

# Quantum Statistical Physics of Glasses at Low Temperatures

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We present a quantum statistical analysis of a microscopic mean-field model of structural glasses at low temperatures. The model can be thought of as arising from a random Born von Karman expansion of the full interaction potential. The problem is reduced to a single-site theory formulated in terms of an imaginary-time path integral using replicas to deal with the disorder. We study the physical properties of the system in thermodynamic equilibrium and develop both perturbative and non-perturbative methods to solve the model. The perturbation theory is formulated as a loop expansion in terms of two-particle irreducible diagrams, and is carried to three-loop order in the effective action. The non-perturbative description is investigated in two ways, (i) using a static approximation, and (ii) via Quantum Monte Carlo simulations. Results for the Matsubara correlations at two-loop order perturbation theory are in good agreement with those of the Quantum Monte Carlo simulations. Characteristic low-temperature anomalies of the specific heat are reproduced, both in the non-perturbative static approximation, and from a three-loop perturbative evaluation of the free energy. In the latter case the result so far relies on using Matsubara correlations at two-loop order in the three-loop expressions for the free energy, as self-consistent Matsubara correlations at three-loop order are still unavailable. We propose to justify this by the good agreement of two-loop Matsubara correlations with those obtained non-perturbatively via Quantum Monte Carlo simulations.

## I. INTRODUCTION

Glasses are known to exhibit distinctive low-temperature properties that differ substantially from those of crystalline solids and are referred to as glassy low-temperature anomalies. For instance, at low temperatures the specific heat and thermal conductivity in crystals show a familiar  $T^3$ -dependence. In glasses the specific heat is found to increase approximately linearly with the temperature at  $T < 1 K$ , while the thermal conductivity increases approximately as  $T^2$  in this low temperature range [1]. At higher temperatures between 1 and 20 K the thermal conductivity is approximately constant, while the specific heat  $C$  shows a peak when displayed as  $C/T^3$ , usually referred to as the Bose-peak. In phenomenological models such as the Standard Tunnelling Model [2, 3] and the soft potential model [4, 5] one postulates that a broad spectrum of tunnelling centres is responsible for the properties at  $T < 1 K$ .

Surprisingly, the glassy anomalies show a noticeable degree of universality at  $T < 1 K$ , whereas between approximately 1 and 20 K these depend more on the specific materials [1]. There are currently two main contending theories to explain this fact. Following ideas of Yu and Leggett [6], it has been suggested as resulting from a collective effect due to interactions between the tunnelling excitations [7]. Alternatively, it is thought to be a property of the potential energy landscape created by glassy freezing at high temperatures. This also defines a phenomenon of collective origin but involves no quantum effects [8]. Universality in the second interpretation is understood as a result of separation of the energy scales involved in glassy freezing on the one hand side, and those relevant for the low-temperature phenomena on the other hand side [8, 9]. Whereas the existence of tunnelling centres is part of the initial assumptions in [7], these are shown to arise naturally as a result of *microscopic* interactions in the model glasses studied in

[8, 9], and do indeed give rise to the characteristic low-temperature anomalies.

The analysis in [8, 9] is still semi-classical in the sense that it is based on an analysis of quantum effects in a glassy potential energy landscape whose properties were determined via classical statistical mechanics. The aim of the present paper is to overcome this deficit and study the system in a full quantum statistical formulation right from the outset. Focus will be here on the translationally invariant model proposed in [9].

We shall proceed along the lines of general methods developed for quantum spin-glasses. In particular, we apply the Matsubara formalism to construct an imaginary-time path integral representation of the partition function and the replica-method to deal with the disorder. The sites are decoupled by introducing order parameters for which the functional integral is evaluated by the method of steepest descent. The result is an effective single-site theory and a set of functional self-consistency relations for the order parameters. These methods are similar to those used for models studying spin-glass transitions in quantum spin-glasses. Examples are the SK-model of spin-glasses generalised to quantum spins [10] and the quantum spherical  $p$ -spin glass model [11, 12]. Here we shall not concern ourselves with the glass transition but concentrate on evaluating the physical properties at low temperatures and in particular the specific heat anomaly in the 1 K region.

To solve the effective single-site theory we first apply a perturbative method in terms of two-particle irreducible (2PI) diagrams, which is based on an expansion in powers of the full interacting correlation functions. This amounts to summing infinite classes of diagrams and can therefore also capture effects of a non-perturbative nature. After this we develop a non-perturbative theory proper. The result is a set of functional self-consistency equations for the order parameters which we first treat with Quantum Monte Carlo simulations.

Following this we construct a *solvable* version of the non-perturbative theory, using a simple approximation known from quantum spin-glass theory as the *static* approximation. This scheme was first introduced as a variational Ansatz in [10] where the time-dependent order parameter was approximated by a time-independent constant.

Given the complications of dealing with quantum fluctuations in this model, we presently restrict the analysis of both perturbative and non-perturbative theory to the replica symmetric approximation. In support of this we mention that the effects of replica symmetry breaking on the low-temperature anomalies were found to be small at the semi-classical level [8, 9].

This paper is organised as follows. In section II we summarise the main ingredients of the proposed glass model. In section III we give the many-particle partition function represented by an imaginary-time path integral and introduce replicas to handle the disorder averaging. Section IV gives an account of the effective single-site formulation, deriving the effective action and the functional self-consistency relations for the order parameters. Then in section V we treat perturbative and in section VI non-perturbative solution methods. The numerical results for the order parameters and the specific heat are discussed in section VII. Finally, the conclusions are drawn in section VIII.

## II. THE GLASS MODEL

Starting point is the microscopic model for a glass-like system at low temperatures, proposed in [9]. To summarise its main ingredients, consider a system of  $N$  degrees of freedom (called particles) with the following model-Hamiltonian

$$H = T + V = \sum_{i=1}^N \frac{p_i^2}{2m_i} + V(\mathbf{u}), \quad (1)$$

where the  $p_i$  denote the momenta and the  $m_i$  the masses, which for simplicity are taken equal for each particle. The variables  $\mathbf{u} = (u_1, \dots, u_N)$  represent coordinate deviations from pre-assigned reference positions. Since glassy low-temperature physics is universal, the interaction potential  $V(\mathbf{u})$  need not contain details of the specific atoms and their specific interactions and is taken as simple as possible, yet containing enough detail to reproduce glassy low-temperature physics. The minimum requirement is that it should respect global translation invariance and have elements of randomness and frustration. Following [9], the potential function is taken to represent the first terms of a Born von Karman expansion of the full interaction energy about the reference positions. A further requirement of global  $Z_2$ -symmetry ( $\mathbf{u} \leftrightarrow -\mathbf{u}$ ) excludes the odd orders in this expansion. Matters are further

simplified by taking the  $u_i$  to be scalar, resulting in

$$V(\mathbf{u}) = \sum_{i < j}^N \left[ \frac{1}{2} J_{ij} (u_i - u_j)^2 + \frac{g}{N} (u_i - u_j)^4 \right]. \quad (2)$$

The glassy properties are represented at the quadratic level, defining a random-interaction term with random interaction strengths  $J_{ij}$ . The quartic term (taken to be non-random) is necessary in order to stabilise the system as a whole, and so  $g > 0$ . The parameters  $J_{ij}$  are quenched and taken independent with equal Gaussian distribution  $\mathcal{N}(0, J^2/N)$  for each combination  $(i, j)$ . The  $1/N$  scaling of the variance and the quartic interaction term in (2) ensures that the thermodynamic energy is proportional to  $N$ . The construction as presented here allows the system to be analysed within replica mean-field theory, similar to that of the SK-model for spin-glasses [13], its generalization to quantum spin-glasses [10] and quantum spherical  $p$ -spin glasses [11, 12].

