Phase transitions of a quasiperiodic Josephson-junction array in magnetic fields

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We have studied both analytically and numerically the phase transitions of a quasiperiodic array of Josephson junctions in transverse magnetic fields. The lattice we consider has Fibonacci quasiperiodicity in one direction and is periodic in the other. Monte Carlo simulation as well as analytical arguments suggest that the phase transition is of the Kosterlitz-Thouless type at certain special magnetic fields. The ground-state configuration is found to be ferromagnetically ordered at these fields, which corresponds to especially weak frustration.

Two-dimensional (2D) periodic arrays of Josephson junctions have shown interesting nonmonotonic behavior as the external magnetic field is varied.[1] The origin of such behavior may be understood as commensurate-incommensurate effects arising from competition between the periodicity of the flux lattice due to the magnetic field and the underlying array periodicity. A number of studies have been carried out on the frustrated XY model, which serves as a model for phase transitions in these systems. These studies have revealed a variety of critical behavior as the value of the magnetic field is varied.[2-7]

In this note, we consider the effects of such frustration in arrays with quasiperiodicity rather than periodicity. Such arrays serve as paradigms for considering phase transitions in quasiperiodic systems. In quasiperiodic lattices, there do exist Bragg peaks, in spite of the absence of translational invariance.[8,9] It therefore seems likely that the behavior of quasiperiodic arrays may not be vastly different from that of periodic arrays. Recently, experiments as well as numerical calculations have been carried out on quasiperiodic superconducting wire networks. These systems, which may be regarded as the mean-field version of the arrays, show a striking, nonmonotonic variation of the transition temperature as a function of applied magnetic field.[10] In case of arrays, however, it seems possible that fluctuations might destroy mean-field behavior. Moreover, the universality class of the transition, as well as the nature of the ground state, is unknown. It therefore seems useful to investigation the behavior of quasiperiodic arrays both numerically and analytically beyond the mean-field theory.

This note presents a first attempt toward such a goal. We consider the frustrated XY model on a quasiperiodic lattice as a model for the quasiperiodic array of Josephson junctions, and present evidence suggesting that at particular values of the frustration, the phase transition is of the Kosterlitz-Thouless (KT) variety. We also argue that phase transitions in this model may occur at finite temperature at every value of applied magnetic field. This feature is analogous to the fact that the Bragg peaks of a quasiperiodic lattice fill the reciprocal lattice space densely.

We consider an $L\times L$ 2D lattice which is periodic in the y direction, but quasiperiodic in the x direction. For simplicity, the lattice constants are set to be 1 in the y direction and to be 1 and τ in the x direction. If we further choose $\tau=(\sqrt{5}-1)/2$, the golden number, then the sequence of the lattice constants along the x direction forms the Fibonacci sequence.

To describe this lattice, we start with the Hamiltonian defined on such a quasiperiodic lattice ($\beta\equiv 1/k_BT$)

$$-\beta H=\sum_{\mathbf{rr}'}K_{\mathbf{rr}'}\cos(\phi_{\mathbf{r}}-\phi_{\mathbf{r}'}-A_{\mathbf{rr}'}) \tag{1}$$

with

$$K_{\mathbf{rr}'}(\equiv\beta J_{\mathbf{rr}'})=\begin{cases}K & \text{for } \mathbf{r} \text{ and } \mathbf{r}' \text{ direct neighbors },\\ 0 & \text{otherwise },\end{cases}$$

where $\phi_{\mathbf{r}}$ is the phase of the superconducting grain at site $\mathbf{r}=(x,y)$, and $A_{rr'}$ is the bond angle given by the line integral of the vector potential,

$$A_{rr'}=\frac{2\pi}{\Phi_0}\int_{\mathbf{r}}^{\mathbf{r}'}\mathbf{A}\cdot d\mathbf{l} \quad \left[\Phi_0\equiv\frac{hc}{2e}\right].$$

In the case of a uniform transverse magnetic field $\mathbf{B}=B\hat{\mathbf{z}}$, it is straightforward to show that

$$A_{\mathbf{rr}'}=\begin{cases}\pm 2\pi f x & \text{for } \mathbf{r}'=\mathbf{r}\pm\hat{\mathbf{y}} ,\\ 0 & \text{otherwise },\end{cases} \tag{2}$$

where the Landau gauge $\mathbf{A}=Bx\hat{\mathbf{y}}$ has been used, and f is the frustration of the larger plaquette, i.e., the flux per larger plaquette in units of Φ_0. The frustration of the smaller plaquette is simply $f\tau$.

