# Interface energies in Ising spin glasses

T. Aspelmeier and M. A. Moore
*Department of Physics and Astronomy, University of Manchester, Manchester M13 9PL, UK*

A. P. Young
*Department of Physics, University of California, Santa Cruz, CA 95064 and*
*Department of Theoretical Physics, 1, Keble Road, Oxford OX1 3NP, England*
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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 spin glasses. At mean-field level the interface free energy vanishes but after allowing for fluctuation effects, a non-zero interface free energy is obtained which is significantly different from numerical expectations.

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A central concept in the droplet picture of spin glasses is the interface free energy [1–5] $\delta F$, and the associated stiffness exponent $\theta$ defined by $\delta F \sim l^\theta$ where $l$ is the length scale of the excitation. If $\theta > 0$ the spin glass state is stable at finite temperature, whereas if $\theta < 0$ at $T = 0$ large scale excitations cost very little energy so the spin glass state will be unstable at finite temperature. The value of $\theta$ at $T = 0$ has been estimated *numerically*, in many calculations, for short range spin glass models from the effects of changes in boundary conditions, see e.g. Refs. [6–9]. It is therefore surprising that no attempt has so far been made to determine the interface free energy from boundary condition changes using the alternative "Replica Symmetry Breaking" (RSB) [10, 11] scenario for the spin glass state. In this paper we calculate $\theta$ *analytically* in high dimensions using the replica method and show that it conflicts with expectations from the droplet picture, and numerical work on systems in lower dimensions.

We define the interface free energy in the standard way as the root mean square change in the free energy of a spin glass when the boundary conditions along one direction (the $z$ direction) are changed from periodic to anti-periodic, i.e. $\delta F = \sqrt{\overline{\Delta F_{P,AP}^2}}$ (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 follows that $\overline{\Delta F_{P,AP}} = 0$. We note that earlier attempts to calculate a defect energy [12, 13] did not employ a definition of it which is relevant to the droplet picture or numerical studies.

It is convenient to replicate the system with periodic boundary conditions $n$ times and the system with anti-periodic boundary conditions $m$ times, and keep $n$ distinct from $m$ for the time being. Expanding the replicated partition function in powers of $m$ and $n$, and taking the logarithm, we have

$$
\begin{aligned}
-\ln \overline{Z_P^n Z_{AP}^m} &= (n+m)\,\beta\overline{F} \\
&\quad - \frac{(n+m)^2}{2}\,\beta^2\overline{\Delta F^2} + \frac{nm}{2}\,\beta^2\overline{\Delta F_{P,AP}^2} + \cdots, \quad (1)
\end{aligned}
$$

where $\overline{\Delta F^2} = \overline{F_P^2} - \overline{F_P}^2 = \overline{F_{AP}^2} - \overline{F_{AP}}^2$ is the (mean square) sample-to-sample fluctuation of the free energy, the same for both sets of boundary conditions $P$ or $AP$, and $\overline{F} = \overline{F_P} = \overline{F_{AP}}$. Hence, to find the variance of the interface free energy, $\overline{\Delta F_{P,AP}^2}$, we expand out $\ln \overline{Z_P^n Z_{AP}^m}$ to 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 $nm$.

Using the standard replica field theory [14], we can write $\overline{Z_P^n Z_{AP}^m} = \int \mathcal{D}q\, \exp(-\beta\mathcal{H}_{\rm rep})$ where $\mathcal{H}_{\rm rep}$ is the replica free energy, expressed in terms of the spin glass order parameter field, $q_{\alpha\beta}(x)$. It is given by

$$
\begin{aligned}
\beta\mathcal{H}_{\rm rep} = \int d^dx\, \Bigg[ &-\frac{\tau}{2}\sum_{\alpha,\beta} q_{\alpha\beta}^2 + \frac{1}{4}\sum_{\alpha,\beta}(\vec\nabla q_{\alpha\beta})^2 \\
&- \frac{w}{6}\sum_{\alpha,\beta,\gamma} q_{\alpha\beta}q_{\beta\gamma}q_{\gamma\alpha} - \frac{y}{12}\sum_{\alpha,\beta} q_{\alpha\beta}^4 \Bigg], \quad (2)
\end{aligned}
$$

