The potential energy landscape of the $\pm J$ Ising spin glass

Sharon C Glotzer†, Naeem Jan‡ and Peter H Poole§

† Polymers Division and Center for Theoretical and Computational Materials Science,
National Institute of Standards and Technology, Gaithersburg, MD 20899, USA
‡ Department of Physics, St Francis Xavier University, Antigonish, Nova Scotia,
Canada, B2G 2W5
§ Department of Applied Mathematics, University of Western Ontario, London, Ontario,
Canada, N6A 5B7

Abstract. We calculate 'inherent structures' (configurations corresponding to local potential energy minima) in the $\pm J$ Ising spin glass over a wide range of temperature T in two and three dimensions. We find that the T-dependence of the average value of the inherent-structure energy E is strikingly similar to that shown recently for a glass-forming liquids. E decreases with T only weakly at high T, but begins to decrease much more rapidly as the spin-glass transition temperature T_{sg} is approached. As in the liquid, we find that the rapid decrease of E with decreasing T occurs in the regime of T in which the relaxation of the spin autocorrelation function becomes increasingly non-exponential. In addition, we show that the inherent structures of the spin glass can be used to identify clusters of strongly correlated 'frozen' spins, and that an incipient percolating cluster of these spins appears (within numerical error) at $T = T_{sg}$.

1. Introduction

Disordered systems cooled toward their glass transition temperature exhibit complex dynamical behaviour. For example, the density autocorrelation function (the intermediate-scattering function) of glass-forming liquids [1] and the spin autocorrelation function of spin glasses [2–4] both decay exponentially at high temperature T, but non-exponentially at lower T. For both systems these autocorrelation functions at large time t are well described by a stretched exponential or Kohlrausch–Williams–Watts (KWW) function $A \exp[-(t/\tau)^{\beta}]$.

Recently, Sastry *et al* [5] showed that the development with decreasing T of non-exponential relaxation in a glass-forming Lennard-Jones liquid is correlated with changes in the system's exploration of its potential energy landscape. In the landscape paradigm as it applies to atomic liquids [6], the state point of the system (given by the $3N$ particle coordinates) moves on a potential energy hypersurface in a $(3N + 1)$-dimensional space. This surface contains many local minima. Basins can be drawn around each minimum such that a steepest-descent minimization of the potential energy maps any state point in that basin to the minimum of the basin. The configuration of the system at such a minimum is termed an 'inherent structure' of the liquid [7]. At sufficiently low T, the dynamics of the liquid can be viewed as a combination of vibrational motion of the state point within a basin, and transitions over barriers between different basins [8]. Sastry *et al* [5] calculated E, the average value of the potential energy of the inherent structures of the liquid as a function of T. They reported that the onset of non-exponential relaxation is correlated with a 'crossover temperature' below which E decreases rapidly with decreasing T, and above which it decreases very slowly. A

change in the T-dependence of the average enthalpy of inherent structures of a supercooled liquid was found in earlier work by Jonsson and Anderson [9]. This phenomenon has also been observed in results from simulation studies of water [10].

The Ising spin glass is an archetypal model of a glass-forming system with quenched disorder [11]. Monte Carlo (MC) computer simulation studies of the $\pm J$ Ising spin glass have shown that increasingly non-exponential relaxation develops in the paramagnetic phase as T decreases toward the spin-glass transition temperature T_{sg} [3]. In the present work we calculate the T-dependence of the average inherent-structure energy E for the $\pm J$ Ising spin glass to determine whether in this system there also exists a correlation between the appearance of complex relaxation dynamics and changes in the potential energy landscape explored by the system. We find that for both dimension $d = 2$ and $d = 3$, there is a striking similarity between the behaviour of E for the spin glass and that reported for liquid simulations. Our results are also consistent with behaviour recently reported for p-spin models of spin glasses [12]. In addition, we find that the results provide an opportunity to realize a quantitative description of the spin-glass transition in terms of the occurrence of a percolation transition of correlated 'frozen' spins.

