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Superconducting arrays in a magnetic field: Effects of lattice structure and a possible double transition

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We report the results of extensive Monte Carlo simulations and mean-field calculations for superconducting arrays in a transverse magnetic field. Two new lattices are studied: triangular and honeycomb. The universality class of the transition is found to depend on both field and lattice type. In the triangular lattice at a field of $\frac{1}{4}$ flux quantum per triangle, there are some indications that the superconducting-normal transformation proceeds by two separate phase transitions.

Two-dimensional arrays of superconducting (S) grains in a nonsuperconducting (N) host show remarkable behavior in a transverse magnetic field B: both resistivity above a transition temperature $T_c(B)$ and critical current below $T_c(B)$ vary periodically in B, with a period of one flux quantum per unit cell of the grain lattice and a great deal of fine structure.[1–4] Current theory[5–7] indicates that this behavior is the manifestation of a novel kind of phase transitions which can be either of the unusual Kosterlitz-Thouless vortex-unbinding variety or of the more conventional Ising type.

The purpose of this Rapid Communication is to extend previous results to two new lattices, the triangular and the honeycomb, which can be readily prepared experimentally. These lattices show a number of new features not seen in the square lattice. In particular, the strong secondary maximum in $T_c(B)$ observed at a field $f=\frac{1}{2}$ (where f is the fractional flux per lattice cell, measured in units of flux quanta) in the square lattice is much weaker, and possibly absent, in the honeycomb lattice, and the universality class of the transition is also different. The triangular lattice exhibits a conspicuous secondary maximum at $f=\frac{1}{4}$, which appears to have been observed experimentally.[8]

Perhaps most intriguing is the suggestion of some of our numerical results, from both Monte Carlo (MC) and mean-field calculations, that at $f=\frac{1}{4}$ in the triangular lattice, superconductivity may disappear by two separate phase transitions. The intermediate-temperature phase seems to be a partially coherent state somewhat similar to that predicted by Blankschtein *et al.*[9] for a type of stacked antiferromagnetic Ising model. However, since the present case has a direct physical realization, a double transition, if present, might have interesting experimental consequences for weakly coupled superconducting arrays. Since the evidence of a double transition is stronger from the mean-field results than from MC, these consequences are perhaps more likely to be observable in superconducting wire networks, such as those studied by Pannetier, Chaussy, and Rammal,[10] than in the weak-coupled arrays. In the wire networks, fluctuation effects are expected to be much weaker and the mean-field predictions are therefore likely to be less inaccurate than in the arrays.

Our calculations are based on the following simplified model Hamiltonian:

$$H=-J\sum_{\langle ij\rangle}\cos(\phi_i-\phi_j-A_{ij}) \ , \tag{1}$$

$$A_{ij}=\frac{2\pi}{\Phi_0}\int_i^j\vec{A}\cdot d\vec{l} \ , \tag{2}$$

where ϕ_i is the phase of the S order parameter on the ith grain, $\Phi_0=hc/2e$ a flux quantum, J the nearest-neighbor coupling energy, $\vec{A}$ the vector potential, and the integral runs between the centers of grains i and j. The thermodynamic properties of the model are determined by treating the phases as classical variables within the canonical ensemble. We have evaluated canonical expectation values [denoted $\langle\ \rangle$] either by MC simulation within the standard Metropolis[11] algorithm, or by mean-field theory,[6] using the asymmetric gauge $\vec{A}=Bx\hat{y}$. We have computed the phase-order parameter $\eta_i=\langle\exp(i\phi_i)\rangle$ using both methods, and a MC or mean-field cell with periodic boundary conditions. In the former, typically 15 000–25 000 passes were made through the entire lattice with the first 5000 discarded for each run, and reported results are generally produced by averaging over 4–6 runs. We have also computed in the MC simulations the specific heat $C=[\langle H^2\rangle-\langle H\rangle^2]/(Nk_BT)$ and the "helicity modulus tensor" $\overleftrightarrow{\gamma}$ as defined in Ref. 12. $\overleftrightarrow{\gamma}$ is a measure of the resistance of the phases to an externally imposed infinitesimal twist, and is nonzero only if the phases are in an ordered configuration. It is the analog of spin-wave stiffness for the present system, and is also proportional to the effective superfluid density of the superconducting array. For the present problem, $\overleftrightarrow{\gamma}=\gamma I$, where I is the 2×2 unit tensor.

