

Freezing Temperature in Dilute Ising Spin Glasses with Long-Range Interactions

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The onset of spin-glass freezing in dilute Ising systems with long-range interactions is investigated with the use of numerical simulations. We show that taking pair correlations explicitly into account results in the renormalization of the interaction matrix and suppression of the density of localized states compared with conventional mean field theory. Application of the theory to the RKKY interaction in the dilute limit raises the question of the appropriate boundary eigenvalue of the effective interaction matrix that separates localized and extended states. We identify the onset of spin-glass freezing with the temperature T_g at which this boundary eigenvalue is equal to one. Numerical simulations reproduces the linear concentration dependence of T_g in the very dilute limit, in agreement with scaling relations, and show a significant improvement over the conventional mean-field theory in the value obtained for the freezing temperature.

KEY WORDS: Spin glasses; long-range interactions; freezing temperature; localized and extended states.

1. INTRODUCTION

In this paper we concentrate on the estimation of the spin-glass freezing temperature T_g of the dilute Ising spin glasses with long-range interactions.

As an example we consider the RKKY interaction

$$J_{ij} = A \frac{\cos(2k_F r_{ij})}{r_{ij}^3} \quad (1)$$

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where $J_{ij} \equiv J(r_{ij})$ is the interaction between spins separated by the distance r_{ij} , k_F is a Fermi vector of the conduction electrons.

Although this issue has been under discussion almost 20 years,⁽¹⁻³⁾ a reliable estimation of T_g has not been given. Moreover, even the apparent scaling law

$$T_g \sim c, \quad c \ll 1 \quad (2)$$

that is a consequence of the special form of RKKY interaction,^(3,4) $J_{ij} \propto r_{ij}^{-3}$, has been reproduced only recently⁽⁵⁾ with the use of computer simulation techniques applied to the mean field equations.

It should be mentioned also that in a major number of previous papers the analyses of the experiment in real spin glasses has been performed in terms of the configurational average value of Edwards–Anderson (EA) order parameter q . The validity of such an assumption implies that spatial fluctuations of q are not very large. However the latter is in apparent contradiction with recent experiments⁽⁶⁾ indicating the inhomogeneous structure in AuFe. Inhomogeneous spin-glass structure has also been found in CuMn.⁽⁷⁾ These experimental findings seems to be consistent with recent Monte Carlo simulations⁽⁸⁾ and earlier mean field analysis⁽⁹⁾ of short range spin glasses. It has been emphasized,⁽⁸⁾ based on the Monte Carlo results, that the description in terms of configurational average value of q is not even qualitatively valid near T_g . (See also ref. 10.)

Another approach to the problem has been proposed long ago by Anderson.⁽¹¹⁾ The straightforward way to find T_g in mean field approximation is the diagonalization of the random matrix J_{ij} and the identifying of T_g with the maximum eigenvalue of the matrix. However, in the applying such a procedure to dilute systems with random interactions additional complications are encountered due to the existence of the localized states of the J_{ij} matrix the latter being associated with small clusters of strongly interacting spins. It is clear however, that localized states are not responsible for the collective behavior of the system which is a property of delocalized, extended states.

In order to estimate the freezing temperature one needs to find a characteristic boundary (or “mobility edge”) between localized and extended states. Although this issue has been widely discussed in the past,⁽¹¹⁻¹³⁾ until recently⁽⁵⁾ there was no implicit implementation of the approach to dilute spin glasses with long-range interactions. In ref. 5 we analysed the linearized local mean field equations

$$\langle S_i \rangle = \frac{1}{T} \sum_j J_{ij} \langle S_j \rangle \quad (3)$$

in terms of the eigenvalues of the matrix J_{ij} . $\langle Si \rangle$ is the thermal average value of the i th spin.

In this paper we go beyond mean field theory and analyze the corrections to the mean field equations using the concept of effective interaction, and replacing the matrix J_{ij}/T in Eq. (3) by the effective interaction matrix Φ_{ij} which takes into account the effect of fluctuations. In order to obtain the effective interaction matrix we use the Zernike approximation,⁽¹⁴⁾ originally proposed for Ising model of regular ferromagnets. Kaneyoshi⁽¹⁵⁾ employed this approximation to spin glasses with nearest neighbors interactions using the techniques of differential operators. We use another approach starting from the evaluation of the distribution function of local field acting on every spin due to its interaction with other spins. The essence of the approximation is in the neglect of correlations between spin contributing to local field, and in this sense we use the terminology “random local field” (RLF) approximation. Contrary to mean field theory we take explicitly into account the pair correlations between the given spin and each of the spins contributing to the local field. The RLF approximation has been applied earlier⁽¹⁶⁾ for dilute ferromagnets and ferroelectrics. It has been shown that for ferromagnetic models the accuracy of RLF approximation is the same as the accuracy of Bethe–Peierls cluster result. The degree of accuracy of RLF approximation to spin glasses with long-range interactions is discussed in Section 4 in comparison with the known results for the Sherrington–Kirkpatrick (SK) model⁽¹⁷⁾ and EA model with nearest neighbor interactions⁽¹⁸⁾

