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 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 crystaline 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 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

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Δ₀ is related with the barrier-height \( V \) between adjacent minima and the distance \( d \) between them. In WKB-approximation one has \( Δ₀ = ħω₀ \exp(-λ) \), with \( λ = \frac{2}{\hbar} \sqrt{2mV/\hbar^2} \). Here \( ω₀ \) 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 \( Δ \) and \( λ \) one has \( P(Δ, λ) \simeq \text{const.} \)

The STM describes experimental data reasonably well at low temperatures, i.e. for \( T < 1 \) K (for an overview, see e.g. [4]). At temperatures above 1 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 \( V(x) = u₀[x² + u₃x³ + x^4] \), with \( u₀ \) a fixed parameter and \( u₂ \) and \( u₃ \) 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 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. \( V(x) = w₂x² + w₃x³ + w₄x^4 \), with all three coefficients \( w₂ \) 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