where $q_{\alpha\beta}$ is a symmetric matrix with $q_{\alpha\alpha} = 0$, we have omitted some unimportant terms of order $q^4$, and set $\tau = 1 - T/T_c$. The fourth order term included is the one responsible for replica symmetry breaking. For the SK model, the coefficients $w$ and $y$ are unity, but we treat them as arbitrary positive parameters here. The replica indices go $\alpha, \beta, \gamma = 1, 2, \cdots, n, n+1, \cdots, n+m$. 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.

We shall assume that there is only spatial variation in the $z$ direction, which we shall take to be of length $L$. All directions perpendicular to the $z$ direction are of length $M$. The volume of the system is $V = M^{d-1}L$. Along the $z$-direction, we impose the boundary condition that the solution is periodic in the Greek and Roman sectors, and is antiperiodic in the mixed sectors reflecting the sign reversal of the plane of bonds in the one sector with respect to the other:

$$\begin{aligned} q_{\alpha\beta}(z) &= q_{\alpha\beta}(z+L) \\ q_{ij}(z) &= q_{ij}(z+L) \\ q_{\alpha i}(z) &= -q_{\alpha i}(z+L). \end{aligned} \tag{3}$$

At mean-field level, there is the following *stable* solution for $\ln \overline{Z_P^n Z_{AP}^m}$:

$$-\ln \overline{Z_P^n Z_{AP}^m} = \beta \mathcal{H}_{\rm rep}\{q^{\rm SP}\}, \tag{4}$$

where

$$q^{\rm SP} = \left( \begin{array}{c|c} Q^{(n)}_{\alpha\beta} & 0 \\ \hline 0 & Q^{(m)}_{ij} \end{array} \right) \tag{5}$$

is independent of the spatial coordinates and $Q^{(s)}$ is a Parisi symmetry broken saddle point solution of size $s \times s$, with the necessary modification for finite positive $s$ as derived in [15], i.e.

$$Q^{(s)} = \lim_{p\to\infty} \underbrace{\begin{pmatrix} \boxed{P^{(s/p)}} & & 0 \\ & \ddots & \\ 0 & & \boxed{P^{(s/p)}} \end{pmatrix}}_{p \text{ blocks}}, \tag{6}$$

where $P^{(s/p)}$ is a 'standard' Parisi matrix. The limit $p \to \infty$ in Eq. (6) should be interpreted in the same sense as for a standard replica symmetry breaking procedure, i.e. as taking $p$ to infinity when it is convenient during a calculation.

It is natural that the diagonal blocks are the same as the regular Parisi ansatz because ordering in the system with periodic boundary conditions, say, should not be affected by there being another *completely independent* copy with different boundary conditions. Choosing the mixed sector to vanish seems to be consistent with the standard interpretation [16] of RSB in short-range systems, namely that changing the boundary conditions changes the system *everywhere*. More precisely the surface of the domain wall separating the regions which flip from the regions which don't flip is space filling. In this situation, one can reasonably expect zero overlap between configurations with different boundary conditions.

This solution is *identical* to the solution one obtains using the correct way of breaking the symmetry, as presented in [15], for a $n+m$-times replicated system ($n+m$ being finite) *without* boundary condition changes. We can therefore immediately use the result from [15] that on mean-field level, there is no term of order $(n+m)^2$, let alone of order $nm$, and thus the interface energy vanishes to this order.

