Interface free energies in p-spin glass models

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The replica method has been used to calculate the interface free energy associated with the change from periodic to anti-periodic boundary conditions in finite-dimensional p-spin glass models in the phase which at mean-field level has one-step replica symmetry breaking (1RSB). In any finite dimension the interface free energy is exponentially small for a large system. This result implies that in finite dimensions, the 1RSB state does not exist, as it is destroyed by thermal excitation of arbitrarily large droplets. The implications of this for the theory of structural glasses are discussed.

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The use of p-spin glass models as models for understanding structural glasses was pioneered in the work of Kirkpatrick, Thirumalai and Wolynes [1]. They found that for the infinite-range version of these models, for which mean-field theory is exact, that there were two important temperatures. At a temperature \(T_d\) there exists a dynamical transition below which an ergodic transition occurs. The dynamical equations which arise are very similar to those of the mode-coupling theory of liquids [2]. At a lower temperature \(T_c\) there is a first-order (discontinuous) transition to a phase with a 1RSB order parameter. As \(T \to T_c\), the entropy goes to zero, so this transition is identified with the Kauzmann glass transition [3], the temperature at which the extrapolated entropy of the supercooled liquid apparently falls to that of the crystalline phase.

It has been realized for many years that outside the mean-field limit there will be no genuine dynamical transition at \(T_d\). This is because the metastable states which trap the system dynamically are unstable because of activation processes over the finite free energy barriers which exist outside the mean-field limit. However, the apparent divergence of the viscosity in fragile glasses at some non-zero temperature, such as that in the Vogel-Fulcher formula [4]

\[
\log \eta = \log \eta_0 + \frac{\Delta}{T - T_{VF}}, \tag{1}
\]

has encouraged the belief that there might be a real thermodynamic glass transition near \(T_{VF}\). The observation that the ratio \(T_K/T_{VF}\) lies between 0.9-1.1 for many glass formers whose \(T_K\) ranges from 50 K to 1000 K [5] is further evidence for this possibility. However, we have recently argued that there is no genuine glass transition [6], and that \(T_K\) and \(T_{VF}\) are just ‘crossover temperatures’. The Ising spin glass in a field seems to provide a satisfactory analogy for supercooled liquids near \(T_{VF}\).

We shall here strengthen these arguments by showing that the 1RSB state simply does not exist in the finite dimensional p-spin glass model! The reasons are similar to those why there is also no real dynamical transition \(T_d\) in finite dimensional systems. There is no transition at \(T_c\) to a state with one-step replica symmetry breaking because that state is destabilized by thermal fluctuations within it of droplets of arbitrarily large size which only cost a finite amount of free energy to produce. When \(p\) is even, the Hamiltonian is left unchanged by flipping the signs of all the spins, and the destabilizing droplets are simple to identify: They are droplets of the time-reversed state. Our basic task then is to calculate the interface free energy for droplets.

There have recently been other attempts to calculate interface free energies in p-spin models [7, 8]. Their results are very different to those reported here, essentially because they are studying a different interface free energy – that appropriate for non-equilibrium effects below \(T_d\). The interface free energy studied here is the one commonly studied in Ising spin glasses which involves changing the boundary conditions along one direction (the \(z\) direction) from periodic to anti-periodic [9]. That is, we study \(\delta F = \sqrt{\Delta F_{P,AP}}\) (here and in the following, the overbar means averaging over bond configurations) where \(\Delta F_{P,AP} = F_P - F_{AP}\), and \(F_P\) and \(F_{AP}\) are the free energies with periodic and anti-periodic boundary conditions respectively. Anti-periodic boundary conditions can be realized by reversing the sign of the bonds crossing a plane whose normal is parallel to the given direction. It will be shown below that \(\Delta F_{P,AP} = 0\). If the system is of length \(L\) in the \(z\) direction, we find that the interface free energy \(\delta F\) decreases to zero as \(\sim \exp(-L/2\xi)\), provided \(L \gg \xi\). \(\xi\) is the correlation length in the 1RSB state. This state will therefore be destabilized by the thermal excitation of large droplets, since the free energy cost of creating them – their interface free energy – can be made arbitrarily small.

