < 1$. The explicit expression for the classical free energy reads

$$2\beta F = -\beta^2 \int_0^1 dx \, \{f(q_d) - f(q(x)\} - \int_0^{q_{\rm EA}} \frac{dq}{I(q)} - \ln(q_d - q_{\rm EA}) - 1 \tag{5.44}$$

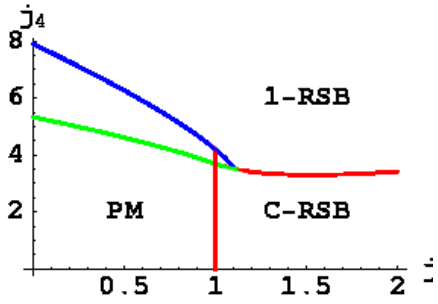


Figure 5.2: *The full phase - diagram of the j - j_4. The green line marks the dynamical phase transition of the model that can be found using the criterion of marginal stability.*

with

$$I(q) = q_d - q_{\rm EA} + \int_q^{q_{\rm EA}} x(q')dq' \ . \tag{5.45}$$

The saddle-point equation reads

$$\beta^2 f'(q(x)) = \int_0^{q(x)} \frac{dq'}{I(q'^2)} \ . \tag{5.46}$$

In the region where $q'(x) \neq 0$ one has $\beta^2 f''(q) = I(q)^{-2}$. It follows that $x(q)$ has an universal shape for all T

$$x(q) = T\frac{f'''(q)}{2(f''(q))^{3/2}} \equiv \frac{6J_4^2 q}{2(J^2 + 3J_4^2 q^2)^{3/2}} \tag{5.47}$$

which gives $q(x,T) = q(\beta x)$ after inversion. The Edwards-Anderson order parameter $q_{\rm EA}$ follows from

$$q_{\rm EA} = q_d - \frac{T}{\sqrt{f''(q_{\rm EA})}} = q_d - \frac{T}{\sqrt{J^2 + 3J_4^2 q_{\rm EA}^2}} \ . \tag{5.48}$$

Now we have to discuss the solutions of (5.48) alone. It is worthwhile to note that (5.48) actually coincides with the equation determining the Edwards-Anderson parameter within the marginally stable spin - glass solution and therefore with the dynamics calculation. The reason is that the Parisi solution is marginally stable intrinsically.

For large values of $j > 1$, equation (5.48) uniquely determines $q_{\rm EA}$ for all values of j_4. For $1 > j > 0.9$ however, there are three solutions to the equation, the one in the middle corresponding to a minimum of the free energy. By increasing j_4 for given j and temperature, there is a discontinuous phase transition where $q_{\rm EA}$ jumps to a nonzero value. For $j < 1.0$, we have no solution to (5.48) in the interval $[0, 1]$ unless $J_4 > J_4^c$, where two solutions appear at some nonzero value of $q_{\rm EA}$. In the for values $J_4 < J_4^c$ the paramagnetic solution is the only one that exists.

In order to determine the transition between the C-RSB and the 1-RSB - solution within the 'dynamical' (i.e. marginally stable) framework, we have to refer to a stability criterion of the C-RSB solution. Requiring $x(q)$ to be monotonously increasing for all values of $q < q_{\rm EA}$ gives us the condition $x'(q_{\rm EA}) = 0$ with $q_{\rm EA}$ determined by (5.48). Translated to our function f, the criterion reads

$$f''''(q_{\rm EA})f''(q_{\rm EA}) - \frac{3}{2}(f'''(q_{\rm EA}))^2 > 0 \tag{5.49}$$

and in terms of the dimensionless parameters the critical line is given by

$$j_4^c = \frac{4j^2}{(1 - 2\sqrt{j})^2} \ . \tag{5.50}$$

This expression is relevant only for the transition between C-RSB and the 1-RSB phase. For j_4 *above* this value we find an 1-RSB scheme. However, a word of caution is in order: In principle, we have used an equilibrium framework in order to determine the C-RSB solution. Therefore we con only talk about the equilibrium phase diagram and the transition between equilibrium 1RSB and C-RSB phase. As we have seen above, the equilibrium 1-RSB state will never be reached by the system because the first order phase transition is preceded by the dynamical phase transition at higher temperatures. We are not aware of a method to calculate the marginally stable C-RSB solution, such that the equivalence between static and dynamic calculations could be continued to the regime of infinite step RSB.

The full phase diagram of the model including the dynamic, static and 1-RSB – C-RSB transition lines is sown in figure 5.2.

5.3 A Toy Approximation

We have seen in the previous section that the equations of our microscopic glass model at its 3-loop approximation differs from the former only by the fact that we have to determine the zero mode of the diagonal part of the correlation matrix $q_d(\omega_0)$ *self-consistently* by minimizing the effective action. In contrast to the spherical models, where q_d is fixed by the spherical constraint, a soft version of the constraint is implemented in our model thanks to the quartic term in the potential. If we *knew* q_d as a function of temperature, given the other parameters J, g and ω^2, it would be very simple to map the models onto each other. In the variational approximation, we *could* determine q_d, but we have seen that the replicon eigenvalue was identically zero in the low-temperature phase and consequently the replica symmetry was exact. Small additional terms would break this marginally stable symmetry as we have seen in the previous section.

However, the *full* 3-loop approximation, obeying the equations of motion derived in the first section of this chapter, is unstable throughout the most interesting range of the parameter space. This is because the 3-loop vacuum diagram contributes a term proportional to $-Q^4$ to the effective action that destabilizes its minimum and leads to diverging paths in the path integral. However, we know that this instability is a spurious product of the 3-loop approximation and is therefore unphysical. In reality, the quartic term in the potential confines the particle irrespective of the quadratic and disorder part of the Hamiltonian. We will see in the next chapter, that in a higher order loop expansion the term arising from the 3-loop vacuum diagram is indeed in a certain sense overcompensated by higher order diagrams.

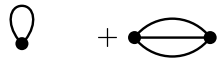
Therefore, we propose a 'toy' approximation in this section, that may seem rather unsystematic at first sight: we will truncate the equations for the diagonal part of the self-energy at 1-loop order and go to 3-loop order in the equations for the off-diagonal part, thereby keeping terms that are small as compared to the terms we neglected in the diagonal part. However, it is important and well justified to keep small terms breaking the replica symmetry and contribute to the replicon eigenvalue because they have to be compared to zero rather than to the contributions to q_d. It will turn out that this approximation captures very interesting physics.

In diagrammatical language we will apply the following approximations for the self-energy:

$$\mathbf{\Sigma_{aa}} = \quad \text{  } \tag{5.51}$$

and

$$\mathbf{\Sigma_{a\neq b}} = \quad + \quad . \tag{5.52}$$



The first term in the last equation vanishes because the quartic vertex is diagonal in the replica indices and consequently the tadpole diagram is proportional to δ_{ab}.

5.3.1 Microscopic Action

We note that the toy approximation can be alternatively understood as follows: as the 3-loop expression displays spurious instabilities we add a stabilizing term $S_{\rm stab}$ to the microscopic action (3.3). The minimal choice for the stabilization is

$$S_{\rm stab} = \frac{g^2}{48\hbar^2} \sum_a \int d\tau \int d\tau' \left(\sum_i x_{a,i}(\tau) x_{a,i}(\tau') \right)^4 \tag{5.53}$$

which is of order x^8 and therefore does not touch our microscopic picture as the latter has been derived as a Born-von-Karman expansion truncated at the order x^4. Equivalently, (5.53) can be seen as a soft version of the constraint usually imposed on p-spin models. The term (5.53) contributes a term

$$S_{\rm stab}[Q] = \frac{3g^2}{(4!)^2\hbar^2} \sum_a \int d\tau \int d\tau' Q_{aa}^4(\tau,\tau')$$

to 3.6. Therefore, the saddle point value of the Lagrange parameter field $\lambda_{ab}(\tau,\tau')$ is modified and we find

$$\lambda_{ab}(\tau,\tau') = -\frac{J^2}{\hbar} Q_{ab}(\tau,\tau') + \frac{g^2}{24\hbar} Q_{aa}^3(\tau,\tau')\delta_{ab} \; . \tag{5.54}$$

This term cancels the diagonal part of the 2-loop contribution to the self-energy exactly.

5.3.2 Schwinger-Dyson Equations

The saddle-point resulting from the expressions (5.51) and (5.52) for the self-energy read

$$(Q^{-1})_{aa}(\omega_0) = \omega^2 + \frac{gz}{2} - J^2 Q_{aa} \tag{5.55}$$

$$(Q^{-1})_{ab}(\omega_0) = J^2 Q_{ab}(\omega_0) + \frac{g^2T^2}{6} Q_{ab}^3(\omega_0) \quad \text{for} \quad a \neq b \tag{5.56}$$

$$q_d(\omega_k)^{-1} = \omega^2 + \omega_k^2 + \frac{gz}{4} - J^2 q_d(\omega_k) \quad \text{for} \quad k \neq 0 \tag{5.57}$$

where we have used shorthand

$$z \;=\; T\sum_k q_d(\omega_k) \equiv Q_{aa}(\tau=0) \tag{5.58}$$

as in the previous chapter.

In the paramagnetic phase, the equations are identical to the variational ones (by construction) and we have

$$q_d(\omega_k) = \frac{1}{2J^2}\left[\omega^2+\omega_k^2+\frac{gz}{2}-\sqrt{(\omega^2+\omega_k^2+\frac{gz}{2})^2-4J^2}\right] \tag{5.59}$$

where z has to be determined self-consistently using (5.58). In the spin-glass phase, (5.59) still holds for $k \neq 0$.