## III. THE PARTITION FUNCTION

The quantum statistical partition function for the fixed disorder configuration  $\{J_{ij}\}$  in a basis of coordinate states  $|\mathbf{u}\rangle = |u_1\rangle \dots |u_N\rangle$  is

$$Z_J = \text{Tr} \exp(-\beta \hat{H}) = \int d\mathbf{u} \langle \mathbf{u} | \exp(-\beta \hat{H}) | \mathbf{u} \rangle, \quad (3)$$

where the Hamiltonian  $\hat{H}$  is defined by (1) with  $u_i$  and  $p_i$  replaced by the operators  $\hat{u}_i$  and  $\hat{p}_i$ . In the Matsubara formalism the path integral representation of (3) is constructed using the Lie-Trotter product formula [14, 15]

$$\exp(-\beta \hat{T} - \beta \hat{V}) = \lim_{r \rightarrow \infty} \left\{ \exp\left(-\frac{\beta \hat{T}}{r}\right) \exp\left(-\frac{\beta \hat{V}}{r}\right) \right\}^r. \quad (4)$$

Insertions of  $\hat{1} = \int d\mathbf{u}_k |\mathbf{u}_k\rangle \langle \mathbf{u}_k|$  and  $\hat{1} = \int d\mathbf{p}_k |\mathbf{p}_k\rangle \langle \mathbf{p}_k|$ , together with definitions of imaginary time  $\tau_k = k\Delta\tau$  ( $k = 0, \dots, r-1$ ) and time-step  $\Delta\tau = \frac{\hbar\beta}{r}$ , leads to the following path integral representation of (3)

$$Z_J = \int \mathcal{D}\mathbf{u} \exp\left(-\frac{1}{\hbar} \mathcal{A}[\mathbf{u}]\right), \quad (5)$$

where the integration is in the functional sense with a measure defined as

$$\mathcal{D}\mathbf{u} = \lim_{r \rightarrow \infty} \prod_{k=0}^{r-1} \prod_{i=1}^N \sqrt{\frac{mr}{2\pi\hbar^2\beta}} du_i(\tau_k). \quad (6)$$

The functions  $u_i(\tau)$  satisfy the periodicity conditions  $u_i(0) = u_i(\hbar\beta)$ . The Euclidean action reads

$$\mathcal{A}[\mathbf{u}] = \int_0^{\hbar\beta} d\tau \left[ \sum_{i=1}^N \frac{m}{2} \left( \frac{du_i(\tau)}{d\tau} \right)^2 + V(\mathbf{u}(\tau)) \right]. \quad (7)$$

The interaction potential  $V(\mathbf{u}(\tau))$  equals the expression in (2) with  $u_i$  replaced by  $u_i(\tau)$ .

In order to study the equilibrium properties of the model we need to compute the disorder averaged free energy density  $f$ . The replica trick [16] allows us to evaluate this as

$$-\beta f = \frac{1}{N} \overline{\log Z_J} = \lim_{n \rightarrow 0} \frac{1}{Nn} \log \overline{(Z_J)^n}, \quad (8)$$

where the overline denotes the average over all realizations of the random interaction. To end this section we list the expression for  $(Z_J)^n$ , i.e. the replicated version of (5)

$$(Z_J)^n = \int \prod_{a=1}^n \mathcal{D}\mathbf{u}^a \exp\left(-\frac{1}{\hbar} \sum_{a=1}^n \mathcal{A}[\mathbf{u}^a]\right). \quad (9)$$

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$$\begin{aligned} \overline{(Z_J)^n} &= \int \prod_{a=1}^n \mathcal{D}\mathbf{u}^a \exp\left[\sum_{i < j} \left\{ \frac{J^2}{8\hbar^2 N} \left( \sum_a \int d\tau [u_i^a(\tau) - u_j^a(\tau)]^2 \right)^2 - \frac{g}{\hbar N} \sum_a \int d\tau [u_i^a(\tau) - u_j^a(\tau)]^4 \right\}\right] \\ &\quad \times \exp\left[-\frac{1}{\hbar} \sum_{ia} \int d\tau \frac{m}{2} \dot{u}_i^a(\tau)^2\right]. \end{aligned} \quad (10)$$

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The expansions of the powers in the first line of (10) contain many terms that vanish due to the following Ansatz. We assume the global  $Z_2$ -symmetry to remain unbroken after quantization:  $1/N \sum_i u_i^a(\tau) = 0$  for all  $\tau \in [0, \hbar\beta]$ .

The index  $a$  numbers the replicas and  $\mathbf{u}^a = (u_1^a, \dots, u_N^a)$ .

#### IV. EFFECTIVE SINGLE-SITE FORMULATION

In order to evaluate (8) we first average over all realizations of the random potential. This is achieved by carrying out the independent Gaussian integrations over the set  $\{J_{ij}\}$ . The result is

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This means that we do not have to consider terms of the kind  $\sum_{ij} \sum_{ab} \int d\tau \int d\tau' u_i^a(\tau)^2 u_i^b(\tau') u_j^b(\tau')$ , which would complicate the formulation considerably. The result after the expansions is

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$$\begin{aligned} \overline{(Z_J)^n} &= \int \prod_{ia} \mathcal{D}u_i^a \exp\left[\sum_{ab} \int d\tau d\tau' \left\{ \frac{J^2}{4\hbar^2 N} \left( \sum_i u_i^a(\tau) u_i^b(\tau') \right)^2 + \frac{J^2}{8\hbar^2} \sum_i u_i^a(\tau)^2 u_i^b(\tau')^2 \right\}\right] \\ &\quad - \frac{1}{\hbar} \sum_a \int d\tau \left\{ \sum_i \left( \frac{m}{2} \dot{u}_i^a(\tau)^2 + g u_i^a(\tau)^4 \right) + \frac{3g}{N} \left( \sum_i u_i^a(\tau)^2 \right)^2 \right\} \right]. \end{aligned} \quad (11)$$

The sites are decoupled with two sets of Gaussian transformations after which (11) becomes

$$\begin{aligned} \overline{(Z_J)^n} &= \int \mathcal{D}\{q_{aa}(\tau, \tau)\} \mathcal{D}\{q_{ab}(\tau, \tau')\} \\ &\quad \exp\left\{N \left( -\frac{1}{\hbar} \mathcal{X}[q] + \log Z_{\text{eff}} \right)\right\}, \end{aligned} \quad (12)$$

where  $Z_{\text{eff}}$  defines the effective single-site partition function

$$Z_{\text{eff}} = \int \prod_a \mathcal{D}u_a \exp\left(-\frac{1}{\hbar} \mathcal{S}_{\text{eff}}[u_a]\right). \quad (13)$$

The non-fluctuating part in (12) is defined as

$$\begin{aligned} \mathcal{X}[q] &= \frac{J^2}{4\hbar} \sum_{ab} \int d\tau d\tau' q_{ab}(\tau, \tau')^2 \\ &\quad - 3g \sum_a \int d\tau q_{aa}(\tau, \tau)^2. \end{aligned} \quad (14)$$

The effective single-site action reads

$$\mathcal{S}_{\text{eff}}[u_a] = \frac{1}{2} \sum_{ab} \int d\tau d\tau' u_a(\tau) q_{0,ab}^{-1}(\tau, \tau') u_b(\tau') + \mathcal{S}_{\text{int}}[u_a]. \quad (15)$$

The interaction part  $\mathcal{S}_{\text{int}}[u_a]$  contains a quartic term non-local in time and quartic term local in time

$$\begin{aligned} \mathcal{S}_{\text{int}}[u_a] = & -\frac{J^2}{8\hbar} \sum_{ab} \int d\tau d\tau' u_a(\tau)^2 u_b(\tau')^2 \\ & + g \sum_a \int d\tau u_a(\tau)^4. \end{aligned} \quad (16)$$

The ‘free’ inverse propagator is

$$\begin{aligned} q_{0,ab}^{-1}(\tau, \tau') = & \left\{ -m \frac{d^2}{d\tau^2} + 12g q_{aa}(\tau, \tau) \right\} \delta_{ab} \delta(\tau - \tau') \\ & - \frac{J^2}{\hbar} q_{ab}(\tau, \tau') \end{aligned} \quad (17)$$

Observe here that  $\mathcal{S}_{\text{eff}}[u_a]$  in (13) and thus also  $Z_{\text{eff}}$ , depend functionally on  $q_{ab}(\tau, \tau')$ .