Information about the critical behavior displayed by the Hamiltonian (1) can be deduced by examining critical modes and constructing accordingly the Landau-Ginzburg-Wilson (LGW) free-energy functional for the system.[4] To obtain the critical modes we first consider the Fourier transform of the interaction matrix $P_{\mathbf{rr}'}\equiv K_{\mathbf{rr}'}\exp(-iA_{\mathbf{rr}'})$:

$$\begin{aligned}P_{\mathbf{qq}'}&\equiv L^{-2}\sum_{\mathbf{rr}'}e^{-i(\mathbf{q}\cdot\mathbf{r}-\mathbf{q}'\cdot\mathbf{r}')}P_{\mathbf{rr}'}\\ &=K\delta_{q_yq_y'}R_{q_xq_x'} ,\end{aligned} \tag{3}$$

where $R_{q_xq_x'}$ involves the summation over x. The x component of lattice site $\mathbf{r}$ can be written in the form

$$x = n_1 + n_2\tau \equiv x(k) ,$$
$$n_1 = [(k-1)\tau] + 1 \equiv n_1(k) , \qquad (4)$$
$$n_2 = (k-1) - [(k-1)\tau] \equiv n_2(k) ,$$

where k is an integer $(0 \leq k < L-1)$, and $[(k-1)\tau]$ is the integer part of the number $(k-1)\tau$. To obtain the explicit form of $R_{q_x q_x'}$, we note that the one-dimensional quasiperiodic lattice given by Eq. (4), the "Fibonacci lattice" can be obtained by the projection of a square lattice onto the line making an angle $\alpha = \arctan\tau$ with the x axis.[9] The 2D lattice in this study then may be regarded as the projected structure of a simple cubic lattice onto the plane parallel to one axis and making the angle α with another axis.

Hence we consider an $L_1 \times L_1$ square lattice with the lattice constant $a = 1/\cos\alpha = (1+\tau^2)^{1/2}$. By projecting it onto the line making an angle α with the x axis, we obtain the projected structure described by

$$x_\parallel = n_1 + n_2\tau \equiv x(k) ,$$
$$q_\parallel = \frac{2\pi}{L_1}\frac{n_1 + n_2\tau}{1+\tau^2} \equiv q_x(k) , \qquad (5)$$

where n_i $(i=1,2)$ has been shown to be equal to $n_i(k)$ given in Eq. (4). With the above assignment it is straightforward to show that both the Fourier transform and the inverse transform are well-defined. $R_{q_x q_x'}$ then takes the explicit form

$$R_{q_x q_x'} = \left[\frac{2}{1+\tau}(\cos q_x + \tau \cos\tau q_x) + 2\frac{\sin z}{z}\cos q_y \delta_{2\pi f, G} \right] \delta_{q_x q_x'} + \frac{\sin z}{z}(e^{iq_y}\delta_{q_x + 2\pi f, q_x' + G} + e^{-iq_y}\delta_{q_x - 2\pi f, q_x' - G})(1 - \delta_{q_x q_x'}) , \qquad (6)$$

where $z = \pi(1+\tau)(n - m\tau)/(1+\tau^2)$ and $G = 2\pi(m + n\tau)/(1+\tau^2)$.

The critical modes are closely related to the ground state energy of the system, as we now show. According to Eq. (1), the ground-state energy may be written

$$\beta E = -\mathrm{Re}\sum_{\mathbf{r}\mathbf{r}'} \eta_{\mathbf{r}}^* P_{\mathbf{r}\mathbf{r}'} \eta_{\mathbf{r}'} ,$$

where $\eta_{\mathbf{r}} = e^{-i\phi_{\mathbf{r}}}$, $P_{\mathbf{r}\mathbf{r}'}$ is the matrix defined above Eq. (3), and $\phi_{\mathbf{r}}$ is the phase of the grain at $\mathbf{r}$ in the ground-state configuration. Thus the largest eigenvalue of $P_{\mathbf{r}\mathbf{r}'}$ is proportional to the ground-state energy, and the corresponding eigenvector describes the ground-state configuration. Information about these eigenvalues and eigenfunctions will enable us to map out the ground state as a function of magnetic field.