There exists simulative evidence as to the validity of the conclusion that the 1RSB state does not exist in the 10-state Potts spin glass [10]. In the infinite-range limit when all the Potts spins are coupled by random interactions, mean-field theory becomes exact and is the same as that for the p-spin model. The simulations of it were consistent with the existence of both a dynamical transition \(T_d\) and a transition to a 1RSB state below
However, in three dimensions using a Gaussian distribution of the couplings, there was no evidence of a dynamical transition $T_d$, nor of a transition to a 1RSB state.

The complete absence in three dimensions of the dynamical behavior found at mean-field level in the Potts glass is perhaps surprising given that in supercooled liquids there is ample evidence that mode-coupling works well. Furthermore we have recently been able to derive the replicated form of the p-spin functional starting directly from the liquid state $\mathbb{R}$. However, this derivation of the p-spin functional provides the answer to the puzzle: Its variables are quantities which are not directly related to the densities whose correlations functions are studied in mode-coupling theory. The derived replicated p-spin functional is useful though when studying whether there might be a genuine glass transition. It can be further transformed to the replicated functional which describes an Ising spin glass in a field $\mathbb{R} [\mathbb{R} \ldots ]$. Then the issue of whether there is or is not a genuine thermodynamic glass transition is the same as whether there is a transition of an Ising spin glass in a magnetic field. But whether there is or is not a transition to a glass state, that state cannot be the 1RSB state as in the mean-field p-spin glass model, since such a state does not exist in finite dimensions.

Numerical studies of p-spin models outside the mean-field limit $\mathbb{R} \ldots$ use Hamiltonians which are of the following form, which is appropriate for the case $p = 3$ $\mathbb{R} \ldots$. Each site is occupied by two Ising spins, $\sigma_i$ and $\tau_i$, and the Hamiltonian is

$$\mathcal{H} = \sum_{<ij>} J^{(1)}_{ij} \sigma_i \tau_i \sigma_j + J^{(2)}_{ij} \sigma_i \tau_i \tau_j + J^{(3)}_{ij} \sigma_j \tau_j \tau_i + J^{(4)}_{ij} \tau_j \sigma_j \tau_i,$$

where $<ij>$ are nearest-neighbor pairs, and the couplings $J^{(n)}_{ij}$ are chosen independently from a Gaussian distribution with zero mean and width $\mathcal{J}$. Note that when the signs of all the spins are reversed, the sign of the Hamiltonian changes, indicating the violation of time reversal symmetry. For models with $p$ even, such as that for $p = 4$ in Ref. $\mathbb{R} \ldots$, the Hamiltonian does not change sign when all the spins are flipped.

Starting from a p-spin Hamiltonian such as that in Eq. $\mathbb{R} \ldots$ it is possible to obtain the ‘generic’ form of the replicated p-spin functional $\mathbb{R} \ldots$ by averaging over the couplings:

$$\beta \mathcal{H}_{\text{rep}} = \int d^d x \left[ \frac{t}{4} \sum_{\alpha, \beta} q_{\alpha \beta}^2 + \frac{1}{4} \sum_{\alpha, \beta} (\nabla q_{\alpha \beta})^2 + \frac{w_1}{6} \sum_{\alpha, \beta, \gamma} q_{\alpha \beta} q_{\beta \gamma} q_{\gamma \alpha} - \frac{w_2}{6} \sum_{\alpha, \beta} q_{\alpha \beta}^3 + \frac{y}{24} \sum_{\alpha, \beta} q_{\alpha \beta}^4 \right],$$

where $q_{\alpha \beta}$ is a symmetric matrix with $q_{\alpha \alpha} = 0$. The coefficients $t, w_1, w_2$ and $y$ are arbitrary positive parameters. This generic functional has the same relationship to the finite dimensional p-spin glass models as (say) the Landau-Ginzburg functional has to the Ising model. It represents a p-spin model with odd values of $p$ as the cubic term with coefficient $w_2$ corresponds to a term which breaks time-reversal invariance. (Terms in which a replica index appears an odd number of times always break time-reversal invariance). The odd $p$ models would seem to be the relevant ones for applications to structural glasses which have no identifiable symmetries. The replica indices go from 1 to $n$, and $q_{\alpha \alpha} = 0$.

