Energy gap of the bimodal two-dimensional Ising spin glass

W Atisattapong and J Poulter
Department of Mathematics, Faculty of Science, Mahidol University, Rama 6 Road, Bangkok 10400, Thailand
E-mail: g4937688@student.mahidol.ac.th and scjpt@mucc.mahidol.ac.th

New Journal of Physics 10 (2008) 093012 (11pp)
Received 13 June 2008
Published 11 September 2008
Online at http://www.njp.org/
doi:10.1088/1367-2630/10/9/093012

Abstract. An exact algorithm is used to compute the degeneracies of the excited states of the bimodal Ising spin glass in two dimensions. It is found that the specific heat at arbitrary low temperature is not a self-averaging quantity and has a distribution that is neither normal nor lognormal. Nevertheless, it is possible to estimate the most likely value and this is found to scale as \( L^3 T^{-2} \exp(-4J/kT) \), for a \( L \times L \) lattice. Our analysis also explains, for the first time, why a correlation length \( \xi \sim \exp(2J/kT) \) is consistent with an energy gap of \( 2J \). Our method allows us to obtain results for up to \( 10^5 \) disorder realizations with \( L \leq 96 \). Distributions of second and third excitations are also shown.

Contents

1. Introduction .................................................. 2
2. Formalism .................................................. 3
3. Results ..................................................... 5
4. Conclusions ............................................... 9
Acknowledgments ............................................. 10
References ............................................... 11
1. Introduction

In spite of its comparative simplicity, the two-dimensional bimodal short-range Ising spin glass model remains an interesting source of controversy. Although it is now widely accepted that the spin glass only exists at zero temperature [1, 2], the nature of excitations, in particular the energy gap with the first excited state, has commanded much interest in the literature.

The bimodal model has bond (nearest-neighbour) interactions of fixed magnitude $J$ and random sign. If we think of an infinite square lattice, without open boundaries, it is easy to appreciate that any finite number of spin flips cannot result in an excitation energy of less than $4J$. Nevertheless, some 20 years ago, Wang and Swendsen [3] gave credible evidence that the energy gap with the first excited state should be $2J$ in the thermodynamic limit. These excitations must involve an infinite number of spin flips. The issue here is the noncommutativity of the zero-temperature and thermodynamic limits. In such a situation, it is imperative to perform the thermodynamic limit first.

Support for the $2J$ energy gap has included studies that have involved exact computations of partition functions [4], a worm algorithm [5] and Monte Carlo simulation [6]. Challenges to $2J$ have also appeared. Saul and Kardar [7] maintained that the energy gap should be $4J$ as naive analysis suggests. More recently [8], it has been reported that the specific heat should follow a power law in temperature. In particular, it was proposed that the critical exponents must be the same as those for the model with a Gaussian distribution of bond interactions, indicating universality with respect to the type of disorder. Fisch [9], using a steepest descent approximation, has also suggested power law behaviour albeit with a different exponent.

An important quantity, intimately involved with studies of the thermodynamic limit at fixed temperature, is the correlation length. Essentially this measures the spatial extent of the influence of one spin on others. The correlation length is infinite at a critical temperature. For the spin glass model of interest here, the correlation length has been determined by reliable Monte Carlo techniques [2, 10] to be $\xi \sim \exp(2J/kT)$. This is in agreement with [7] and consistent with a qualitative study [11]. If this is true then hyperscaling predicts that the energy gap should be $4J$. A $2J$ gap would be consistent with $\xi \sim \exp(J/kT)$ as proposed in [6]. Another scenario is power law behaviour [8].

A good current review of the issues involved here has been given in [12]. The power law behaviour of [8] is discussed in the light of new Monte Carlo data. The conclusion is that the suggested universality cannot be reliably proven with the computational facilities currently available. Further, it is stated that extrapolation of the data of [6] to zero temperatures may not be plausible. The main message of this paper is to argue, for the first time, why a correlation length $\xi \sim \exp(2J/kT)$ is perfectly consistent with an energy gap $2J$, in apparent violation of hyperscaling.