It is also important to note that in the framework of RLF approximation one takes explicitly into account the nonlinear coupling between eigenmodes of the matrix J_{ij} that leads to the renormalized effective interaction Φ_{ij} . Such an effective interaction was originally discussed in the model calculations⁽¹²⁾ based on φ (4) theory with the use of independent modes approximation. It has been shown⁽¹²⁾ that nonlinear coupling leads to the suppression of the weight of localized states. We will show in Section 3 that our approach reproduces for the first time this effect for the RKKY spin glasses and takes into account nondiagonal interactions in the J_{ij} basis as well as diagonal interactions.

2. RANDOM LOCAL FIELD APPROXIMATION

In order to understand at least qualitatively how crucial is the effect of thermal fluctuations on the freezing temperature in spin glasses with long-range interactions we consider below the first order corrections to mean field theory based on the random local field approximation.

In the development of random local field approximation we start from the identity^(19, 20)

$$\langle S_i \rangle = \left\langle \tanh \left(\frac{H_i}{T} \right) \right\rangle \quad (4)$$

here $S_i = \pm 1$,

$$H_i = \sum_j J_{ij} S_j \quad (5)$$

is the local field acting on every spin due to interaction with its neighbors. Equation (4) can be written in the form

$$\langle S_i \rangle = \int dH \tanh \left(\frac{H}{T} \right) f_i(H) \quad (6)$$

where

$$f_i(H) = \langle \delta(H - H_i) \rangle \quad (7)$$

Note that the function $f_i(H)$ in Eq. (7) is the exact distribution function of local field acting on spin i . Local mean field equation (3) corresponds to the approximation $f_i(H) = \delta(H - \langle H_i \rangle)$.

Using the integral representation of the delta function and the fact that one has $S_i^{2n} = 1$ and $S_i^{2n+1} = S_i$, we rewrite Eq. (7) as

$$f_i(H) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\rho e^{i\rho H} f_{ip} \quad (8)$$

in which

$$f_{ip} = \langle \exp[-i\rho H_i] \rangle = \left\langle \prod_k [\cos(\rho J_{ik}) - i S_k \sin(\rho J_{ik})] \right\rangle \quad (9)$$

In order to calculate the spin-glass transition temperature it is sufficient in Eq. (9) to keep only terms linear in $\langle S_i \rangle$. We also neglect correlations between different spins k, k', \dots interacting with spin i , which is equivalent to Zernike approximation. When this is done, the expression for f_{ip} assumes the form

$$f_{ip} = \prod_k \cos(\rho J_{ik}) - i \sum_j \prod_{k \neq j} \cos(\rho J_{ik}) \sin(\rho J_{ik}) \langle S_j \rangle \quad (10)$$

Only the second term in Eq. (10) which depends on $\langle S_j \rangle$ contributes to Eq. (6). We make the replacement

$$\prod_{k \neq j} \cos(\rho J_{ik}) \approx \overline{\prod_{k \neq j} \cos(\rho J_{ik})} \quad (11)$$

where overbar denotes the configurational average over random spin positions, based on the fact that the cosine function partially suppresses the effect of fluctuations in J_{ij} that originates from the variable sign interactions. Equation (11) is the exact result for the infinite range SK model with

$$J_{ij} = \pm \frac{J}{\sqrt{N}} \quad (12)$$

and for $\pm J$ nearest neighbor interaction.

In dilute systems ($c \ll 1$) in which the randomness in the interaction stems from the random occupation of the lattice sites (as in the case of RKKY interaction), the result of the configurational average in Eq. (11) can be written in the form $\exp[-F_1(\rho)]$, where $F_1(\rho)$ is given by

$$F_1(\rho) = c \sum_j [1 - \cos(\rho J(\mathbf{r}_{ij}))] \quad (13)$$

where the summation in Eq. (13) is taken over all lattice sites.