In order to calculate interface free energies between systems which differ as to whether they have periodic or anti-periodic boundary conditions, we will follow the procedure used in Ref. $\mathbb{R} \ldots$. This requires one to replicate the system with periodic boundary conditions $n$ times and the system with anti-periodic boundary conditions $m$ times, where as usual we will take $n$ and $m$ to zero at the end of the calculation.

Expanding the replicated partition function in powers of $m$ and $n$, we have

$$- \ln Z_p Z_{\mathbb{R} \ldots}^{\alpha} = (n + m) \beta F + \frac{(n + m)^2}{2} \beta^2 \Delta F^2 + \frac{nm}{2} \beta^2 \Delta F_{\mathbb{R} \ldots}^{\alpha} + \cdots,$$

where $\Delta F^2 = \mathbb{F}_P^2 - \mathbb{F}_P^2$ and $\Delta F_{\mathbb{R} \ldots}^{\alpha}$ is the (mean square) sample-to-sample fluctuation of the free energy, the same for both sets of boundary conditions $P$ or $\mathbb{R} \ldots$, and $\mathbb{F} = \mathbb{F}_P = \mathbb{F}_{\mathbb{R} \ldots}$. Thus $\Delta F_{\mathbb{R} \ldots}^{\alpha} = 0$. To find the variance of the interface free energy, $\Delta F_{\mathbb{R} \ldots}^{\alpha}$, we expand out $\ln Z_p Z_{\mathbb{R} \ldots}^{\alpha}$ in second order in the numbers of replicas, $n$ and $m$, separate out the pieces involving the total number of replicas $n + m$, and take the remaining piece, which is proportional to $nm$.

The replica indices in the generalization of Eq. $\mathbb{R} \ldots$ go $\alpha, \beta, \gamma = 1, 2, \ldots, n, n + 1, \ldots, n + m$. The order parameter $q$ divides naturally into blocks of size $n$ and $m$. From now on, Greek indices will label the first block, Roman ones the second block, so, for example, $q_{\alpha i}$, means $\alpha \in [1, n]$ and $i \in [n + 1, n + m]$, and refers to the respective entry in the off-diagonal, or mixed, sector.

The boundary condition which results from the flipping the sign of the bonds in the plane perpendicular to the $z$-axis is that $q$ must be periodic in the Greek and Roman sectors, and anti-periodic in the mixed sectors:

$$q_{\alpha \beta}(z) = q_{\alpha \beta}(z + L)$$
$$q_{ij}(z) = q_{ij}(z + L)$$
$$q_{\alpha i}(z) = -q_{\alpha i}(z + L).$$

In the directions perpendicular to the $z$-axis, which we will take to be all of length $M$, the system is periodic.

At mean-field level, the stable solution for $\ln Z_p Z_{\mathbb{R} \ldots}^{\alpha}$ is
given by
\[ -\ln Z_P Z_{AP} = \beta \mathcal{H}_{\text{rep}} \{ q^{SP} \}, \]
where \( q^{SP} \) denotes the solution of the Euler-Lagrange equations:
\[
\frac{d^2 q_{\alpha \beta}}{dz^2} = t q_{\alpha \beta} - w_1 \sum_{\gamma=1}^n q_{\alpha \gamma} q_{\gamma \beta} - \sum_{i=1}^m q_{\alpha i} q_{i \beta} \\
- w_2 q_{\alpha \beta}^2 + y q_{\alpha \beta}^3 / 3,
\]
\[
\frac{d^2 q_{ij}}{dz^2} = t q_{ij} - w_1 \sum_{k=1}^m q_{ik} q_{kj} - \sum_{\gamma=1}^n q_{i \gamma} q_{\gamma j} \\
- w_2 q_{ij}^2 + y q_{ij}^3 / 3,
\]
\[
\frac{d^2 q_{\alpha i}}{dz^2} = t q_{\alpha i} - w_1 \sum_{\gamma=1}^n q_{\alpha \gamma} q_{\gamma i} - \sum_{k=1}^m q_{\alpha k} q_{ki} \\
- w_2 q_{\alpha i}^2 + y q_{\alpha i}^3 / 3.
\]

Notice that there is a solution of these equations which satisfies the boundary conditions in which the mixed overlaps \( q_{\alpha i} = 0 \) and where in the all Greek or all Roman sectors \( q_{\alpha \beta} \) and \( q_{ij} \), the solutions are \( z \) independent. We believe that this is the physically relevant solution as it is stable. Thus at mean-field level the free energy of the \( n+m \) replicated system with the boundary conditions breaks up into the sum of the free energies of the \( n \) and \( m \) replicated systems without boundary conditions, so that there can be no term of order \( nm \) in Eq. \( \text{(6)} \), so that the interface energy vanishes to this order.

