A Solvable Model of a Glass

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Abstract

An analytically tractable model is introduced which exhibits both, a glass–like freezing transition, and a collection of double–well configurations in its zero–temperature potential energy landscape. The latter are generally believed to be responsible for the anomalous low–temperature properties of glass–like and amorphous systems via a tunneling mechanism that allows particles to move back and forth between adjacent potential energy minima. Using mean–field and replica methods, we are able to compute the distribution of asymmetries and barrier–heights of the double–well configurations analytically, and thereby check various assumptions of the standard tunneling model. We find, in particular, strong correlations between asymmetries and barrier–heights as well as a collection of single–well configurations in the potential energy landscape of the glass–forming system — in contrast to the assumptions of the standard model. Nevertheless, the specific heat scales linearly with temperature over a wide range of low temperatures.

1 Introduction

The present contribution is primarily concerned with the anomalous low–temperature properties of amorphous and glass–like materials. A prominent example of such an anomaly is the roughly linear temperature dependence of the specific heat at $T < 1$ K, which is in stark contrast to the $T^3$ behaviour known to originate from lattice vibrations in crystalline materials. Further anomalies are reported for the temperature dependences of the thermal conductivity and other transport properties.

To explain these anomalies, a phenomenological model — the so–called standard tunneling model (STM) [1, 2, 3] — has been introduced. It is based on two assumptions, which are plausible but until today are still lacking an analytic foundation based on microscopic modelling. First, it is assumed that even at temperatures well below the glass temperature, small local rearrangements of single atoms or of small groups of atoms are possible via tunneling between adjacent local minima in the potential energy surface.

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of the system. Second, individual local double–well configurations of the potential energy surface are taken to be randomly distributed, and a specific assumption is advanced concerning the distribution \( P(\Delta, \Delta_0) \) of asymmetries \( \Delta \), and tunneling–matrix elements \( \Delta_0 \), viz., \( P(\Delta, \Delta_0) \sim \Delta_0^{-1} \). The value of \( \Delta_0 \) is related with the barrier–height \( V \) between adjacent minima and the distance \( d \) between them. In WKB–approximation one has \( \Delta_0 = \hbar \omega_0 \exp(-\lambda) \), with \( \lambda = d^2 \sqrt{2mV/\hbar^2} \). Here \( \omega_0 \) is a characteristic frequency (of the order of the frequency of harmonic oscillations in the two wells forming the double well structure), \( m \) the effective mass of the tunneling particle, and \( d \) the separation between the two minima of the double well. In terms of \( \Delta \) and \( \lambda \) one has \( P(\Delta, \lambda) \approx \text{const} \).

The STM describes experimental data reasonably well at low temperatures, i.e. for \( T < 1 \text{ K} \) (for an overview, see e.g. [4]). At temperatures above \( 1 \text{ K} \), one observes a (non–phonon) \( T^3 \) contribution to the specific heat and a plateau in the thermal conductivity which cannot be accounted for within the set of assumptions of the STM. To model these phenomena, alternative assumptions concerning the distribution of local potential energy configurations have been advanced, such as those leading to the so–called soft–potential model [5, 6], where it is assumed that locally the potential energy surface can be described by fourth order polynomials of the form \( V(x) = u_0[u_2x^2 + u_3x^3 + x^4] \), with \( u_0 \) a fixed parameter and \( u_2 \) and \( u_3 \) independently distributed in a specific way. Under certain assumptions about these distributions, these systems also exhibit a collection of ‘soft’ (an)harmonic single–well potentials, supporting localized soft vibrations which can reasonably well account for both, the crossover to \( T^3 \)–behaviour of the specific heat above \( 1 \text{ K} \) as well as the plateau in the thermal conductivity.

On the other hand, simulations that tried to detect double–well potentials in quenched Lenard–Jones mixtures [7] produced results which did not fit well with the assumptions of the soft–potential model, but could be described by an ansatz that leads to a generalized soft–potential model, viz. \( V(x) = w_2x^2 + w_3x^3 + w_4x^4 \), with all three coefficients \( w_\alpha \) independently distributed in a specific way. Evaluations are, however, as yet based on rather moderate statistics.

For the time being, it is perhaps safe to say that both, the STM and the soft–potential model provide phenomenological descriptions, based on assumptions which — while plausible in many respects — are still lacking analytic support based on more microscopic approaches.

Here we propose a microscopic model inspired by spin–glass theory which exhibits both, a glass–like freezing transition at a certain glass–temperature \( T_g \), and a collection of double–well configurations in its zero–temperature potential energy surface. Within this model, we shall not only be able to compute the full statistics of double–well configurations believed to be responsible for the low–temperature anomalies but also exhibit relations between low–temperature and high–temperature phenomena, e.g. between the low–temperature specific heat and the value of the glass–transition temperature itself.