The replicated partition function (12) can be treated with the saddle-point method. At the saddle-points we have

$$\overline{(Z_J)^n} \sim \exp \left\{ N \left( -\frac{1}{\hbar} \mathcal{X}[q] + \log Z_{\text{eff}} \right) \right\}, \quad (18)$$

where the saddle-point fields  $q_{ab}(\tau, \tau')$  are the order parameters of the theory. The saddle-point equations result in the following functional self-consistency relations for the order parameters

$$q_{ab}(\tau, \tau') = \langle u_a(\tau) u_b(\tau') \rangle. \quad (19)$$

The angular brackets  $\langle \dots \rangle$  denote the quantum thermodynamical average mediated by the effective action (15). The order parameters  $q_{ab}(\tau, \tau')$  are the full interacting correlation functions of the single-site theory, from here on called Matsubara correlations.

The Matsubara correlations are time-translational invariant since we are studying an equilibrium problem. They are also symmetric in time due to the time-reversal invariance of the action (15), i.e. we have

$$q_{ab}(\tau, \tau') = q_{ab}(\tau - \tau') = q_{ab}(\tau' - \tau). \quad (20)$$

Furthermore the Matsubara correlations  $q_{ab}(\tau - \tau')$  are  $\hbar\beta$  time-periodic.

We should mention that the first interaction term in (16) defines a complete square, which could be linearised at the cost of introducing a Gaussian family of systems. However, we have chosen not to do this at this stage. It would lead to more complicated saddle-point equations for the order parameters when solving the single-site theory perturbatively. However, we shall linearise this interaction term in the *non-perturbative* treatment.

## V. PERTURBATION THEORY

### A. 2PI-effective action formalism

To solve the single-site theory perturbatively, we need a formalism that expands the path integral (13) in terms

of a further effective (classical) action  $\Gamma_{\text{eff}}[q]$

$$\begin{aligned} Z_{\text{eff}}[q] = & \int \prod_a \mathcal{D}u_a \exp \left( -\frac{1}{\hbar} \mathcal{S}_{\text{eff}}[u_a, q] \right) \\ = & \exp \left( -\frac{1}{\hbar} \Gamma_{\text{eff}}[q] \right). \end{aligned} \quad (21)$$

Here we have explicitly referred to the functional dependences on the Matsubara correlations in  $\mathcal{S}_{\text{eff}}[u_a, q]$  and in  $Z_{\text{eff}}[q]$ . Remember, this dependence is due to the appearance of  $q_{ab}(\tau, \tau')$  in the inverse propagator (17). The  $q_{ab}(\tau, \tau')$  define the *full interacting* correlations as we saw in the previous section. As regards to a perturbative expansion of the path integral, the most efficient way is to also express  $\Gamma_{\text{eff}}[q]$  entirely in terms of the full interacting correlations, which was already assumed in the notation in (21). For this we choose the two-particle irreducible (2PI) effective action approach, developed in field theory [17, 18], which is indeed based on an expansion of  $\Gamma_{\text{eff}}[q]$  in powers of the full interacting correlators  $q_{ab}(\tau, \tau')$  and involves only 2PI diagrams. The 2PI nature of the diagrams has the additional advantage of considerably reducing the number of diagrams that need to be included in the expansion. Also, as the expansion is in terms of the full interacting correlators, the 2PI approach effectively amounts to summing infinite classes of diagrams of a conventional perturbation expansion, thus enabling it to capture effects of a *non-perturbative* nature. Usefulness of the 2PI effective action approach for the study of stochastic dynamical systems was advocated in [19]. Its application to the analysis of glassy systems was suggested in [20].

Before presenting the series expansion of  $\Gamma_{\text{eff}}[q]$ , we discuss the key ingredients of the 2PI effective action approach, in a formulation appropriate for the present problem. Following [17], one first adds a two-body source term to the action  $\mathcal{S}_{\text{eff}}$ . This defines a generating functional

$$\begin{aligned} Z_{\text{eff}}[K, q] = & \int \prod_a \mathcal{D}u_a \exp \left( -\frac{1}{\hbar} \left\{ \mathcal{S}_{\text{eff}}[u_a, q] \right. \right. \\ & \left. \left. + \frac{1}{2} \sum_{ab} \int d\tau d\tau' u_a(\tau) K_{ab}(\tau, \tau') u_b(\tau') \right\} \right) \\ \equiv & \exp \left( -\frac{1}{\hbar} W_{\text{eff}}[K, q] \right), \end{aligned} \quad (22)$$

giving

$$\frac{\delta W_{\text{eff}}[K, q]}{\delta K_{ab}(\tau, \tau')} = \frac{1}{2} q_{ab}(\tau, \tau'). \quad (23)$$

From (22) and (14) follows

$$\frac{\delta W_{\text{eff}}[K, q]}{\delta q_{ab}(\tau, \tau')} + \frac{\delta \mathcal{X}[q]}{\delta q_{ab}(\tau, \tau')} = 0, \quad (24)$$

We shall need this in the equations of motion for  $q_{ab}(\tau, \tau')$ , to be constructed next. In order to eliminate

$K$  in favour of the full interacting correlations  $q$ , one performs the following Legendre transformation

$$\Gamma_{\text{eff}}[q] = W_{\text{eff}}[K, q] - \frac{1}{2} \sum_{ab} \int d\tau d\tau' q_{ab}(\tau, \tau') K_{ab}(\tau, \tau'), \quad (25)$$

giving

$$\frac{\delta \Gamma_{\text{eff}}[q]}{\delta q_{ab}(\tau, \tau')} = \frac{\delta W_{\text{eff}}[K, q]}{\delta q_{ab}(\tau, \tau')} - \frac{1}{2} K_{ab}(\tau, \tau'). \quad (26)$$

Then setting the source field  $K_{ab}(\tau, \tau')$  to zero and using (24) results in the following ‘equations of motion’ for  $q_{ab}(\tau, \tau')$

$$\frac{\delta \Gamma_{\text{eff}}[q]}{\delta q_{ab}(\tau, \tau')} + \frac{\delta \mathcal{X}[q]}{\delta q_{ab}(\tau, \tau')} = 0. \quad (27)$$

Next is to describe the series expansion of  $\Gamma_{\text{eff}}[q]$ , which we present in the standard form as derived in [17, 18]

$$\Gamma_{\text{eff}}[G] = \frac{\hbar}{2} \text{Tr} q_0^{-1} G + \frac{\hbar}{2} \text{Tr} \log G^{-1} + \sum_{p=2}^{\infty} \Gamma_p[G], \quad (28)$$

with Green’s function  $G_{ab}(\tau, \tau') \equiv q_{ab}(\tau, \tau')/\hbar$ . As already mentioned, the variable  $q_{ab}(\tau, \tau')$  defines the full interacting correlation functions and satisfies the equations of motion (27). The traces are taken in the functional sense. The first two terms in (28) define what is called the one-loop contribution. The terms denoted by  $\Gamma_p[G]$  define the  $p$ -loop contributions. These are represented by 2PI diagrams containing  $p$  loops. In the next section we shall discuss the rules for constructing such diagrams. A diagram is said to be 2PI if it does not become disconnected upon cutting two lines. The fact that the contributions  $\sum_{p=2}^{\infty} \Gamma_p[G]$  define 2PI diagrams is understood from the following argument. The equations of motion (27) with substitutions of (14) and (28) just result in the Dyson equations

$$G^{-1} = q_0^{-1} + 2 \frac{\delta}{\delta G} \left( \sum_{p=2}^{\infty} \Gamma_p[G] \right). \quad (29)$$

Since the second part of (29) defines the proper self-energy, the diagrams of which are known to be One-Particle-Irreducible, clearly the diagrams of the terms  $\Gamma_p[G]$  must be two-particle irreducible. In the expansion of 2PI diagrams we shall consider two orders, the two-loop and the three-loop order. They are analysed in section VC and VD below.

One should mention that (28) is only valid for the special case  $\langle u_a(\tau) \rangle = 0$ . If  $\langle u_a(\tau) \rangle \equiv \mathcal{U}_a \neq 0$  a further source term in (22) is needed. This would lead to extra terms depending on  $\mathcal{U}_a$  in the effective action (28), and a further equation of motion  $\delta \Gamma_{\text{eff}}/\delta \mathcal{U}_a = 0$  [17]. We shall not concern ourselves with this case since we have assumed global symmetry to remain unbroken, i.e.  $\langle u_a(\tau) \rangle = 0$  (see section IV).

In the 2PI effective action formalism the classical form (21) results in the following expression for free energy

$$\beta f^{(2PI)} = \lim_{n \rightarrow 0} \frac{1}{n} (\mathcal{X}[q] + \Gamma_{\text{eff}}[q]), \quad (30)$$

where we have used (8) and (18).

