Spin glass behavior of frustrated 2-D Penrose lattice in the classical planar model

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Via extensive Monte Carlo studies we show that the frustrated XY Hamiltonian on a 2-D Penrose lattice admits of a spin glass phase at low temperature. Studies of the Edwards-Anderson order parameter, spin glass susceptibility, and local (linear) susceptibility point unequivocally to a paramagnetic to spin glass transition as the temperature is lowered. Specific heat shows a rounded peak at a temperature above the spin glass transition temperature, as is commonly observed in spin glasses. Our results strongly suggest that the critical point exponents are the same as obtained by Bhatt and Young in the $\pm J$ XY model on a square lattice. However, unlike in the latter case, the critical temperature is clearly finite (nonzero). The results imply that a quasiperiodic 2-D array of superconducting grains in a suitably chosen transverse magnetic field should behave as a superconducting glass at low temperature.

75.10.Hk, 75.10.Nr, 64.70.Pf

The notion of frustration, first introduced by Toulouse, has played a key role in the theoretical understanding of spin glasses. It is now believed that frustration is a necessary condition for the existence of a spin glass phase. However, all real systems (alloys) exhibiting spin glass behavior have an additional common feature, namely the topological disorder of magnetic component(s). On the theoretical front, models of uniformly frustrated spin systems without disorder have often failed to show spin glass behavior, and the debate as to whether disorder, in addition to frustration, is necessary in a spin glass continues. In this paper we present strong evidence that a frustrated XY Hamiltonian on a 2-D quasiperiodic lattice admits of a low temperature spin glass phase. The degree of frustration in this case varies widely from one lattice point to another, but in a predictable way determined by the quasiperiodic structure.

We consider the Hamiltonian for the XY model describing the interaction between 2-D spin vectors with orientations $\theta_i$ and $\theta_j$ situated at lattice sites $i$ and $j$ via a nearest neighbor coupling parameter $J$:  

$$H = -J \sum_{[ij]} \cos(\theta_i - \theta_j + A_{ij}), \quad (1)$$

where the summation is restricted to nearest neighbor pairs $[ij]$. The parameter $A_{ij}$ controls the frustration in the model. In the context of an array of superconducting grains, $\theta_i$ is the phase of the grain $i$ and the above Hamiltonian can be seen as describing the resulting Josephson junction of the grains “minimally coupled” to a transverse magnetic field with vector potential $\mathbf{A}$ with

$$A_{ij} = \frac{2\pi}{\Phi_0} \oint_{r_i} \mathbf{A} \cdot d\mathbf{l}. \quad (2)$$

$\Phi_0$ is the elementary flux quantum $\frac{2\pi}{\Phi_0}$ associated with the Cooper pairs, and $r_i$ denotes the lattice sites. Here the magnetic field acts as the source of frustration: an $A_{ij}$ which is an odd multiple of $\pi$ essentially renders the bond $[ij]$ negative.

The directed sum of $A_{ij}$ about a plaquette in a 2-D lattice can be written as $2\pi f$, where $f$ is the flux through the plaquette in units of $\Phi_0$. The 2-D Penrose lattice is composed of two (fat and thin) rhombic unit cells (plaquettes). Since the ratio of the areas of the fat and the thin rhombuses in the Penrose lattice is the Golden Mean ($\tau$), only one set of plaquettes can be fully frustrated at a time with a suitable choice of the magnetic field giving $f = 1/2$. The flux $f$ through the individual plaquettes in the other set will then be an irrational number.

In what follows we will present results for the case where the ‘thin rhombus’ is fully frustrated, mentioning at the outset that the results for the fully frustrated ‘fat rhombus’ case are qualitatively similar. All our results are obtained via Monte Carlo (MC) simulation based on the Metropolis algorithm using periodic boundary conditions on periodic Penrose lattices. We have cooled our systems in a quasi-static manner, starting from a high temperature ($T$(in units of $J$) > 2.0) random configuration and then heated the system in the same quasi-static fashion. Since we performed the simulation in $n$ blocks, the heating and cooling data are obtained by averaging over these blocks, with the error bars representing the standard deviation, obtained by dividing the square root of sum of squares of the deviations from the mean by $\sqrt{n-1}$, instead of $\sqrt{n}$. We then perform a ‘grand average’ over the heating and cooling data.