Our line of reasoning is as follows. In Sec. 2, we propose an expression for the potential energy of a collection of particles forming an amorphous model system, which is taken to be random in its harmonic part, and which includes anharmonic on–site potentials to stabilize the system as a whole. We choose our setup in such a way that it can be analysed exactly within mean–field theory, and the replica method is used to deal with the disorder.
By these means, the phase diagram of the model can be computed (Sec. 3), and we observe that it has a glass–like frozen phase at sufficiently low temperatures.

In mean–field theory, the system is described by an ensemble of effective single–site problems, characterized by single–site potentials which contain random parameters; replica theory in this context can be understood as a method to compute the distribution of these parameters self–consistently. The potential energy surface of the original model is thereby represented as the zero temperature limit of the aforesaid ensemble of independent single–site potentials, and we are able to identify regions of parameter space where some members of this ensemble have double–well form. The distribution of the parameters characterizing the double–well potentials (DWPs) — asymmetries and barrier heights — can be computed analytically within replica theory (Sec. 4). Taking these distributions as input of a tunneling model, we are able to compute the contribution of the tunneling states to various low–temperature anomalies. In the present paper we shall restrict our attention to the specific heat at low temperatures. Section 5 contains a summary of our achievements and an outlook on open problems.

## 2 The Model

Consider the following expression for the potential energy of a collection of $N$ degrees of freedom (particles for short) forming an amorphous or glass–like system,

$$ U_{\text{pot}}(v) = -\frac{1}{2} \sum_{i,j} J_{ij} v_i v_j + \frac{1}{\gamma} \sum_i G(v_i), \tag{1} $$

in which $v_i$ ($1 \leq i \leq N$) may be interpreted as the deviation of the $i$-th particle from some preassigned reference position. We propose to model the amorphous aspect of the system by taking the first, i.e. the harmonic contribution to $U_{\text{pot}}(v)$ to be random, so that the reference positions and thereby the entire system would quite generally turn out to be unstable in the harmonic approximation. This is why a set of anharmonic on–site potentials $G(v_i)$ is added to stabilize the system as a whole.

To be specific, we take the $J_{ij}$ to be independent Gaussians with mean $J_0/N$ and variance $J^2/N$. In order to fix the energy- and thus the temperature scale, we specialize to $J = 1$ in what follows. For the on–site potential we choose

$$ G(v) = \frac{1}{2} v^2 + \frac{a}{4!} v^4. \tag{2} $$

That is, $G$ also creates a harmonic restoring force, and by varying the parameter $\gamma$ in (1) we can tune the number of modes in the system which are unstable at the harmonic level of description. Other forms of $G(v)$ may be contemplated; our method to solve the model does not depend on the particular shape of $G$. The only requirement is that it increases faster than $v^2$ for large $v$ for the system to be stable.

The harmonic contribution to (1) is reminiscent of the SK spin–glass model [8], apart from the fact that we are dealing with continuous ‘spins’ here, without any local or global constraints imposed on them. Models of the type introduced above — albeit with different
couplings and different choices for $G(v)$ — have, however, been studied in the context of analogue neuron systems [3, 4]. A model with Gaussian couplings, but different $G$ has been considered by Bös [11].

The choice of quenched random couplings in (1) certainly puts our model outside the class of glass–models in the narrow sense. In view of recent ideas concerning the fundamental similarity between quenched disorder and so–called self–induced disorder as it is observed in glassy systems proper [13], it may nevertheless be argued that our choice should capture essential aspects of glassy physics at low temperatures.

To analyze the potential energy surface, we compute the (configurational) free energy of the system

$$f_N(\beta) = -(\beta N)^{-1} \ln \int \prod_i dv_i \exp[-\beta U_{pot}(v)]$$

and take its $T = 0$ limit, using replica theory to average over the disorder, so as to get typical results. Standard arguments [8] give

$$n f_n(\beta) = \lim_{n \to 0} f_n(\beta)$$

for the quenched free energy, with

$$f_n(\beta) = \frac{1}{2} J_0 \sum_a m_a^2 + \frac{1}{4} \beta \sum_{a,b} q_{ab}^2 - \beta^{-1} \ln \int \prod_a dv^a \exp [-\beta U_{eff}(\{v^a\})].$$

Here

$$U_{eff}(\{v^a\}) = -J_0 \sum_a m_a v^a - \frac{1}{2} \beta \sum_{a,b} q_{ab} v_a v_b + \frac{1}{\gamma} \sum_a G(v^a)$$

is an effective replicated single–site potential, and the order parameters $m_a = N^{-1} \sum_i \langle v_i^a \rangle$ and $q_{ab} = N^{-1} \sum_i \langle v_i^a v_i^b \rangle$ are determined as solutions of the fixed point equations

$$m_a = \langle \langle v^a \rangle \rangle_z, \quad a = 1, \ldots, n$$

$$q_{ab} = \langle \langle v^a v^b \rangle \rangle_z, \quad a, b = 1, \ldots, n ,$$

where angular brackets denote a Gibbs average corresponding to the effective replica potential (5), and where it is understood that the limit $n \to 0$ is eventually to be taken.