We have performed exact calculations of the degeneracies of excited states at a fixed arbitrarily low temperature. Each disorder realization consisted of a frustrated $L \times L$ patch with periodic boundary conditions in one dimension, embedded in an infinite unfrustrated environment in the second dimension. This choice of boundary conditions, with even $L$, definitely does not allow any first excitation with energy gap less than $4J$. There are no open boundaries and no diluted bonds. A $2J$ energy gap can only arise in the thermodynamic limit.
2. Formalism

Any planar Ising model is isomorphic to a system of interacting fermions. The Pfaffian formalism [13] is particularly convenient for disordered systems [14, 15]. Each bond is decorated with two fermions, one either side, so that a square plaquette has four; left, right, top and bottom. The partition function is given by \( Z \sim (\det D)^{1/2} \) where \( D \) is a real skew-symmetric \( 4N \times 4N \) matrix for a lattice with \( N \) sites. Perturbation theory is used to determine ground state properties. Basically we require the low-temperature behaviour of the defect (meaning zero at zero temperature) eigenvalues of \( D \). Exactly, \( D = D_0 + \delta D_1 \) where \( \delta = 1 - t \) with \( t = \tanh(J/kT) \). The temperature dependence appears in \( \delta \) only. \( D_0 \) is singular in the ground state and has eigenvectors \( |d⟩ \) corresponding to zero eigenvalue, that is \( D_0|d⟩ = 0 \), localized on each frustrated plaquette. These eigenvectors form the subbasis for the perturbation theory.

At first order, the matrix \( D_1 \), which is \( 2 \times 2 \) block diagonal across bonds, is diagonalized in the subbasis. To continue at second order requires the continuum Green’s function \[ G_c = (1 - P)g_c(1 - P) \] where \( P = \sum_d |d⟩⟨d| \) and \( g_c = g_{c1} + g_{c2} \). The first term \( g_{c1} = 4 \times 4 \) block diagonal in the four fermions in each plaquette and allows us to connect frustrated plaquettes across two bonds. At second order we diagonalize \( D_2 = D_1 g_{c1} D_1 \). The matrix \( g_{c2} \) is, just like \( D_1 \), \( 2 \times 2 \) block diagonal across bonds and only relevant for excited states. For higher orders, we require the Green’s functions \( G_r \) constructed at previous orders. At third order, the matrix to be diagonalized is \( D_3 = D_2(1 + G_1 D_1)g_{c1} D_1 \) and, generally at arbitrary order \( D_r = D_{r-2}(1 + G_{r-2} D_{r-2}) \cdots (1 + G_1 D_1)g_{c1} D_1 \) until all degeneracy is lifted. Here we define, for \( r \geq 1 \),

\[
G_r = \sum_{i=1}^{N(r)} \frac{\langle \alpha^i_r \rangle \langle \beta^i_r | - | \beta^i_r \rangle \langle \alpha^i_r |}{\epsilon^i_r},
\]

where \( D_r|\alpha^i_r⟩ = -\epsilon^i_r|\beta^i_r⟩ \) and \( D_r|\beta^i_r⟩ = \epsilon^i_r|\alpha^i_r⟩ \) with \( \epsilon^i_r \neq 0 \) and there are \( N(r) \) such pairs at order \( r \). Note that \( G_r \) is real here, as are all matrices; in contrast to [15] where they are imaginary.

The internal energy of the system is

\[
U = -J \sum_{\langle ij \rangle} \zeta_{ij} \langle \sigma_i \sigma_j⟩,
\]

where \( \sigma_i \) is an Ising spin, \( \zeta_{ij} \) represents the sign of the bond and the nearest-neighbour correlation function can be written [14]

\[
\zeta_{ij} \langle \sigma_i \sigma_j⟩ = t - (1 - i^2)\mathcal{G}^{-+},
\]

where \( \mathcal{G}^{-+} \) means the matrix element of \( \mathcal{G} = -D^{-1} \) between the two nodes decorating the bond \( \langle ij⟩ \).