Magnetic moment per lattice point calculated for periodic Penrose lattices of various sizes is found to be small (< 0.02) over the entire temperature range. The magnitude of the moment decreases steadily with the size of the cluster, suggesting that the magnetization is strictly zero in the thermodynamic limit. To study the freezing of the spins at the lattice sites we calculate the Edwards-Anderson order parameter, a measure of breakdown of ergodicity in the system. In Fig.1 we show this order parameter defined by

$$q_{EA} = \sum_i (\vec{S}_i)^2, \quad (3)$$
where $\vec{S}_i = (\cos \theta_i, \sin \theta_i)$, and $\langle \rangle$ denotes a canonical ensemble average. In a completely frozen system $q_{EA}$ is unity, while for a completely ergodic system it is zero.

This order parameter shows a monotonic decrease with increasing temperature, clearly vanishing at temperatures beyond 0.5 for the 4,414 site periodic Penrose lattice shown in Fig.1. These results were obtained by averaging over 5 blocks of 60,000 configurations, generated after equilibrium was achieved. Since the vanishing of the order parameter with a long tail is a consequence of the finite system size, it is expected that the tail region will decrease with increasing system size and eventually disappear in the thermodynamic limit. However, we find that this tail persists, even for our largest system ($N = 11,556$) and, consequently, the spin glass transition temperature cannot be appropriately determined from Fig.1. Thus, we use other quantities to provide an estimate of the transition temperature $T_f$. It is clear, however, that the system has a low temperature phase with a nonzero order parameter $q_{EA}$.

Local (linear) susceptibility per spin, calculated from the fluctuations in the magnetization (net magnetic moment $m$ for a lattice of $N$ sites),

$$\chi = \frac{\langle m^2 \rangle - \langle m \rangle^2}{Nk_BT}, \quad (4)$$

is shown in Fig.2. At low temperatures, $0.02 - 0.2$ the results are obtained by averaging over 5 blocks of 125,000 MC steps, while 5 blocks of 15,000-45,000 steps were used for higher temperatures. The large hysteresis in the low temperature region indicates a high number of metastable states, which is a characteristic of spin glasses. These metastable states give rise to large error bars in $\langle m^2 \rangle - \langle m \rangle^2$ at low temperatures, which are further accentuated by a division by $T$ in Eq.(4). Although we feel that it might be possible to reduce the size of these error bars, this would require very long runs and one must also ensure that the system does not become trapped in one of these metastable states. Nevertheless, despite the large error bars, a cusp-like feature in $\chi$ is clearly visible at $T_f \sim 0.15$. We find a saturation in this cusp with respect to system size, which is consistent with spin glass behavior. Note that the high temperature (above $T_f$) phase is strictly paramagnetic. Here the decrease in $\chi$ is Curie-like, with $T\chi$ becoming a constant as shown in the inset of Fig.2.

Specific heat obtained from the fluctuations in the energy is shown in Fig.3 for various system sizes. The results are averages between heating and cooling, with the low temperature results having a somewhat larger hysteresis. All averages were obtained after equilibrating, however, the high temperature values were obtained by averaging over 5 blocks of 15,000 steps, whereas 5 blocks of 45,000 steps were used for the low temperatures. The result for the unfrustrated case is shown in the inset. Both frustrated and unfrustrated cases show saturation in specific heat with respect to system size. In the unfrustrated case the peak in the specific heat is at 1.10, which is beyond the Kosterlitz-Thouless (KT) transition.
perature $T_{KT}$. The specific heat peak for the frustrated case is more rounded relative to the unfrustrated case and occurs at a temperature lower than $T_{KT}$. This temperature is, however, higher than the temperature $T_f$ at which, we believe, the Edwards-Anderson order parameter goes to zero or a cusp appears in the linear susceptibility.

The saturation in the peak height of the specific heat is a consequence of the fact that it appears at a temperature at which the spin glass correlation is finite. Note that in both the unfrustrated and the frustrated cases the zero temperature specific heat approaches a value of $0.5k_B$, consistent with a linear spin-wave theory.

In a ferromagnet, the approach to the ferromagnetic phase from temperatures above the Curie temperature $T_C$ is accompanied by a dramatic increase in the range of the spin correlations, which then diverges at $T_C$. A corresponding phenomenon occurs in spin glasses. However, it is not the spin correlation function $\langle \vec{S}_i \cdot \vec{S}_j \rangle$, but rather its square that acquires a long-range. This leads to the divergence, at the spin glass transition temperature $T_f$, of the spin glass susceptibility

$$\chi_{SG} = \frac{1}{N} \sum_{ij} (\vec{S}_i \cdot \vec{S}_j)^2 \quad (T > T_f).$$

(5)