So far we have evaluated (4)–(7) only in the replica symmetric approximation by assuming $m_a = m$ for the ‘polarization’–type order parameter, and $q_{aa} = \hat{q}$ and $q_{ab} = q$ for $a \neq b$ for the diagonal and off–diagonal entries of the matrix of Edwards-Anderson order parameters. These are determined from the fixed point equations

$$m = \langle \langle v \rangle \rangle_z ,$$

$$\hat{q} = \langle \langle v^2 \rangle \rangle_z ,$$

$$q = \langle \langle v^2 \rangle \rangle_z .$$

Here $\langle \ldots \rangle_z$ denotes an average over a zero-mean unit-variance Gaussian $z$ while $\langle \ldots \rangle$ without subscript is a Gibbs average corresponding to the effective replica-symmetric single–site potential

$$U_{RS}(v) = -[J_0 m + \sqrt{q} z] v - \frac{1}{2} C v^2 + \frac{1}{\gamma} G(v)$$

with $C = \beta(\hat{q} - q)$. The replica symmetric approximation thus describes a Gaussian ensemble of independent single-site potentials $U_{RS}(v)$, with parameters $m$, $q$ and $C$ which are determined self-consistently through (8).
3 Phase Diagram

The system described by (8)–(9) exhibits a glass-like freezing transition from an ergodic phase with $m = q = 0$ to a frozen phase with $q \neq 0$ at some temperature $T_g$ depending on the parameters $J_0$ and $\gamma$ of the model. If $J_0$ is sufficiently large, a transition to a macroscopically polarized phase with $m \neq 0$ may also occur.

![Phase Diagram](image)

Figure 1: $T = 0$ phase diagram. $E$ denotes the $T = 0$–limit of the ergodic phase, $G$ the glassy phase, and $P$ a phase with macroscopic polarization. The bold line is the AT line. Below the (small) dotted line is the region with DWPs. The bigger dots separate the glassy phase $G$ from the phase $P$ with macroscopic polarization.

The assumption of replica symmetry is not always correct. Spontaneous replica symmetry breaking (RSB) occurs at low temperatures (large $\beta$) and large $\gamma$. The precise location of the instability against RSB is given by the AT criterion \cite{12}

$$1 = \beta^2 \left\langle \left( \langle v^2 \rangle - \langle v \rangle^2 \right)^2 \right\rangle_z = \frac{1}{q} \left\langle \left( \frac{d}{dz} \langle v \rangle \right)^2 \right\rangle_z,$$

the second expression being more appropriate for an evaluation in the $T = 0$-limit.

Phase boundaries between ergodic and non-ergodic phases are increasing functions of $\gamma$, diverging as $\gamma \to \infty$, and approaching zero for finite values of $\gamma$ which can be read off from the $T = 0$ phase diagram of the model in Fig. 1.

Interestingly, the system can also exhibit a collection of DWPs in its zero-temperature potential energy surface. The following Sect. is devoted to extracting their statistics, and to analyzing their contribution to the low-temperature specific heat.

4 Double–Well Potentials and Specific Heat

We take the $T \to 0$ ($\beta \to \infty$) limit of the above set (8) of fixed point equations to compute the $T \to 0$ limit of the order parameters characterizing the ensemble (9) of effective replica symmetric single–site potentials, which in turn represents the potential energy surface of
Figure 2: Effective replica–symmetric single–site potential for two different values of $\tilde{h} = J_0m + \sqrt{q}z$. (a) $\tilde{h} = 0.1$. (b) $\tilde{h} = 0.5$. In (a), the asymmetry $\Delta$ is the difference between the two minima, the barrier height $V$ is the difference between the maximum and the (lower) minimum, and $d$ is the separation between minima on the $v$ axis. In both cases we have $\gamma^{-1} = 0.5$ and $J_0$ such that $m = 0$.