2. Methods

The $\pm J$ Ising spin glass is described by the Hamiltonian $H = -\sum_{\langle ij \rangle} J_{ij} s_i s_j$, on a square ($d = 2$) or simple cubic lattice ($d = 3$). In our simulations the external magnetic field is zero. Lattices are prepared by randomly assigning exchange interactions $J_{ij} = \pm J$ to the edges of the lattice, and placing on the vertices (sites) Ising spins s with values ± 1. The sum in H is taken over all nearest-neighbour (nn) pairs of sites. Our simulations are performed using the heat-bath Monte Carlo algorithm [13] with helical boundary conditions for lattices of size 32^3 and 128^2 (except where otherwise indicated). For this model the transition temperature $kT_{sg}/J = 1.175 \pm 0.025$ ($d = 3$) [4] and 0 ($d = 2$) [14]; k is Boltzmann's constant. As a reference, it is useful to note the Curie temperature T_c of the corresponding ferromagnetic Ising model, in which $J_{ij} = +J$ for all nn interactions: for $d = 2$, $kT_c/J = 2.269$ [15] while for $d = 3$, $kT_c/J = 4.51154$ [16]. All the results reported here use one specific random arrangement of exchange interactions. We have confirmed that using a different random arrangement of exchange interactions does not change our results.

In general, a steepest-descent minimization of the energy of a spin system proceeds by successively locating and flipping that spin with the largest positive energy [17]. The minimization procedure ends when only sites with negative energy remain; that is, when flipping any single spin would raise the energy of the system. Due to the discrete nature of the exchange interactions in the $\pm J$ Ising spin glass studied here, the site with the largest positive energy is in general not unique, and so a steepest-descent minimization procedure is not defined. Despite this, many configurations of the $\pm J$ Ising spin glass exist for which the energy cannot be further decreased via single spin flips and we define these configurations to be inherent structures of the system. Any procedure for quenching the energy of an equilibrium configuration via a path in configuration space along which the energy decreases monotonically will terminate in such an inherent structure. If the procedure is deterministic, then the potential energy surface of the system in configuration space can be unambiguously partitioned into basins surrounding inherent-structure minima.

With these considerations in mind, we choose the following procedure to map equilibrium configurations of the $\pm J$ Ising spin glass to inherent structures: starting from a given configuration of spins, a quench is carried out by setting $T = 0$ in the Boltzmann factor that controls the probability for spin flips in heat-bath dynamics, and performing MC iterations until

the energy no longer changes. Setting $T = 0$ in the Boltzmann factor has the result that spin flips that lower the energy are always accepted, spin flips that raise the energy are never accepted, and spin flips that keep the energy unchanged are accepted with probability $1/2$. This algorithm ensures that during the quench, the system energy decreases monotonically. The absence of changes that increase the energy prevents the system from moving over barriers separating one basin from another on the potential energy landscape. The system thus approaches a local minimum of the potential energy, i.e. an inherent structure, and not the absolute global minimum. To have a deterministic procedure, we update sites in 'typewriter' order, starting in one corner of the system and proceeding from site to site, row by row. As a check, we have also updated sites in random order, and confirmed that the results reported here for averaged quantities are unchanged.

Our quench algorithm is not as efficient as might be expected of a steepest-descent procedure. For example, we find that even after 10^5 Monte Carlo steps per spin (MCS), infrequent small decreases of the energy are occasionally observed. Our quench algorithm therefore generates an approximate value for the local minimum energy of a basin. Extrapolation of our results to an infinite number of quench steps suggests that this estimate is within 0.1% of the actual value. We also note that for the spin-glass model studied here, the inherent-structure configuration corresponding to a local minimum of the energy is not in general unique. At all times during our quench procedure, and in the final inherent structure, a set of sites exists for which a change of spin state does not change the potential energy.

3. Temperature dependence of inherent-structure energy

For both $d = 2$ and 3 we study T-values from $kT/J = 0.2$ to 6.0. Simulations are carried out first at the highest T; simulations at successively lower T are then initiated using a configuration generated at higher T. We fix the maximum time to attempt to equilibrate the system at all T to 10^7 MCS. Relaxation times increase rapidly as $T \rightarrow T_{sg}$ and exceed this fixed equilibration time at approximately $kT/J = 1.0$ for $d = 2$ and $kT/J = 1.6$ for $d = 3$. That is, the system is in equilibrium above this T, but incompletely relaxed and out of equilibrium below. For each T a 'production' stage is then initiated. The MC evolution of the system is continued at the given T, and every 10^3 MCS the current configuration of the system is quenched using the algorithm described above to obtain the corresponding inherent-structure energy. The number of lattice updates required for the quenches ranges from 10^4 at high T to 10^5 at our lowest T. The average inherent-structure energy E is calculated for each T from approximately 1000 quenches.