New features appear in the spin-glass phase, where we choose an 1-RSB ansatz, that is $Q_{ab}(\omega_0) = (q_d - q)\delta_{ab} + q\epsilon_{ab}^m$, for the zero mode of the correlation matrix first. The above equations have to be supplemented by an equation for the breakpoint parameter m. We use the condition of marginal stability instead of the equilibrium condition as discussed in the previous section. Taking the formulas from appendix C, the full set of equations reads

$$\frac{1}{q_d-q}-\frac{q}{(q_d-q)(q_d+(m-1)q)} \;=\; \omega^2+\frac{gz}{2}-J^2q_d \tag{5.60}$$

$$\frac{q}{(q_d-q)(q_d+(m-1)q)} \;=\; J^2q+\frac{g^2T^2}{6}q^3 \tag{5.61}$$

$$\frac{1}{(q_d-q)^2} \;=\; J^2+3\frac{g^2T^2}{6}q^2 \tag{5.62}$$

supplemented by equation (5.58) for z. Using 5.61 in 5.60 gives

$$\frac{1}{q_d-q} = \omega^2+\frac{gz}{2}+\frac{g^2T^2}{6}q^3-J^2(q_d-q)\;. \tag{5.63}$$

One has to find the zeros of a second order polynomial to solve 5.62 for $q_d(q)$. Introducing $f''(q) = J^2+\frac{g^2T^2}{2}q^2$, equation (5.60) can be written as

$$\sqrt{f''(q)} = \omega^2+\frac{gz}{2}+\frac{g^2T^2}{6}q^3-\frac{J^2}{\sqrt{f''(q)}}\;. \tag{5.64}$$

This can be solved numerically for $q(z)$. Multiplying with $\sqrt{f''(q)}$ and taking the square gives

$$(2J^2+\frac{\gamma}{2}q^2)^2 = (J^2+\frac{\gamma}{2}q^2)\left[\omega^2+\frac{gz}{2}+\frac{\gamma}{6}q^3\right]^2 \tag{5.65}$$

with $\gamma = g^2T^2$. There will be either no solution or two solutions with positive q. We choose the larger solution because we infer its stability by virtue of the analogy to the equivalent spherical model.

The breakpoint parameter can then be found from 5.61 as a function of q_d and q. We find

$$m = 1 - \frac{q_d}{q} + \frac{1}{(q_d - q)(J^2 q + \frac{\gamma q^3}{6})} \ . \tag{5.66}$$

The criterion for the stability of the 1-RSB solution with respect to C-RSB can be taken from the considerations in the previous section. We find that the critical line is determined by

$$J^2 = 3\gamma q^2 \ . \tag{5.67}$$

5.3.3 The Equilibrium Spin-Glass Solution

For the equilibrium spin-glass solution we have

$$\frac{1}{q_d - q} - \frac{q}{(q_d - q)(q_d + (m-1)q)} = \omega^2 + \frac{gz}{2} - J^2 q_d \tag{5.68}$$

$$\frac{q}{(q_d - q)(q_d + (m-1)q)} = J^2 q + \frac{\gamma^2}{6} q^3 \tag{5.69}$$

$$\frac{q}{m(q_d + (m-1)q} - \frac{1}{m^2}\log(1 + \frac{mq}{q_d - q}) = -\frac{1}{2}J^2 q^2 - \frac{\gamma^2}{24} q^4 \tag{5.70}$$

which we have to solve for m, q and q_d given z. The latter has to be determined self-consistently. Using the second equation in the first, we get a relation between q_d and q that does not depend on the breakpoint parameter m. This can be solved for $q_d(q)$ or $q(q_d)$ as one likes. We decide to take $\Delta = q_d - q$ as an independent variable and find

$$\Delta(q) = \frac{1}{2J^2}\left[\Omega^2(q) \pm \sqrt{\Omega^2(q)^2 - 4J^2}\right] \ , \tag{5.71}$$

where

$$\Omega^2(q) \equiv \omega^2 + \frac{gz}{2} + \frac{\gamma^2}{6} q^3 \ . \tag{5.72}$$

We choose the solution with the negative sign because we expect $\Delta(q) \to 0$ for $q \to \infty$.

Equations 5.69 and 5.70 are most conveniently written in terms of $\Delta = q_d - q$, $x \equiv \frac{mq}{q_d - q}$ and q. We find

$$\frac{1}{1+x} = J^2\Delta^2 + \frac{\gamma^2}{6}\Delta^2 q^2 \tag{5.73}$$

$$\frac{x}{1+x} - \log(1+x) = -\frac{1}{2}J^2x^2\Delta^2 - \frac{\gamma^2}{24}x^2\Delta^2q^2 \ . \tag{5.74}$$

Now q can be eliminated from the last equation using the first. This allows us to get x as a function of Δ, solving

$$\frac{x(1+\frac{1}{4}x)}{1+x} - \log(1+x) = -\frac{1}{4}J^2\Delta^2x^2 \ . \tag{5.75}$$

Besides the trivial solution $x = 0$ corresponding to the paramagnetic phase, this equation has a nonzero solution only for $J^2\Delta^2 < 1$, signaling the phase transition. The maximum value of x, $x_{\max} = 4.115..$ is found when $J\Delta = 0$.

Given $x(\Delta)$ we can easily determine

$$q(\Delta) = \sqrt{\frac{6}{\gamma^2\Delta^2}\left(\frac{1}{(1+x(\Delta))} - J^2\Delta^2\right)} \tag{5.76}$$

and insert it into 5.68. This means that we have a single real positive solution for all $\Delta < 1/J$.

5.3.4 The Marginally Stable Spin-Glass Solution

For the marginally stable spin-glass solution we have to replace 5.70 with

$$\frac{1}{(q_d - q)^2} = J^2 + \frac{\gamma^2}{2}q^2 \equiv \tilde{J}(q) \ . \tag{5.77}$$

This means

$$\tilde{\Delta}(q) = \frac{1}{\sqrt{\tilde{J}(q)}} \ . \tag{5.78}$$

The expression for the breakpoint 5.66 remains unaltered and q can be determined by solving $\tilde{\Delta}(q) = \Delta(q)$ with $\Delta(q)$ taken from 5.71.

5.3.5 Discussion of the Phase Diagram

The numerical solution shows different behavior depending on the quadratic part ω^2 of the bare single-site potentials. For $\omega^2 > 0$, there is a second order phase transition, whereas for $\omega^2 < 0$ there is a first order phase transition.

If $\omega^2 < 0$, that is if we start with double-well potentials, there is a first order phase transition occurring with a value $m = 1$ of the breakpoint parameter and a nonzero value of the Edwards-Anderson parameter. However, there is an important difference to the spherical p-spin models. In both cases, the internal energy depends on q_d and the product $(m-1)q$ alone. As in the spherical models, q_d is held fixed, a jump of the Edwards-Anderson parameter does not produce latent heat as long as $m = 1$. This means that the phase transition is not first order in the Ehrenfest sense. In our model, the jump in q induces a jump in q_d as well as both of the parameters depend on each other. This produces latent heat *even if* $m = 1$ at the transition.

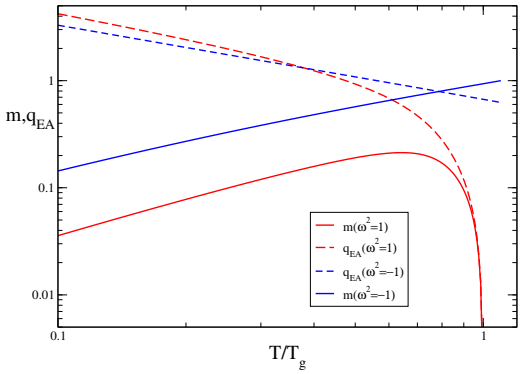


Figure 5.3: *Behavior of the Edwards-Anderson order parameter and the breakpoint m in the case of a first order (blue, $\omega^2 = -J$) and second order (red, $\omega^2 = J$) phase transition. The parameter ω^2 is the quadratic part of the bare potential.*

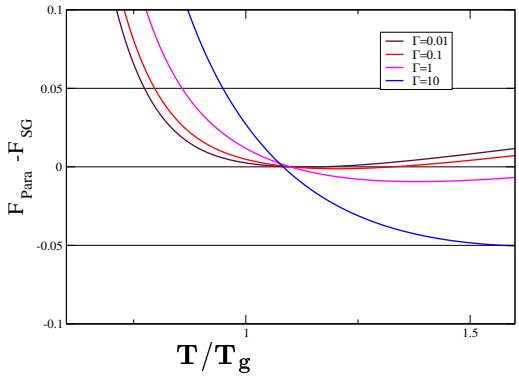


Figure 5.4: *The difference between the paramagnetic and spin-glass free energy for different strengths of quantum fluctuations Γ and $\omega^2 = -1$ as a function of T/T_g. For $\Gamma = 0$ we recover a second order phase transition, whereas for nonzero Γ it is weakly first order.*

It has been shown [24] that in spherical models, the quantum fluctuations can drive the transition from second to first order by producing a phase transition where the breakpoint parameter m jumps to a value different from one. This may occur in our model as well, if only the quantum fluctuations are strong enough. However, there will be no qualitative change in the

behavior because the phase transition is first order for any finite value of $\hbar$. Only in the limit $\hbar \to 0$ the transition becomes second order.

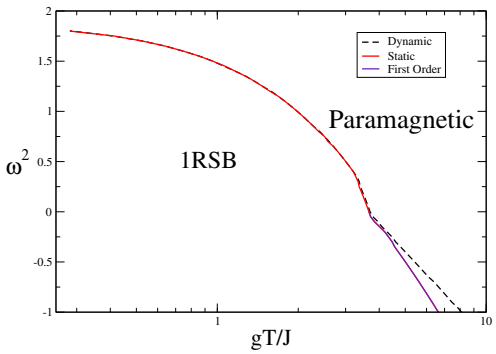


Figure 5.5: *1-RSB phase diagram of the toy approximation for $g = 1.0$ and $\Gamma = 0.1$ within a equilibrium 1RSB ansatz and the marginally stable solution corresponding to the dynamical phase diagram.*

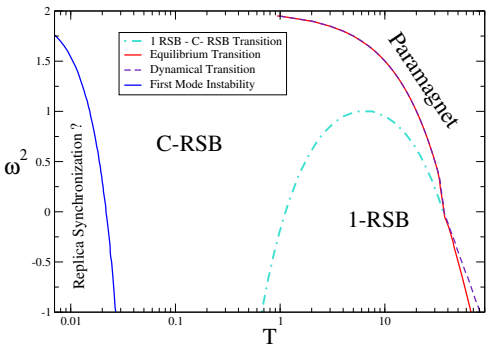


Figure 5.6: *1-RSB phase diagram of the toy approximation for $g = 0.1$ and $\Gamma - 0.01$ extended to lower temperatures. The blue line determines the temperature where the toy approximation breaks down because the first Matsurbara mode becomes unstable. The dash-dotted line indicates a transition form 1-RSB to C-RSB.*

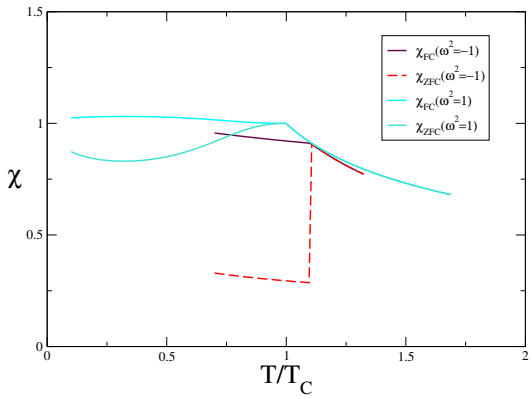


Figure 5.7: *Susceptibilities calculated within the 'toy' approximation for $\omega^2 = -1$ and $\omega^2 = 1$, where in the latter case the phase transition is of second order. We remind that ω^2 is the quadratic part of the bare potential and that we are* not *calculating frequency dependent susceptibilities.*

As expected from the spherical p-spin models, the dynamical phase transition occurs at a higher temperature than the first-order phase transition

and the transition lines are identical in the case of a second order phase transition. Interestingly, the free energies of the paramagnetic and the marginally stable spin-glass solution are identical within our numerical precision in the temperature range where they coexist.