Figure 1 shows γ and C for two representative transitions, the triangular and honeycomb lattices at $f=\frac{1}{2}$. In the first case, γ drops smoothly to zero at $T_c(f)$, while C has a pronounced peak which sharpens with increasing MC sample size. γ also has clear size dependence and we interpret these results as indicating an "Ising-like" (i.e., conventional continuous) transition with a singularity in C at T_c. Of course, our calculations do not cover a size range sufficient to confirm a logarithmic specific heat singularity as in the 2D Ising model. In the honeycomb lattice at $f=\frac{1}{2}$, C has no size dependence near T_c, indicating no singularity at T_c. We label this transition "Kosterlitz-Thouless–like" although

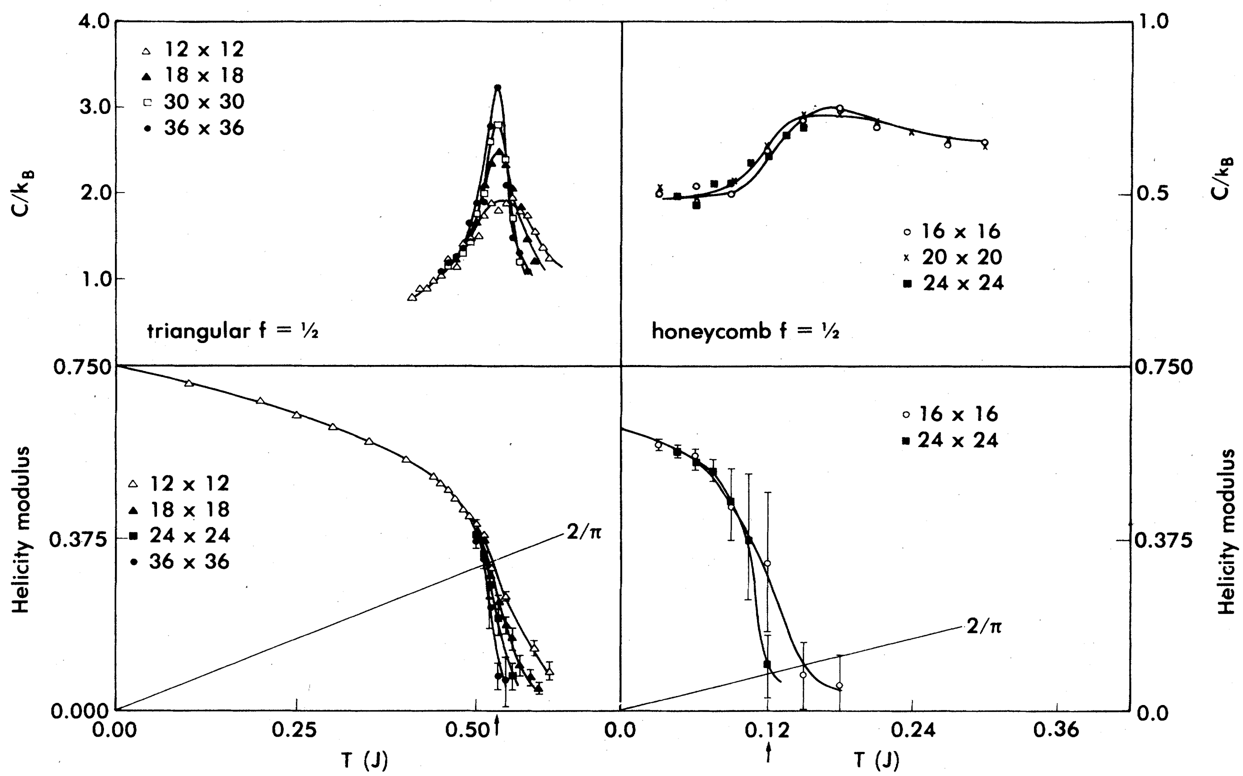

FIG. 1. Monte Carlo specific heat per grain C and helicity modulus γ, for (a) triangular and (b) honeycomb lattice at field $f=\frac{1}{2}$. Different symbols denote different MC cell sizes. Arrows denote estimated transition temperatures.

we cannot determine if γ has a universal jump of $2k_BT_c/\pi$ at T_c, as would be expected at such a transition, or goes smoothly to zero.