The full Green’s function \( \mathcal{G} \) can be expanded for a finite system in powers of \( \delta \)

\[
\mathcal{G} = \sum_{m=-\infty}^{r_{\text{max}}} \delta^{-m} K_m
\]

where \( r_{\text{max}} \) is the highest order of perturbation theory required. It is obvious that \( K_m \), for \( m > 1 \), has no direct physical meaning. We provide here a brief outline of how the perturbation theory for the Green’s function allows us to expand the internal energy exactly.

\[1\] It is convenient to use the bond basis \( |±⟩ = \frac{1}{\sqrt{2}}(|\alpha⟩ ± \zeta_{ij}|\beta⟩) \) where \( |\alpha⟩ \) and \( |\beta⟩ \) are as shown in figure 4 of [15].
Equating powers of δ in GD = −1, we obtain (for \( m < r_{\text{max}} \))

\[
D_0 K_m + D_1 K_{m+1} = -\delta_{m0}. \tag{5}
\]

Since PD_0 = 0, we can show that for \( m \leq 0 \),

\[
K_m = (1 + K_1 D_1) g_c (\delta_{m0} + D_1 K_{m+1}). \tag{6}
\]

It also can be proved that (1 + K_1 D_1) is idempotent, that is

\[
(1 + K_1 D_1)^2 = (1 + K_1 D_1). \tag{7}
\]

Since both \( g_{c2} \) and \( D_1 \) are bond diagonal and \( g_{c2} D_1 = \frac{1}{2} \) [16], we get \( K_0 = (1 + K_1 D_1) g_{c1} (1 + D_1 K_1) + g_{c2} + \frac{1}{2} K_1 \) and for \( m < 0 \)

\[
K_m = \left( (1 + K_1 D_1) g_{c1} D_1 + \frac{1}{2} \right) K_{m+1}. \tag{8}
\]

Substituting \( t = 1 - \delta \) and the Green’s function in (3), the correlation function can be expressed in terms of \( K_1 \) as

\[
\zeta_{ij} \langle \sigma_i \sigma_j \rangle = (1 - 2K_1^{-}) - 2 \sum_{m=1}^{\infty} \delta^m \left[ ((1 + K_1 D_1) g_{c1} D_1 + \frac{1}{2})^{m-1} (1 + K_1 D_1) g_{c1} (1 + D_1 K_1) \right]^{-}. \tag{9}
\]

We can now use the binomial theorem to expand in exp \((-2J/kT)\) instead of \( \delta \), which eliminates the explicit effect of \( g_{c2} \) and the internal energy can be expressed as

\[
U = \sum_{m=0}^{\infty} e^{-2Jm/kT} U_m, \tag{10}
\]

where \( U_0 = -2J N + 2J \sum_{\langle ij \rangle} K_1^{-} \) and for \( m > 0 \)

\[
U_m = 2^{m+1} J \sum_{\langle ij \rangle} \left[ ((1 + K_1 D_1) g_{c1} D_1)^{m-1} (1 + K_1 D_1) g_{c1} (1 + D_1 K_1) \right]^{-}. \tag{11}
\]

Since \( D_1^{-} = -1 \), it is obvious that \( 2 \sum_{\langle ij \rangle} A^{-} = - \sum_{\langle ij \rangle} (D_1 A)^{++} - \sum_{\langle ij \rangle} (A D_1)^{-} = -\text{Tr}(AD_1) \) for any skew-symmetric matrix \( A \). We can then show under the trace that for \( m > 0 \),

\[
U_m = -2^m J \text{Tr}\left[ ((1 + K_1 D_1) g_{c1} D_1)^m (1 + K_1 D_1) \right]. \tag{12}
\]

This can be rewritten using the idempotence relation (7) to get

\[
U_m = -2^m J \text{Tr}(D_1 g_{c1} (1 + D_1 K_1))^m. \tag{13}
\]