Using Eqs. (8) and (10) in Eq. (6), along with the identity

$$\int_{-\infty}^{\infty} dH \tanh\left(\frac{H}{T}\right) \sin(\rho H) = \frac{\pi T}{\sinh(\pi \rho T/2)} \quad (14)$$

we obtain the equation

$$\langle S_i \rangle = \sum_j \Phi_{ij}(T) \langle S_j \rangle \quad (15)$$

where

$$\Phi_{ij}(T) = T \int_0^{\infty} \frac{d\rho \exp[-F_1(\rho)] \sin(J_{ij}\rho)}{\sinh(\pi \rho T/2)} \quad (16)$$

It follows from Eqs. (15), (16) that effect of thermal fluctuations, explicitly taken into account in Eq. (6), (7), leads to the renormalization of interaction matrix in linearized equations for local magnetization. This results is consistent with the earlier discussions.⁽¹³⁾

Note that the linearized Thouless–Anderson–Palmer (TAP) equations⁽²¹⁾ obtained for SK model can be written in the form of Eq. (15) with the effective interaction

$$\phi_{ij}^{TAP} = \frac{J_{ij}/T}{1 + J^2/T^2}, \quad J^2 = \sum_j \overline{J_{ij}^2} \quad (17)$$

Φ_{ij}^{TAP} takes into account the effect of thermal Gaussian fluctuations of the local field, characterized by the variance J^2 , and reproduces the effect of the Onsager reaction field. The TAP approach can not be generalized on non-Gaussian fluctuations of the local field as takes place in the case of the RKKY interaction. In contrast to TAP approach, our approach allows to consider in approximate manner Gaussian as well as non-Gaussian fluctuations.

It follows from Eq. (16) that the linear dependence Φ_{ij}/T (corresponding to mean field theory) is approximately valid only for $J_{ij}/T \ll 1$. At higher values of J_{ij}/T the effective interaction matrix Φ_{ij} deviates significantly from J_{ij}/T and saturates to $\Phi_{ij} = 1$. As we show below, this results in the suppression of the effect of local clusters on the distribution of eigenvalues of matrix Φ_{ij} (compared with that in mean field theory)⁽⁵⁾ and in the relative decrease of the density of localized states.

3. RESULTS OF NUMERICAL SIMULATIONS

We have performed the numerical solution of Eqs. (15) using computer simulation techniques. We randomly distributed approximately $N = 900$ Ising spins on a simple cubic lattice with periodic boundary conditions, where the size of the lattice had been adjusted to the spin concentration. We then calculated all eigenvalues E_k ($k = 1, \dots, N$) of the matrices $\Phi_{ij}(T)$. The value $k_F = 3/d$ (d is the lattice constant) has been chosen in Eq. (1) which corresponds approximately to the Cu in a sense that the product of k_F^3 and the volume per lattice site is approximately the same as in real material.

The crossover between localized and extended states has been extensively studied^(22–24) in connection with the problem of Anderson localization. It has been shown that the boundary between localized and extended states is usually rather sharp, and the characteristic eigenvalue of the effective interaction matrix for which a relative variance in the distribution of eigenvalues is equal to 1/2 can be considered as a simple criterion determining the crossover between localized and extended states. The relative variance (that is the ratio between the variance and the distribution function)

approaches 1 for Poisson statistics, that are a characteristic of localized states, and is much less than 1 for extended states.

In order to calculate the distribution function of the eigenvalues we divided the interval $[-R, R]$ into 200 subintervals and collected the number $n(E)$ of eigenvalues in each subinterval. This was repeated for 100 different random configurations of the spins and the results averaged. The distribution function was written as

$$\sigma(E) = \frac{1}{M} [n(E)]_{av} \quad (18)$$

where M is the normalizing coefficient.

In the same manner we calculated the variance of the eigenvalue distribution

$$var(E) = \frac{1}{M} ([n(E)^2]_{av} - [n(E)]_{av}^2) \quad (19)$$

We have tested the effect of finite lattice size by comparing the results obtained for 900 spins with those for 1300 spins. No noticeable difference in eigenvalue distribution was found.

We have also considered another very common localization measure, the inverse participation ratio, $IPR(E)$, for the eigenvalue E , defined as

$$IPR(E) = \sum_j \Psi_j(E)^4 \quad (20)$$

where $\Psi_j(E)$, $j = 1, \dots, N$, are the corresponding eigenvector components. Because $\sum_j \Psi_j^2 = 1$, the IPR should be very small, i.e. proportional to $1/N$ for very delocalized states, and approaching 1 only in the opposite limit of extreme localization. The results of a numerical diagonalization of the matrix $\Phi_{ij}(T)$ are presented in Figs. 1, 2 for two concentration of spins $c = 0.02$ and $c = 0.04$ and different temperatures. For convenience we present on the same graph the values of distribution function $\sigma(E)$, variance $var(E)$, and inverse participation ratio $IPR(E)$.