## B. Rules for 2PI diagrams

The two interaction terms in (16) determine the following rules for constructing 2PI diagrams and their expressions. Vertices are labelled by a replica index and a time variable. Two vertices labelled by  $(a, \tau)$  and  $(b, \tau')$  are connected by a solid line contributing a factor  $\hbar G_{ab}(\tau, \tau') = q_{ab}(\tau, \tau')$ . The two interaction terms define two types of vertices. Firstly, there is a  $g$ -type vertex which is represented by a dot  $\bullet$  and contributes a factor  $-g/\hbar$ . Secondly, there is a  $J$ -type vertex which is represented by a cross  $\times$ . The  $J$ -type vertices always come in sets of two. The two are connected by a dashed line  $\times \text{---} \times$ . A dashed line contributes a factor  $J^2/8\hbar^2$ . Each diagram gets an extra factor  $-\hbar$  due to the prefactor  $-1/\hbar$  in (13). Then there is a further permutational factor to consider which we write in front of the diagram. Next is to collect all factors of a diagram and multiply them. Finally, one needs to sum over all replica indices and integrate over all time variables.

When constructing diagrams of order  $p$ , all distinct diagrams containing  $p$  loops are added together, resulting in the final expression for  $\Gamma_p[q]$ . When counting loops, both solid lines and dashed lines need to be considered. The number of loops in a diagram is equal to the power of  $\hbar$  in its expression. A subtlety here is that when counting powers of  $\hbar$ , one factor  $\hbar$  in the contribution of each dashed line  $J^2/8\hbar^2$  must not be taken into account. This is the factor  $\hbar$  that originates from the coupling constant  $J^2/8\hbar$  of the non-local interaction term in (16), which represents an interaction parameter as a whole. Finally, it should be noted that each expansion order  $\Gamma_p[q]$  contains diagrams of  $\mathcal{O}(n)$  in replica and diagrams of  $\mathcal{O}(n^2)$  or higher order. Since  $n \rightarrow 0$  the latter can be ignored. The 2PI diagrams for two-loop order ( $p = 2$ ) and three-loop order ( $p = 3$ ) are given in Fig. 1. The prefactors here result from permutations.

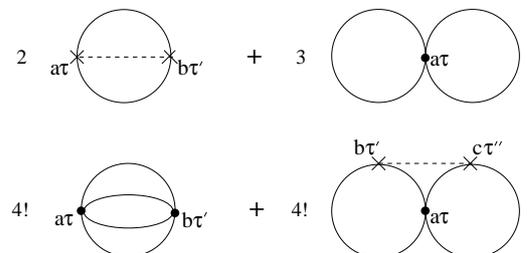


FIG. 1: Two-loop and three-loop 2PI diagrams

### C. Two-loop order

The two-loop 2PI diagrams are shown in the first line of Fig. 1. According to the rules listed in section VB these diagrams represent the following expressions

$$\begin{aligned} \Gamma_2[q] = & -\frac{J^2}{4\hbar} \sum_{ab} \int d\tau d\tau' q_{ab}(\tau, \tau')^2 \\ & + 3g \sum_a \int d\tau q_{aa}(\tau, \tau)^2, \end{aligned} \quad (31)$$

where we have used  $q_{ab}(\tau, \tau') = \hbar G_{ab}(\tau, \tau')$ . The equations for the two-loop Matsubara correlations  $q_{ab}(\tau, \tau')$  are derived from the equations of motion (27), resulting in

$$\begin{aligned} 0 = & \frac{1}{2} q_{0,ab}^{-1}(\tau, \tau') - \frac{\hbar}{2} q_{ab}^{-1}(\tau, \tau') - \frac{J^2}{2\hbar} q_{ab}(\tau, \tau') \\ & + 6g \delta_{ab} \delta(\tau - \tau') q_{aa}(\tau, \tau). \end{aligned} \quad (32)$$

These were solved in a replica symmetric approximation, and using Fourier transform techniques as described in section VII B 1 below.

### D. Three-loop order

The three-loop 2PI diagrams are shown in the second line of Fig. 1. These diagrams represent the following expressions

$$\begin{aligned} \Gamma_3[q] = & -\frac{12g^2}{\hbar} \sum_{ab} \int d\tau d\tau' q_{ab}(\tau, \tau')^4 \\ & + \frac{3J^2g}{\hbar^2} \sum_{abc} \int d\tau d\tau' d\tau'' q_{ab}(\tau, \tau')^2 q_{ac}(\tau, \tau'')^2 \end{aligned} \quad (33)$$

Again, we derive the equations for the three-loop Matsubara correlations  $q_{ab}(\tau, \tau')$  from the equations of motion (27), resulting in

$$\begin{aligned} 0 = & \frac{1}{2} q_{0,ab}^{-1}(\tau, \tau') - \frac{\hbar}{2} q_{ab}^{-1}(\tau, \tau') - \frac{J^2}{2\hbar} q_{ab}(\tau, \tau') \\ & + 6g \delta_{ab} \delta(\tau - \tau') q_{aa}(\tau, \tau) - \frac{48g^2}{\hbar} q_{ab}(\tau, \tau')^3 \\ & + \frac{12J^2g}{\hbar^2} q_{ab}(\tau, \tau') \sum_c \int d\tau'' q_{ac}(\tau, \tau'')^2. \end{aligned} \quad (34)$$

Solutions of the self-consistency equations (32) and (34) were attempted in a replica symmetric approximation, and using Fourier transform techniques as described below. First, however let us turn to a description of the two non-perturbative approaches we have looked at, both also in a replica symmetric version.

## VI. NON-PERTURBATIVE THEORY

### A. Replica symmetry

The non-perturbative theory is constructed in the replica symmetric (RS) approximation. We mention here that the effects of replica symmetry breaking on the low-temperature anomalies have been small for the *semi*-classical treatments [8, 9]. The RS form of the Matsubara correlations is

$$q_{aa}(\tau, \tau') = q_d(\tau, \tau'), \quad (35a)$$

$$q_{ab}(\tau, \tau') = q \text{ (for } a \neq b), \quad (35b)$$

independent of the replicas  $a, b$ . The off-diagonal Matsubara correlation (35b) is assumed time-independent. The argument is that the replicas are independent and time-translationally invariant, and that the origin of time could be chosen independently for each replica [10].

The RS Ansatz allows us to decouple the replicas in the effective single-site action (15). This concerns 2 terms. The first term to decouple is the non-local quartic interaction given in (16). We linearise this with a Gaussian variable  $\bar{z}$ . The second term to consider comes from the part of  $q_0^{-1}$  in (17) that involves  $q_{ab}(\tau, \tau')$ . This is decoupled by means of the Gaussian variable  $z$ . After decoupling, the effective single-site partition function (13) becomes

$$Z_{\text{eff}} = \int \mathcal{D}z \mathcal{D}\bar{z} \left\{ \int \mathcal{D}u \exp\left(-\frac{1}{\hbar} \mathcal{S}_{\text{RS}}[u; z, \bar{z}]\right) \right\}^n, \quad (36)$$

where  $\mathcal{D}z = dz/\sqrt{2\pi} \exp(-\frac{1}{2}z^2)$  and the same form for  $\bar{z}$ . The decoupled RS action reads

$$\begin{aligned} \mathcal{S}_{\text{RS}}[u; z, \bar{z}] = & \int d\tau \left[ \frac{m}{2} \left( \frac{du(\tau)}{d\tau} \right)^2 - Jz\sqrt{q} u(\tau) \right. \\ & + \frac{1}{2} \left( 12g q_d(\tau, \tau) + J\bar{z} \right) u(\tau)^2 + g u(\tau)^4 \\ & \left. - \frac{J^2}{2\hbar} \int d\tau' (q_d(\tau, \tau') - q) u(\tau) u(\tau') \right] \end{aligned} \quad (37)$$