We now turn to the loop expansion about the saddle point, which is expected to be valid for dimension $d$ greater than 6. The first correction is due to Gaussian fluctuations around the saddle point solution. They are given by

$$-\ln \overline{Z_P^n Z_{AP}^m} = \beta \mathcal{H}_{\rm rep}\{q^{\rm SP}\} + \frac{1}{2}\sum_k I(k^2), \tag{7}$$

where

$$I(k^2) = \sum_\mu d_\mu \ln(k^2 + \lambda_\mu), \tag{8}$$

$k$ is a $d$-dimensional wave vector and $\lambda_\mu, d_\mu$ are the eigenvalues of the Hessian, evaluated at the saddle point solution, and their degeneracies. The eigenvalues $\lambda_\mu$ and degeneracies $d_\mu$ are the same as for a system of size $n+m$ without boundary condition changes (because the saddle point solution 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 $k = (2n_1\pi/M, \ldots, 2n_{d-1}\pi/M, (2n_d+1)\pi/L)$ (with $n_i \in \mathbb{Z}$) in the mixed sector as opposed to $k = (2n_1\pi/M, \ldots, 2n_{d-1}\pi/M, 2n_d\pi/L)$ in the Greek or Roman sectors.

It was shown in [15] for a system without boundary condition changes that it is initially easier to compute $\partial I/\partial(k^2)$ than $I$ itself , and that it is given in terms of the diagonal propagators $G_{\alpha\beta,\alpha\beta}$ (or $G_{11}^{xx}$ in the limit of infinitely many replica symmetry breaking steps [14]) as

$$\frac{\partial I_P}{\partial(k^2)} = \sum_{\alpha<\beta} G_{\alpha\beta,\alpha\beta} = -\frac{n}{2}\int_n^1 dx\, G_n^{xx}, \tag{9}$$

where we have dropped the subscript 11 from the propagators as it is irrelevant here and replaced it by $n$ since the propagators depend on it.

Therefore the contribution to $\partial I/\partial(k^2)$ from those eigenvectors that are nonzero in the Greek or Roman sectors (the periodic sectors, hence the subscript $P$ below) is

$$\frac{\partial I_P}{\partial(k^2)} = -\frac{n}{2}\int_n^1 dx\, G_n^{xx} - \frac{m}{2}\int_m^1 dx\, G_m^{xx} \tag{10}$$

$$= -\frac{n+m}{2}\int_0^1 dx\, G_0^{xx} + \frac{n^2+m^2}{2} G_0^{00}, \tag{11}$$

The last line follows from the modified symmetry breaking procedure (Eq. (6)), as was shown in [15]. The origin of the term linear in $n+m$ in Eq. (10) is the eigenvectors that are nonzero in a Parisi block $P^{(n/p)}$ or $P^{(m/p)}$ on the diagonal [15], while the origin of the $n^2+m^2$-term is the eigenvectors that are nonzero in the off-diagonal blocks. This observation facilitates calculating the contribution from the mixed sector as there are only eigenvectors of the latter type present, i.e. there is no term of linear order. Therefore $\partial I_{AP}/\partial(k^2)$ is given by

$$\frac{\partial I_{AP}}{\partial(k^2)} = nmG_0^{00}, \tag{12}$$

where the prefactor $nm$ reflects the number of eigenvectors in the mixed sector.

The integral $\int d(k^2)\, G_0^{00}$ and the constant of integration have been worked out in [15], resulting in

$$J(k^2) := \int d(k^2) G_0^{00} = \ln(k^2 + \frac{x_1^2 w^2}{2y}) - \frac{4w(4yk^2 + wx_1)}{4yk^2\sqrt{4yk^2 + w^2x_1^2}} \tan^{-1} \frac{wx_1}{\sqrt{4yk^2 + w^2x_1^2}}, \tag{13}$$

where $x_1$ is the breakpoint of the Parisi $q$-function. We can now assemble in $I$ the terms of quadratic order,

$$I = (n+m)C + \frac{n^2+m^2}{2} J_P(k^2) + nmJ_{AP}(k^2) \tag{14}$$

$$= (n+m)C + \frac{(n+m)^2}{2} J_P(k^2) + nm(J_{AP}(k^2) - J_P(k^2)). \tag{15}$$

The constant $C$ is of no interest to us. 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 antiperiodic.

We can now identify the term that gives rise to the interface energy. Comparison with Eq. (1) shows

$$\beta^2\overline{\Delta F_{P,AP}^2} = \left(\sum\nolimits_{AP} - \sum\nolimits_{P}\right) J(k^2) = \sum_{l} \sum_{r=-\infty}^{\infty} \left( J(l^2 + \frac{(2r+1)^2\pi^2}{L^2}) - J(l^2 + \frac{(2r)^2\pi^2}{L^2}) \right) \tag{16}$$

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 has been extended to $\pm\infty$, introducing only exponentially small errors for large $L$.