Formally, the spin-glass solution can be continued into the paramagnetic phase and the paramagnetic solution can be continued into the spin-glass phase. However, the breakpoint parameter m becomes bigger than 1 for the continuation of the spin-glass solution into the paramagnetic phase such that there is no clear physical meaning to this continuation. This has the consequence that one would expect an hysteresis cycle for the *zero field cooled susceptibility* [17, 37]

$$\chi_{\mathrm{ZFC}} \equiv \int d\tau q_d(\tau) - q_{\mathrm{EA}} \tag{5.79}$$

living entirely in the low temperature phase. The authors of [24] state that the quantum spherical p-spin model has a hysteretic behavior of the *field cooled* susceptibility

$$\chi_{\mathrm{FC}} = \int d\tau q_d(\tau) + (m-1)q_{\mathrm{EA}} \tag{5.80}$$

on both sides of the phase transition. We do not observe this in our approximation.

The spin-glass phase is divided into two regions, one with a 1-RSB scheme, and one with a continuous replica symmetry breaking. The toy approximation displays unphysical reentrant behavior for $0 \leq \omega^2 \leq 1$. We think that this is an artifact of our approximation. We note that this transition is an *equilibrium* transition between two equilibrium states and occurs at a temperature much lower than the dynamical transition temperature. Indeed, the dynamical calculation reveals another criterion than the one we applied [42].

For very small temperatures, the solution presented above no longer exists and a new type of solution to our toy approximation appears. It is worthwhile to comment on this. At the critical temperature, the first mode $Q(\omega_1)$ becomes unstable and reaches a critical value $1/J$. This means that below this temperature there is a spin-glass solution with nonzero off- diagonal elements $q_1 = Q(\omega_1)_{ab}$ with $a \neq b$. If taken seriously, this would indicate an instability with respect to *replica synchronization* transition as discussed in section 4.6.2. If such a phase transition would happen to exist in more serious spin-glass models, it would surely be a candidate for an explanation of the low temperature phase transition in structural glasses observed by

Strehlow and collaborators [10] as it is manifestly a quantum phase with transition temperature scaling with $\hbar$.

Chapter 6

Non Perturbative Approach

In this section, we want to develop a resummed perturbation theory for the model. We will sum a series of 'ring' type 2PI diagrams and finally will find an approximation that is closely related to the random-phase approximation known form strongly correlated electron systems.

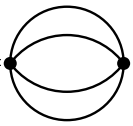
6.1 Summation of Ring Diagrams

First, we will consider the 2- and 3-loop contributions to the two-particle irreducible part of the free energy Γ_2:

$$\Gamma_1 = \frac{g}{8} \sum_a \int d\tau Q_{aa}^2(\tau, \tau) = \qquad (6.1)$$

and to order g^2:

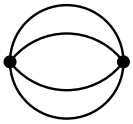
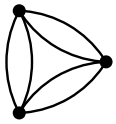
$$\Gamma_2 = \frac{g^2}{48} \sum_{ab} \int \int d\tau d\tau' Q_{ab}^4(\tau, \tau') = \qquad (6.2)$$



.

Concerning higher order terms, we content ourselves with the series of ring - diagrams represented in (6.3). The diagram to order n of this series can be transformed into itself by $2n$ symmetry operations consisting in rotations and combined rotations and reflexions of the whole figure and additional 2^n symmetry operations corresponding to exchanges of the double lines between

the neighboring vertices. That is, the overall symmetry factor of the n'th order diagram is given by $\frac{1}{(2n)2^n}$.

$\mathbf{\Gamma_R = \frac{1}{4}}$  $\mathbf{-\frac{1}{16}}$  $\mathbf{+\frac{1}{48}}$  $+\cdots$. (6.3)

The above series is summed by the function

$$\Gamma_{\rm R} = \frac{1}{2}{\rm Tr}\ln(\mathbb{1} + \frac{g}{2}\hat{Q}_2) \tag{6.4}$$

with the double - line propagator defined as

$$(\hat{Q}_2)_{ab}(\tau,\tau') = Q^2_{ab}(\tau,\tau') \tag{6.5}$$

where the trace is understood to be taken over replica and time indices and the logarithm is taken in the sense of its Taylor expansion. The products in this expansion are convolutions with respect to time and matrix products with respect to replica indices. We have introduced $\mathbb{1} \equiv \delta_{ab}\delta(\tau - \tau')$.

Comparing the symmetry factors appearing for the diagram to order g^2 in (6.5) with (6.1) and(6.2), we find that the prefactors arising from the series expansion of the logarithm overestimate the order g and g^2 - contribution. This is due to the additional symmetries of (6.2) under exchanges of lines which have not been taken into account in the above derivation of the symmetry factors for the ring-type diagrams. This has to be compensated by subtracting a term $\frac{g\beta^2}{8}Q^2_d(\tau = 0) \equiv \frac{\beta g z^2}{8}$ and adding a term $\frac{g^2}{24}{\rm Tr}\hat{Q}^2_2$ to (6.5).

Finally, the 2PI - part of the free energy given by

$$\Gamma_{\rm Ring} = \frac{1}{4}{\rm Tr}\ln(\mathbb{1} + \frac{g}{2}\hat{Q}_2) - \frac{\beta g z^2}{8} + \frac{g^2}{24}{\rm Tr}\hat{Q}^2_2 \equiv \Gamma_R + \frac{2}{3}\Gamma_2\ . \tag{6.6}$$

6.2 The Paramagnetic Phase

In the paramagnetic phase, we assume $Q_{ab}(\omega_k) = q_d(\omega_k)\delta_{ab} = \frac{\lambda_d}{J^2}$ and the 2PI effective action is given by

$$\Gamma \;=\; -\frac{1}{2}\sum_k \ln q_d(\omega_k) + \frac{1}{2}\sum_k((\omega_k^2 + \omega^2)q_d(\omega_k) - 1) - \frac{\beta g z^2}{8}$$

$$
\begin{aligned}
- \quad & \frac{1}{2}\sum_k q_d(\omega_k)\lambda_d(-\omega_k) + \frac{g^2}{24}\int d\tau \int d\tau' Q_d^4(\tau-\tau') \\
+ \quad & \frac{1}{2}\sum_k \ln\left(1+\frac{gT}{2}\sum_l q_d(\omega_l)q_d(\omega_k-\omega_l)\right) \ . \qquad (6.7)
\end{aligned}
$$

The Schwinger-Dyson equations we have to solve in the paramagnetic phase can be obtained by deriving (6.7) with respect to $q_d(\omega_k)$ and setting λ to its saddle point value afterwards. We find

$$
\begin{aligned}
\frac{1}{q_d(\omega_k)} \quad = \quad & \omega^2+\omega_k^2 - J^2 q_d(\omega_k) - \frac{gz}{2} \\
+ \quad & \frac{(gT)^2}{3}\sum_{l,m} q_d(\omega_l)q_d(\omega_m)q_d(\omega_k-\omega_l-\omega_m) \qquad (6.8) \\
+ \quad & gT\sum_l q_d(\omega_k-\omega_l)\frac{1}{1+\frac{gT}{2}\sum_m q_d(\omega_m)q_d(\omega_l-\omega_m)} \ .
\end{aligned}
$$

The above equations can be solved numerically in a straightforward way. It is worthwhile to note that the last and next to last terms include the Fourier components of $q_d(\tau)^2$ and $q_d(\tau)^3$ respectively. These contributions can be evaluated much faster numerically by Fourier transforming to imaginary time and back again.

The strategy for the numerics is thus as follows: start with some initial guess for the $q_d(\omega_k)$ and calculate $q_d(\tau)$ by Fourier transforming. From this calculate $q_d(\tau)^2$ and $q_d(\tau)^3$ and Fourier transform them in order to find their Fourier modes $Q_d^2(\omega_k)$ and $Q_d^3(\omega_k)$. Knowing this, we can easily calculate the gradient of Γ which we will follow using some minimization algorithm. This is numerically more convenient than solving the Schwinger-Dyson equations, because it is simpler to find a minimum in multi-dimensions than solving a large number of coupled nonlinear equations simultaneously, especially because we have gradient information from the Schwinger-Dyson equations at our disposal.