In contrast to the assumptions of the STM, we find that $\Delta$ and $\lambda$ are strongly correlated random variables; in the RS approximation both are functions of one Gaussian random variable, viz. $z$, as shown in Fig. 3. The distributions $P(\lambda)$ and $P(\Delta)$ are depicted in Fig. 4. Both have singularities at their upper boundary, the former an integrable divergence, the latter a cusp singularity. A notable feature here is that upper and lower limits of the $\lambda$ and $\Delta$ ranges are given within our approach, and the total mass under either distribution gives the fraction of degrees of freedom which ‘see’ DWPs.
Despite the differences in the shape of $P(\Delta, \lambda)$ from that assumed in the STM, we find that the contribution of the tunneling states to the specific heat – taking the tunnel splitting to be given by $\epsilon = \sqrt{\Delta^2 + \Delta_0^2}$, and ignoring higher excitations – exhibits an extended range of temperatures where it scales linearly with $T$, and we find this phenomenon to be more pronounced, as we move deeper into the DWP phase, i.e., deeper also into the glassy phase as it is described in our model (see Fig. 5). At very low temperatures exponential behaviour of the specific heat is observed which is due to the cutoff in the $\lambda$ distribution, which in turn creates a cutoff in the density of states at low energies.

5 Summary and Outlook

We have proposed and solved a simple model which exhibits both, a glass–like freezing transition, and a collection of DWPs in its zero temperature potential energy landscape. The latter are generally believed to give rise to a number of low-temperature anomalies in glassy and amorphous systems via a tunneling mechanism that allows particles to move back and forth between the wells forming the DWP structure at temperatures where thermally activated classical motion would still be rather unlikely. Within our model, we were able to compute the distribution of the parameters characterizing the DWPs analytically, and we found, in particular, strong correlations between asymmetries $\Delta$ and the parameter $\lambda$ which determines the magnitude of the tunneling matrix element $\Delta_0$. Nevertheless, we observe an extended range of low temperatures at which the contribution of the two-level tunneling systems to the specific heat scales linearly with temperature. The correlations between $\lambda$ and $\Delta$ can be weakened (but most likely not eliminated) by introducing local randomness, i.e., by introducing either a randomly $i$–dependent $\gamma$ or by making other parameters of the on–site potentials $i$–dependent in a random fashion. It has been demonstrated elsewhere [10] that the model remains solvable with these modifications.

So far, we have evaluated only the replica symmetric approximation. At the same time we know that RSB is observed in the interesting region of the phase diagram where
Figure 4: Distributions $P(\Delta)$ (for positive $\Delta$), and $P(\lambda)$. Here $\gamma = 4$, while $J_0$ is as in Fig. 2. The total mass under either distribution is 0.138 and gives the fraction of particles which ‘see’ DWPs.

DWP’s actually do occur. However, it can be shown that DWPs and even the correlation between asymmetries and tunneling matrix element persist at all finite levels of RSB [16]; the distribution of the parameters characterizing them may of course change in details. The one- and two-step RSB approximations [14] as well as Parisi’s full RSB scheme [15] for this model are currently being evaluated [16].

Concerning the motivation of (1) via the idea of an expansion of the potential energy about a set of reference positions, it should be noted that in principle a linear random–field type term should be added to $U_{pot}$. While such a term does change details of the low-temperature properties of the system, we find that the main physics is left invariant [16].

Up to now we have not investigated relations between high–temperature and low–temperature properties of our system in any detail, but it should be obvious that they exist — all properties are determined from the two model–parameters $\gamma$ and $J_0$ — and that they are within relatively easy reach of our approach; they are currently under study [16]. Moreover, we have as yet treated the DWPs only as two–level systems, which entails that their contribution to the specific heat levels off and eventually decreases to zero as
the temperature is further increased. Clearly, the contribution of higher excitations as well as that of the single well configurations to physical quantities must finally be taken into account as well.

It should be pointed out that our model will also exhibit interesting dynamical properties at or near its glass transition temperature and very likely throughout the glassy phase, which are worth investigating. Indeed, formally such an investigation already exists [17], albeit for the Langevin dynamics of a model with $G$ chosen differently, so as to describe Ising spins. It would be interesting to see which features of that model will survive in the present context, and which will turn out to be altered.

In the present paper we have chosen to quantize our system only after a mean-field decoupling. For ordered, translationally invariant systems, the validity of this procedure has been rigorously proven by Fannes et al. [18]. A corresponding proof for disordered systems is still lacking. Therefore, it would be interesting to study the system in a full quantum statistical context right from the outset, using imaginary time path integrals in conjunction with the replica method. It would seem feasible to solve the system along these lines at least within the so called static approximation. The clear connection to the DWP
concept, to which we have access precisely through the mean–field decoupling scheme is, however, likely to be lost in a solution along these lines.

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