We note a potential pitfall in this result: the contribution to Eq. (16) from the $k = 0$ term (in $\sum_P$) diverges. Usually, this problem is removed by converting the sums to integrals converging in high enough dimensions, and arguing that the divergence is, in reality, only a subdominant contribution. However, since $\theta < (d-1)/2$ [4], the interface energy is subdominant itself, so it is not clear whether the subdominant terms from the $k = 0$ mode are in fact dominating over the terms we kept. Therefore we need to treat the $k = 0$ mode properly before proceeding. The way to do this is to go to the equation of state for $q_{\alpha\beta}$ and include the $k = 0$ mode exactly, while treating the other modes perturbatively as before. The complete equation of state is given by Eq. (15) from [14], and restricted to the $k = 0$ mode it reads

$$2\tau q_{\alpha\beta} + w(q^2)_{\alpha\beta} + \frac{2y}{3}q_{\alpha\beta}^3 = -\frac{1}{V}\left( w \sum_{\gamma\neq\alpha,\beta} G_{\alpha\gamma,\beta\gamma}(k=0) + 2yq_{\alpha\beta}G_{\alpha\beta,\alpha\beta}(k=0) \right). \tag{17}$$

This equation is highly nontrivial since $G$ in this expression is the *full* propagator. We do not propose to solve this formidable self-consistency equation, but we note that the presence of the right hand side shifts $q_{\alpha\beta}$ by an amount $\epsilon_{\alpha\beta}$ from the mean-field value, which in turn shifts the eigenvalues of the Hessian. The left hand side is given by $\sum_{\gamma\delta} G^{-1}_{\alpha\beta,\gamma\delta}(k=0)\epsilon_{\gamma\delta} = \mathcal{O}(\epsilon)$ (recalling that $G^{-1}(k=0)$ is equal to the Hessian), the right hand side is of order $1/V\lambda_{\min}$, where $\lambda_{\min}$ is the smallest eigenvalue of the Hessian. If $\lambda_{\min} = \mathcal{O}(\epsilon)$, which is the natural expectation, it follows that $\lambda_{\min} \sim V^{-1/2}$. Therefore $G(k=0)$ has changed from being infinite to being of order $V^{1/2}$. This argument is not rigorous, however, therefore we prefer to denote the exponent more generally by $2\mu$. The upshot of this treatment is that we can exclude the divergent $k = 0$ terms from the sums over wave vectors (as they have been dealt with non-perturbatively), provided a term of order $V^{2\mu}$, where $\mu$ may be 1/4, is introduced in the $n^2$ and $m^2$ terms in Eq. (14). This additional term is *identical* to the free energy fluctuations in the Sherrington-Kirkpatrick model which has only the $k = 0$ mode, and will be denoted by $\Delta f_{\rm SK}^2 V^{2\mu}$. This observation allows us to obtain estimates of $\mu$ from existing numerical work [17–19], which supports $\mu = 1/4$.

Since we are expecting that the changes to the eigenvalues are of order $V^{-1/2}$, while the changes due to the different boundary conditions are of order $1/L^2$, our treatment of the non-zero $k$ modes will be satisfactory in the range of dimensions where the loop expansion applies, i.e. $d > 6$.