6.3 The RS Solution

Assuming an RS structure for the zero mode of the propagator and using the notation $q = Q_{ab}(\omega_0)$ for $a \neq b$ and $q_d = Q_{aa}(\omega_0)$, the full effective action can be expressed as a function of q_d, $q_d(\omega_k)$ for $k \neq 0$ and of q. We derive the saddle-point equations

$$
\frac{1}{q_d-q} - \frac{q}{(q_d-q)^2} \quad = \quad \omega^2 - J^2 q_d + \frac{g^2T^2}{3}Q_3(\omega_0)
$$

$$+ \quad gT \sum_k Q(\omega_k) I(-\omega_k) \tag{6.9}$$

$$\frac{q}{(q_d - q)^2} = J^2 q + g^2 T^2 q^3 (I_q - \frac{1}{3}) \; . \tag{6.10}$$

Here

$$I_q = \frac{1}{(1 + \frac{q}{2}(Q_2(\omega_0) - Tq^2))^2} \tag{6.11}$$

$$I(\omega_k) = \frac{1 + \frac{q}{2}(Q_2(\omega_k) - 2q^2\delta(\omega_k))}{(1 + \frac{q}{2}(Q_2(\omega_k) - q^2\delta(\omega_k)))^2} \tag{6.12}$$

and

$$Q_l(\omega_k) \equiv \int_0^{\beta\hbar} q_d^l(\tau) e^{-i\omega_k \tau} d\tau \tag{6.13}$$

is the Fourier transform of the l'th power of $Q(\tau)$. Equation (6.10) can be solved numerically for q for fixed values q_d and $Q_2(\omega_0)$. These parameters have to obey $Q_2(\omega_0) >= Tq_d^2$ due to a simple Schwartz inequality. besides the zero solution we find a nonzero solution as soon as $q_d > 1/J$, just as in the variational approximation. This solution can be taken into the full effective action which is then a function of q_d and $Q(\omega_k)$, $k \neq 0$, alone and can be minimized numerically using gradient methods. Because q is a continuous function of q_d, there will be no first order phase transition and the phase diagram as well as the critical behavior is very similar to the behavior we found in the variational approximation.

6.4 Stability of the RS solution

It turns out that $m = 0$ is the only solution to the Schwinger-Dyson equations within an 1-RSB ansatz. The derivation of this result is relegated to appendix D. This result is surprising because one would not expect a symmetry to be restored in a higher order loop expansion once it is broken at some finite loop level. However, we are not dealing with any finite loop order. In appendix D we propose to include a vertex renormalization into the effective acton in order to find replica symmetry breaking solutions.

Concerning the rich phase space structure of the 3-loop toy approximation we have to admit that the appearence of the first-order transition and the transition from 1-RSB to C-RSB is probably an artifact of the approximations done. This could have been anticipated anyway because we would expect to recover the Sherrington-Kirkpatrick (SK) model in the limit of deep double wells $\omega^2 \ll 0$.

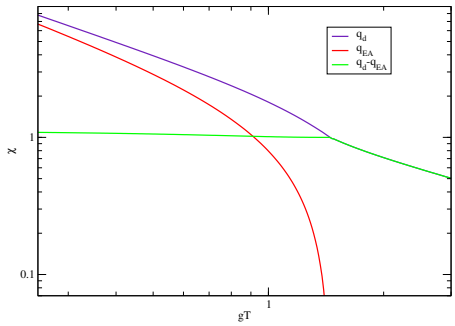


Figure 6.1: *The temperatures dependence of the parameters in the RS solution here shown for* $\omega^2 = J = 1$ *and* $\Gamma = 0.1$. *Note the definition of the Fourier transform for the factors* β.

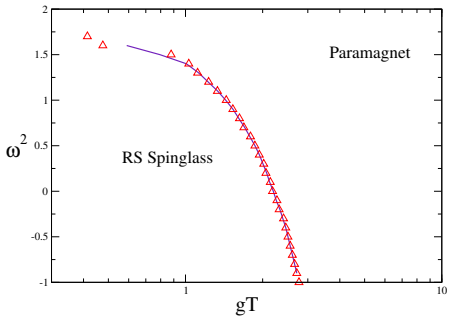


Figure 6.2: *Phase diagram of the RS - solution for* $J = 1$ *and* $\Gamma = 0.1$ *and* $g = 0.1$. *The solid line is a smooth interpolation to the transition points found numerically.*

The toy approximation remains interesting by itself because it reveils a close relationship between the equivalent p-spin model and our microscopic glass model and finally it is exact for a microscopic action different from the oringinal one of our model.

6.4.1 Replica Synchronization

At very low temperatures, the solution newly becomes instable because the first mode $q_d(\omega_1)$ reaches a the critical value $1/J$. This means that the off-diagonal elements $Q_{ab}(\tau, \tau')$ become time dependent. As the effective action mixes all modes it is numerically hard to determine the precise time - dependence and we will merely state here that *there is a replica synchronized low -temperature phase*, the critical temperature being determined by $q_d(\omega_1) = 1/J$. The investigation of the physical properties of this phase will be left to future studies. This transition is probably the one we would have expected least to survive from the toy approximation. The fact that we still find it within this elaborate version of perturbation theory justifies some optimism. If this transition would happen to take place in real glasses, we would have found a new type of coherent quantum state in glasses. However, there will be a lot of work to do on the intepretational side before we

will be able to have a physical understanding of what an imaginary time dependence of the Edwards-Anderson order parameter could stand for in the non-replicated world.

Chapter 7

Conclusions

We have presented several approximations to one simple microscopic spin glass model and have found a profound relationship between models dealing with low-temperature properties, being of soft-potential type and models known to be very good close to the glass transition, such as p-spin models.

The variational approximation investigated in the first part has the major advantage of being solvable analytically to a large extent. We find an exact correspondence to a system consisting of an ensemble harmonic oscillators in a random field coupled to a super-ohmic bath of oscillators with a spectral function that can be determined exactly. Due to its solubility, we were able to analytically continue the imaginary time correlation function of the model to real times for this approximation. We find the well known features of dissipative quantum systems such as damping and an algebraic decay. Furthermore, assuming the random field to be static on experimental time scales, we find a linear component in the specific heat even though there is no real tunneling involved in the variational Hamiltonian. At zero temperature, the nonlocal effective single-site action can be interpreted as an average over independent particles in quartic potentials subject to random external fields. This justifies a posteriori the quasi-classical approach applied to the same model [9]. In the variational approximation, the permutation symmetry of replicas is exact and marginally stable. The temperature of the transition to the RS phase is lowered by quantum fluctuations and can become zero at a critical strength of the quantum fluctuations depending on the ratio between disorder energy and the harmonic part of the stabilizing potential.

The main methodological point in this work is the introduction of the two-particle irreducible effective action formalism into the field of quantum spin-glass theory. It provides a very simple and elegant way of dealing with

functional self-consistency problems. We stress that the applicability of this method is not restricted to the model investigated in this work but applies to virtually all mean-field spin-glass models.

The 3-loop approximation introduces a term breaking the replica symmetry. We have shown that for *fixed* diagonal part q_d of the correlation matrix, we recover a equations identical to those of a spherical p- spin model with 2-spin and 4-spin interactions showing a 1-RSB or C-RSB phase depending on the dimensionless coupling constants. In our model however, q_d is temperature dependent and the situation is slightly more involved. At 3-loop level, there is no stable solution for q_d in the most interesting part of the parameter space. However, this instability is a spurious product of the approximation as we know that the initial model must have a solution everywhere.

In order to have a stable solution, we present an approximation extending the variational approach by the term breaking the replica symmetry and neglecting the term giving rise to the instability of the 3-loop approximation. This approximation is partially justified a posteriori in the discussion of the higher order loop expansions. The 'toy' approximation has very interesting features by itself. It shows a phase diagram similar to the equivalent p-spin model, with a second order phase transition if the 'bare' potentials in our initial model are of single-well type and a first order phase transition precessed by a dynamical phase transition if the bare potentials are of double-well type. At very low temperatures, there is a second order transition from 1-RSB to C-RSB just as in the case of discontinuous spherical p-spin models [39]. Concerning the influence of quantum fluctuations on the first order line, we find that quantum fluctuations drive the phase transition first order in the Ehrenfest sense, as weak as they may be. Only for $\hbar = 0$, the phase transition becomes second order in the thermodynamical sense. This is to be contrasted with the results of pure quantum spherical p - spin models [24] where the quantum fluctuations drive the phase transition to first order only if they exceed a critical strength.

The non perturbative approach, originally devised to substantiate the toy approximation, surprisingly shows a much simpler critical behavior again. The thermodynamical phase transition is of second order throughout the critical line and the glass phase is of RS type. However, collective features occur at very low temperatures and we argue that we are facing a phase transition involving the loss of independence of the replicas concerning translations in time. The detailed investigation of this *replica synchronization transition*, and of its physical meaning is left to further studies.

Appendix A

1 PI Effective Action Formalism

A.1 General Formalism

Going back to 3.1 we see that we have to evaluate functional integrals of the form

$$Z_n = \int \mathcal{D}x \exp\{-S[x]\} \tag{A.1}$$

with $S[x]$ given in (3.6) and x a n- component vector. The disorder destabilizes the minimum of the effective action at $x_a(\tau) \equiv 0$ such that below a critical temperature the inverse propagator in the variational approach gets negative eigenvalues. This means that there are is a new path $\Phi(\tau) \neq 0$ minimizing the effective action. Clearly, $\Phi(\tau) \equiv < x(\tau) >$. Consequently, we will have do set up a variational theory by expanding around this path.

In order to do so, we write the Generating functional

$$Z_n[\xi] = \int \mathcal{D}x \exp\{-S[x] - \sum_a \int d\tau x_a(\tau)\xi_a(\tau)\} \tag{A.2}$$

and define the 1 PI effective action as the Legendre Transform of $Z_n[\xi]$ with respect to the generating field $\xi(\tau)$. We find

$$\Gamma[\Phi] = -\ln(Z_n[\xi]) - \sum_a \int d\tau \xi_a(\tau)\Phi_a(\tau) \tag{A.3}$$

This gives

$$\exp\{-\Gamma[\Phi]\} = \int \mathcal{D}x \exp\left\{-S[x] - \sum_a \int d\tau (x_a(\tau) - \Phi_a(\tau))\xi_a(\tau)\right\} \tag{A.4}$$

Shifting the integration variable $x_a \to x_a + \Phi_a$ gives

$$\exp\{-\Gamma[\Phi]\} = \int \mathcal{D}x \exp\left\{-S[x+\Phi] - \sum_a \int d\tau x_a(\tau)\xi_a(\tau)\right\} \qquad (A.5)$$

and we are left with a 'shifted' effective action

$$\begin{aligned} S[x+\Phi] &= \frac{1}{2}\left[xG^{-1}(Q)x + xG^{-1}(Q)\Phi + \Phi G^{-1}(Q)x + \Phi G^{-1}(Q)\Phi\right] \\ &+ \frac{g}{4!}\left[x^4 + 4x^3\Phi + 6x^2\Phi^2 + 4x\Phi^3 + \Phi^4\right] \end{aligned} \qquad (A.6)$$

where we have used shorthand

$$G^{-1}_{ab}(Q) = (\frac{\partial^2}{\partial\tau^2} + \omega^2)\delta_{ab}\delta(\tau-\tau') + \omega^2 - 2JP^2Q^{(p-1)}_{ab}(\tau,\tau')$$

and suppressed all sums and integrals for matrix multiplications. We note that we can partially integrate the $\Phi G^{-1}(Q)x$-term twice to make it equal to $xG^{-1}(Q)\Phi$. Now we arrange the different terms according to their power in x. We find

$$\begin{aligned} S[x+\Phi] &= \frac{1}{2}\left[x(G^{-1}(Q) + \frac{g}{2}\Phi^2)x\right] + \frac{g}{3!}\Phi x^3 + \frac{g}{4!}x^4 \\ &+ x\left[G^{-1}(Q)\Phi + \frac{g}{6}\Phi^3\right] \ . \end{aligned} \qquad (A.7)$$

It is now obvious that we can cancel all terms linear in x if only we choose for Φ a solution of the equation

$$G^{-1}(Q)\Phi + \frac{g}{6}\Phi^3 = -\xi \qquad (A.8)$$

such that the linear term in (A.7) cancels the source term!

