First-order flux-lattice melting of a frustrated XY model with a [111] magnetic field

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We have studied a three-dimensional isotropic Josephson-junction array in a simple cubic lattice with a magnetic field $\mathbf{B} = \Phi_0(\frac{1}{3},\frac{1}{3},\frac{1}{3})$, using Monte Carlo simulation. There is a clear first-order phase transition with a latent heat of melting of about $0.11k_B T_m$ per superconducting grain at a melting temperature $T_m \approx 0.70J$, where J is the intergrain coupling energy. We briefly discuss the possible relation of this transition to flux-lattice melting in high-T_c superconductors. [S0163-1829(96)00746-1]

Several recent experiments have suggested that melting of the Abrikosov flux lattice,[1] in a sufficiently clean high-T_c material, is first order, with a finite latent heat and magnetization jump. For example, Safar *et al.*[2] have observed a sharp drop to zero resistivity, in clean YBa$_2$Cu$_3$O$_{7-\delta}$ in an applied magnetic field, which they interpreted as a discontinuous transition from a resistive flux liquid to a zero-resistance flux solid phase. Zeldov *et al.*[3] directly observed a magnetization jump at the flux-liquid–flux-solid interface, using a two-dimensional network of Hall microprobes to measure local magnetization. More recent measurements have reported resistivity hysteresis at the melting transition, a phenomenon which again strongly suggests first-order melting.[4]

The first theoretical suggestion that the Abrikosov transition might be first order[5] has been supported by several numerical studies. Hetzel *et al.*[6] found a first-order transition in a uniformly frustrated XY model on a three-dimensional (3D) stacked triangular lattice at a frustration $f = \frac{1}{6}$, with an entropy jump of about $0.3k_B$ per vortex pancake. Domínguez *et al.*,[7] studying a dynamical version of the model, found resistivity hysteresis, similar to that observed by Ref. 4. Several workers have found a first-order phase transition in a lowest Landau level (LLL) representation of a Ginzburg-Landau free energy functional[8–11] in both two[8–10] and three dimensions.[11,12] For YBa$_2$Cu$_3$O$_{7-\delta}$, Šášik and Stroud[11] calculated both the magnetization and the specific heat near melting in the LLL approximation. They obtained good agreement for both the melting curve and the magnetization near melting, but an entropy jump of only about $0.034k_B$ per pancake at a field $B \approx 5$ T. Ryu and Stroud[13] found a first-order transition in a "layered London model,"[14] using both Monte Carlo and Langevin dynamical simulations, with an entropy jump similar to that of Ref. 11 at the parameters of YBa$_2$Cu$_3$O$_{7-\delta}$.

In this paper, we study the uniformly frustrated XY model[15] on a simple cubic lattice,[16] but with a field equal to $(\Phi_0/3)(\hat{x}+\hat{y}+\hat{z})$, where $\Phi_0 = hc/2e$ is the flux quantum. Our main finding is that, just as in the stacked triangular lattice of Hetzel *et al.*,[6] there is a first-order superconducting-insulating phase transition.

We consider the model Hamiltonian[16]

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

Here ϕ_i represents the phase of the local superconducting order parameter on the ith grain, and we assume that the grains are arranged on the sites of a simple cubic lattice. The sum runs over the nearest-neighbor pairs of sites. The phase factor $A_{i,j} = 2\pi/\Phi_0 \int_i^j \mathbf{A} \cdot d\mathbf{l}$, where $\mathbf{A}$ is the vector potential, $\mathbf{B} = \nabla \times \mathbf{A}$ is the local magnetic induction. We assume weak screening, so that $\mathbf{B} \approx \mathbf{H}$, the uniform applied magnetic field. The lattice constant is a, in units of which the lattice has dimensions $N_x \times N_y \times N_z$. The field is conveniently described by the *frustration* $\mathbf{f} \equiv (f_x, f_y, f_z)$. If Φ_i is the flux through a plaquette perpendicular to the ith coordinate axis, then f_i is the fractional part of the flux per plaquette perpendicular to the ith axis, in units of Φ_0, i.e., $\Phi_i = (n_i + f_i)\Phi_0$, where n_i is an integer.

We have carried out calculations for $f = (\frac{1}{3},\frac{1}{3},\frac{1}{3})$. In this [111] direction, the simple cubic lattice is a stack of two-dimensional planes perpendicular to the [111] axis, each containing a network of grains arranged on a triangular lattice with lattice constant $\sqrt{2}a$. Successive planes are offset from one another to generate the familiar $ABCABC\ldots$ stacking. The flux through one triangular plaquette is $\Phi_0/2$. A single triangular lattice of this kind, with nearest-neighbor interactions, forms an alternating structure with two triangles per unit cell,[17] which may be viewed as a kind of checkerboard arrangement of two-dimensional vortices. For the case of staggered stacked lattices, the equilibrium state is less obvious.