One can clearly see that extended states responsible for the collective behavior are confined within a region inside the central peak. In this region both criteria for extended states are satisfied: ratio $var(E)/\sigma(E) < 1/2$ and $IPR(E)$ is very small. Also, in spite of the noticeable fluctuations of the $var(E)$ inside the central peak, one can see that the variance undergoes a crossover behavior near the value E_m for which the ratio $var(E_m)/\sigma(E_m) \approx 1/2$. Above E_m $var(E)$ rapidly approaches the values of $\sigma(E)$ which is an

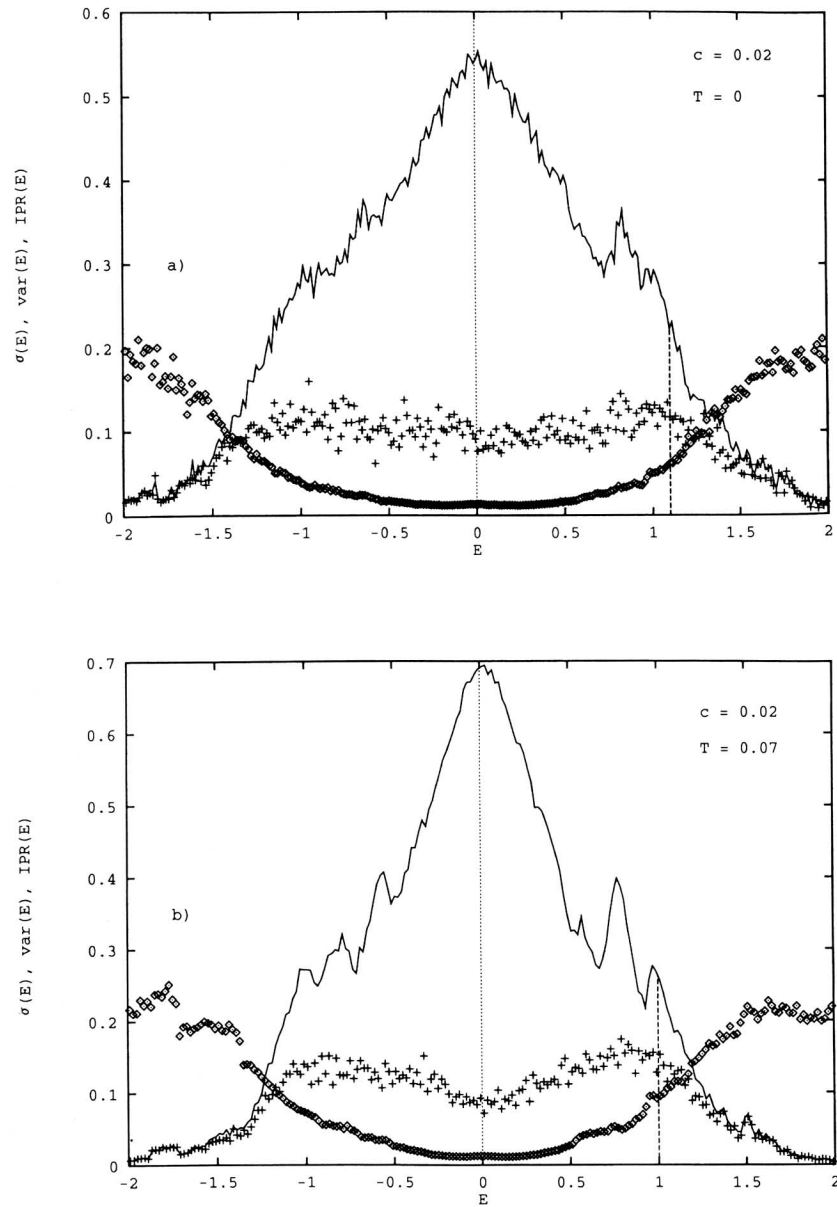


Fig. 1. Eigenvalue distribution function, $\sigma(E)$ (solid line), variance, $var(E)$ (crosses) and inverse participation ratio $IPR(E)$ (diamonds) corresponding to random local field matrix Φ_{ij} , Eq. (21) for $c = 0.02$ and different temperatures. Vertical dashed line denote the position of crossover eigenvalue E_{III} .