Substituting (36) in (18) gives for the free energy (8)

$$\begin{aligned} \beta f = & - \int \mathcal{D}z \mathcal{D}\bar{z} \log \left\{ \int \mathcal{D}u \exp\left(-\frac{1}{\hbar} \mathcal{S}_{\text{RS}}\right) \right\} \\ & + \frac{1}{\hbar} \mathcal{X}_{\text{RS}}[q], \end{aligned} \quad (38)$$

where the non-fluctuating part is now defined as

$$\mathcal{X}_{\text{RS}}[q] = \frac{J^2}{4\hbar} \int d\tau d\tau' (q_d(\tau, \tau')^2 - q^2) - 3g \int d\tau q_d(\tau, \tau)^2. \quad (39)$$

Finally, the RS saddle-point equations (19) become

$$q_d(\tau, \tau') = \langle\langle u(\tau) u(\tau') \rangle\rangle_{z\bar{z}}, \quad (40a)$$

$$q = \langle\langle u(\tau) \rangle^2 \rangle_{z\bar{z}}, \quad (40b)$$

where  $\langle \dots \rangle$  denotes an average mediated by the action  $\mathcal{S}_{\text{RS}}$ , and  $\langle \dots \rangle_{z, \bar{z}}$  the averages w.r.t. the Gaussians  $z$  and  $\bar{z}$ . The theory defined by (37-40) is non-local in Matsubara time. There are currently no analytic techniques available to solve the self-consistency problem for the Matsubara correlations in this theory non-perturbatively while keeping the full complexity arising from this fact. Two different methods will be used to deal with this problem, a numerical approach using Quantum Monte Carlo simulations as proposed in [21], and the so-called static approximation due to Bray and Moore [10].

## B. Static approximation

In this approximation the non-local term (the third line in (37)) is approximated by taking for the diagonal Matsubara correlations a simple time-independent trial function

$$q_d(\tau, \tau') = q_d, \quad (41)$$

which may but need not assumed to be equal to  $q_d(\tau, \tau) \equiv q_d(0)$ . Such static approximation scheme was introduced as a variational Ansatz in [10] when studying the spin-glass transition for the SK-model generalised to quantum spins. After applying (41) we are able to linearise the non-local term of (37) by means of a further Gaussian transformation, defined by a Gaussian variable  $v$ . This results in the following static action

$$\begin{aligned} \mathcal{S}_{\text{st}}[u, v; z, \bar{z}] = & \int d\tau \left[ \frac{m}{2} \left( \frac{du(\tau)}{d\tau} \right)^2 + \frac{1}{2} v^2 \right. \\ & - J\sqrt{C} v u(\tau) + d_1(z) u(\tau) \\ & \left. + d_2(\bar{z}) u(\tau)^2 + g u(\tau)^4 \right], \quad (42) \end{aligned}$$

with  $C = \beta(q_d - q)$ . The random parameters  $d_1$  and  $d_2$  are defined as

$$\begin{aligned} d_1(z) &= -Jz\sqrt{q} \\ d_2(\bar{z}) &= \frac{1}{2}(12gq_d(0) + J\bar{z}), \quad (43) \end{aligned}$$

with  $q_d(0) = q_d(\tau, \tau)$ . The free energy (38) becomes

$$\begin{aligned} \beta f = & - \int \mathcal{D}z \mathcal{D}\bar{z} \log \left\{ \int \mathcal{D}u \int \frac{dv}{\sqrt{2\pi/\beta}} \exp \left( -\frac{1}{\hbar} \mathcal{S}_{\text{st}} \right) \right\} \\ & + \frac{1}{\hbar} \mathcal{X}_{\text{RS}}[q] \quad (44) \end{aligned}$$

with the non-fluctuating part  $\mathcal{X}_{\text{RS}}[q]$  given by (39).

Before presenting the self-consistency relations for the order parameters, let us first take a closer look at the static action (42). The parameters  $d_1(z)$ ,  $d_2(\bar{z})$  and  $g$  are the coupling constants of a potential energy for the system defined by the local *quantum* variable  $u(\tau)$ . The (quenched) Gaussians  $z$  and  $\bar{z}$  imply that we have here a heterogeneous family of such systems. This results in a

broad spectrum of *tunnelling* and *vibrational excitations*, which we shall discuss in a separate section below. Interestingly, there is another term in the action namely  $-J\sqrt{C} v u(\tau)$ , which is of a different nature. The constant  $J\sqrt{C}$  defines a coupling constant for the bilinear interaction between the variable  $u(\tau)$  and the *classical* (annealed) degree of freedom  $v$ . The latter is indeed a classical variable since it has no kinetic term associated with it. The coupling to an additional dynamic (albeit classical) variable  $v$  is reminiscent of a coupling of local degrees of freedom to a ‘heat-bath’, as it is postulated in the phenomenological models [2, 3, 4, 5] of glassy low-temperature anomalies, though the details are of course different. Whereas phenomenological models *postulate* a coupling of local degrees of freedom to the strain-field of a heat-bath of phonons as an additional ingredient, the coupling to a harmonic classical variable  $v$  in the present case *emerges* through the (approximate) mathematical treatment of quantum fluctuations.

Next we evaluate the free energy as a variational estimate w.r.t. the static Matsubara correlations  $q_d(0)$ ,  $q_d$  and  $q$ . The static formulation (42-44) defines a theory local in time. We were able to find numerical solutions for the Matsubara correlations in two different approaches, a *three-variable* approach in terms of the variables  $q_d(\tau, \tau) \equiv q_d(0)$ ,  $q_d$  and  $q$ , and a *two-variable* approach in terms of the variables  $q_d$  and  $q$ , assuming  $q_d(0) = q_d$ . The variational equations in the three-variable approach are

$$q_d(0) = \langle \langle u(\tau)^2 \rangle \rangle_{z\bar{z}}, \quad (45a)$$

$$Jq_d\sqrt{C} = \langle \langle v u(\tau) \rangle \rangle_{z\bar{z}}, \quad (45b)$$

$$q = \langle \langle u(\tau) \rangle \rangle_{z\bar{z}}^2. \quad (45c)$$

Here  $\langle \dots \rangle$  denotes an average mediated by the static action (42), while  $\langle \dots \rangle_{z, \bar{z}}$  denotes the Gaussian averages over  $z$  and  $\bar{z}$ . In the two-variable approach the variational equations are

$$J^2 C = -12g \left( \langle \langle u(\tau)^2 \rangle \rangle_{z\bar{z}} - q_d \right) + \frac{J}{\sqrt{q}} \langle z \langle u(\tau) \rangle \rangle_{z\bar{z}}, \quad (46a)$$

$$q = \langle \langle u(\tau) \rangle \rangle_{z\bar{z}}^2. \quad (46b)$$

We will solve the functional self-consistency equations (45) and (46) reverting to an operator description, and using truncated Hilbert-spaces as described in section VII B 3 below.

### 1. Tunnelling and vibrational excitations

The potential energy in the action (42) contains an ensemble of single-well and (asymmetric) double-well potentials because of the stochastic nature of the parameters  $d_1(z)$  and  $d_2(\bar{z})$  as defined in (43). These single-well and double-well potentials are responsible for respectively vibrational excitations and the characteristic

tunnelling excitations in the system [9]. We see that this potential structure arises naturally as a result of *microscopic* interactions defined by the model. In this context we mention the phenomenological soft potential model [4, 5] in which one *postulates* the existence of an ensemble of *classical* potentials  $V(u) = d_1 u + d_2 u^2 + g u^4$ , providing a semi-classical analysis of its tunnelling- and vibrational states. Whereas that model assumes a *uniform* distribution of the parameters  $d_1$  and  $d_2$ , the quantum statistical treatment of the microscopic model as presented here predicts a *Gaussian* distribution of the parameters  $d_1(z)$  and  $d_2(\bar{z})$ . Furthermore,  $d_1(z)$  and  $d_2(\bar{z})$  are parameterised by the disorder strength  $J$  and the order parameters  $q$  and  $q_d(0)$ . The *collective* nature of the latter can be seen as the origin of universality of the low-temperature physics predicted by the model.