In the high-temperature phase the solution to the stationarity equations is \( q_{\alpha \beta} = q_{ij} = q_{\alpha i} = 0 \). A spatially constant 1RSB solution appears discontinuously at a temperature \( t_K = 2 w^2 / (3 y) \) where to simplify the algebra the following notational changes have been made: \( w_1 = 1, w_2 = 1 + w \) with \( w > 0 \). For the specific model of Eq. \( \text{(2)} \) \( w \) is actually negative \( [12] \). There is, for temperatures \( t \leq t_K \), a 1RSB solution in which \( q_{\alpha \beta} \) is zero everywhere except in \( n/\tilde{m} \) boxes of size \( \tilde{m} \) along the leading diagonal, where it takes the value \( q_1 \). \( q_{ij} \) similarly is zero everywhere except in \( m/\tilde{m} \) boxes of size \( \tilde{m} \). \( q_{\alpha i} = 0 \). For a review of 1RSB see Ref. [13]. Right at \( t_K \), on letting \( n,m \) go to zero, \( q_1 = 2 w/y \) and \( \tilde{m} = 1 \). For temperatures \( t < t_K \), \( q_1 \) increases and \( \tilde{m} \) decreases.

To get the leading non-vanishing contribution to the interface free energy we need to go to one-loop order. The first correction is due to Gaussian fluctuations around the stationary 1RSB solution:
\[ -\ln Z_P Z_{AP} = \beta \mathcal{H}_{\text{rep}} \{ q^{SP} \} + \frac{1}{2} \sum_k I(k^2), \]
where
\[ I(k^2) = \sum_{\mu} d_\mu \ln(k^2 + \lambda_\mu). \]
\( k \) is a \( d \)-dimensional wave vector, \( \lambda_\mu \) are the eigenvalues of the Hessian, evaluated at the stationary point, and their degeneracies are \( d_\mu \). The eigenvalues and degeneracies are the same as for a system of size \( n + m \) without boundary condition changes (because the stationary point is the same), only the nature of the \( k \)-vectors changes for the terms involving eigenvalues whose corresponding eigenvectors \( f \) are nonzero exclusively in the mixed sector (i.e. \( f_{\alpha \beta} = f_{ij} = 0 \): the wave vectors have to respect the imposed boundary conditions, which implies \( \tilde{k} = (2 n_1 \pi / M, \ldots, 2 n_{d-1} \pi / M, (2 n_d + 1) \pi / L) \) (with \( n_i \in \mathbb{Z} \) in the mixed sector as opposed to \( \tilde{k} = (2 n_1 \pi / M, \ldots, 2 n_{d-1} \pi / M, 2 n_d \pi / L) \) in the Greek or Roman sectors).

While it is possible to compute the eigenvalues \( \lambda_\mu \) and their degeneracies \( d_\mu \), it is much easier to follow the procedures of Ref. \([8, 17]\). One computes \( \partial I / \partial (k^2) \) rather than \( I \) itself. This helps because it is possible to express the terms in this derivative of order \( n^2 \), \( m^2 \) and \( nm \) directly in terms of a single propagator of the mixed sector calculated for the system without boundary condition changes:
\[ \frac{\partial I_{AP}}{\partial (k^2)} = n m G_{\alpha i, \alpha i} \]
where the prefactor \( n m \) reflects the number of eigenvectors in the mixed sector. The subscript AP indicates that its argument \( k \) must have values appropriate to the mixed sector. Defining the integral
\[ J(k) := \int d(k^2) G_{\alpha i, \alpha i} \]
and obtaining the constant of integration via Ref. \([17]\) enables one to write the terms of order \( n^2 \), \( m^2 \) and \( nm \) in \( I \) as
\[ \frac{n^2 + m^2}{2} J_P(k^2) + n m J_{AP}(k^2) = \frac{(n + m)^2}{2} J_P(k^2) + n m (J_{AP}(k^2) - J_P(k^2)). \]
The subscripts \( P \) and \( AP \) on \( J \) mean that \( J \) must be taken as 0 when the argument is not of the required type, i.e. periodic or anti-periodic.