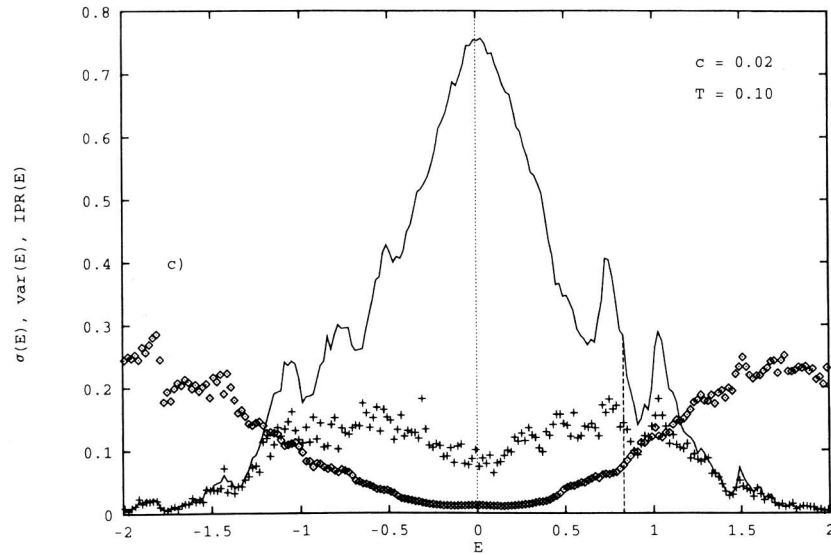


Fig. 1. (Continued)

indication of complete localization so we consider the eigenvalues E_m as the edge of extended states for the given spin concentration and temperature.

First of all one should verify that the freezing transition does exist within the approach used. Note that this problem is not in question within the conventional mean field theory, Eq. (3), for which all eigenvalues are proportional to $1/T$ and the criterion $E_m = 1$ can always be satisfied. In contrast, as we discussed above, the matrix Φ_{ij} has a well defined finite limit $(\Phi_{ij})_{\max} \rightarrow 1$ as $T \rightarrow 0$ and in this case the existence of the thermodynamic freezing transition is the intrinsic property of the model and is characterized by the maximum eigenvalue of the Φ_{ij} matrix at $T=0$ corresponding to extended states. (Note that Φ_{ij} is a monotonically decreasing function with increasing T .)

In Fig. 1a, and Fig. 2a we present the spectrum of eigenvalues, $\text{var}(E)$ and $\text{IPR}(E)$ of Φ_{ij} matrix for $c = 0.02$ and $c = 0.04$ at $T = 0$. One can clearly see that the eigenvalue $E = 1$ is below the edge of extended states, that is $E_m \approx 1.2$ for both concentrations. This shows that a freezing transition associated with the extended states does exist for 3 dimensional RKKY Ising spin glasses in agreement with the Monte Carlo results.⁽²⁵⁾

In order to find the estimate for the T_g we have performed numerical simulations for different temperatures using the values of Φ_{ij} matrix given by Eq. (16). We then identified T_g with the temperature for which $E_m = 1$.