In the end, we are always interested in the case of a vanishing source term $\xi = 0$. Then there is always a solution $\Phi \equiv 0$ to the above equation. If this solution does not exist anymore, we would assume $\Phi = \text{const}$ for a first try. This gives

$$\omega^2\Phi_a - 2pJ^2\sum_b Q^{(p-1)}_{ab}(0)\Phi_b + \frac{g}{6}\Phi^3_a = 0 \ . \qquad (A.9)$$

This sheds a new light on the instability we encountered in the previous section. In the high-temperature phase $Q_{ab} \equiv Q\delta_{ab}$ and we have the the only solution $\Phi = 0$ that becomes unstable whenever $pJ^2Q^{(p-1)}(0) \geq \omega^2$. In

the case $pJ^2Q^{(p-1)}(0) \geq \omega^2$ we find an additional solution corresponding to a macroscopic polarization of the system.

$$\Phi^2 = \frac{6}{g}\left[2pJ^2Q^{(p-1)}(0) - \omega^2\right] \tag{A.10}$$

if Q was still diagonal in this case. Assuming a replica symmetric structure $Q(0) = (Q-q)\delta_{ab}+q$ for the zero mode of the connected correlation function Q gives for $n \to 0$

$$\Phi^2 = \frac{6}{g}\left[2pJ^2(Q-q)^{(p-1)} - \omega^2\right] \ . \tag{A.11}$$

If there are higher modes for which $\omega^2 + \omega_k^2 - Q(\omega_k)$ becomes negative, the situation becomes considerably more involved because one mode different from zero would create nonzero values of the other modes as well.

It turns out to be convenient to translate the above equations to equations for Φ and the *connected* correlation function $G = Q - \Phi\Phi$. In the case $p = 2$ we find

$$\omega^2\Phi_a - 4J^2\left[\sum_b (G_{ab}\Phi_b) - \underbrace{\Phi_a \sum_b \Phi_b^2}_{\mathcal{O}(n)}\right] + \frac{g}{6}\Phi_a^3 = 0 \tag{A.12}$$

such that we could have been using the connected correlation function directly in order to determine Φ.

At this point it is important to note that there are, besides of the obvious replica symmetric solution $\Phi_a \equiv \Phi$ other solutions as well [46]. Now the disconnected two-point function Q_{ab} *depends* on the Φ such that a non symmetric structure of the vector Φ would manifest in a breaking of the replica symmetry of the correlation function as well. However, Q is defined as the *average* correlation function such that an ansatz with a replica symmetric Q and more than one non replica symmetric vectors Φ distributed in a *globally replica symmetric way* is no contradiction.

Appendix B

The 2PI Effective Action Formalism

B.1 General Framework

In order to go beyond the variational approach, we have to devise new approximation methods. The 2PI effective action formalism will be shown to be a very powerful tool for the treatment of disordered systems in general and for the microscopic glass model treated in this work in special. The ideas presented here have been introduced for fermion systems by Martin and DeDominicis [44] long time ago footing on ideas of Luttinger and Ward [43]. We want to follow a generalized notation for general quantum fields introduced by Cornwall *et. al.* [45] .

We translate the 2PI-effective action formalism known from field theory into the language of quantum statistical physics and show that it is especially well suited for the treatment of disordered systems.

We consider the partition function

$$\begin{aligned} Z[J,R] &\equiv e^{-W[J,R]} \qquad\qquad (B.1)\\ &= \int \mathcal{D}\varphi \exp\left\{-\left[S[\varphi] + \int_x \varphi(x)J(x) + \frac{1}{2}\int_{xy}\varphi(x)R(x,y)\varphi(y)\right]\right\} \end{aligned}$$

where the integrals in the exponent are meant to be over the whole $n(d+1)$-dimensional configuration space: $\int_x \equiv \sum_a \int d^d x_a \int_0^{\beta\hbar} d\tau$. The quantum statistical problems investigated in this work correspond to $d = 0$.

We obviously have $W = -\ln(Z)$ and $W[0,0] = \beta F$ where F is the free energy. As in statistical mechanics, we can generate expectation values from

the function W:

$$\frac{\delta W[J,R]}{\delta J(x)} =< \varphi(x) >_{J,R} \equiv \Phi(x) \tag{B.2}$$

and

$$\frac{\delta W[J,R]}{\delta R(x,y)} = \frac{1}{2} < \varphi(x)\varphi(y) > \equiv \frac{1}{2}(\Phi(x)\Phi(y) + G(x,y)) \ . \tag{B.3}$$

We proceed stepwise: first we take the Legendre transform with respect to J:

$$\Gamma^R[\Phi] = W[J,R] - \int_x \Phi(x)J(x) \ . \tag{B.4}$$

This is nothing but the 'standard' 1PI effective action for a theory with action

$$S^R[\varphi] = S[\varphi] + \frac{1}{2}\int_{xy} \varphi(x)R(x,y)\varphi(y) \ . \tag{B.5}$$

In deriving the properties of this effective action, we have to take care of the fact that the relation between Φ and J is now R- dependent: $J = J^R[\Phi]$.

Calculating the properties of Γ^R we find:

$$\begin{aligned} \frac{\delta\Gamma^R[\Phi]}{\delta R(x,y)} &= \frac{\delta W[J,R]}{\delta R(x,y)} + \int_z \underbrace{\frac{\delta W[J,R]}{\delta J(z)}}_{\equiv\Phi(z)} \frac{\delta J(z)}{\delta R(x,y)} - \int_z \Phi(z)\frac{\delta J(z)}{\delta R(x,y)} \\ &= \frac{\delta W[J,R]}{\delta R(x,y)} = \frac{1}{2}(\Phi(x)\Phi(y) + G(x,y)) \end{aligned} \tag{B.6}$$

and in complete analogy to the 1PI effective action

$$\frac{\delta\Gamma^R[\Phi]}{\delta\Phi(x)} = -J(x) \ . \tag{B.7}$$

We now want to decompose $\Gamma^R[\Phi]$ into two parts:

$$\Gamma^R[\Phi] = S^R[\Phi] + \Gamma_1^R[\Phi] \tag{B.8}$$

where

$$\begin{aligned} \Gamma_1^R[\Phi] &= \Gamma^R[\Phi] - S^R[\Phi] \\ &= W[J,R] - \int_x \Phi(x)J(x) - S^R[\Phi] \\ &= -\ln\left(\int \mathcal{D}\varphi exp\left\{-\left[S[\varphi] + \int_x \varphi(x)J(x) + \frac{1}{2}\int_{xy}\varphi(x)R(x,y)\varphi(y)\right]\right\}\right) \\ &\quad -\ln\left(\int \mathcal{D}\varphi exp\left\{\int_x \Phi(x)J(x) + S^R(\Phi)\right\}\right) \ . \end{aligned} \tag{B.9}$$

After a shift $\varphi \to \varphi + \Phi$ in the first integral we find:

$$\Gamma_1^R[\Phi] \;=\; -\ln\Big(\int \mathcal{D}\varphi exp\Big\{-\Big[S^R[\Phi+\varphi] - S^R[\Phi] + \int_x \varphi(x)J(x)\Big]\Big\}\Big)\ . \tag{B.10}$$

In this expression we insert $J(x) = -\frac{\delta\Gamma^R[\Phi]}{\delta\Phi(x)} = -\frac{\delta S^R[\Phi]}{\delta\Phi(x)} - \frac{\delta\Gamma_1^R[\Phi]}{\delta\Phi(x)}$ to find

$$\begin{aligned}\Gamma_1^R[\Phi] \;=\; -\ln\Big(\int \mathcal{D}\varphi exp\Big\{-\Big[S^R[\Phi+\varphi] \;- S^R[\Phi] - \int_x \underbrace{\varphi(x)\frac{\delta S^R[\Phi]}{\delta\Phi(x)}}_{(*)} \\ +\quad \varphi(x)\frac{\delta\Gamma_1^R[\Phi]}{\delta\Phi(x)}\Big]\Big\}\Big)\ .\end{aligned} \tag{B.11}$$

Now we expand the difference $S^R[\varphi+\Phi] - S^R[\Phi]$ in a Taylor series

$$S^R[\varphi+\Phi]-S^R[\Phi] = \underbrace{\varphi(x)\frac{\delta S^R[\Phi]}{\delta\Phi(x)}}_{\text{cancels with } (*)} + \frac{1}{2}\varphi(x)[G_0^{-1}(x,y)+R(x,y)]\varphi(y)+S_{\rm int}[\Phi,\varphi] \tag{B.12}$$

where G_0^{-1} is the quadratic part of the bare action S and $S_{\rm int}$ contains cubic and higher order terms in $\varphi(x)$.