## VII. NUMERICAL RESULTS

### A. Scaling

For numerics and representation of results we represent the theory constructed in the previous sections in terms of dimensionless variables and parameters. Starting from a microscopic length scale  $u_0$  we define the following energy scales

$$E_0 = \frac{\hbar^2}{m u_0^2}, \quad E_g = g u_0^4, \quad E_J = J u_0^2, \quad (47)$$

where  $E_0$  defines the quantum energy scale. The dimensionless ratios of the variables are

$$\tilde{u} = \frac{u}{u_0}, \quad \tilde{q} = \frac{q}{u_0^2}. \quad (48)$$

Those for the parameters are defined as

$$\tilde{g} = \frac{E_g}{E_0}, \quad \tilde{J} = \frac{E_J}{E_0}, \quad \tilde{T} = \frac{k_B T}{E_0} = \tilde{\beta}^{-1}. \quad (49)$$

Let us consider the relation between the dimensionless temperature  $\tilde{T}$  and the absolute temperature  $T$  for the simple example of vitreous silica, the amorphous state of  $SiO_2$ . Taking a microscopic length scale  $u_0 = 10^{-10} m$  and substituting the values of  $\hbar$ ,  $k_B$  and the mass  $m$  of  $SiO_2$  in the definitions above, implies for this case that  $\tilde{T} = 1$  corresponds approximately to  $T = 1$  K. In this context we shall from here on look at the dimensionless temperature  $\tilde{T}$  as an approximate representation of the absolute temperature.

In what follows we shall ignore writing the tildes on the dimensionless variables and parameters. One can show that the scaled form of all equations given in the previous sections is then obtained by setting  $\hbar = k_B = m = 1$  and  $u_0 = 1$ .

## B. Matsubara correlations

### 1. Perturbative solutions at two-loop order

The perturbative Matsubara correlations were computed at two-loop order in the RS approximation. This requires solving the saddle-point equations (32) with  $q_{aa}(\tau - \tau') = q_d(\tau - \tau')$  which is an  $\hbar\beta$ -periodic function, and  $q_{a \neq b}(\tau - \tau') = q$ . We treated them in a Fourier transformed representation. Our convention for the Fourier transform of  $\hbar\beta$ -periodic functions  $f(\tau)$  is as follows

$$f(\tau) = \sum_k e^{i\omega_k \tau} \hat{f}(\omega_k), \quad (50a)$$

$$\hat{f}(\omega_k) = \frac{1}{\hbar\beta} \int d\tau e^{-i\omega_k \tau} f(\tau), \quad (50b)$$

with Matsubara frequencies  $\omega_k = \frac{2\pi}{\hbar\beta} k$  ( $k = 0, \pm 1, \dots$ ). The advantage of this convention is that the dimension of the transformed quantity is equal to its original dimension. The Fourier transform of the saddle-point equations (32) requires computing the Fourier transform  $\hat{q}_{ab}^{-1}(\omega_k)$  of the (functional) inverse kernel  $q_{ab}^{-1}(\tau, \tau')$ . Note that the latter defines an inverse w.r.t. both replica structure and Matsubara-time integration satisfying

$$\sum_c \int d\tau'' q_{ac}^{-1}(\tau - \tau'') q_{cb}(\tau'' - \tau') = \delta_{ab} \delta(\tau - \tau'). \quad (51)$$

Using Fourier transform relations requires that

$$\sum_c \hat{q}_{ac}^{-1}(\omega_k) \hat{q}_{cb}(-\omega_k) = \delta_{ab} / (\hbar\beta)^2, \quad (52)$$

for all  $k$ , i.e. up to a factor  $1/(\hbar\beta)^2$  the Fourier transforms  $\hat{q}_{ac}^{-1}(\omega_k)$  of the inverse kernel are equal to the corresponding elements of the matrix inverse  $\hat{q}(\omega_k)_{ac}^{-1}$  of the  $\hat{q}(\omega_k)$  matrix in replica space,

$$\hat{q}_{ab}^{-1}(\omega_k) = \hat{q}(\omega_k)_{ab}^{-1} / (\hbar\beta)^2. \quad (53)$$

The RS representation of the matrix elements  $\hat{q}(\omega_k)_{ac}^{-1}$  in the  $n \rightarrow 0$  limit are given by [16]

$$\hat{q}(\omega_k)_{aa}^{-1} = \frac{1}{\hat{q}_d(\omega_k) - \hat{q}(\omega_k)} - \frac{\hat{q}(\omega_k)}{(\hat{q}_d(\omega_k) - \hat{q}(\omega_k))^2}, \quad (54a)$$

$$\hat{q}(\omega_k)_{a \neq b}^{-1} = - \frac{\hat{q}(\omega_k)}{(\hat{q}_d(\omega_k) - \hat{q}(\omega_k))^2}, \quad (54b)$$

where  $\hat{q}(\omega_k) = \hat{q}_{k,0}$ . Using (54) and (53) in the Fourier transform of (32) leads to the following equations for the two-loop RS Matsubara correlations. First, for  $k = 0$  we have of (32)

$$\frac{1}{\hat{q}_d(\omega_0) - \hat{q}} - \frac{\hat{q}}{(\hat{q}_d(\omega_0) - \hat{q})^2} = -2(\beta J)^2 \hat{q}_d(\omega_0) + 24g\beta \sum_k \hat{q}_d(\omega_k), \quad (55a)$$

$$- \frac{\hat{q}}{(\hat{q}_d(\omega_0) - \hat{q})^2} = -2(\beta J)^2 \hat{q}, \quad (55b)$$

where (55a) represents the replica-diagonal and (55b) the replica off-diagonal case. For  $k \neq 0$  we only have to consider the replica-diagonal case, giving

$$\frac{1}{\hat{q}_d(\omega_k)} = \beta \omega_k^2 - 2(\beta J)^2 \hat{q}_d(\omega_k) + 24g\beta \sum_k \hat{q}_d(\omega_k) \quad (56)$$

In the high-temperature phase where  $\hat{q} = 0$  the  $\hat{q}_d(\omega_k)$  are found numerically from (55) and (56) by solving a single self-consistency equation for the variable  $\hat{z}_1 = \sum_k \hat{q}_d(\omega_k) = q_d(0)$ , namely

$$\hat{z}_1 = \frac{1}{4\beta J^2} \sum_k \left( B_k - \sqrt{B_k^2 - 8J^2} \right), \quad (57)$$

in which  $B_k = \omega_k^2 + 24g\hat{z}_1$ . In the low-temperature phase where  $\hat{q} \neq 0$ ,  $\hat{z}_1$  can be determined analytically, entailing that the  $\hat{q}_d(\omega_k)$  can be expressed in closed form as

$$\beta(\hat{q}_d(\omega_0) - \hat{q}) = \frac{1}{J\sqrt{2}}, \quad (58a)$$

$$\hat{q}_d(\omega_{k \neq 0}) = \frac{1}{4\beta J^2} \left( B_k - \sqrt{B_k^2 - 8J^2} \right), \quad (58b)$$

$$\hat{z}_1 = \frac{\sqrt{2}J}{12g}, \quad (58c)$$

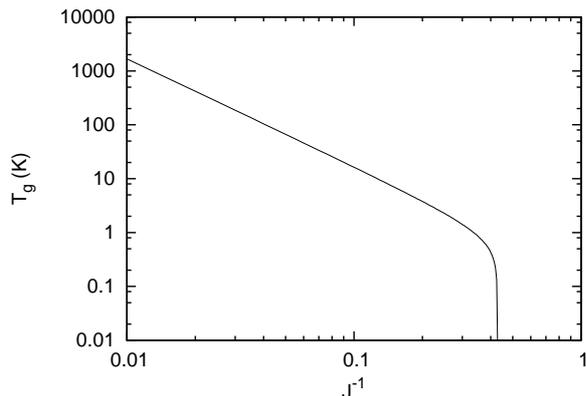


FIG. 2: Glass transition temperatures  $T_g$  vs.  $J^{-1}$  at two-loop perturbation theory for  $g = 1$ .

The glass transition temperature  $T_g$  as a function of  $J$  (at  $g = 1$ ) is shown in Fig. 2. Glass transition temperatures for structural glasses are typically in the range between 500 K and 1500 K. Clearly this requires  $J$  to be large. The majority of our results in the present study were therefore computed for a typical large  $J$ ,  $J = 50$  giving  $T_g \approx 500$  K.