To obtain the critical modes, we would in principle need to diagonalize the $L \times L$ matrix R, whose elements are given by Eq. (6). Although we cannot diagonalize explicitly the matrix R, which is infinite in extent ($L \to \infty$ in the thermodynamic limit), it could be done approximately by numerical methods by truncating the matrix above a certain cutoff wave vector. Here, however, we confine ourselves to approximate analytic results. Some information on the largest eigenvalue λ can be obtained through the use of hermiticity of R. In particular, it is possible to show that the largest eigenvalue λ depends on the wave vector (q_x, q_y) through the functional relation

$$\lambda = \begin{cases} \lambda(\cos q_x, \cos\tau q_x, \cos q_y, \cos L q_y) & \text{for } 2\pi f = G , \\ \lambda(\cos q_x, \cos\tau q_x, \cos L q_y) & \text{otherwise} . \end{cases}$$

In case $2\pi f = G$ or $f = (m + n\tau)/(1+\tau^2)$, it is obvious that λ reaches its maximum value at $\mathbf{q} = (0,0)$ or at $\mathbf{q} = (0,\pi)$ according to the sign of $\sin z/z$, which implies only one critical mode. In particular, when $\sin z/z > 0$, we predict a nondegenerate ferromagnetic ground state, i.e., the ground states have no degeneracy other than the trivial one involving rotation of all the phases by the same constant angle. Thus no discrete symmetry is present in the system, and the corresponding LGW free-energy functional would take the same form as that of an ordinary XY model. This formal similarity suggests the possibility of an ordinary KT transition. On the other hand, the maximum value of at such fields is proportional to $\tilde{J}$, the integration strength of the corresponding XY model. Since the KT transition temperature is known to be proportional to $\tilde{J}$,[11] this argument suggests that the transition temperature T_c will also be proportional to that maximum eigenvalue. Moreover, the maximum eigenvalue is exactly twice the mean-field transition temperature, T_c^{MF}. Consequently, the mean-field approximation should give a correct trend for the variation of the transition temperature with the frustration in this model. However, T_c^{MF} would be substantially higher than T_c for each value of f due to strong fluctuations, a characteristic of 2D systems.

The transition temperature T_c in this case is expected to depend very sensitively on the frustration since $z \propto n - m\tau$ in Eq. (6). In general T_c becomes higher when the factor $\sin z/z$ is large. Particularly high T_c's are expected when $z \propto n - m\tau \approx 0$, i.e., when n and m are two successive Fibonacci numbers. Since $n - m\tau$ becomes closer to zero as the two successive Fibonacci numbers n and m become larger, the transition temperature becomes higher as the magnetic field is increased in this case. In the limit $m,n \to \infty$ (i.e., $B \to \infty$), we have $n - m\tau \to 0$ and recover the result for an ordinary XY model with no frustration. These results are consistent with both experiments and numerical Ginzburg-Landau calculations on superconducting networks,[10] which are equivalent to the mean-field version of Josephson-junction arrays.

If $2\pi f \neq G$, then λ reaches its maximum value at $\mathbf{q} = (0, 2l\pi/L)$ $(l = 0, 1, \ldots, L-1)$. Therefore there exists an infinite number of critical modes in the thermodynamic limit ($L \to \infty$), and no finite-temperature transition is expected.[5]

These results in turn imply that the transition temperature is a highly discontinuous function of the frustration or the magnetic field. Finite-temperature transition points in particular would form a countable but dense set on the interval of the frustration.