Finally, with recursive expansion, this can be expressed as

\[
U_m = -2^m J \text{Tr}(D_1 g_{c1} (1 + D_1 K_1))^m
= -2^m J \text{Tr}(D_1 g_{c1} (1 + D_1 G_1) (1 + D_2 K_2))^m
= \cdots
= -2^m J \text{Tr} R^m. \tag{14}
\]
Figure 1. The degeneracy of the first excitations for the Villain model as a function of lattice size $L$. The curve is a guide for the eye.

where

$$R = D_1 g_{c1} (1 + D_1 G_1) (1 + D_2 G_2) \cdots (1 + D_{r_{\text{max}}} G_{r_{\text{max}}})$$ \hfill (15)

This is sensible since it includes all the features of the ground-state calculation. It is also exact.

We can imagine colouring plaquettes black and white; like a chess board. Matrices $D_r$ and $G_r$ are colour diagonal for even $r$: otherwise they are off-diagonal. Since $g_{c1}$ is colour diagonal, $R$ is off-diagonal and it follows that $U_m = 0$ for odd $m$. This explicitly excludes any $2J$ excitations involving a finite number of spins.

The specific heat per spin can be derived in terms of the internal energy as

$$c_v = \frac{1}{L^2} \frac{dU}{dT} = \frac{1}{L^2} \left( \frac{4J}{kT^2} \right) \sum_{m=1}^{\infty} m e^{-4Jm/kT} U_{2m}.$$ \hfill (16)

We denote the degeneracy of the $i$th excited state as $M_i$. Expanding $\ln Z$ by Taylor series $\ln(1+x) = x - x^2 + \frac{x^3}{3} - \cdots$, we obtain, for example, $U_2 = 4J \left( \frac{M_1}{M_0} \right)$, $U_4 = 8J \left( \frac{M_2}{M_0} - \frac{1}{2} \left( \frac{M_1}{M_0} \right)^2 \right)$ and $U_6 = 12J \left( \frac{M_3}{M_0} - \frac{M_2}{M_0} \frac{M_1}{M_0} + \frac{1}{2} \left( \frac{M_1}{M_0} \right)^3 \right)$.

3. Results

As a means of establishing bearings, we first report a study of the first excitations of the fully frustrated Villain model \[17, 18\]. Figure 1 shows clearly that the ratio $\frac{M_1}{M_0} \sim \frac{2}{\pi} L^2 \ln L$. The correlation length is known to be $\bar{\xi} \sim \delta^{-1}$ \[19\]. Replacing $\ln L$ with $-\ln \delta \sim T^{-1}$, the correct form for the specific heat is obtained, that is $c_v \sim T^{-3} \exp (-4J/kT)$. The degeneracy per spin of the first excited state is infinite in the thermodynamic limit, although only weakly (logarithmically) so.
In figure 2, we show the distribution of $\frac{M_1}{M_0}$ for the spin glass. It is clear that the most likely value scales as $L^3$. In this case we have an extra factor $L$, unlike $\ln L$ for the Villain model. In consequence, taking $\xi \sim \exp (2J/kT)$, the specific heat varies like $c_v \sim T^{-2}\exp \left( -2J/kT \right)$ explaining why a $2J$ energy gap arises from the form of the correlation length obtained from Monte Carlo calculations [2, 10]. Hyperscaling fails here. We also emphasize that the Villain model is not a spin glass and comparisons, such as in [7], are not meaningful.

The distributions are scaled with a factor of $L$, probably indicating that the amount of effort required for an experiment to find the mode of the distribution scales like $L$. This is consistent with the known difficulties that arise when trying to extrapolate Monte Carlo data to zero temperature. Also, the distributions are obviously neither normal nor lognormal. Further, the data is not self-averaging. In fact, the relative variance grows quickly with $L$ which is unusually severe; convergence to a constant is normally expected [20].