Figures 1 and 2 show E as a function of T for $d = 2$ and 3. As stated above, at low T the relaxation time of the system exceeds our observation time and the system is no longer in equilibrium. Equilibrium data are shown in figures 1 and 2 as filled circles, whereas data points obtained for incompletely relaxed states are shown with open circles. We find that E decreases weakly with T for high T, and then begins to decrease more rapidly with decreasing T for T substantially above T_{sg}. We emphasize that this effect is well established in the equilibrium data, and is not an artifact due to loss of ergodicity in the system. Comparison of these figures with figure 1 of reference [5] and figure 2(b) of reference [9] shows that the change in topography of the potential energy landscape with decreasing T in the Ising spin glass (as measured by E) is qualitatively the same as that observed in simulations of glass-forming liquids.

In the non-equilibrium regime, the decrease of E with T slows as $T \rightarrow 0$, and (particularly for $d = 3$) shows a crossover to a nearly constant value, again similarly to the liquid simulations. This behaviour is due, at least in part, to freezing in of the configurational properties of
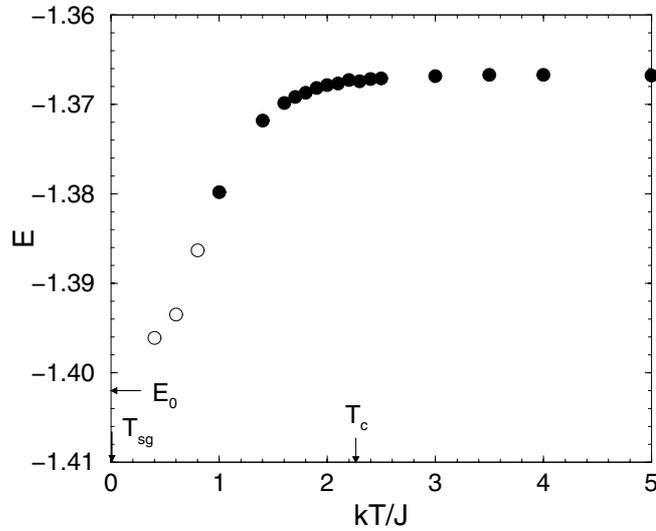
Figure 1. Average inherent-structure energy E versus T for $d = 2$. Both equilibrium data (•) and data points for incompletely relaxed states (○) are shown.
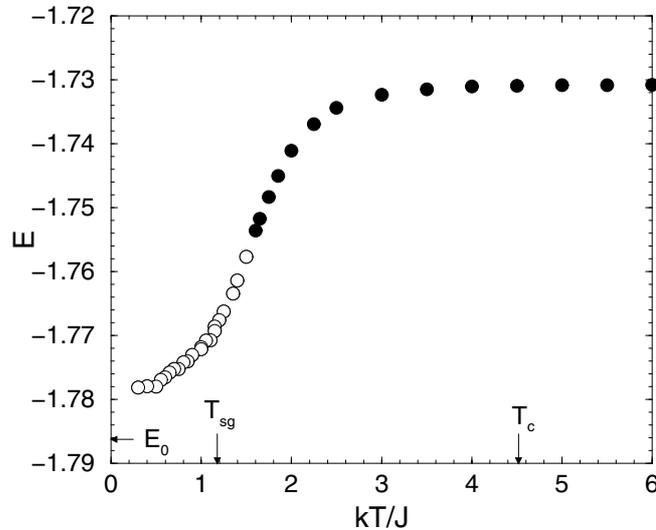
Figure 2. Average inherent-structure energy E versus T for $d = 3$. Both equilibrium data (•) and data points for incompletely relaxed states (○) are shown.