The existence of finite-temperature transitions at values of the frustration satisfying $2\pi f = G$ is completely analogous to the existence of Bragg peaks at wave vectors $q = G$ in the Fibonacci lattice. The preservation of KT transitions at $2\pi f = G$ is analogous to the preservation of δ peaks at $q = G$ in spite of the absence of translational invariance. When $2\pi f = G$, the frustration is weak enough to preserve the KT transition while at "other" values of the frustration ($2\pi f \neq G$), the transition is destroyed. In numerical calculations or experiments, however, such highly singular behavior would, of course, not be observed because the fields for which $2\pi f = G$ densely fill the interval.

In order to test these conjectures, we have carried out numerical studies for several pairs of successive Fibonacci numbers (m,n). The pairs $(m,n)=(1,1),(2,1),(3,2),\ldots$ correspond to the magnetic fields $B/B_0=(1/\tau)^0,(1/\tau)^1,(1/\tau)^2,\ldots$, in the notation used by Behrooz *et al.* in Ref. 10. Here B_0 denotes a field corresponding to an average flux of one quantum per plaquette. At the field denoted by (m,n) the average field is the same as would be produced by exactly m flux quanta in the larger plaquettes, n in the smaller. For larger and larger Fibonacci pairs, the flux through each plaquette more and more closely approximates an integer, and the frustration becomes weaker and weaker. To isolate effects which might arise from the finite size of the lattice, we have carried out all calculations on $N \times N$ lattice, with N the Fibonacci numbers, 3,5,8,13,.... As N increases, we obtain a better and better approximation to the asymptotic ratio τ of the number of larger plaquettes to the number of smaller ones.

We have calculated mean-field transition temperatures by directly applying the mean field approximation to the Hamiltonian (1) on $N \times N$ lattices (up to $N=13$) with periodic boundary conditions,[12] and solving the resulting N^2 coupled nonlinear complex equations for the order parameters. Since the mean-field transition temperatures have been obtained in detail for this geometry by Behrooz *et al.* and by Nori *et al.* (Ref. 10), we have not concentrated on calculating these temperatures, but have considered principally the ground state energies and configuration, which we have obtained by an iteration method. This procedure is equivalent to minimizing the Hamiltonian[3] and gives, in principle, the exact ground state energy within numerical accuracy. We have also carried out MC annealing to confirm the ground-state configuration down to $T=0.01J/k_B$. Both types of calculations have been carried out for lattice sizes as large as 34×34. Once the ground-state configuration is found we can calculate the ground-state energy E_g.

MC simulation has been done via the standard Metropolis algorithm[13] on 8×8 and 21×21 lattices with periodic boundary conditions.[12] The first 5000 MC steps per spin have been discarded for the equilibration and thermodynamic variables have been obtained by averaging over next 10 000 MC steps per "spin." Final averages have been performed over the values from several independent runs with different random number seeds.

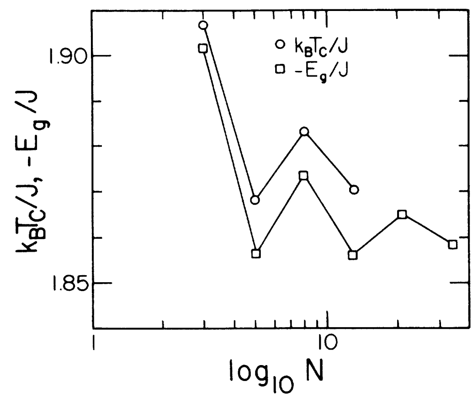

FIG. 1. Variation of the mean-field transition temperature and the ground-state energy as functions of the lattice dimension N for $(m,n)=(3,2)$.

Typical results for $T_c^{\rm MF}$ and E_g as functions of lattice size for a fixed field $(m,n)=(3,2)$ are plotted in Fig. 1. These results show that for fixed field $T_c^{\rm MF}$ and E_g converge as N increases, but with a characteristic oscillatory behavior. This is the result of approximating τ by the ratio of two successive Fibonacci numbers. Because of the oscillatory convergence, we expect the values of $T_c^{\rm MF}$ and E_g for the infinite system will lie between the two values for the largest and the next largest systems studied. One would also expect that the amplitude of the oscillations (that is, the size dependence) will become smaller for larger integer k at fields $B/B_0=(1/\tau)^k$ (we have found this to be true in calculations). This can be understood as follows: as the field increases with the form $f=(m+n\tau)/(1+\tau^2)$, frustration effects decrease because f is closer to an integer. Thus the Hamiltonian becomes more and more similar to that of an unfrustrated XY model (with a unit cell of 1×1), for which there is no size dependence in the calculation of $T_c^{\rm MF}$.