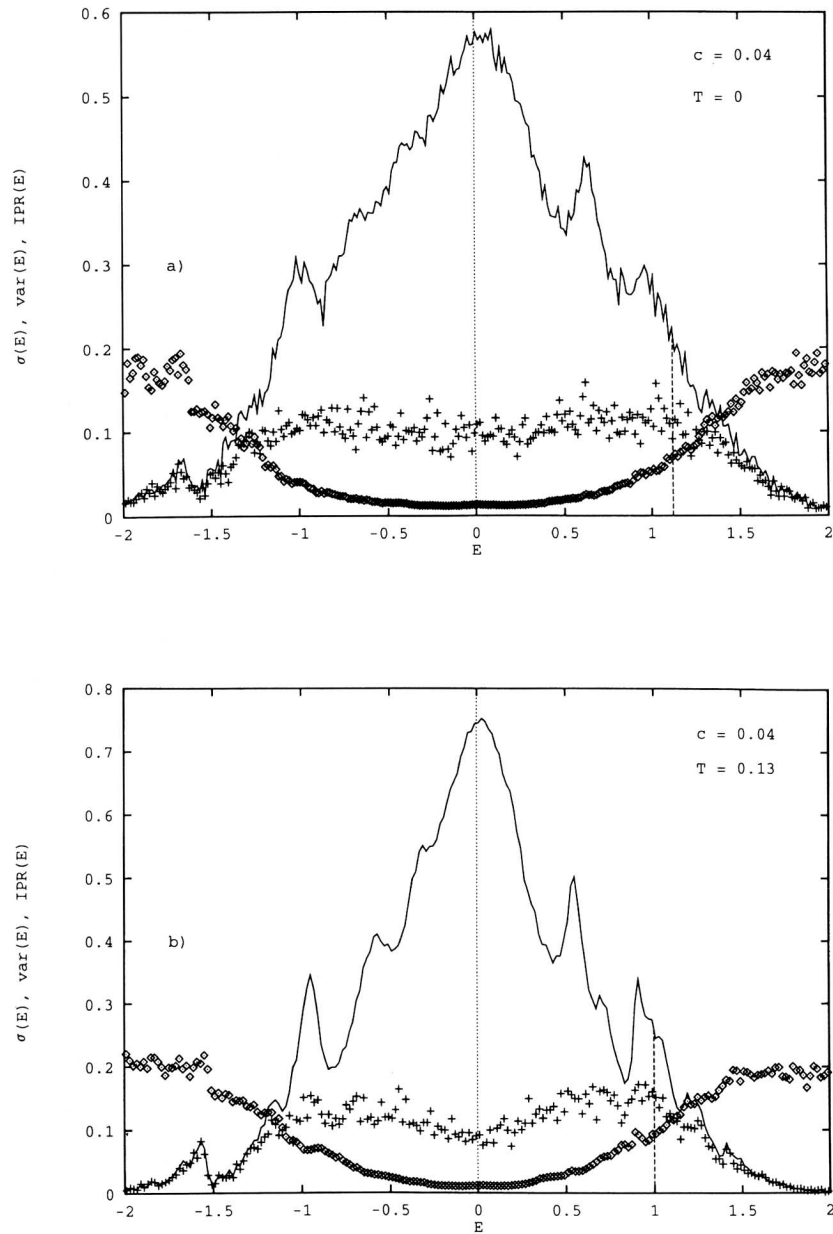


Fig. 2. Eigenvalue distribution function, $\sigma(E)$, variance, $\text{var}(E)$ and inverse participation ratio $\text{IPR}(E)$ corresponding to random local field matrix Φ_{ij} , Eq. (21) for $c = 0.04$ and different temperatures.

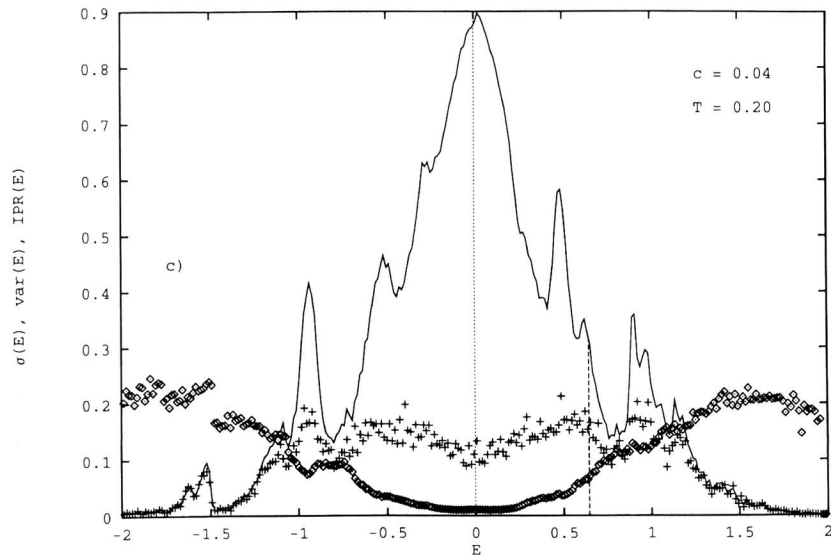


Fig. 2. (Continued)

Spectra of eigenvalues at $T = T_g$, are presented on Fig. 1b and Fig. 2b. From Fig. 2c and Fig. 3c one can see how different the spectra are at T well above T_g , where $E_m < 1$. I.e. the relative weight of the localized states decreases while temperature approaches T_g from above. This property of the localized states in spin glasses has been already discussed⁽¹²⁾ in model calculations.