A summary of the MC and mean-field results is given in Table I. Besides critical temperatures $T_c(f)$, we show also ground-state energies $-E_g$ and critical currents I_c at $T=0$, calculated by the methods of Refs. 6 and 5, respectively. In the triangular and honeycomb lattices, the critical currents, unlike the helicity moduli, are anisotropic. Also shown are values of γ at $T=0$, calculated as the second derivative of $-E_g$ with respect to an imposed twist of the phases at the boundary of the sample. The notations "KT" and "Ising"

TABLE I. Mean-field transition temperature $T_c^{\rm MF}$, Monte Carlo transition temperature $T_c^{\rm MC}$ (both in units of J), ground-state energy $-E_g$ per grain in units of J, zero-temperature critical current density I_c $(T=0)$, zero-temperature helicity modulus γ $(T=0)$, and transition class, for (a) triangular and (b) honeycomb. Where two critical current densities are shown, they refer to currents in two perpendicular directions; the larger critical current involves flow perpendicular to some of the lattice bonds. Critical current densities are given in units of I_c^0/a, where I_c^0 is the critical current of a single junction and a is the spacing between grains.

f	$T_c^{\rm MC}$	$T_c^{\rm MF}$ (J)	$-Eg$ (J)	$I_c(T=0)$	$\gamma(T=0)$	Transition
			(a) Triangular			
0	1.45	3	3	2,2	1.5	KT
$\frac{1}{4}$	~0.13,0.3	1.73	1.5	0.43,0.43	0.75	KT
$\frac{1}{3}$	0.16	1.5	$1\frac{1}{3}$			KT
$\frac{1}{2}$	0.53	1.5	1.5	0.43,0.83	0.75	Ising
			(b) Honeycomb			
0	0.65	1.5	1.5	$1/\sqrt{3}$,2/3	0.75	KT
$\frac{1}{4}$	0.17	1.3	1.2771	0.18,0.28	0.62	KT
$\frac{1}{3}$	0.23	1.266	1.266	0.28,0.36	0.62	KT
$\frac{1}{2}$	0.12	1.2071	1.2071	0.24,0.28	~0.58	KT

are merely intended to indicate the absence or presence of size dependence in C, and do not imply that we have actually demonstrated the universality class of the transition. A secondary maximum in $T_c(f)$ is present at $f=\frac{1}{2}$ in both the square[5,6] and triangular lattices (besides the principal maxima at integer f), whereas the secondary maximum is at $f=\frac{1}{3}$ for the honeycomb lattice. Mean-field results generally follow the MC simulations qualitatively, but differ considerably at small f.

The ground-state vortex configuration for $f=\frac{1}{4}$ in the triangular lattice is shown in Fig. 2; the unit cell consists of eight elementary triangles, two of which contain vortex charge $+\frac{3}{4}$, and six, charge $-\frac{1}{4}$. (Vortex charges are always $n-f$, with n integer; we determine the sign of the vortex charge by calculating the current around each elementary triangle in the ground-state configuration.) The $T=0$ configuration is easily destabilized, because it contains triangles of like charge grouped in a hexagon. At temperature T_{c1}, therefore, mean-field theory predicts that the grain in the center of the hexagon loses phase coherence, probably via a first-order transition. Above this point, the junctions between this grain and the vertices of the hexagon are normal (Fig. 2). This intermediate phase, if it exists, is thus *inhomogeneous,* with some bonds superconducting and some normal. At a slightly higher temperature T_{c2}, there is a second phase transition above which all the superconducting grains lose phase coherence. The two mean-field transitions occur for this field and lattice at temperatures about a factor of 10 above the MC transitions, indicating that fluctuations are very important here. Figure 3 shows $|\eta_i|$ for a grain i in the center of the hexagon, and for one of the perimeter grains, as calculated from MC; corresponding mean-field results are shown in Fig. 2. The MC results give some suggestions of a first-order transition at about $T=0.12\ J$, but this suggestion cannot be relied on because of some numerical instability (i.e., time dependence) in these order parameters. Also shown in Fig. 3 are γ and C as obtained

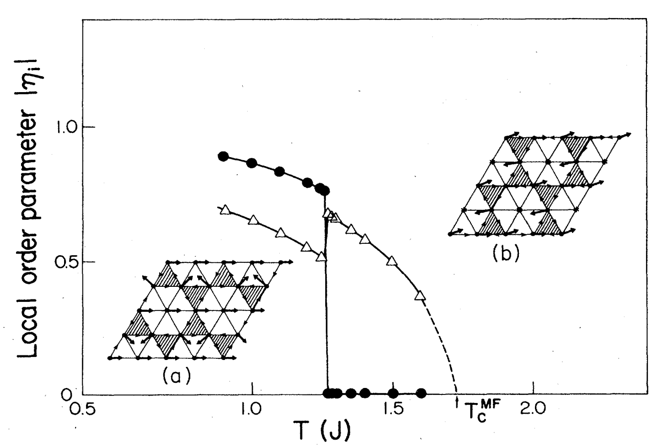

FIG. 2. Phase-order parameters $|\eta_i|$ for grains in center of hexagon (●) and on perimeter of hexagon (Δ) in triangular lattice at $f=\frac{1}{4}$, as calculated by mean-field theory. Order parameter of center goes to zero at T_{c1}. Inserts: phase and vortex configurations in low- and intermediate-temperature states. Heavy arrows denote orientation of phases; light arrows, the current directions. Shaded areas represent locations of positive vortex charge.