For a theory with interaction $\sim \frac{\lambda}{4!}\int_x \varphi(x)^4$ we would simply find

$$S_{\rm int}[\varphi,\varphi] = \int_x \frac{\lambda}{6}\Phi(x)\varphi(x)^3 + \frac{\lambda}{4!}\varphi(x)^4 \tag{B.13}$$

and

$$G_0^{-1} = \frac{\delta^2 S}{\delta\varphi(x)\delta\varphi(y)}|_{\varphi=\Phi} = (m\frac{\partial^2}{\partial\tau^2} + m\omega^2 + \frac{\lambda}{6}\Phi(x^2))\delta(x-y)\ . \tag{B.14}$$

As usual in field theory, we write the full (R-dependent) inverse Propagator in Terms of a Schwinger-Dyson equation which, in our case *defines* the proper self-energy Σ^R:

$$\frac{\delta^2\Gamma^R[\Phi]}{\delta\Phi(x)\delta\Phi(y)} = G^{-1}(x,y) + R(x,y) - \Sigma^R(x,y;\Phi)\ . \tag{B.15}$$

The proper self-energy defined in this way clearly contains *only one particle irreducible* (1PI) diagrams.

In order to complete the derivation, we take the Legendre transform with respect to R in order to get the full 2PI effective action:

$$\begin{aligned}
\Gamma[\Phi,G] &= \Gamma^R[\Phi] - \int_{x,y} \frac{\delta\Gamma^R[\Phi]}{\delta R(x,y)} R(x,y) \\
&= \Gamma^R[\Phi] - \int_{x,y} \underbrace{\frac{\delta W[J,R]}{\delta R(x,y)}}_{=\frac{1}{2}(\Phi(x)\Phi(y)+G(x,y))} R(x,y) \qquad \text{(B.16)} \\
&= \Gamma^R[\Phi] - \frac{1}{2}\int_{xy} \Phi(x)R(x,y)\Phi(y) - \frac{1}{2}\underbrace{\int_{xy} R(x,y)G(x,y)}_{\mathrm{Tr}(RG)} \\
&= \Gamma_1^R[\Phi] + \underbrace{S^R[\Phi] - \frac{1}{2}\int_{xy} \Phi(x)R(x,y)\Phi(y)}_{S[\Phi]} - \frac{1}{2}\mathrm{Tr}(RG) \\
&= \Gamma_1^R[\Phi] + S[\Phi] - \frac{1}{2}\mathrm{Tr}(RG)\ .
\end{aligned}$$

The derivatives of $\Gamma[\Phi,G]$ are easily found:

$$\frac{\delta\Gamma[\Phi,G]}{\delta\Phi(x)} = -J(x) - \int_y R(x,y)\Phi(y) \qquad \text{(B.17)}$$

$$\frac{\delta\Gamma[\Phi,G]}{\delta G(x,y)} = -\frac{1}{2}R(x,y)\ . \qquad \text{(B.18)}$$

In most physical applications, the external fields $J(x)$ and $R(x,y)$ are zero and the above equations state that the full propagator G and the 'classical' field Φ are saddle points of the 2PI effective action $\Gamma[\Phi,G]$.

We motivate the common way of writing the 2PI effective action by considering the 1-loop result first. In order to do so, we denote with $S^{(2)}$ the part bilinear in the fluctuating fields of the action. Taking only the '*tree level*' and the quadratic bilinear part of the action into account we find

$$\Gamma[\Phi,G]^{(1-loop)} = S[\Phi] + \frac{1}{2}\mathrm{Tr}\ln[S^{(2)}] + \frac{1}{2}\mathrm{Tr}RG \qquad \text{(B.19)}$$

denoting $S^{(2)} = G^{-1} = G_0^{-1} - R$ and consequently $R = G_0^{-1} - G^{-1}$ we find the following expression for the one-loop effective action:

$$\Gamma[\Phi,G]^{(1-loop)} = S[\Phi] + \frac{1}{2}\mathrm{Tr}\ln\left(G^{-1}\right) + \frac{1}{2}\mathrm{Tr}\left(G_0^{-1}G - 1\right)\ . \qquad \text{(B.20)}$$

Using this result we decompose the 2PI effective action into one part which is of the form of the one-loop expression and into another part Γ_2 which contains all the rest.

$$\Gamma[\Phi,G] = \underbrace{S[\Phi] + \frac{1}{2}\mathrm{Tr}(\ln G^{-1}) + \frac{1}{2}\mathrm{Tr}(G_0^{-1}G - 1)}_{\text{one-loop expression}} + \underbrace{\Gamma_2[\Phi,G]}_{\text{all the rest}} \quad . \tag{B.21}$$

The first terms are reminiscent of the one-loop result and $\Gamma_2[\Phi,G]$ stands for all the rest. A simple comparison with the definition of the proper self-energy B.15 reveals that from $\frac{\delta\Gamma[\Phi,G]}{\delta G(x,y)} = -\frac{1}{2}R(x,y)$ one immediately gets the identity

$$\Sigma(x,y;\Phi) = 2\frac{\delta\Gamma_2[\Phi,G]}{\delta G(x,y)} \tag{B.22}$$

as we know that $\Sigma(x,y;\Phi)$, being a proper self-energy, contains only one particle irreducible diagrams we immediately know that Γ_2 can only contain two-particle irreducible diagrams. Else, the derivative with respect to G -namely Σ - would contain a one-particle *reducible* diagram.

This is all the importance of the 2PI effective action, because the restriction to only 2PI diagrams diminishes the number of diagrams one has to calculate at a given order enormously. We finally restate this important result:

$\Gamma_2[\Phi,G]$ *is given by all two particle irreducible Graphs with propagator lines set equal to G; the 2PI Graphs are constructed from* $S[\Phi+\varphi]$. *Terms cubic and quartic in* Φ *give the vertices:*

$$\Sigma(x,y;\Phi,G) = \Sigma^R(x,y;\Phi) \tag{B.23}$$

We note that setting $R = 0$ and $J = 0$ we find $\Gamma[\Phi,G] = W[0,0] = \beta F$. This means that finding the Extrema of the effective action is equivalent to finding the extrema of the free energy.

The generalization to the case of non vanishing source fields $R_{ab} = \lambda_{ab}$ as it is required in our case is obvoius. Either one solves the saddle point equations for finite R_{ab} or one includes the bilinear and nonlocal part of the action in the quadratic part of the action, the bare inverse porpagator G_0^{-1}.

B.2 Loop Expansion of the 2PI Effective Action

B.2.1 Feynman Rules for Quantum statistical Mechanics

The Generation Functional $Z(\beta, j)$ can be written as

$$\begin{aligned} Z(\beta,j) &= \mathcal{N}\exp\left\{-\sum_a \int_0^\beta d\tau \mathcal{V}(\frac{\delta}{\delta j_a(\tau)})\right\} \\ &\times \exp\left\{\frac{1}{2}\sum_{ab}\int d\tau d\tau' j_a(\tau)G_{ab}(\tau,\tau')j_b(\tau')\right\} \end{aligned} \tag{B.24}$$

The Feynman rules derived from this are identical to those for $T = 0$, provided one takes the Matsurbara propagator G_{ab} to represent the lines. Because of the periodicity in imaginary time it is most convenient to work with Matsurbara Frequencies ω_k. The energy conservation will be given by a $\beta\delta(\sum_{i=1}^4 \omega_i)$ at each vertex, where ω_i are the frequencies of the incoming lines.

We will now give the Feynman Rules for a quartic potential with 'interaction $\mathcal{V}x = \frac{g}{4!}x^4$.

1. Draw all topologically inequivalent diagrams to a given order of perturbation theory.

2. Assign a replica index a and a factor $-g\beta\delta(\sum_{i=1}^4 \omega_i)$ to every vertex of the diagram.

3. Assign a factor $G_{ab}(\omega_k)$ to every line of the diagram, where a and b are the replica indices of the endpoints of the line.

4. Sum over the frequencies of every internal and line with the measure $T\sum_n$.

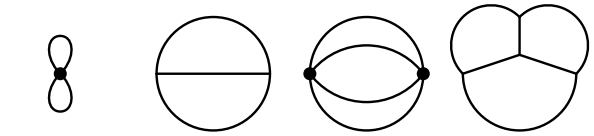
5. Sum over the replica indices of the vertices.

6. Multiply by the symmetry factor.

B.2.2 Loop Expansion of the Quartic Model

In this section we want to discuss the loop expansion of the 2PI effective action in quantum statistical problems.

The contributions corresponding to the different Feynman graphs given in Figs. (a)- (d) are as follows:



(a) (b) (c) (d)

$$\Gamma_2^a[\Phi, G] = \frac{g}{8}\int_0^\beta d\tau G^2(\tau,\tau) \tag{B.25}$$

$$\Gamma_2^b[\Phi, G] = -\frac{g^2}{12}\int_0^\beta d\tau \int_0^\beta d\tau' G^3(\tau,\tau')\Phi(\tau)\Phi(\tau') \tag{B.26}$$

$$\Gamma_2^c[\Phi, G] = -\frac{g^2}{48}\int_0^\beta d\tau \int_0^\beta d\tau' G^4(\tau,\tau') \tag{B.27}$$

$$\Gamma_2^d[\Phi, G] = \frac{g^3}{8}\int_0^\beta d\tau \int_0^\beta d\tau' \int_0^\beta d\tau'' G^2(\tau,\tau')G^2(\tau',\tau'')G(\tau,\tau'')\Phi(\tau)\Phi(\tau'') \tag{B.28}$$

At the 2-loop level in the symmetric phase, ($\Phi = 0$), we have to consider graph (a) only. The resulting expression for the 2PI effective action reads

$$\Gamma^{2-\text{loop}} = -\frac{1}{2}\text{Tr}\ln(G) + \frac{1}{2}\text{Tr}(G_0^{-1}G - 1) + \frac{g}{8}\int_0^\beta d\tau G^2(\tau,\tau) \tag{B.29}$$

which gives us just the expression for the free energy we had found in the variational approach.

Appendix C

1-RSB Formulary

In this appendix we want to derive the relevant expressions for the logarithm and the inverse of ultrametric matrices with 1-RSB structure described by the ansatz:

$$Q_{ab} = (q_d - q_1)\delta_{ab} + (q_1 - q_0)\epsilon^m_{ab} + q_0 \tag{C.1}$$

where

$$\epsilon^m_{ab} = \begin{cases} 1 & \text{when} \quad \lfloor \frac{a}{m} \rfloor = \lfloor \frac{b}{m} \rfloor \\ 0 & \text{else} \end{cases} \tag{C.2}$$

and $\lfloor \cdot \rfloor$ denotes the largest integer smaller than the argument of the brackets (Gauss brackets or floor function).