We found $T_g \approx 0.07 \pm 0.01$ ($|A|/d^3$) for $c = 0.02$ and $T_g = 0.13 \pm 0.01$ ($|A|/d^3$) for $c = 0.04$. Also we performed additional calculations for $c = 0.03$ and found $T_g \approx 0.1 \pm 0.01$ ($|A|/d^3$). T_g scales practically linearly with concentration and can be written as

$$T_g^{RLF} \approx 3c \frac{|A|}{d^3} \quad (21)$$

Note that the values of T_g given by Eq. (21) are approximately one-half of the corresponding values for T_g in the mean field simulations,⁽⁵⁾ that is a significant improvement over the conventional mean field theory.

As regards the experimental situation, almost linear concentrational dependence of freezing temperature has been observed in very dilute CuMn

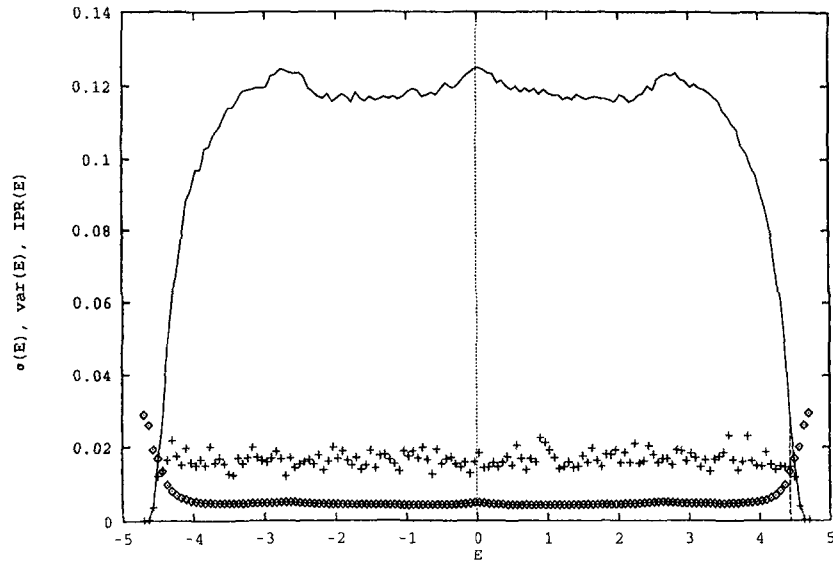


Fig. 3. Eigenvalue distribution function, $\sigma(E)$, variance, $var(E)$ and inverse participation ratio $IPR(E)$ corresponding to ζ_{ij} , Eq. (27) for nearest neighbor interaction on a 3d cubic lattice.

and AgMn alloys.^(3, 26) See also recent results.⁽²⁷⁾ Unfortunately, we are not able to compare numerically Eq. (21) with the experiment due to the Heisenberg rather than Ising nature of canonical spin glasses. However, the concentration dependence of T_g should be the same for both Heisenberg and Ising models, since it is caused by the specific form of RKKY interaction $J(r) \sim r^{-3}$.

4. DISCUSSION

1. The results obtained in the preceding section establish apparently the upper limit for the freezing transition temperature in RKKY Ising spin glasses (that is twice lower its mean field value). A question arises how far this upper limit is from the true value of T_g . A qualitative answer to this question can be given by applying the method used to other models for which the values of T_g are known. We will consider below the SK model with J_{ij} given by Eq. (12), and EA model with $\pm J$ nearest neighbor interactions.

SK model. Substituting Eq. (12) into Eq. (10) we obtain $F(\rho) = \rho^2 J^2/2$, while $\sin(\rho J_{ij})$ can be replaced by its argument. The matrix Φ_{ij} then assumes the form

$$\phi_{ij}(T) = \left\{ T \int_0^\infty \frac{d\rho \exp[-\rho^2 J^2/2] \rho}{\sinh(\pi\rho T/2)} \right\} J_{ij} \quad (22)$$

We note that for infinite range interactions all eigenvectors of the random matrix Φ_{ij}^{RLF} are delocalized,^(21, 28) and the transition temperature can be identified with the temperature at which the largest eigenvalue of the matrix Φ_{ij} is equal to one. Since the largest eigenvalue of the matrix (12) is equal to $2J$, one obtains an expression for T_g by numerically evaluating the integral in Eq. (22). The result is

$$T_g^{\text{RLF}} \simeq 1.5J \quad (23)$$

which is half way between the mean field and exact results, and, thus, is a significant improvement of the former. The same result for T_g is obtained for SK model with a gaussian distribution of J_{ij} as well.