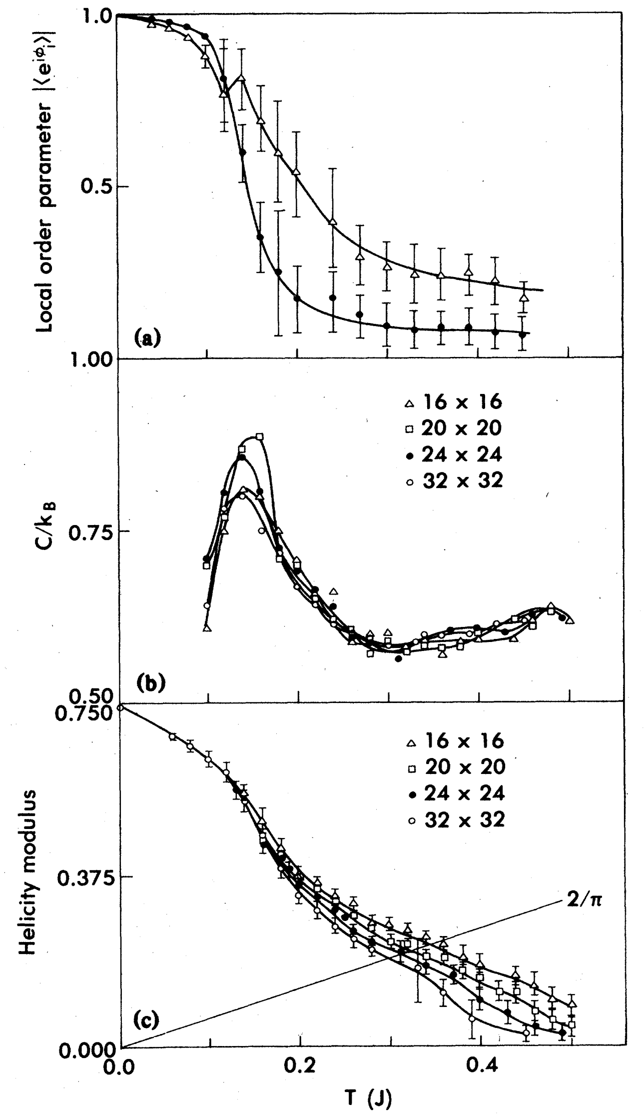

FIG. 3. (a) Phase-order parameters $|\langle e^{i\phi_i}\rangle|$; (b) specific heat C per grain; (c) helicity modulus γ, for triangular lattice at $f=\frac{1}{4}$, as calculated by MC. In (a), (●) represents the center of hexagon and (Δ) the perimeter of hexagon on a 12×12 sample.

from MC. γ appears to show a change of slope at T_{c1}, the temperature of the principal peak in C. T_{c2} is arbitrarily chosen as the temperature of intersection of the curve for $\gamma(T)$ with a straight line of slope $2/\pi$; the residual part of γ above T_{c2} is probably a finite-size artifact and would disappear in a sufficiently large MC cell. Although there is a distinct peak in C near T_{c1}, T_{c2} is associated with at most a much weaker anomaly.

Clearly, the MC evidence for a double transition is inconclusive and further work is required to establish the nature of the transition to superconductivity at $f=\frac{1}{4}$ in a triangular lattice. Nonetheless, the experimental implications of any double transition are of interest. At the upper transition at T_{c2}, the array would acquire zero resistance to an infinitesimal external current, while the transition at T_{c1}

would most likely be accompanied by a jump in critical current. The intermediate phase between T_{c1} and T_{c2} could have ac properties of an impedance network composed of pure inductive elements (the Josephson junctions) and resistors (the normal links) regularly distributed on a two-dimensional lattice, and could exhibit substantial absorption below the superconducting energy gap. Moreover, similar transitions seem likely to occur in other lattices and at other magnetic fields, as well as in superconducting wire networks.

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