$\chi_{SG}$ satisfies a finite-size scaling relation of the form\(^6\)

$$\chi_{SG} = L^{2-\eta} \bar{\chi}(L^{1/\nu}(T-T_f)),$$

(6)

where $\bar{\chi}$ is the scaling function, $L$ is the system length, $\nu$ is the exponent for spin glass correlation length $\xi$ for $T \geq T_f$, and $\eta$ describes the power law decay of the spin glass correlation at $T_f$. For a square lattice $L = \sqrt{N}$, and the above scaling relation can also be expressed in terms of $N$. We have used this scaling relation, expressed in terms of $N$, for periodic Penrose lattices of various size to study $\chi_{SG}$. To ensure a proper convergence of $\chi_{SG}$, we have averaged over 5 blocks of 40,000-60,000 steps at low temperatures ($< 0.2$) and 5 blocks of 60,000-80,000 steps at higher temperatures. By examining our results every 5,000 steps, we find little change in $\chi_{SG}$ over the last 5,000-10,000 steps. Thus, we estimate that these chain lengths produced at least a 95% convergence in $\chi_{SG}$.

FIG. 3. Specific heat as a function of temperature. The inset shows the specific heat for the unfrustrated case with the peak slightly beyond the KT transition temperature.

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FIG. 4. Scaling plot for spin glass susceptibility. The inset shows the log-log plot of the Edwards-Anderson order parameter with $(T-T_f)$ with $T_f=0.137$ obtained from the fit to the scaling relation (6) with $\eta=0.02$ and $\nu=2.6$, as given by Bhatt and Young\(^5\). The slope of this plot yields a value of 0.26 for the exponent $\beta$, in agreement with the hyperscaling relation $\beta = \nu\eta/2$.

In Fig.4, we show the scaling behavior of $\chi_{SG}$ in terms of $N$ for $T_f = 0.137$, where we have used the values of $\nu = 2.6$ and $\eta = 0.2$ reported by Bhatt and Young\(^6\) in their study of $J$ XY model on square lattices. These results represent the average over cooling and heating and lie within the 0.02 – 0.45 temperature range. A choice of $T_f = 0$ results in 4 distinctly separate curves, indicating a clear breakdown of the scaling relation. If we try to obtain a good fit to the scaling curve with $T_f = 0$, then the exponents $\nu$ and $\eta$ deviate drastically from the values obtained by Bhatt and Young\(^6\) and others (see ref-
ferences in Bhatt and Young), obtained for 2-D XY spin glass models.

Furthermore, we have examined the Edwards-Anderson parameter in the vicinity of \( T_f \), where the relation \( q_{EA} \sim (T - T_f)^{\beta} \) is supposed to hold. We find that our value of \( T_f = 0.137 \) yields a value of \( \beta = 0.26 \), (see inset of Fig.4) which satisfies the hyperscaling relation \( \beta = \frac{2\nu}{D} \) valid for our 2-D system. Note that this value of \( T_f \) is clearly consistent with our results for the susceptibility \( \chi \), which shows a cusp at \( T \sim 0.15 \) (Fig.2). The inescapable conclusion seems to be that the frustrated 2-D Penrose lattice has a spin glass transition temperature above zero with exponents that are equal (similar) to those obtained for random XY models on square lattices.

In summary, we have shown, via the Edwards-Anderson order parameter, spin glass susceptibility and local (linear) susceptibility, the existence of a low temperature spin glass phase in frustrated 2-D Penrose lattice. Our results for magnetization and specific heat also support this picture. Our detailed study of the unfrustrated case (not reported here) reveal a behavior similar to that of a square lattice with a somewhat higher KT transition temperature. We would like to add that similar studies by us performed on other frustrated quasiperiodic lattices (such as the octagonal lattice) also show a low temperature spin glass phase.

A few comments are in order at this stage. Our results are consistent with those of Halsey\(^8\), who finds a spin glass phase for the frustrated XY model on a square lattice with an irrational flux through the plaquettes. Note that we can fully frustrate only one of the two elementary plaquettes at one time, the corresponding flux through the other plaquette being irrational. In both cases, the model studied by Halsey\(^8\) and the frustrated Penrose lattice, the parameter \( \cos(A_{ij}) \), which determines the nature of the coupling along the bond \([ij]\), shows a similar distribution in its values, varying widely between 1 and -1. This is different from most of the fully frustrated regular lattices studied so far. For example, the fully frustrated square lattice studied by Teitel and Jayaprakash\(^9\) or the triangular lattice studied by Shih and Stroud\(^10\), where the nature of the transition is seen to change from KT to the Ising type, has a much narrower distribution of \( \cos(A_{ij}) \).