the system as ergodicity is lost. However, it is helpful to compare the low-T values of E with estimates of the global ground-state energy E_0 of the $\pm J$ Ising spin glass. E_0 is, by definition, a lower bound on E. In $d = 2$ dimensions, a recent study [18] found that $E_0 = 1.401\,93 \pm 0.000\,02$, while in $d = 3$ dimensions, $E_0 = 1.7863 \pm 0.0004$ has been reported [19]. Figures 1 and 2 show that if these estimates of E_0 are correct (and assuming that E is a monotonic function of T), then the underlying equilibrium behaviour of E at low T must be qualitatively the same as that shown in the plots. That is, the overall shape of the E-versus-T curve can be described as approaching a constant both in the high- and low-T

limits, continuously connected by a crossover region centred at a value of T above T_{sg} but below T_c. The data exhibit an inflection point at $kT/J \approx 0.8$ for $d = 2$ and $kT/J \approx 1.5$ for $d = 3$. We note that the equilibrium energy has an inflection point (i.e. a maximum of the specific heat) at $kT/J = 1.6$ for $d = 2$ [20] and $kT/J = 1.8$ for $d = 3$ [3]. A model for the functional variation of E with T has been proposed in reference [21].

Sastry *et al* [5] reported that the value of T where E for the liquid begins to change rapidly as T decreases coincides with the T where relaxation becomes increasingly non-exponential, and where the relaxation time begins to increase strongly. For the spin-glass model studied here, Ogielski [3] showed that unambiguous non-exponential relaxation appears in the vicinity of T_c. Figures 1 and 2 show that E is not yet varying strongly, relative to its overall variation, at T_c. Hence, while a qualitative correspondence between changes in E and non-exponential relaxation holds for both the spin glass and liquid, the details of this relationship differ for the two systems [3, 22, 23].

We also note that the onset of a rapid decrease in E with decreasing T corresponds to the emergence of other complex dynamical phenomena observed recently for the ±J Ising spin glass. These phenomena include the appearance of a subset of sites having a spin relaxation rate that *increases* as T decreases [24], and the appearance and growth of spatially heterogeneous dynamics [25]. The emergence of spatially heterogeneous dynamics and enhanced mobility in simulations of supercooled liquids has also been demonstrated to occur in the same region of T in which E decreases rapidly with T, for both Lennard-Jones systems [26] and polymers [27]. Hence, for both spin glasses and molecular liquids, an interrelated set of complex dynamical behaviour emerges and grows in strength as the topography of the potential energy landscape explored by the system changes.

4. Percolation of 'frozen' spins near T_g

Comparison of individual spins in equilibrium and in quenched configurations yields insight into the microscopic details of the spin-glass transition. In particular, this comparison provides an opportunity to realize a quantitative description of the spin-glass transition in terms of a percolation transition [28–30]. To achieve this, an equilibrium configuration at a given T is selected, and a configuration X is generated from it by carrying out one MC step of the quench procedure. The configuration X is similar to the equilibrium configuration, but individual sites at which the spin state is locally unfavourable energetically (due to thermal fluctuations) have relaxed to their preferred state. We then measure the local 'overlap' q_i between a spin i in the configuration X and in the corresponding fully quenched configuration Y, averaged over M independent X, Y pairs:

$$q_i = \frac{1}{M} \sum_{m=1}^{M} s_i^{X_m} s_i^{Y_m}$$

where m labels the pair. Independent X, Y pairs are generated by quenching independent equilibrium configurations. Note that q_i should be evaluated for a fixed configuration of exchange interactions; if averaged over different interaction configurations, all q_i will converge to the same value.

With this definition for q_i, $q_i = 0$ when s_i^X and s_i^Y are uncorrelated on average, and $q_i = 1$ when $s_i^X = s_i^Y$ in every X, Y pair. We define a 'frozen' spin as any spin i for which $q_i = 1$. Note that a site for which $q_i = 1$ can change state during the normal equilibrium updating of the system. Hence, by 'frozen' we do not mean a site whose spin does not flip in equilibrium [30]. Rather, a frozen spin is a spin whose typical state in equilibrium (with transient thermal effects approximately removed) is unchanged by quenching. However, we expect that frozen spins

would tend to be sites having a particularly large relaxation time, and would thus be related to the spatially heterogeneous dynamics of the spin glass described e.g. in reference [25]. Further work is required to quantify this expectation.