We can discuss our choice of correlation length in the light of [12]. Two crossover temperatures are defined. Below $T^*(L)$ the ground state behaviour dominates. Above the finite-size crossover temperature $T_\xi (L)$ no size limitations are expected. It is clearly stated that, in all situations, $T_\xi > T^*$. This immediately rules out $\xi \sim \exp (J/kT)$. For our case, we can in fact make the definite prediction $T_\xi = 1.5T^*$. A power law behaviour for $\xi$ must also be ruled out if we also expect similar behaviour for the specific heat.

Pfaffians are also computed, for the partition function, in [4] at definite finite temperatures. For comparison, we have computed the mean of $\ln (\frac{M_1}{M_0})$ and find fairly close agreement. Nevertheless, we do not believe that this is physically meaningful. The distributions of $\frac{M_1}{M_0}$ are not lognormal and the most likely value scales as $L^3$, not $L^4$. We emphasize here that we are not computing the entire Pfaffians.

In figure 2, we show the distribution of $\frac{M_1}{M_0}$, scaled with a factor $L$, for $\frac{M_1}{M_0} L^3$ with various values of lattice size $L$. Each distribution includes $10^5$ disorder realizations, except for $L = 96$ which has 20 000.
We also analyse the distributions of $M_1/M_0$ according to a generalized extreme-value distribution. The Fréchet distribution is feasible for fat-tailed distributions as found in [21] where the probability density function is given by

$$f_{\xi,\mu,\beta}(x) = \frac{1}{\beta} \left(1 + \xi \left(\frac{x - \mu}{\beta}\right)\right)^{-(1/\xi)-1} \exp\left(-\left(1 + \xi \frac{x - \mu}{\beta}\right)^{-1/\xi}\right)$$  \hspace{1cm} (17)

which has the mode:

$$\bar{x} = \mu + \beta \frac{(1+\xi)^{-\xi} - 1}{\xi}.$$  \hspace{1cm} (18)

The parameters of the distribution $\mu$ (location), $\xi$ (shape) and $\beta$ (scale) are determined by a maximum likelihood estimator [22, 23]. It is useful to also present our distributions in figure 3 scaled with respect to

$$f(\bar{x}) = \frac{1}{\beta} (1+\xi)^{(1+\xi)} \exp\left(-(1+\xi)\right)$$ \hspace{1cm} (19)

obtained using fitted parameters. The fitted distributions, again divided by $f(\bar{x})$, are shown in figure 4 for comparison. The corresponding modes are shown in figure 5. Nevertheless, it is found that the quality of the fit is quite poor even for $L = 8$ and this gradually deteriorates with respect to increasing $L$ as shown in figure 6. The fit for $L = 96$ is the worst of all. We believe that, for larger $L$, more disorder realizations are necessary for a smooth distribution. However, it is reasonable to believe that convergence of the mode from the actual distributions occurs. There is no real contradictory evidence.

We have also checked distributions for second excitations. The most likely value of $M_2/M_0 - N$ scales as $L^6$. We have subtracted off here the (infinite) total number of spins $N$. Single spin flips
Figure 4. Fréchet distributions obtained from fitting actual disorder realizations for $\frac{M_1}{M_0} L$ by the algorithm of Hosking [22], divided by $f(\bar{x})$.

Figure 5. The mode of the fitted distributions.

can occur anywhere and it is sensible to measure the internal energy relative to the unfrustrated system. However, the appropriate contribution to the internal energy is $\frac{M_1}{M_0} L - \frac{1}{2} \left( \frac{M_1}{M_0} L \right)^2 - N$. As shown in figure 7, the most likely value is close to zero. We note that the mode of $\frac{1}{2} \left( \frac{M_1}{M_0} L \right)^2$ is roughly 0.002; indicating a close cancellation. Note also that the shapes of the distributions show clearly the dominant effect of the first excitations. The distributions for third excitations,
Figure 6. Distributions, scaled with a factor $L$, for $\frac{M_1}{M_0}$, The lines use the parameters resulting from the algorithm of Hosking [22] fitted to actual disorder realizations.

that is of $\frac{M_3}{M_0} - \frac{M_2}{M_0} \frac{M_1}{M_0} + \frac{1}{3} \left( \frac{M_1}{M_0} \right)^3 - 2N$, also show a most likely value close to zero as shown in figure 8. Here, the mode of $\frac{M_3}{M_0} - 2N$ scales as $L^9$ and the unfrustrated system has $M_3 = 2N$. It is also clear in this case, again from the skewness, that the first excitations are dominant. It is unlikely that higher excitations will interfere with our arguments based on first excitations.