The behaviors of the large-N limit of $T_c^{\rm MF}$ and E_g, are depicted as functions of field in Fig. 2(a). Evidently the difference between $T_c^{\rm MF}$ and $-E_g$ becomes smaller as the field is increased. This may again be explained as the result of diminishing frustration, since $T_c^{\rm MF}$ and $-E_g$ are both equal to $2J$ in the unfrustrated limit ($k\to\infty$). This mean-field result agrees with the experimental results on networks,[10] which are a mean-field version of a Josephson junction. The trend is also consistent with the analytic prediction above.

In carrying out ground state calculations for $N\times N$ lattices with $N=3$, 5, 8, 13, 21, and 34, we find that both the iteration method and MC annealing give the same results, although MC annealing displays some fluctuations. The ground states proves to be ferromagnetic with U(1) symmetry for all fields of the form $(1/\tau)^k$ for all sizes studied except the case $(m,n)=(1,1)$ with $N\geq 13$. In this case, a lower energy configuration has been found in which the phases along the y direction gradually rotate completing a full rotation after N sites while phases along the x direc-

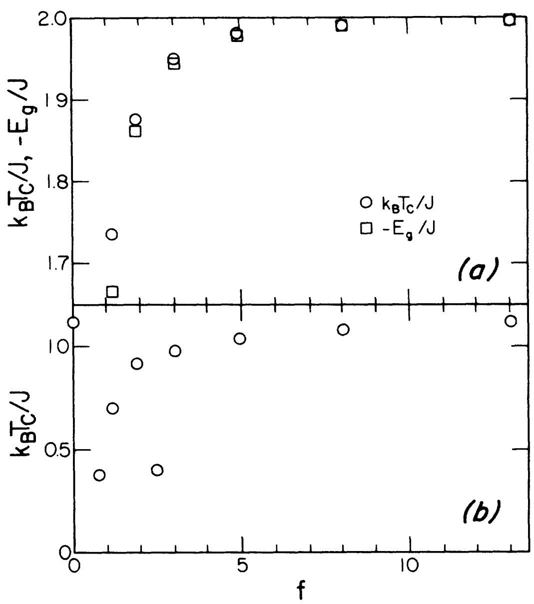

FIG. 2. (a) Variations of the transition temperature $k_B T_c$ and the ground-state energy E_g as functions of the flux $f = \Phi/\Phi_0$ through the larger plaquette, as determined by mean-field theory. The values plotted for each field are arithmetic means of the values for the two largest systems investigated. (b) Upper limits of $k_B T_c$, as determined by Monte Carlo simulation on 21×21 lattices with periodic boundary conditions. The upper limits are estimated from the positions of the specific heat peaks.

tion remain the same. However, as the size grows, the discrepancy in energy between this configuration and the ferromagnetic one decreases, leading to the realistic expectation that it will vanish in case of the infinite system. Therefore, we conclude that the ground state of the infinite system will be ferromagnetic with no discrete degeneracy at all fields of the form $B/B_0 = (1/\tau)^k$ studied, in agreement with the analytic results. This suggests that the transition at fields of the form $B/B_0 = (1/\tau)^k$ is of the KT type.

We have also investigated two values of f in the form $(m + n\tau)/(1+\tau^2)$ but for which m and n are not successive Fibonacci numbers, namely $f \approx 0.79$ and $f \approx 2.51$. At these fields, the iteration method leads to several different configurations with different energies. This suggests the possibility of many metastable states, consistent with the usual behavior of strongly frustrated systems.

