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Spin-glass approach to low-temperature anomalies in glasses

Uta Horstmann, Reimer Kühn*

Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 19, 69120 Heidelberg, Germany

Abstract

We discuss a spin-glass-type approach to the physics of structural glasses, which leads to a class of models that exhibit both glassy low-temperature phases and double- and single-well configurations in their potential energy landscape. The low-temperature anomalies characteristic of amorphous systems are reproduced, and within our model the universality issue can be illuminated. We consider the interaction between localized excitations and phonons, and we present a general expression for the dynamic susceptibility, from which dynamic properties such as the internal friction can be calculated. © 1999 Elsevier Science B.V. All rights reserved.

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It is well known that at low-temperatures glassy systems exhibit anomalies in almost all their thermodynamic, transport and dynamic properties, see e.g. Refs. [1,2]. Below 1 K they are *universal* in the sense that they are shared by virtually *all* glassy and amorphous systems. They have found their phenomenological explanation in the standard tunneling model (STM) [3,10] (for $T < 1$ K) and in its extension, the soft potential model (SPM) [4,11,12] (up to around 10 K). While both models assume specific ensembles of random local potential energy configurations, they do not provide a *mechanism* to explain *how* these would arise.

The very existence of universality is the starting point of our microscopic approach, because it implies that the detailed form of the interaction between the particles should play a subordinate role in the emergence of glassy low temperature anomalies. Inspired by spin-glass physics (see e.g. Ref. [5]), we choose a model with *random interactions* to produce a glassy phase. Their specific form is taken such that the model can be solved via mean-field and replica techniques. The details of this ansatz were elaborated elsewhere [6], so that here we just give a brief review. We start out from N degrees of freedom (described by their deviations v_i from certain reference positions) forming a glass-like system which are subject to an interaction energy given by

$$U_{\text{int}}(\{v_i\}) = -\tfrac{1}{2}\sum_{i\neq j} J_{ij}v_iv_j + \sum_i G(v_i). \tag{1}$$

The first part represents the interactions, chosen to be random with a Gaussian distribution of the couplings J_{ij} of mean J_0/N and variance $1/N$. The second part represents local anharmonic on-site potentials of the form $G(v) = (a_2/2)v^2 + (a_4/4!)v^4$. It is natural to take their harmonic part a_2, which can

* Corresponding author. Fax: + 49-6221-549331; e-mail: kuehn@tphys.uni-heidelberg.de.

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be viewed as contributing to the J_{ii}, to be random as well [8].

In a mean-field setting the system is described by an ensemble of effective single-site problems, $U_{\rm int} \to \sum U_{\rm eff}$, with

$$U_{\rm eff}(v) = -h_{\rm eff}\, v - \tfrac{1}{2}Cv^2 + G(v). \qquad (2)$$

Here $h_{\rm eff}$ is random and both, C and $P(h_{\rm eff})$, are computed self-consistently. The system can be shown to exhibit glassy and (for sufficiently large J_0) polarized low-temperature phases [6–8]. The potential energy landscape described by Eq. (2) comprises both, double-well configurations (DWPs) as in the STM as well as single-well configurations as in the SPM. The former occur if C in Eq. (2) is sufficiently large compared to a_2. Since C is of *collective* origin this can result in a purely *dynamic* creation of DWPs. Their spectrum of asymmetries is determined by $P(h_{\rm eff})$ and thus also of *collective* origin in contrast to contributions of the *local* potentials $G(v)$. Moreover, we find amorphous phases *without* low-energy tunneling excitations which might be discussed in the context of the experiments of Liu et al. [9].

The specific heat follows from the spectra of excitations in the $U_{\rm eff}$-ensemble. We find (Fig. 1) $C(T) \sim T$ at low T due to tunneling excitations, largely determined by *collective* effects (thus *universal*), and a subsequent boson peak at higher T, mainly determined by *local* quantities (thus *non-universal*). These results are rather insensitive to the presence or absence of randomness in the $G(v)$.

For the calculation of dynamic properties we must consider the interaction between the localized excitations and phonons, which manifests itself in resonance and relaxation phenomena. The basic assumption is a bilinear interaction between the local coordinates v_i and the phonon bath, mediated by the strain-field,

$$H = H_{\rm S} + H_{\rm B} + H_{\rm SB} = \frac{p^2}{2m} + U_{\rm eff}(v) + \sum_{ks} \hbar\omega_{ks} b_{ks}^\dagger b_{ks} + v\sum_s \gamma_s e_s\,, \qquad (3)$$

with s labelling the acoustic branches of the phonon spectrum, e_s denoting the contribution of branch s to the strain field at site i, and appropriate

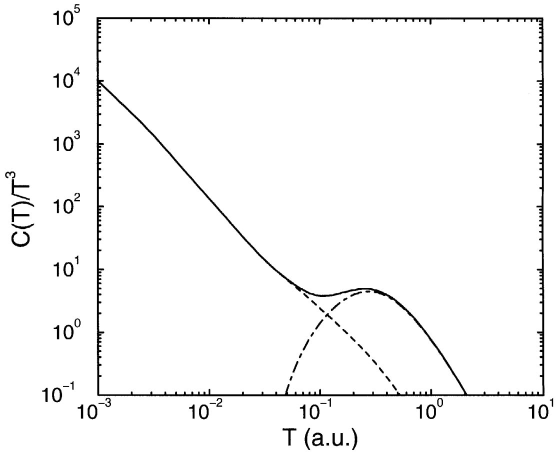

Fig. 1. C/T^3 plot of specific heat: (dashed line) = contribution of tunnel regime; (dot-dashed line) = contribution of quasiharmonic excitations ($J_0 = 0$, $a_4 = 0.25$, $\bar{a}_2 = 0.25$, $\sigma_{a_2} = 1.25$).

coupling constants γ_s. A Debye model is assumed for the phonon bath.