On approach to T_{sg}, the number and connectivity of nearly frozen sites (i.e. sites with q_i-values approaching unity) should increase. To test this we evaluate the largest value q^* of q_i necessary to obtain an incipient spanning cluster of nearest-neighbour spins that have $q_i \geqslant q^*$. The T-dependence of q^* for both $d = 2$ and $d = 3$ is shown in figure 3. The dotted lines indicate linear extrapolations of q^* to low T. For $d = 3$, this extrapolation gives $q^* = 1$ at $kT/J \approx 1.16$, numerically indistinguishable from T_{sg}. Thus the data show that the spin-glass transition for $d = 3$ is coincident, within numerical error, with a percolation transition of frozen spins. For $d = 2$, extrapolation is less reliable because of the lack of equilibrated data near $kT_{sg}/J = 0$. However, we see from the dashed line that the $d = 2$ data are also consistent with a percolation transition at $T = 0$. A percolation transition of frozen spins at T_{sg} has been previously suggested [28–31].
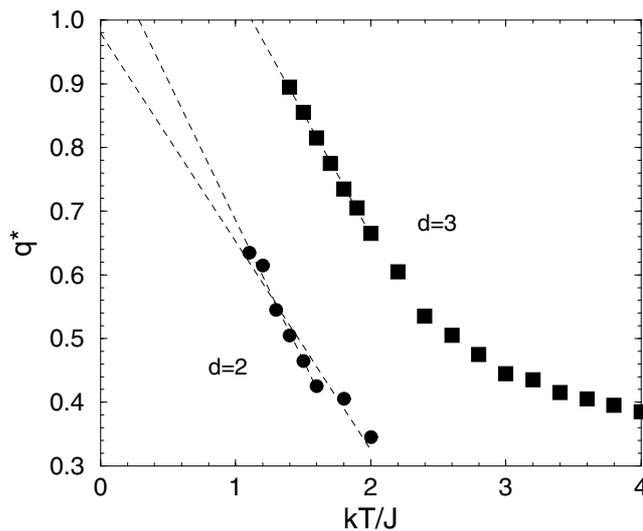
Figure 3. The threshold value q^* of the overlap yielding an incipient spanning cluster, plotted versus kT/J, for both $d = 2$ and $d = 3$. The dashed lines indicate linear extrapolation of the data to low T. For $d = 2$ we fit to different numbers of low-T data points in order to estimate confidence limits for the T at which $q^* = 1$. The data presented in this figure for $d = 3$ are generated from a 48^3 system.

5. Discussion

Our results confirm the universality expected for landscape descriptions of glass-forming systems, regardless of whether the disorder and frustration present in the system is quenched, as in spin glasses, or annealed, as in liquids. They also suggest that the connection between landscape behaviour and non-exponential dynamics may be universal. Our observation of a percolating cluster of frozen spins at T_{sg} suggests that evaluation of a suitably defined overlap function for liquids may also prove fruitful. We also remark that the changing topography of the potential energy landscape with T in both spin glasses and liquids should have implications for studies of aging in glasses following temperature quenches [32].