Comparison with Eq. \( \text{(6)} \) shows
\[ \beta^2 \Delta F_{P, AP}^2 = \left( \sum_{AP} - \sum_{P} \right) J(k^2) = \sum_{i} \sum_{r=-\infty}^{\infty} \left( J(l^2 + \frac{(2r + 1)^2 \pi^2}{L^2}) - J(l^2 + \frac{(2r)^2 \pi^2}{L^2}) \right) \]
where the subscripts on the sums indicate the nature of the allowed \( k \)-vectors, as made explicit in the second part of the equation where the \( z \) component of the \( k \)-vector has been split off, leaving the \( d - 1 \)-dimensional wave.
vector \( l \). The sum over the \( z \) component can be extended to \( \pm \infty \), introducing only exponentially small errors for large \( L \).

The calculation of \( \Delta F_{\beta, AP} \) is readily accomplished using the methods of Ref. [18]. Right at the transition \( t_K \), the propagator is very simple because \( \bar{m} = 1 \): \( \Delta w_{\beta,\alpha i} = 1/(k^2 + t) \), so \( J(k^2) = \ln(k^2 + t) \). We shall for simplicity work in the limit where the sums over the first \( d - 1 \) directions can be converted to integrals (renaming the integration variable \( q \)). Then

\[
\beta^2 \Delta F_{\beta, AP}^2 = M^{d-1} \int \frac{d^{d-1}q}{(2\pi)^{d-1}} \sum_{r=-\infty}^{\infty} \left( \ln(q^2 + \frac{(2r + 1)^2\pi^2}{L^2} + t) - \ln(q^2 + \frac{(2r)^2\pi^2}{L^2} + t) \right).
\]

The sum over \( r \) can be done analytically when the right-hand side becomes

\[
2 \frac{S_{d-1}}{(2\pi)^{d-1}} M^{d-1} \int_0^\infty dq q^{d-2} \ln \coth[\sqrt{q^2 + tL/2}],
\]

\( S_d \) is the surface area of a \( d \)-dimensional unit sphere. In the limit when \( L \gg \xi \), where \( \xi = 1/\sqrt{t} \) is the correlation length, the integral is simple to evaluate:

\[
\beta^2 \Delta F_{\beta, AP}^2 \approx 2 \frac{S_{d-1}}{(2\pi)^{d-1}} \frac{d-1}{2} \frac{S_{d-1}}{(2\pi)^{d-1}} \times \left( \frac{M}{L} \right)^{d-1} \left( \frac{L}{\xi} \right)^{d-1} \exp \left( -\frac{L}{\xi} \right).
\]

This result is valid in the limits \( M \gg L \gg \xi \). By going back to Eq. (12), however, any desired aspect ratio can be studied for any value of \( L/\xi \).

While we have produced an explicit expression for the interface energy \( \delta F \) at one particular temperature, \( t_K \), at which the system jumps into the 1RSB state, the same methods can be used at any temperature. The origin of the exponentially small free energy is the presence of positive non-zero eigenvalues in the Hessian matrix. The stationary point needs to be marginally stable in order to get interface free energies of the form \( \delta F \sim L^{\theta} \), with \( \theta > 0 \), which is what happens for the Ising spin glass. In both the temperature regions above and below \( t_K \), the eigenvalues are positive so the interface free energy in \( p \)-spin models is at all temperatures exponentially small. This conclusion will also be true of the 1FRSB state which exists for some generalizations of the \( p \)-spin model, where the order parameter \( q(x) \) has both a jump, characteristic of 1RSB, but in addition varies with \( x \), like in full replica symmetry breaking. It has also only non-zero Hessian eigenvalues [18].

The methods used here can also be used to calculate the interface free energy appropriate to the dynamical questions studied in Ref. [7, 8]. To locate the dynamical transition one imposes the condition that the stationary point solution \( q^{SP} \) has a Hessian with a null eigenvalue [18]. This will guarantee that the associated interface free energy will not be exponentially small. The calculation is very similar to that of Ref. [6, 20].

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