We describe our numerical results in terms of various equilibrium quantities. The internal energy per site, $E/N_s \equiv e$, where N_s is the total number of sites, is expressed in units of J, and length in units of a. One interest quantity is the helicity modulus tensor,[18] which measures stiffness against long-wavelength twists of the phase of ϕ. General expressions for the components of γ_{xx} are given, for example, in Ref. 15.

We can also define a *vortex number* for each plaquette. In a plaquette in the xy plane, for example, the vortex number is defined as

$$n_z = f_z + \frac{1}{2\pi}\sum_{\text{plaquette}}(\phi_i - \phi_j - A_{i,j}), \tag{2}$$

where the gauge-invariant phase difference for each junction $(\phi_i - \phi_j - A_{i,j})$ is defined to lie in the range $(-\pi, \pi]$, and
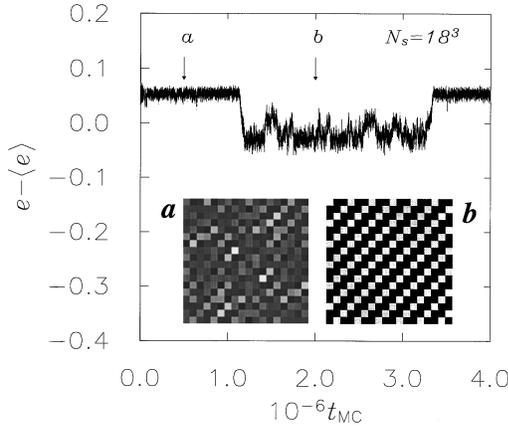
FIG. 1. Evolution of the internal energy per superconducting grain with MC ''time,'' at the melting temperature $T = 0.703$, and frustration $\mathbf{f} = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, as obtained by MC simulation. Insets (a) and (b) are intensity plots of the correlation function $g_{zz}(x,y,N/2)$.

the summation is taken around the plaquette boundary in the counterclockwise direction (viewed from the positive z axis). Similar definitions hold for plaquettes in other planes. Also of interest are the (vector) density-density correlation function, defined by

$$g_{ij}(\mathbf{r}) = \frac{1}{N_s f_i} \frac{1}{N_s f_j} \sum_{\mathbf{r} = \mathbf{r}' - \mathbf{r}''} \langle n_i(\mathbf{r}') n_j(\mathbf{r}'') \rangle, \qquad (3)$$

and its Fourier transform, the vortex structure factor, $S_{ij}(\mathbf{k}) = \Sigma_{\mathbf{r}} g_{ij}(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r})$. Here $\langle \cdots \rangle$ denotes an average in the canonical ensemble. In practice, we have considered mostly the zz component of both g and S.

To calculate these quantities, we carry out Monte Carlo simulations using the standard Metropolis algorithm, assuming periodic boundary conditions in all three directions and a cubic simulation cell, so that the number of grains $N_s = N_x N_y N_z$, where $N_x = N_y = N_z \equiv N$. We initialize the phases of the superconducting grains in a random configuration. Thereafter, all Monte Carlo moves are made in terms of the gauge-invariant phase differences $\phi_i - \phi_j - A_{i,j}$, and it is unnecessary ever to calculate either the phases ϕ_i or the line integrals $A_{i,j}$ individually, or to define an explicit gauge. A similar procedure has been previously used in Ref. 6. The ground state energy we finally obtain by annealing from high temperature is very close to that obtained by Ref. 16, using a molecular-field approximation. Typically, we make 5×10^5 MC passes through the entire system for equilibration, followed by an additional 2×10^5 MC passes for averaging at $N_s = 12^3$ (this choice varied somewhat with N_s). Since the system typically equilibrates more slowly near melting, we usually average at such temperatures over $4 - 8 \times 10^6$ sweeps through the entire sample at a size of $N_s = 18^3$.

Figure 1 shows the evolution of internal energy e with respect to MC time at a temperature $T = 0.703J$. For $N_s = 18^3$, the system slowly oscillates between two different values during the MC run. At a slightly smaller system size, $N_s = 12^3$, there are about $4 - 5$ oscillations between the two states during 2×10^6 passes through the entire system. The correlation function $g_{zz}(x,y,N/2)$, which is shown in insets
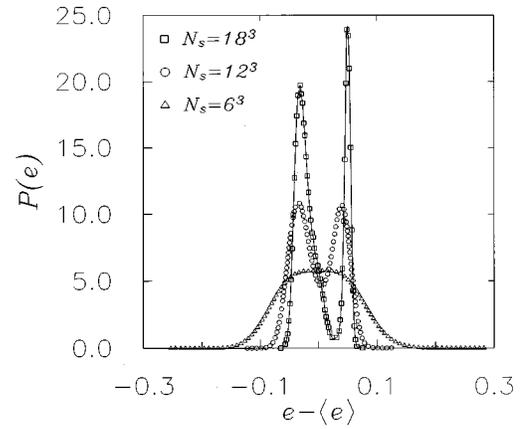

FIG. 2. MC Probability distribution $P(e)$ of internal energy per superconducting grain at the finite-size melting point.