Acknowledgments

References

[1] Ediger M D, Angell C A and Nagel S R 1996 *J. Phys. Chem.* **100** 13 200
   Glotzer S C 1995 *Comput. Mater. Sci.* **4** 283
[2] Ogielski A T and Morgenstern I 1985 *Phys. Rev. Lett.* **54** 928
   Ogielski A T and Stein D L 1985 *Phys. Rev. Lett.* **55** 1634
   Ogielski A T and Huse D A 1986 *Phys. Rev. Lett.* **56** 1298
   Ogielski A T 1986 *Phys. Rev. Lett.* **57** 1251
[3] Ogielski A T 1985 *Phys. Rev.* B **32** 7384
[4] Rieger H 1995 *Annu. Rev. Comput. Phys.* **2** 295
[5] Sastry S V, Debenedetti P G and Stillinger F H 1998 *Nature* **393** 554
[6] Goldstein M 1969 *J. Chem. Phys.* **51** 3728
   Goldstein M 1977 *J. Chem. Phys.* **67** 2246
   Stillinger F H 1995 *Science* **267** 1935
[7] Stillinger F H and Weber T A 1982 *Phys. Rev.* A **25** 978
[8] Schrøder T B, Sastry S, Dyre J and Glotzer S C 1999 *Preprint* cond-mat/9901271
[9] Jonsson H and Anderson H C 1988 *Phys. Rev. Lett.* **60** 2295
[10] Starr F W, Sastry S, Sciortino F and Stanley H E 2000 *Preprint*
   Scala A, Starr F W, La Nave E, Sciortino F and Stanley H E 2000 *Preprint*
[11] Mezard M, Parisi G and Virasoro M A 1987 *Spin Glass Theory and Beyond* (Singapore: World Scientific)
[12] Crisanti A and Ritort F 1999 *Preprint* cond-mat 9907499
[13] In heat-bath dynamics, a spin at site i is given a value $s_i = 1$ with a probability $p = \exp(h_i/kT)$
   $\times[\exp(-h_i/kT) + \exp(h_i/kT)]^{-1}$, where $h_i = \sum_j J_{ij}s_j$ is the local field at site i. See
   Binder K 1986 *Monte Carlo Methods in Statistical Physics* ed K Binder (Berlin: Springer)
   Derrida B and Weisbuch G 1987 *Europhys. Lett.* **4** 657
[14] Bhatt R N and Young A P 1988 *Phys. Rev.* B **37** 5606
[15] Onsager L 1944 *Phys. Rev.* **65** 117
[16] Salman Z and Adler J 1998 *Int. J. Mod. Phys.* C **9** 195
[17] Cieplak M and Jäckle J 1987 *Z. Phys.* B **66** 325
[18] Palmer R G and Adler J 2000 *Int. J. Mod. Phys.* C at press
[19] Pal K P 1996 *Physica* A **223** 283
   Celik T, Hartmann U H E and Berg B 1993 *Computer Simulation Studies in Condensed Matter Physics VI* ed
      D P Landau, K K Mon and H B Schuttler (Heidelberg: Springer) p 173
[20] Morgenstern I and Binder K 1980 *Phys. Rev.* B **22** 288
   Fischer K H and Hertz J A 1991 *Spin Glasses* (Cambridge: Cambridge University Press)
[21] Kieffer J 1999 *J. Phys. Chem.* B **103** 4153
[22] Hukushima K and Nemoto K 1995 *J. Phys. Soc. Japan* **64** 2183
   Hukushima K and Nemoto K 1993 *J. Phys.: Condens. Matter* **5** 1389
[23] Franzese G and Coniglio A 1998 *Phys. Rev.* E **58** 2753
   Fierro A, Franzese G, de Candia A and Coniglio A 1999 *Phys. Rev.* E **59** 60
[24] Poole P H, Glotzer S C, Coniglio A and Jan N 1996 *Phys. Rev. Lett.* **78** 3394
[25] Glotzer S C, Jan N, Lookman T, MacIsaac A B and Poole P H 1998 *Phys. Rev.* E **57** 7350
[26] Kob W, Donati C, Plimpton S J, Poole P H and Glotzer S C 1997 *Phys. Rev. Lett.* **79** 2827
   Donati C, Douglas J F, Kob W, Plimpton S J, Poole P H and Glotzer S C 1998 *Phys. Rev. Lett.* **80** 2338
   Donati C, Glotzer S C and Poole P H 1999 *Phys. Rev. Lett.* **82** 5064
   Glotzer S C and Donati C 1999 *J. Phys.: Condens. Matter* **11** A285
   Donati C, Glotzer S C, Poole P H, Kob W and Plimpton S J 1999 *Phys. Rev.* E **60** 3107
[27] Bennemann C, Donati C, Baschnagel J and Glotzer S C 1999 *Nature* **399** 246
[28] Coniglio A 1990 *Correlations and Connectivity* ed H E Stanley and N Ostrowsky (Dordrecht: Kluwer) p 21
   Coniglio A, Liberto F, Monroy G and Peruggi F 1991 *Phys. Rev.* B **44** 12 605
[29] Glotzer S C and Coniglio A 1995 *Comput. Mater. Sci.* **4** 325
[30] Kinzel W 1982 *Z. Phys.* B **46** 59

Stauffer D 1993 *J. Phys. A: Math. Gen.* **26** L525
Ray T S and Jan N 1993 *J. Physique* I **3** 2125
[31] Stevens M, Cleary M and Stauffer D 1994 *Physics* A **208** 1
[32] Kob W, Sciortino F and Tartaglia P 1999 *Preprint* cond-mat/9905090