Typical results of MC simulations are shown in Fig. 3 for $(m,n) = (3,2)$. Both the helicity modulus and the specific heat peaks are consistent with a KT transition. The helicity modulus may exhibit a jump near $k_B T = 0.85J$, though the size of the jump cannot easily be estimated from our data. The specific heat data display little growth in the peak height with increasing lattice size, and therefore, also suggest a KT transition. (In a regular KT transition, the height of the specific heat peak saturates at a finite value as the size of the lattice grows.) The height of our peak is comparable to that reported for the conventional unfrustrated XY model for comparable lattice sizes.[14] The behavior of the helicity modulus near $T = 0$ also resembles that of the pure KT transition in that the helicity modulus extrapolates to unity at $T = 0$.[15] In transitions of mixed KT and Ising character, by contrast, the zero-temperature helicity modulus generally extrapolates to a lower value.[2,7,14]

In Fig. 2(b), we show an upper limit to the transition temperatures T_c, as estimated by MC simulation. The two very low T_c's correspond to values $f \approx 0.79$ and $f \approx 2.51$. At these fields, the transitions are probably not KT like (because the helicity modulus neither tends to unity at low temperature nor shows a jump at a finite temperature), and the frustration is much larger than at the other fields shown, which are of the form (m,n). For the fields (m,n), the transition temperatures follow the trends of T_c^{MF} and E_g.

It would be most interesting to have experimental confirmation of these results on physically realized

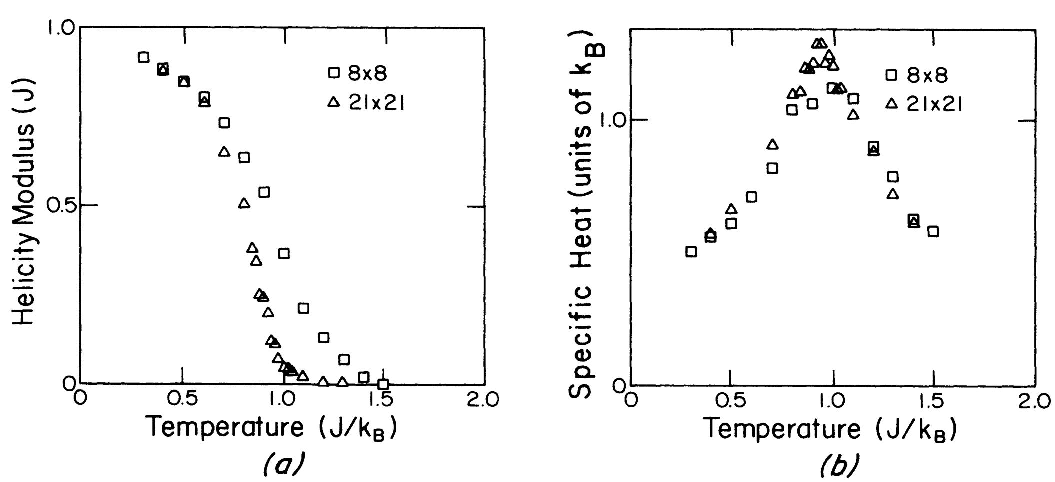

FIG. 3. Typical results of MC simulation for (a) the x component of the helicity modulus and (b) the specific heat with $(m,n) = (3,2)$. Typical rms errors (not shown), defined as the standard deviation of the five to ten MC runs taken for each point, are of order 5–10 % in the transition region and less than 2% elsewhere.

Josephson junction arrays. It is also interesting to speculate that similar KT transitions take place at analogous fields in Penrose tilings of Josephson junction arrays, such as have been studied by VanHarlingen and collaborators.[10]

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[12]The precise effects of using periodic boundary conditions are not known. In our gauge, $A = Bx\hat{\mathbf{y}}$, and therefore, the phase factor $A_{\mathbf{rr}'} = 0$ for all horizontal bonds. Imposing periodic boundary conditions thus means attaching the grains of the Nth column to those of the first column by horizontal "ferromagnetic" bonds. For the particular fields studied in this paper, the extra frustration produced by imposing periodicity is very weak. This implies that the value of $A_{\mathbf{rr}'}$ for the $(N+1)$th vertical bond is nearly zero. The periodic boundary condition is equivalent to approximating this value by zero. Thus the boundary conditions probably do not change our results much from the infinite-sample limit, for these particular fields.

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