In order to map out the physics in the relevant subspace we applied Mori–Zwanzig projection techniques to compute the symmetrized centered correlation function $\hat{C}_{vv}(t)$ of the fluctuation operators $\Delta v = v - \langle v \rangle$. Its spectral function is related to that of the dynamic susceptibility $\chi''_{vv}(\omega)$ via a fluctuation dissipation theorem. In the weak coupling limit we get a resonant contribution

$$\chi''^{\rm res}_{vv}(\omega) = \frac{1}{\hbar}\tanh\left(\frac{\hbar\omega}{2k_{\rm B}T}\right)\sum_{m\neq n} v_{mn}^2(p_m + p_n) \times \frac{1/\tau_{mn}}{(\omega - \Omega_{nm})^2 + 1/\tau_{mn}^2} \qquad (4)$$

from the transitions between any two different energy levels in $U_{\rm eff}$ (not exceeding some highest excitation $n_{\max}$), where v_{nm} are transition matrix elements, $\hbar\Omega_{nm} = E_n - E_m$, $p_n = {\rm e}^{-E_n/k_{\rm B}T}/Z$, and where the widths of the levels are related to the quantum mechanical transition rates $\Gamma_{mn} = v_{nm}^2 \pi\alpha\Omega_{nm}^3({\rm e}^{\beta\hbar\Omega_{nm}} - 1)^{-1}$ via $1/\tau_{mn} = \frac{1}{2}\sum_k(\Gamma_{mk} + \Gamma_{nk})$ (with $\alpha = \sum_s \hbar\gamma_s^2/4\pi^2\rho c_s^5$). The relaxational contribution

$$\chi''^{\rm rel}_{vv}(\omega) = \frac{2}{\hbar}\tanh\left(\frac{\hbar\omega}{2k_{\rm B}T}\right)\sum_{m,n} v_{mm}v_{nn} \times \sum_k \frac{\lambda_k}{\omega^2 + \lambda_k^2} U_{mk} U_{kn}^{-1} p_n \qquad (5)$$

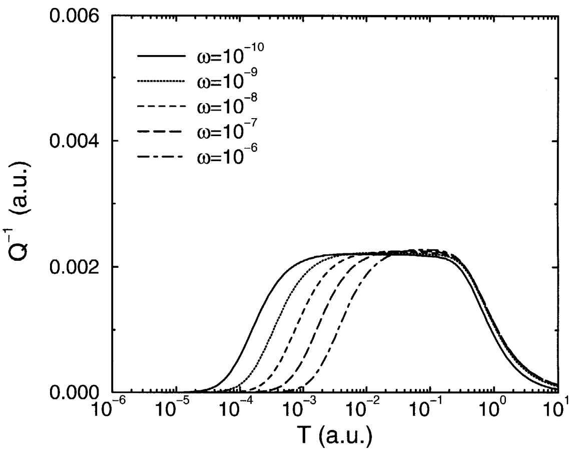

Fig. 2. Internal friction for different external frequencies ($J_0 = 0$, $a_4 = 0.25$, $\bar{a}_2 = 0.25$, $\sigma_{a_2} = 1.25$).

comprises $n_{\max} - 1$ relaxation channels. Here the relaxation rates λ_k are the eigenvalues of the rate matrix $W_{mn} = \delta_{mn}\sum_k \Gamma_{mk} - \Gamma_{nm}$, and U is its diagonalizing matrix. For low T the contributions of the higher levels are thermally suppressed and thus our model obviously approaches the TLS-physics in that temperature range. There the dynamics are governed by slow inter-well transitions via tunneling, but for higher T the fast intra-well transitions between 'quasiharmonic' levels must be taken into account, too.

As a first quantity we calculated the internal friction $Q^{-1} = \gamma^2/\rho c^2 \overline{\chi''_{vv}(\omega)}$ as an average over h_{eff} and a_2. A fluctuating a_2 in $G(v)$ was proven nesessary to reproduce the experimental data, specifically the rise with T^3 at very low T and a plateau of 1 to 3 orders of magnitude in T, depending on the external frequency (see Fig. 2). As Eqs. (4) and (5) only include one-phonon processes we are not able to reproduce the peak observed at the upper end of the plateau which is usually attributed to thermally activated processes over the barrier.

We have presented a model-based rather than phenomenological approach to glassy physics. It provides insights into microscopic mechanisms responsible for the emergence of low-temperature anomalies, and allows to understand their degree of universality.

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