$\pm J$ nearest neighbor interactions. This model can be considered as an opposite limit to SK model in a sense of effect of thermal fluctuations. The fluctuations decrease significantly the numerical value of T_g for 3 dimensional systems and completely destroy the spin glass equilibrium phase for $d=2$.⁽²⁹⁾ Very precise calculations⁽³⁰⁾ of T_g for $\pm J$ is nearest neighbor interactions model give $T_g \approx 1.2$ for 3d cubic lattice. Let us compare this value with that given by RLF approximation.

In order to perform numerical calculations we write the matrix Φ_{ij} in the form

$$\Phi_{ij} = \Phi(T) \xi_{ij} \quad (24)$$

where

$$\Phi(T) = T \int_0^\infty \frac{d\rho}{\sinh(\pi\rho T/2)} \cos(J\rho)^{z-1} \sin(J\rho) \quad (25)$$

and

$$\xi_{ij} = \pm 1 \quad (26)$$

z is the number of nearest neighbors.

Calculations have been performed in the same way as discussed in Sec. 3. According to Eq. (24) each eigenvalue of the matrix Φ_{ij} is equal to

the product of $\Phi(T)$ and the corresponding eigenvalue of the matrix ξ_{ij} . Spectrum of the eigenvalues of the matrix ξ_{ij} is presented in Fig. 3. One can see that almost all eigenvalues are extended and the maximum eigenvalue of the ξ_{ij} matrix is equal to 4.5. This value has been reported earlier.⁽⁹⁾ However, from the ratio between the distribution function of the eigenvalues and the variance we conclude that the boundary between localized and extended states $E_m \approx 4.3$. In order to find the spin-glass freezing transition temperature one should numerically solve the equation

$$\Phi(T_g) E_m = 1 \quad (27)$$

that gives

$$T_g^{RLF} \approx 2.9J \quad (28)$$

One can argue that the value $T_c = 2.9J$ is higher than $T_c = 2.45J$ for $z = 6$ that would be obtained by simply scaling the SK result by the square root of the number of nearest neighbors. However, the latter estimate is purely phenomenological since it includes Onsager reaction field, obtained for infinite range SK model, in short range EA model.

2. One can speculate further about the actual value of the transition temperature T_g for RKKY interaction. Due to the long-range nature of the RKKY interaction one can expect that the ratio between exact (presently unknown) value of T_g and T_g^{RLF} , Eq. (21), should be greater than that for nearest neighbor interactions and less than that for infinite range SK model. T.e

$$\frac{1.2}{2.9} < \frac{T_g}{T_g^{RLFA}} < \frac{1}{1.5} \quad (29)$$

or, using Eq. (21),

$$1.2c \frac{|A|}{d^3} < T_g < 2c \frac{|A|}{d^3} \quad (30)$$

One can expect that in inequality (30) the values of T_g should be closer to the right hand side limit due to the long-range nature of the RKKY interaction.

3. Finally, we discuss the question of the sensitivity of the RLF to the dimension of the system. In the framework of mean field equations (3) $T_g \neq 0$ for any dimension. At the same time RLF approximation establishes the well defined criterion for the existing of freezing transition.

Taking into account that function $\Phi(T)$ in Eq. (27) monotonically increases as T approaches to zero, we can write the criterion that $T_g \neq 0$ in the form

$$\zeta \equiv \Phi(T=0) E_m > 1 \quad (31)$$

We have performed numerical simulations of Eq. (15) for $d=1$ and $d=2$. We found that for $d=1$ $\zeta < 1$ meaning that equilibrium freezing transition does not exist. For $d=2$ the boundary eigenvalue separating localized and extended states $E_m \approx 3.2$ that gives $\zeta \approx 1.1$. This results is in apparent contradiction with presently established fact that for Ising spin glasses the lower critical dimension is between 2 and 3 and indicates the limitation of RLF approximation to low dimensional systems. However, the obtained value $\zeta \approx 1.1$ for $d=2$ is lower the value $\zeta \approx 1.3$ for $d=3$ reproducing qualitatively the increasing role of thermal fluctuation with the decrease of the dimension of the system.

5. CONCLUSION

In conclusion, we have shown that the RLF approximation combined with the computer simulation technique allows to find a crossover between localized and extended states and estimate the freezing temperature in Ising spin glasses with long-range interactions. The analysis suggested can be easily applied to the situations where the interaction J_{ij} has the more complicated form than considered above, e.g., when the mean free path of conduction electrons λ is comparable with the average distance R between spins and the dependence of T_g on the concentration c changes with the change of the parameter R/λ .

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