(a) and (b) for $N = 18$ at the same temperature and different time windows. Larger magnitudes are indicated by greater brightnesses. Each inset is an average over 4×10^3 passes through the entire system, but over different time windows (cf. arrows). Inset (b) corresponds to the lower-energy state. It exhibits periodic maxima corresponding to an ordered solid phase. The period of the maxima perpendicular to the z direction is proportional to $f_z = \frac{1}{3}$. Inset (a) averages over the higher energy state. The periodic structure is now washed out, suggesting a liquid. The presence of two coexisting states, of different internal energies and structures, is further evidence of a *first order transition*.

Figure 2 shows the size-dependent probability distribution $P(e)$ of internal energy per site at melting. The size-dependent melting temperatures are 0.707, 0.677, and 0.656 for system sizes $N_s = 18^3$, 12^3, and 6^3. The smallest size shows only a single peak, but there are two distinct peaks at the two larger sizes. Figure 1 shows that the low-energy peak of $P(e)$ corresponds to the ordered state, while the high-energy peak is the disordered (liquid) state. For the largest system ($N_s = 18^3$), the transition between the two states is so slow that $P(e)$ is asymmetrical — the system is more likely to be solid than liquid for the limited time window considered. Greater symmetry would have been achieved in this case with a longer MC run. For $N_s = 6^3$, the system flips so frequently between phases, and the difference in internal energy is comparable to the variance of the individual gaussian distributions,[6] that the double-peaked feature is masked. Although we have not carried out detailed scaling studies of this distribution as a function of size, Fig. 1 shows that the dip is growing larger with increasing size, as expected of a first order phase transition.[19]

From either Fig. 1 or 2, we infer a latent heat of about 0.08 per superconducting grain for $N_s = 18^3$. The corresponding entropy jump $\Delta S = \Delta E / T$ is $0.08/0.703 \approx 0.11 k_B$ per grain, or $0.19 k_B$ per unit *length* per vortex.

Figure 3 shows average helicity modulus $\gamma \equiv (\gamma_{xx} + \gamma_{yy} + \gamma_{zz})/3$. Since the field is in the [111] direction and the coupling is isotropic, $\gamma_{xx} = \gamma_{yy} = \gamma_{zz}$. By plotting $\gamma = (\gamma_{xx} + \gamma_{yy} + \gamma_{zz})/3$ rather than the individual components, we improve the statistics. Note that the transition occurs *above* the intersection of $\gamma(T)$ with a straight line of
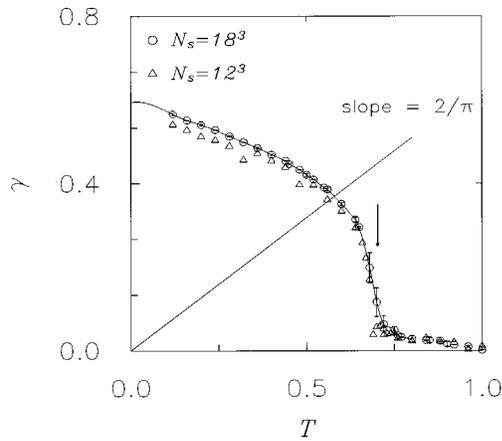
FIG. 3. Helicity modulus $\gamma = (\gamma_{xx} + \gamma_{yy} + \gamma_{zz})/3$. The smooth curve through the data is a guide to the eye. Arrow denotes the estimated transition temperature for $N_s = 18^3$.

slope $2/\pi$, indicating that this transition is not of the Kosterlitz-Thouless universality class.[20]

Figure 4 shows the internal energy $e(T)$ on cooling and on heating. Each plot is obtained by averaging over 8×10^4 passes through the entire lattice, with an initial 3×10^4 passes for equilibration at each temperature. We use a temperature step, ΔT, of 1×10^{-3} for $N_s = 18^3$, and $\Delta T = 5 \times 10^{-3}$ for $N_s = 24^3$. Both plots show clear hysteresis, again suggesting a first-order melting transition. For the larger system, $N_s = 24^3$, we cannot localize the melting point with precision inside the hysteresis loop, because of slow relaxation (much slower at this size than at $N_s = 18^3$).