The above matrix has the following eigenvalues:

$$\lambda_s = q_d + (m-1)q_1 + (n-m)q_0 \quad \text{with 1- fold degeneracy} \tag{C.3}$$

$$\lambda_{a_1} = q_d + (m-1)q_1 - mq_0 \quad \text{with } \tfrac{n}{m} - 1 \text{ fold degeneracy} \tag{C.4}$$

$$\lambda_{a_2} = (q_d - q_1) \quad \text{with } (m-1)\tfrac{n}{m} \text{ fold degeneracy} \tag{C.5}$$

where the eigenvectors are common eigenvectors of ϵ^m with eigenvalue m, m and 0 respectively and of $\tilde{1}_n$, the $n \times n$ - matrix with all elements equal to 1 and with eigenvalues $n, 0$ and 0 respectively.

We construct the projectors on the eigenspaces in terms of ϵ_m , $\tilde{1}_n$ and $\mathbb{1}$ and write the inverse matrix as

$$Q^{-1} = -\frac{q_0}{\lambda_s \lambda_{a_1}} \tilde{1}_n - \frac{q_d - q_1}{\lambda_{a_1} \lambda_{a_2}} \epsilon^m + \frac{1}{\lambda_{a_2}} \mathbb{1}. \tag{C.6}$$

Note that $\lambda_s \to \lambda_{a_1}$ for $n \to 0$.

The Trace of the logarithm of the matrix is just the sum of the logarithms of the eigenvalues multiplied with their degeneracy and we find:

$$\begin{aligned} \mathrm{Tr}\ln Q &= \ln\left(1+\frac{nq_0}{m(q_1-q_0)+(q_d-q_1)}\right) \\ &+ \frac{n}{m}\ln\left(1+\frac{m(q_1-q_0)}{(q_d-q_1)}\right)+n\ln(q_d-q_1). \end{aligned} \tag{C.7}$$

In absence of external fields we always have the solution $q_0 = 0$. Now the derivatives with respect to the remaining parameters read:

$$\frac{\delta \mathrm{Tr}\ln Q}{\delta q_d} = \frac{q_d+(m-2)q_1}{(q_d-q_1)\left[(q_d-q_1)+mq_1\right]} \tag{C.8}$$

$$\frac{\delta \mathrm{Tr}\ln Q}{\delta q_1} = \frac{(1-m)q_1}{(q_d-q_1)\left[(q_d-q_1)+mq_1\right]} \tag{C.9}$$

$$\frac{\delta \mathrm{Tr}\ln Q}{\delta m} = \frac{1}{m^2}\ln\left[\frac{q_d-q_1}{q_d-q_1+mq_1}\right]-\frac{1}{m}\frac{q_1}{q_d-q_1+mq_1}. \tag{C.10}$$

We note that for $m = 0$ we recover the RS ansatz.

Appendix D

Stability of the RS solution

In this appendix we want to investigate the stability of the replica symmetric solution to the resummed perturbation theory presented in chapter 6. We will find that the replica symmetric solution is exact and outline an additional 2PI -vertex correction that presumably has to be taken into account in order to break this spurious symmetry.

Assuming a 1-RSB structure for the correlation function Q immediately leads to a 1-RSB structure of the argument of the logarithm in (6.6), such that the trace over the replica indices can be taken using the well known eigenvectors of ultra-metric matrices.

Doing this, we end up with

$$\begin{aligned} \frac{1}{n}\Gamma_R &= \frac{1}{2}\mathrm{Tr}\left[\frac{1}{m}\ln(\mathbb{1}+\frac{g}{2}(\hat{Q}_d^2+(m-1)q_{\mathrm{EA}}^2)) \right. \qquad \text{(D.1)} \\ &+ \left. \frac{m-1}{m}\ln(\mathbb{1}+\frac{g}{2}(\hat{Q}_d^2-q_{\mathrm{EA}}^2))\right] \\ &= \frac{1}{2}\mathrm{Tr}\left[\frac{1}{m}\ln(\mathbb{1}+\frac{g}{2}\frac{mq_{\mathrm{EA}}^2}{1+\frac{g}{2}(\hat{Q}_d^2-q_{\mathrm{EA}}^2)}) \right. \\ &+ \left. \ln(\mathbb{1}+\frac{g}{2}(\hat{Q}_d^2-q_{\mathrm{EA}}^2))\right] \qquad \text{(D.2)} \end{aligned}$$

Note that whenever correlation functions appear in the denominator of a fraction, this has to be interpreted as the inverse in the matrix sense. Moreover, the logarithms are functional ones and $\mathbb{1} = \delta(\tau - \tau')$. In the expression (D.1), the trace is over the time - arguments only. The second formulation of Γ_{R} in (D.1) points out that in the limit of vanishing Edwards-Anderson - Order - Parameter $q_{\mathrm{EA}} \to 0$, Γ_R becomes independent of m and

equal to its paramagnetic expression:

$$\Gamma_R^{\rm para} = \frac{1}{2}{\rm Tr}\ln(\mathbb{1} + \frac{g}{2}Q^2(\tau,\tau')) \tag{D.3}$$

D.1 1-RSB Saddle Point Equations

In the end, we are interested in the extrema of the 2PI effective action and we have to take the derivatives of Γ_R with respect to its parameters. We find

$$\begin{aligned}
\frac{1}{n}\frac{\partial\Gamma_R}{\partial q_d(\tau,\tau')} &= \frac{g q_d(\tau,\tau')}{2} I_d(\tau,\tau') && \text{(D.4)}\\
\frac{1}{n}\frac{\partial\Gamma_R}{\partial q_{\rm EA}} &= -\frac{g^2 q_{\rm EA}^3 (m-1)}{4} I_q && \text{(D.5)}\\
\frac{1}{n}\frac{\partial\Gamma_R}{\partial m} &= -\frac{1}{2m^2}{\rm Tr}\ln(\mathbb{1} + m\frac{g q_{\rm EA}^2}{2}U^{-1}) \\
&+ \frac{g q_{\rm EA}^2}{4m}{\rm Tr}\Big(\Big[U + m\frac{g q_{\rm EA}^2}{2}\Big]^{-1}\Big)\ . && \text{(D.6)}
\end{aligned}$$

Here we have introduced the functions

$$\begin{aligned}
I_d(\tau,\tau') &= \int d\tau'' d\tau''' \Big[U(\tau,\tau'') + (m-1)\frac{g q_{\rm EA}^2}{2}\Big] \\
&\times \Big[U(\tau'',\tau''') + m\frac{g q_{\rm EA}^2}{2}\Big]^{-1} [U(\tau''',\tau')]^{-1} && \text{(D.7)}\\
U(\tau,\tau') &= \delta(\tau-\tau') + \frac{g}{2}(q_d^2(\tau,\tau') - q_{\rm EA}^2) && \text{(D.8)}\\
I_q &= \int d\tau d\tau' d\tau'' \Big[U(\tau,\tau') + m\frac{g q_{\rm EA}^2}{2}\Big]^{-1} [U(\tau',\tau'')]^{-1}\ . && \text{(D.9)}
\end{aligned}$$

In order to get rid of the excessive convolutions, it is again convenient to pass to Fourier space. As always, assume time translational invariance in time for all time dependent quantities: $Q(\tau,\tau') = Q(\tau-\tau')$ and use the following conventions of the previous chapters for the Fourier transform. We find

$$U(\omega_l) = 1 + \frac{gT}{2}\sum_k q_d(\omega_k) q_d(\omega_l - \omega_k) - \frac{gT}{2}\tilde{q}_{\rm EA}^2\delta(\omega_l) \tag{D.10}$$

where $\tilde{q}_{\rm EA} \equiv \beta q_{\rm EA}$ is the Fourier transform of $q_{\rm EA}$. The convolutions in equations (D.4)-(D.9) become simple products in Fourier space and we find

$$
\begin{aligned}
I_d(\omega_k) &= \frac{U(\omega_k) + \frac{(m-1)gTq_{\rm EA}^2}{2}\delta(k)}{U(\omega_k)(U(\omega_k) + \frac{mgTq_{\rm EA}^2}{2}\delta(k))} && \text{(D.11)}\\
&= \frac{1}{U(\omega_k)} - \delta(k)\frac{gT}{2}q_{\rm EA}^2 I_q && \text{(D.12)}\\
I_q &= \frac{1}{(U(\omega_0) + \frac{mgTq_{\rm EA}^2}{2})U(\omega_0)} && \text{(D.13)}\\
\frac{1}{n}\frac{\partial \Gamma_R}{\partial m} &= -\frac{1}{2m^2}\ln\left[1 + \frac{mgTq_{\rm EA}^2}{2U(\omega_0)}\right] + \frac{gTq_{\rm EA}^2}{4m}\frac{1}{U(\omega_0) + \frac{mgTq_{\rm EA}^2}{2}}\\
\Sigma^2(\omega_k) &\equiv 2\frac{\delta\Gamma^2}{n\delta Q(\omega_k)} = \frac{g^2T^2}{3}\sum_{lm} Q(\omega_l)Q(\omega_m)Q(-\omega_l-\omega_m)\ . && \text{(D.14)}
\end{aligned}
$$

Using these expressions and the shorthand $x = \frac{mq_{\rm EA}}{q_d - q_{\rm EA}}$ and $y = \frac{mgTq_{\rm EA}^2}{2U(\omega_0)}$, we can write the full set of saddle- point equations for the zero modes:

$$
\begin{aligned}
\frac{1}{q_d - q_{\rm EA}} &- \frac{q_{\rm EA}}{(q_d - q_{\rm EA})(q_d + (m-1)q_{\rm EA})} = \omega^2 - J^2 q_d - \frac{gz}{2}\\
&+ gT\sum_l Q(\omega_l)I_d(-\omega_l) + \Sigma^{(2)}(\omega_0) && \text{(D.15)}
\end{aligned}
$$

and for the off-diagonal elements:

$$
\frac{q_{\rm EA}}{(q_d - q_{\rm EA})(q_d + (m-1)q_{\rm EA})} = J^2 q_{\rm EA} + \frac{g^2T^2q_{\rm EA}^3}{2}(I_q - \frac{1}{3}) \quad \text{(D.16)}
$$

or

$$
\frac{x^2}{1+x} - \frac{2y^2}{1+y} = J^2m^2q_{\rm EA}^2 - \frac{m^2g^2T^2q_{\rm EA}^4}{6}\ . \quad \text{(D.17)}
$$

The saddle point equation with respect to m can be written as

$$
-\frac{1}{2}J^2q_{\rm EA}^2 + \frac{g^2T^2}{24}q_{\rm EA}^4 = -\frac{1}{2m^2}\left[\ln(1+y) + \frac{y}{1+y}\right] + \frac{1}{2m^2}\left[\ln(1+x) + \frac{x}{1+x}\right] \quad \text{(D.18)}
$$

where the last equation holds at equilibrium only and has to be replaced by a condition of marginal stability for the 'dynamic' calculation.