4. Conclusions

In conclusion, we have reported exact results for the excitations of the bimodal two-dimensional Ising spin glass by expanding in arbitrary temperature from the ground state. All other treatments, except [7], have required extrapolation from definite finite temperatures. We have argued that an energy gap of $2J$ is consistent with $\xi \sim \exp (2J/kT)$ as found from Monte Carlo simulations. The manner in which our model is arranged excludes the possibility of any $2J$ excitation for a finite system. Nevertheless, it should also be interesting to study systems with obvious $2J$ excitations, for example the hexagonal lattice or square lattice with open boundaries or diluted bonds, and investigate the distributions.
**Figure 7.** Distributions, scaled with a factor $L$, for the second term in the specific heat. Each includes $10^5$ disorder realizations, except for $L = 64$ which has $35\,000$.

**Figure 8.** Distributions, scaled with a factor $L$, for the third term in the specific heat. Each includes $10^5$ disorder realizations.

**Acknowledgments**

W A thanks the Commission on Higher Education Staff Development Project, Thailand for a scholarship. J P acknowledges fruitful conversations with J A Blackman. Some of the computations were performed on the Tera Cluster at the Thai National Grid Center.
References

[1] Hartmann A K and Young A P 2001 Phys. Rev. B 64 180404
[2] Houdayer J 2001 Eur. Phys. J. B 22 479
[3] Wang J-S and Swendsen R H 1988 Phys. Rev. B 38 4840
[4] Lukic J, Galluccio A, Marinari E, Martin O C and Rinaldi G 2004 Phys. Rev. Lett. 92 117202
[5] Wang J-S 2005 Phys. Rev. E 72 036706
[6] Katzgraber H G, Lee L W and Campbell I A 2005 Nontrivial critical behavior of the free energy in the two-dimensional Ising spin glass with bimodal interactions arXiv:cond-mat/0510668
[7] Saul L and Kardar M 1993 Phys. Rev. E 48 R3221
Saul L and Kardar M 1994 Nucl. Phys. B 432 641
[8] Jörg T, Lukic J, Marinari E and Martin O C 2006 Phys. Rev. Lett. 96 237205
[9] Fisch R 2007 J. Stat. Phys. 128 1113
[10] Katzgraber H G and Lee L W 2005 Phys. Rev. B 71 134404
[11] Sungthong R and Poulter J 2003 J. Phys. A: Math. Gen. 36 6347
[12] Katzgraber H G, Lee L W and Campbell I A 2007 Phys. Rev. B 75 014412
[13] Green H S and Hurst C A 1964 Order-Disorder Phenomena (London: Interscience)
[14] Blackman J A 1982 Phys. Rev. B 26 4987
[15] Blackman J A and Poulter J 1991 Phys. Rev. B 44 4374
[16] Poulter J and Blackman J A 2005 Phys. Rev. B 72 104422
[17] Villain J 1977 J. Phys. C: Solid State Phys. 10 1717
[18] André G, Bidaux R, Carton J-P, Conte R and de Seze L 1979 J. Physique 40 479
[19] Lukic J, Marinari E and Martin O C 2006 Europhys. Lett. 73 779
[20] Wiseman S and Domany E 1998 Phys. Rev. Lett. 81 22
[21] Dayal P, Trebst S, Wessel S, Würtz D, Troyer M, Sabhapandit S and Coppersmith S N 2004 Phys. Rev. Lett. 92 097201
[22] Hosking J R M 1985 Appl. Stat. 34 301
[23] Macleod A J 1989 Appl. Stat. 38 198

New Journal of Physics 10 (2008) 093012 (http://www.njp.org/)