The experimental implication of our study is that a quasiperiodic array (such as the Penrose or octagonal lattice) of Josephson junctions in a suitably chosen transverse magnetic field should behave as a superconducting glass at low temperature. Via advanced microfabrication techniques\(^11\), it should be possible to generate such quasiperiodic arrays of superconducting grains. Experimental investigation on a 2-D fractal (Sierpinski-gasket) network has been reported\(^12\). Halsey\(^8\) has pointed out that for superconducting arrays with low normal-state resistivities the glass transition should basically appear as a mean-field transition, with fluctuation effects being barely observable. For arrays with high normal-state resistivities the fluctuation effects will cause the glass transition to deviate substantially from a mean-field transition, with noticeable system-dependent details. An important feature of such glassy superconductors, as pointed out by Ebner and Stroud\(^13\), is a large difference between their dc and ac susceptibilities.

Finally, a comment about the lower critical dimension for the spin glass phase. It is widely believed that the lower critical dimension for the spin glass phase is greater than two\(^14\). This is corroborated by Monte Carlo studies by Binder and co-workers\(^15\) (see also ref. 14) and Young and co-workers\(^6\) on square lattices. Our results indicate that quasiperiodic 2-D lattices may provide an exception. The glassy behaviour we are reporting is truly the behavior of macroscopic systems and not a reflection of some other model masked by the finite system size. This behavior is guaranteed for the particular choice of frustration considered in this paper, dictated by the quasiperiodic lattice structure and the magnetic field. Unlike in the above studies\(^6,14,15\) with completely random distributions of the coupling constants along the bonds, the effective coupling constants in our model are nonrandom. However, our results obtained for the particular magnetic field considered are amenable to experimental verification and merit attention.

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\(^{1}\) G. Toulouse, Commun. Phys. 2, 115 (1977).
\(^{2}\) K.J. Strandburg, Computers in Physics, Sep/Oct 520 (1991).
\(^{3}\) N.C. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, and E. Teller, J. Chem. Phys. 21, 1087 (1953).
\(^{4}\) S.F. Edwards and P.W. Anderson, J. Phys. F 5, 965 (1975).
\(^{5}\) J.M. Kosterlitz and D.J. Thouless, J. Phys. C 6, 1181 (1973); J.M. Kosterlitz, ibid. 7, 1046 (1974).
\(^{6}\) R.N. Bhatt and A.P. Young, Phys. Rev. B 37, 5606 (1988); see also S. Jain and A.P. Young, J. Phys. C: Solid State Phys. 19, 3913 (1986).
\(^{7}\) J. Tobocznik and G.V. Chester, Phys. Rev. B 20, 3761 (1979).
\(^{8}\) T.C. Halsey, Phys. Rev. Lett. 55, 1018 (1985).
\(^{9}\) S. Teitel and C. Jayaprakash, Phys. Rev. B 27, 598 (1983).
\(^{10}\) W.Y. Shih and D. Stroud, Phys. Rev. B 30, 6774 (1984).
\(^{11}\) D.E. Prober in Percolation, Localization, and Superconductivity, NATO ASI Series B: vol. 109, ed. A.M. Goldman and S.A. Wolf (Plenum, 1984).
\(^{12}\) J.M. Gordon, A.M. Goldman, J. Maps, D. Costello, R. Tiberio, and B. Whitehead, Phys. Rev. Lett. 56, 2280 (1986).
\(^{13}\) C. Ebner and D. Stroud, Phys. Rev. B 31, 165 (1985).
\(^{14}\) K. Binder and A.P. Young, Rev. Mod. Phys. 58, 801 (1986).
\(^{15}\) I. Morgenstern and K. Binder, Phys. Rev. B 22, 288 (1980).

ERRATUM
The authors regret that the following errors remained undetected during the proof stage.

(1) In the abstract ‘±J XY model’ should read ‘±J Ising model’.

(2) Ref. 6 should read:
(a) R.N. Bhatt and A.P. Young, Phys. Rev. B 37, 5606 (1988); (b) S. Jain and A.P. Young, J. Phys. C: Solid State Phys. 19, 3913 (1986).

(3) In the caption of Fig. 4, Ref. 5 should be changed to Ref. 6(a), and η = 0.02 should be changed to η = 0.2.

(4) Ref. 5 immediately preceding Eq. (6) should be changed to Ref. 6(a).

(5) Regarding the exponents, note that our results agree much better with those of Bhatt and Young 6(a) (±J Ising model) than with those of Jain and Young 6(b) (±J XY model). Accordingly, references to ±J XY model study by Bhatt and Young 6 should be changed to ±J Ising model study by Bhatt and Young 6(a) at appropriate places in the main body of the paper.

One final comment: It is not clear to us at this stage whether the agreement with the ±J Ising model is purely coincidental, or there is a connection with the result of S. Teitel and C. Jayaprakash, Phys. Rev. B 27, 598 (1983) (Ref. 9) on square lattice, where the nature of the transition is seen to change from KT to the Ising type as a result of frustration.

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