Using $\Delta \equiv q_d - q_{\rm EA}$ as in the toy approximation we can relate x, y and Δ by an equation independent of m and of the temperature:

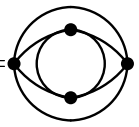
$$-J^2x^2\Delta^2 = -\left[\frac{y}{1+y} + \frac{y^2}{1+y} + \ln(1+y)\right] + \left[\frac{x}{1+x} + \frac{1}{2}\frac{x^2}{1+x} + \ln(1+x)\right] . \tag{D.19}$$

It turns out that the equations (D.16) and (D.19) have only one solution corresponding to $m = 0$, i.e. the replica symmetric solution. The solution $m = 0$ corresponds to $x = y = 0$ and is obvious from (D.19) We must conclude that the replica symmetry is not broken in the non perturbative approach presented in this section and that therefore the replica symmetry is exact in thermal equilibrium at this level of approximation.

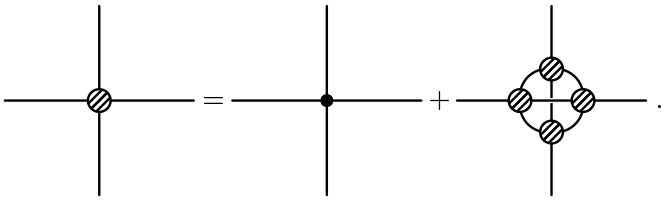
This is surprising because one would expect the solution presented above to be fairly good because we have summed a large class of diagrams. In the classical limit however, our model should become equivalent to the Sherrington-Kirkpatrick (SK) model in the limit of deep double wells, when ω^2 is negative and large in absolute value. The SK-model however is well known to display full replica symmetry breaking. At the level of approximation presented here, we have not included an order parameter q_0 (c.f. appendix C) in the 1-RSB ansatz. It is possible that including such a parameter would allow for an 1-RSB solution. However, most probally we have to include a vertix renormalization of the type presented in the next section in order to find replica symmetry breaking for the effective field theory presented in this work.

D.2 The First 2PI vertex correction

The first vacuum diagram we have not taken into account in the non perturbative approach is of order g^4 and is sometimes called the 'eye' diagram for obvious reasons. It reads

$\Gamma_{\rm eye} =$  (D.20)

This term gives rise to the first two-particle irreducible vertex correction:

 (D.21)

We suppose that this diagram would contribute to the replicon eigenvalue and thereby break the replica symmetry just as the three loop term did on top of the variational approximation. However, (D.21) generates vertices g_{aabb} with $a \neq b$ and a systematic self-consistent treatment of this vertex renormalization scheme is very involved and beyond the scope of this work.

Bibliography

[1] R.C. Zeller and R.O. Pohl Phys. Rev. **B 4**, 2029 (1971)

[2] *Tunneling Systems in Amorphous and Crystalline Solids*, edited by P. Esquinazi (Springer, Berlin 1998)

[3] S. Hunklinger and C.Enss in *Insulating and Semiconducting Glasses*, edited by P. Boochland (World Scientific, Singapore 2000)

[4] P. W. Anderson, B. I. Halperin, and C. M. Varma, Philos. Mag. **25** 1 (1972)

[5] W. A. Phillips, J. Low Temp. Phys, **7**, 351 (1972)

[6] V.G. Karpow, M. I. Klinger and F. N. Ignat'ev, Zh. Eksp. Teor. Fiz. **84**, 760 (1983) [Sovj. Phys. JETP **57**, 439 (1983)]

[7] R. Kühn, Europys. Lett. **62**, 313, (2003)

[8] C.C. Yu, A. Leggett, Comments Cond. Mat. Phys. **14**, 231 (1988)

[9] R. Kühn and U. Horstmann, Phys. Rev. Lett. **78**, 4967 (1997)

[10] P. Strehlow, C. Enss and S. Hunklinger Phys. Rev. Lett. **80** 5361 (1998)

[11] P. Strehlow, M. Wohlfahrt, A.G.M. Janssen, R. Haueisen, G. Weiss, C. Enss and S. Hunklinger, Phys. Rev. Lett. **84**, 1938 (2000)

[12] C. Enss in Proceedings of Phonons 2001 , (Physica B (Amsterdam))

[13] S. Ludwig, C. Enss, P. Strehlow, and S. Hunklinger, Phys. Rev. Lett. **88** Nr. 7 to be published 18. Feb. 2002

[14] R. Kühn and J. Urmann, J. Phys. C **12**, 6359, U. Horstmann and R. Kühn, Physica B **263 - 264**, 290 (1999)

[15] A. Heuer,R.J. Silbey,"Collective dynamics in glasses and its relation to the low-temperature anomalies, Phys. Rev. B **55**, 609-619 (1999), A. Heuer, R.J. Silbey, "Tunneling in real structural glasses: A universal theory", Phys. Rev. B **49**, 1441 (1994)

[16] R.O. Pohl, X. Liu and E. Thompson, Rev. Mod. Phys. **74**, 991 (2002)

[17] M. Mézard, G. Parisi and M. A. Virasoro *Spin Glass Theory and Beyond* (World Scientific, Singapore 1987)

[18] B. Derrida Phys. Rev. Lett. **45**, 79 (1980)

[19] D. J. Thouless, P. W. Anderson and R. G Palmer, Phil. Mag. **35** (1997) 593

[20] A. L. Fetter and J. D. Walecka *Quantum Theory of Many Particle Systems* (McGraw-Hill, New York 1971)

[21] John W. Negele, H. Orland *Quantum Many Particle Systems* (Addison Wesley, New York 1988)

[22] Michel Le Bellac, *Thermal Field Theory*, Cambridge Monographs on Mathematical Physics 1996

[23] L. F. Cugliandolo, D. R. Grempel and C. A. da Silva Santos Phys. Rev. **B 64** 014403 (2001), cond-mat/0012222

[24] L. F. Cugliandolo, D. R. Grempel and C. A. da Silva Santos, Phys. Rev. Lett. **85** 2589 (2000), cond-mat/0003268

[25] Fisher Hertz, *Spin Glasses*, Cambridge University Press

[26] A. Bray and M. Moore, J. Phys. **C 13**, L655 (1980)

[27] G. Parisi, J. Phys. A: Math. Gen. **13** 1887 (1980)

[28] R.P. Feynamn and A.R. Hibbs, *Quantum mechanics and path integrals* (McGraw-Hill, New York 1965)

[29] Press, William H., et. al, *Numerical Recipes in C, 2nd Edition*, Cambridge University Press 1992

[30] L. P. Kadanoff and G. Baym *Quantum Statistical Mecahnics* (Benjamin, New York 1962)

[31] G. Baym N.D. Mermin, J. Math. Phys. **2** (1961)

[32] A. C. Leggett *et. al.* Rev. Mod. Phys. **59**, 1 (1987)

[33] H. Horner, lecture notes *Stochastische Dynamik klassischer und quantenmechanischer Systeme* WS 1994/95

[34] U. Weiss *Quantum Dissipative Systems* (World Scientific, Singapore 1993)

[35] T.R. Kirkpatrick and D. Thirumalai, Phys. Rev. **B 36**, 5388 (1987)

[36] J. P. Bouchaud, L. F. Cugliandolo, J, Kurchan, M. Mézard in *Spin Glasses and Random Fields* edited by A. P. Young, (World Scientific, Singapore 1997)

[37] Th. M. Nieuwenhuizen, Phys. Rev. Lett. **74** 4289 (1995)

[38] A. Crisanti and H. J. Sommers, Z. Phys. **B 87** 341 (1992),A.Crisanti, H.Horner and H. J. Sommers, Z. Phys. **B 92**, 257 (1993)

[39] E. Gardner, Nucl. Phys. **B 257** 747 (1985)

[40] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989)

[41] A. Georges, G. Kolitar, W. Krauth and M. Rozenberg, Rev. Mod. Phys. **68** 13, (1996)

[42] H. Horner, private communication, unpublished.

[43] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960)

[44] P. Martin and C. De Dominicis, J. Math. Phys. **5**, 14 (1964); 31 (1964)

[45] J. M. Cornwall, R. Jackiw and E. Tomboulis, Phys. Rev. **D 10**, 2428 (1974)

[46] V. Dotsenko, M. Mézard J. Phys. A **30** (1997) 3363.

Dankeschön

Allen, die mich bei meiner Promotion unterstützt haben möchte ich von Herzen danken.

Allen voran natürlich Reimer Kühn, der immer ein offenes Ohr und viel Zeit für meine Probleme hatte und mir in langen Diskussionen geholfen hat meine Ideen zu ordnen.

Meiner Frau Sonja danke ich für ihr Verständnis für meine zeitwelige Zerstreutheit und dafür, dass ich manchmal auch beim Abendessen noch über Physik nachdenken durfte. Noch mehr danke ich ihr allerdings dafür, letzteres meistens verhindert zu haben.

Außerdem danke ich Herrn Prof. H. Horner für die Aufnahme in seine Arbeitsgruppe und die Übernahme des Zweitgutachtens sowie der gesamten Belegschaft des Instituts für theoretische Physik für die nette Athmosphäre.

Der Deutschen Forschungsgemeinschaft danke ich für die Finanzielle Unterstützung meiner Promotion im Rahmen des Projektes *Quantenstatistische Physik mikroskopischer Glasmodelle*.

Schließlich bin ich auch meinen Eltern großen Dank schuldig, die mich während des Studiums immer unterstützt und in meinen Entscheidungen begleitet haben.