Next is to discuss the solutions of (58) for the Matsubara correlations. The  $q_d(\tau)$  were computed from a numerical inverse Fourier transformation of  $\hat{q}_d(\omega_k)$ . In Fig. 3 we plot the results for  $q_d(\tau) - q$  for a number of low temperatures. A selection of them is compared with the results of Quantum Monte Carlo (QMC) simulations

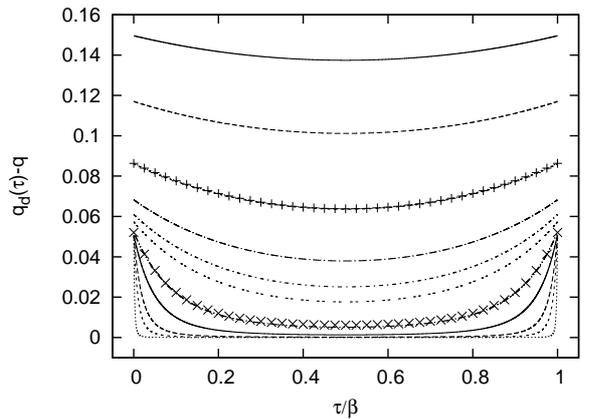


FIG. 3: Two-loop perturbative data for the function  $q_d(\tau) - q$ . Inverse temperatures (in  $K^{-1}$ ) from top to bottom are  $\beta = 0.1, 0.13, 0.2, 0.3, 0.4, 0.5, 1, 2, 5, 10, 50$ . Comparison with QMC solutions of the non-perturbative theory for  $\beta = 0.5$  and  $\beta = 1$  (marked by + and  $\times$ ).

of the *non*-perturbative theory, which will be discussed in a subsection below. The solutions for the Matsubara correlation  $q$  are plotted in Fig. 4 in the low-temperature phase. From both Fig. 3 and 4 we conclude that the two-

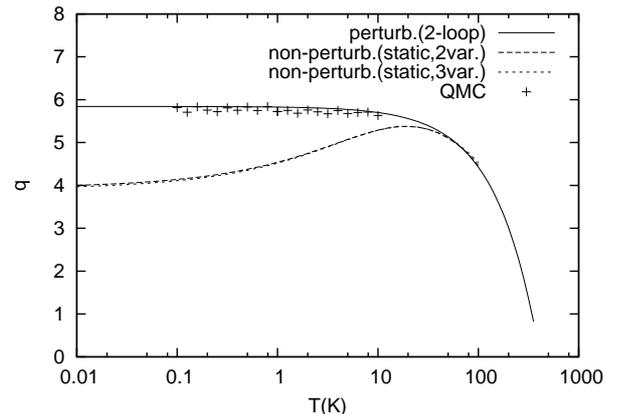


FIG. 4: Perturbative and non-perturbative data for the Matsubara correlation  $q$  in the low-temperature phase. Note the good agreement of two-loop perturbative data with non-perturbative data from Quantum Monte Carlo simulations. Data of non-perturbative static approximations deviate from these in the low-temperature region.

loop results are in reasonably good agreement with the QMC results.

The Fourier-representation of the self-consistency equations for the Matsubara correlations in the low-temperature phase at three-loop order is given in the appendix. Unlike the two-loop equations which only require the self-consistent solution of a single equation for the variable  $\hat{z}_1 = q_d(0)$ , the coupling between the Fourier modes at three-loop order contains a truly functional element via the function  $\hat{z}_3(\omega_k)$ . Although we suc-

ceeded in simplifying the problem to solving a set of only four coupled transcendental equations for the variables  $\hat{z}_1, \hat{z}_2, \hat{q}_d(\omega_0)$  and  $q$ , we have so far been unable to solve them. In fact we suspect that physically acceptable solutions may not exist at three-loop order and an expansion to higher loop order might be necessary.

## 2. Non-perturbative Quantum Monte Carlo simulations

The Matsubara correlations  $q_d(\tau)$  and  $q$  of the non-perturbative RS theory defined in section VIA above, were evaluated with Quantum Monte Carlo simulations. This involved solving the functional self-consistent relations (40). We used iterative QMC-techniques along the lines of [21], starting with a set of initial values of  $q_d(\tau)$  and  $q$  to be used as input for the action (37), after which they were updated in a path integral Monte Carlo algorithm. This procedure was repeated 10 times, resulting in reasonably good convergence of the Matsubara correlations. As regards to the algorithm, an update contained  $10^5$  Monte Carlo sweeps (taking data every 10th sweep),  $5 \cdot 10^4$  equilibration sweeps and  $5 \cdot 10^3$  Gaussian  $z, \bar{z}$  samples. The imaginary time axis was discretised into 40 time slices. The results for  $q_d(\tau) - q$  at a selected number of temperatures are plotted in Fig. 3. The results for the off-diagonal Matsubara correlation  $q$  are plotted separately in Fig. 4. As mentioned previously, they were found to be in good agreement with the solutions of the two-loop perturbative theory given in (58). The conclusion from the simulations is that they confirm the validity of the perturbative *two-loop* results for the Matsubara correlations.

## 3. Non-perturbative static solutions

The Matsubara correlations of the static approximation treated in section VIB, were computed numerically. This involved solving the functional self-consistency relations (45) and (46). They were solved in the operator representation, for which the required Hamiltonian  $\hat{H}_{\text{st}}(\hat{p}, \hat{u}, v; z, \bar{z})$  is reconstructed from the action (42). Path integrals are then re-expressed in terms of traces over a suitable truncated Hilbert space. We used a bases of harmonic oscillator eigenstates. The Gaussian integrals were computed with Gauss-Legendre quadratures.

The results for the replica off-diagonal Matsubara correlations  $q$  are plotted in Fig. 4 over a large temperature range. We believe the differences with the two-loop perturbative and QMC results seen here to be an artifact of the static approximation, which after all does not represent the true self-consistent solutions of the saddle-point equations (40).

Differences between the results of the two-variable and three-variable approach are not visible on the scale used in Fig. 4. They are plotted separately in Fig. 5 for a

selected range of low temperatures. The combination of order parameters  $C = \beta(q_d - q)$ , which can be seen as a susceptibility-like variable, was found to be approximately equal for both, the two-variable and the three-variable approach, with nearly constant numerical value  $C \approx 17 \cdot 10^{-3}$  for  $0 < T < 100 K$ . Since this is very small, the values of  $q_d$  and  $q$  barely differ at low temperatures, as is indicated in Fig. 5. On the other hand, the two-variable and three-variable approaches do give rise to different values for the  $(q_d, q)$  pairs: Introduction of a third variable  $q_d(0)$  in the three-variable approach leads to a depression of the values of  $q_d$  and  $q$  relative to those in the two-variable approach, whereas  $q_d(0)$  in the three-variable approach turns out to be larger than  $q_d$  and  $q$  within the two-variable solution.

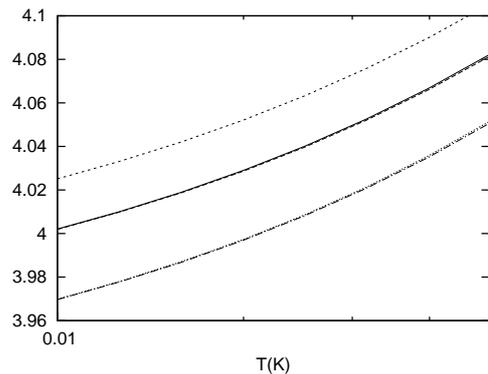


FIG. 5: The upper line shows  $q_d(0)$  in the three-variable approach. The lowest pair of lines correspond to  $q_d$  and  $q$  in the three-variable approach, whereas the pair of lines in the middle correspond to  $q_d$  and  $q$  in the two-variable approach.