Upon completing the square as in Eq. (15) the contribution $\Delta f_{\rm SK}^2 V^{2\mu}$ appears in the $nm$ term, so from Eq. (16) we get

$$\beta^2\overline{\Delta F_{P,AP}^2} = \sum_{l\neq 0} \sum_{r=-\infty}^{\infty} \left( J(l^2 + \frac{(2r+1)^2\pi^2}{L^2}) - J(l^2 + \frac{(2r)^2\pi^2}{L^2}) \right) + 2\sum_{r=1}^{\infty} \left( J(\frac{(2r-1)^2\pi^2}{L^2}) - J(\frac{(2r)^2\pi^2}{L^2}) \right) + \Delta f_{\rm SK}^2 V^{2\mu} \tag{18}$$

The sums over $r$ in Eq. (18) can be calculated exactly, in principle, and the sum over $l$ can be converted to an integral with a lower cutoff and carried out, but the result is too long to show here. The important feature of it is that the leading behaviour as a function of $L$ is determined by the divergent part of $J$ as $k^2 \to 0$. The other parts of $J$ only give exponentially small corrections. Since $J(k^2) \approx -\pi w/4yk^2$ for small $k^2$, it is sufficient to work out the term

$$\frac{-w\pi}{4y} \sum_{r=-\infty}^{\infty} \left( \frac{1}{l^2 + \frac{(2r+1)^2\pi^2}{L^2}} - \frac{1}{l^2 + \frac{(2r)^2\pi^2}{L^2}} \right) = \frac{w\pi L}{4yl \sinh lL}. \tag{19}$$

Together with $\sum_{r=1}^{\infty}(\frac{1}{(2r-1)^2} - \frac{1}{(2r)^2}) = \pi^2/12$ this gives

$$\beta^2 \overline{\Delta F^2_{P,AP}} = M^{d-1} \frac{S_{d-1}}{(2\pi)^{d-1}} \int_{\frac{2\pi}{M}}^{\infty} dl\, l^{d-2} \frac{w\pi L}{4yl \sinh lL} - \frac{w\pi}{24y} L^2 + \Delta f^2_{\mathrm{SK}} V^{2\mu} \tag{20}$$

$$= L^2 f^2(L/M) - \frac{w\pi}{24y} L^2 + \Delta f^2_{\mathrm{SK}} V^{2\mu}, \tag{21}$$

where

$$f^2(L/M) = \frac{w\pi S_{d-1}}{4y(2\pi)^{d-1}} \left(\frac{M}{L}\right)^{d-1} \int_{\frac{2\pi L}{M}}^{\infty} \frac{dx\, x^{d-3}}{\sinh x} \tag{22}$$

is an exponentially decreasing scaling function and $S_d$ is the surface of a $d$-dimensional unit sphere.

Only the first term in Eq. (21) has a form compatible with aspect ratio scaling [20], according to which $\sqrt{\overline{\Delta F^2_{P,AP}}} = L^\theta f(L/M)$. On the face of it, this would give rise to $\theta = 1$ for all dimensions. The other two terms, however, do not have aspect ratio scaling form. In particular, the term $\Delta f^2_{\mathrm{SK}} V^{2\mu}$, which is dominant in $d > 6$ if $\mu > 1/6$, depends only on volume but not on shape.

Our calculation is exact in high dimensions within the replica symmetry breaking scenario for spin glasses. It is quite unusual and contradicts all expectations one might have about the interface energy based on experience from other systems and numerical data. It is significantly different from that found in, for instance, ferromagnets. There, the defect energy comes from the gradient term in the analogue of Eq. (2). Here, on the other hand, the mean-field solution is independent of $z$ so there is no contribution from the gradient term. A difference between the interface energy in spin glasses and ferromagnets is, however, that in ferromagnets there is a 'real' domain wall, whereas in spin glasses, the interface can only be defined by comparing one system to a reference system with the opposite set of boundary conditions. Thus strictly speaking, the interface in spin glasses is not a physical system itself, which may account for the absence of an interface energy on the mean field level.

The failure of aspect ratio scaling is a strong prediction which contradicts numerical evidence for $d = 2$ [20, 21]. The replica symmetry breaking scenario predicts space-filling domain walls [16, 22], therefore the dependence of the interface energy on volume but not on shape (to leading order) appears natural since the interface explores even the remote corners of the sample and would be likely to exist in some form down to three dimensions, even though the loop expansion used in this paper will need modification below six dimensions. This suggests a simple test of replica symmetry breaking ideas. If they are valid in three dimensions, then aspect ratio scaling will fail. To date, there is (weak) evidence that aspect ratio scaling *works* in three dimensions [20].

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