## C. Thermodynamics

### 1. Perturbative specific heat

To obtain an expression for the perturbative free energy we substitute (14) and (28) in (30). We consider Fourier transforms as defined in (50) and the scaling introduced in section VII A. The trace  $\frac{1}{2}\text{Tr} \hat{q}_0^{-1} \hat{q}$  diverges when substituting  $\hat{q}_0^{-1}$  from its definition (17). Instead we substitute the expression for  $\hat{q}_0^{-1}$  determined by the saddle-point equations (32) or (34). The result is then finite up to an irrelevant infinite constant  $\frac{1}{2}\text{Tr} \hat{q}^{-1} \hat{q}$ . The trace  $\frac{1}{2}\text{Tr} \log \hat{q}^{-1}$  can be shown to have the following RS representation [16]

$$\frac{1}{2}\text{Tr} \log \hat{q}^{-1} = -\frac{n}{2} \sum_k \left\{ \frac{\hat{q}(\omega_k)}{\hat{q}_d(\omega_k) - \hat{q}(\omega_k)} + \log(\hat{q}_d(\omega_k) - \hat{q}(\omega_k)) \right\}, \quad (59)$$

where  $n$  defines the number of replicas. Observe that when substituting  $\hat{q}(\omega_k) = \hat{q} \delta_{k,0}$  the second part of (59)

contains the divergent sum  $-\frac{1}{2} \sum_{k \neq 0} \log \hat{q}_d(\omega_k)$ . To deal with this we first substitute  $\hat{q}_d(\omega_k)$  from (56) or (62). From the result we isolate a divergent contribution of the following form  $\frac{1}{2} \sum_k \log \{\beta(\omega_k^2 + 24g\hat{z}_1)\}$  with  $\hat{z}_1 = \sum_k \hat{q}_d(\omega_k)$ . This term, as part of (59) and  $\Gamma_{\text{eff}}$  in (28), should be exponentiated according to (21), defining the partition function of a simple harmonic oscillator with frequency  $\omega_0 = \sqrt{24g\hat{z}_1}$ . Consequently, we may replace  $\frac{1}{2} \sum_k \log \{\beta(\omega_k^2 + \omega_0^2)\}$  by ( $\beta$  times) the free energy of a simple harmonic oscillator, giving  $\log \sinh(\frac{1}{2}\beta\omega_0)$  which is now finite.

To compute the RS free energy numerically we have only the two-loop data from (58) at our disposal. The specific heat computed from the two-loop free energy did *not* result in a glassy low-temperature anomaly. Only vibrational excitations of the system featured here (see Fig. 6). On the other hand, when evaluating the free

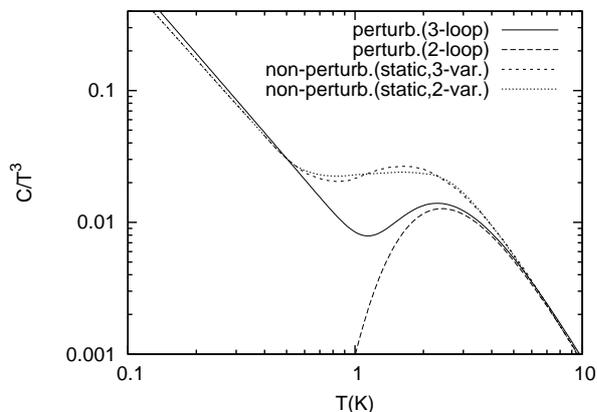


FIG. 6: Approx. linear specific heat  $C \sim T^{1.02}$  ( $T < 0.8 K$ ) and  $C \sim T^{1.1}$  ( $T < 0.5 K$ ) for resp. perturbative (three-loop) and non-perturbative (static) theory and a Bose-peak at higher temperatures. The two-loop perturbative theory described only the vibrational excitations.

energy at three-loop order, a specific heat exhibiting the characteristic glassy low-temperature anomalies was obtained ( $C \sim T^{1.02}$  for  $T < 0.8 K$ ), though we had to use two-loop results for the Matsubara correlations in those expressions (as three-loop results are so far unavailable). The good agreement between two-loop Matsubara correlations and QMC results is thought to provide a reasonable justification for this approach.

## 2. Non-perturbative specific heat

The non-perturbative thermodynamics was evaluated in the *static* approximation. For this we used the free energy expression (44) and the numerical results determined from (45) and (46). This indeed reproduced the characteristic glassy low-temperature specific heat anomaly for both the two-variable and three-variable approach (see Fig. 6). Again the low-temperature spe-

cific heat showed an approximately linear (in fact super-linear) temperature dependence  $C \sim T^{1.1}$  for  $T < 0.5 K$ , in reasonable agreement also with experimental data [1][22]. We found little difference in these results for the two-variable and three-variable approach at higher temperatures, as can be seen in Fig. 6. Differences between the three-loop perturbative specific heat and the non-perturbative ‘static’ specific heat are restricted to the  $0.5 - 5 K$  temperature region. This could be at least partly because of the strong temperature dependence of the ‘static’ Matsubara correlations in this region, as displayed in Fig. 4 for the order parameter  $q$ .

## VIII. CONCLUSIONS

In summary, we have provided a fully quantum statistical analysis of a microscopic model of a glass, respecting global translation invariance. Until now such analysis was available only at a semi-classical level. We formulated an effective theory in terms of single-site path integrals and constructed perturbative and non-perturbative solutions of a set of self-consistency equations describing the system. Both resulted in an approximately linear specific heat at low temperatures, in good agreement with experiment.

The perturbation theory was formulated in terms of two-particle irreducible diagrams at two-loop and three-loop order for the effective action. As solutions of the self-consistency equations at three-loop order remained unavailable, we resorted to investigating the reliability of our two-loop results using Quantum Monte Carlo simulations. We found surprisingly good agreement of the Matsubara correlations obtained perturbatively and via QMC simulations.

Within a non-perturbative static approximation we obtain a description in terms of a glassy potential energy landscape containing an ensemble of effective single-well and double-well potentials, much as in the soft-potential model [4, 5] and in the semi-classical approach [9]. Interestingly there is an important difference, namely the emergence of a coupling to an additional classical variable in a manner reminiscent of a coupling of local excitations to a heat bath as postulated within phenomenological models [23].

It would be interesting to carry the perturbative approach to higher loop order, or in fact attempt summations of infinite classes of 2PI diagrams. On another front, effects of replica symmetry breaking have not yet been looked at and are worth investigating (though in a semi-classical approach RSB effects were found to be weak [9]).

One of the motivations for the present investigation was to understand a phase transition observed in ultra-cold glasses more than a decade ago [24], which has so far not found an explanation. Regrettably, the present study has not produced any progress in that particular direction. It might well be the case that an expansion of the

present investigation in *both* directions mentioned above — including effects of replica symmetry breaking and inclusion of diagrams up to arbitrarily high loop order — would be required to reveal pertinent signatures of that phase transition.

## IX. APPENDIX

Here we present the Fourier transformed RS representation of the *three*-loop perturbative equations (34) in the low-temperature phase. Considering the scaling introduced in section VII A and using (53) and (54), the Fourier transformation leads to the following set of equations. First, for  $k = 0$  we have

$$\frac{1}{\hat{q}_d(\omega_0) - \hat{q}} - \frac{\hat{q}}{(\hat{q}_d(\omega_0) - \hat{q})^2} = -2(\beta J)^2 \hat{q}_d(\omega_0) + 24g\beta \hat{z}_1 - 96(\beta g)^2 \hat{z}_3(\omega_0) + 24(\beta J)^2 g \hat{q}_d(\omega_0) \beta (\hat{z}_2 - \hat{q}^2), \quad (60a)$$

$$-\frac{\hat{q}}{(\hat{q}_d(\omega_0) - \hat{q})^2} = -2(\beta J)^2 \hat{q} - 96(\beta g)^2 \hat{q}^3 + 24(\beta J)^2 g \hat{q} \beta (\hat{z}_2 - \hat{q}^2), \quad (60b)$$

where (60a) represents the replica-diagonal and (60b) the replica off-diagonal case. The last two terms in these equations define the *three*-loop extensions of the two-loop equations (55). Here we used the following definitions

$$\hat{z}_2 = \sum_k \hat{q}_d(\omega_k)^2, \quad (61a)$$

$$\hat{z}_3(\omega_k) = \sum_{lm} \hat{q}_d(\omega_l) \hat{q}_d(\omega_m) \hat{q}_d(\omega_k - \omega_l - \omega_m). \quad (61b)$$

For  $k \neq 0$  we only have to consider the replica-diagonal case, giving

$$\frac{1}{\hat{q}_d(\omega_k)} = \beta \omega_k^2 - 2(\beta J)^2 \hat{q}_d(\omega_k) + 24g\beta \hat{z}_1 - 96(\beta g)^2 \hat{z}_3(\omega_k) + 24(\beta J)^2 g \hat{q}_d(\omega_k) \beta (\hat{z}_2 - \hat{q}^2), \quad (62)$$

where the last two terms again represent the three-loop extensions of the two-loop equations. The solutions of (60) can no more be expressed in analytic form as was the case for the two-loop perturbative equations (58).

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