Figure 5 shows the structure factor $S_{zz}(k_{||})$ for various temperatures and a range of $k_{||}$, where $\mathbf{k}_{||} = 2\pi(n,n,n)/N$, $k_{||} = |\mathbf{k}_{||}|$ and $n = 0, \ldots, N-1$. Labels $0.703a$ and $0.703b$ both correspond to a temperature $T = 0.703 = T_m$, but averaged over solid and liquid time windows as in Fig. 1. Clearly, there is a sharp drop in vortex correlations parallel to the magnetic field as solid melts, suggesting that melting produces simultaneous vortex disordering both parallel and perpendicular to the magnetic field.

We turn now to the significance of these results. The greatest interest of this calculation lies in the possible con-
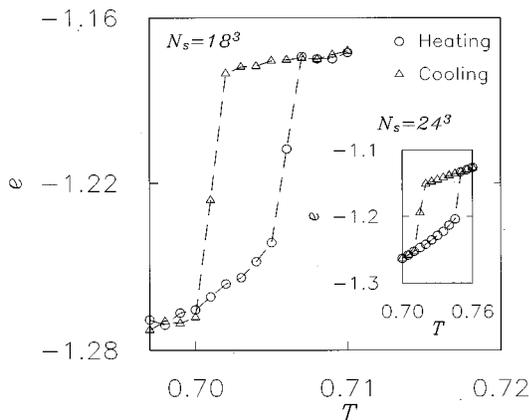

FIG. 4. Internal energy $e(T)$ per superconducting grain, as measuring on cooling and heating.
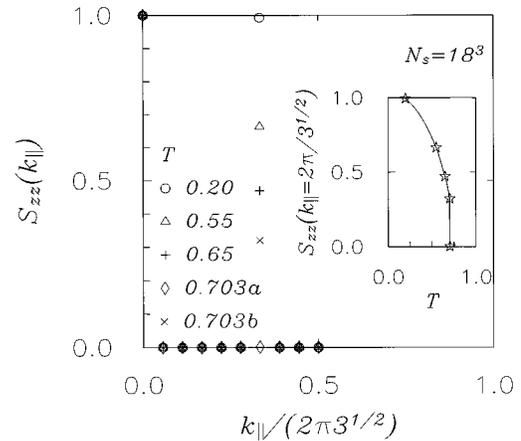

FIG. 5. Structure factor $S_{zz}(k_{||})$ parallel to the magnetic field at several T. The full line is a quasi-Hermite spline fit to the data; other parameters as in Fig. 1.

nection to flux lattice melting in high-T_c materials. The model is most appropriate at low-screening limit, where the flux line separation $\ell_0 \ll \lambda$ (the penetration depth), and the approximation of a uniform magnetic field is most reasonable. In the high-T_c materials, this inequality is satisfied in much of the H-T phase diagram. The XY model also ignores amplitude fluctuations in the order parameter, but these are small compared to the phase fluctuations.

Of greater concern is the spurious pinning of the periodic lattice. By choosing a magnetic field in the [111] direction, we minimize these effects. In that direction, as already noted, the system is a stack of planes, each with a triangular lattice structure. The pinning barrier for motion of a single two-dimensional vortex in a triangular lattice is only about 0.03 J.[21] This should be further reduced for our stacked array of planes which are offset: a minimum energy configuration in one plane is a maximum in another. Thus, the pinning energy may be even smaller for this system and the calculated results may nearly reflect the behavior of the unpinned vortex lattice.

It is also of interest to compare our results to those of Hetzel et al.,[6] calculated for a different lattice structure. Our field has magnitude $\Phi_0/(a^2\sqrt{3})$, where a is the lattice constant, while that of Ref. 6 is $2\Phi_0/(a^23\sqrt{3})$. Alternatively, one might calculate the field in units of Φ_0/λ^2. For our model, λ is isotropic and given by $\sqrt{a\Phi_0^2/(16\pi^3 J)}$. For the stacked triangular lattice, λ is also isotropic and given by $\sqrt{\sqrt{3}a\Phi_0^2/(32\pi^3 J)}$. In units of Φ_0/λ^2, therefore, our field is larger than theirs by a factor of $\sqrt{3}$.

Our melting parameters also differ somewhat from Ref. 6: our $T_c \approx 0.70 J$ (compared to $0.11 J$), and our $\Delta S = 0.11\sqrt{3}k_B = 0.19 k_B$ per vortex per unit length, taking $a = 1$ (compared to $\Delta S \approx 0.3 k_B$ per vortex per unit length). These differences are reasonable: our magnetic field is higher than Ref. 6, and, therefore, both the melting temperature and $\Delta S/k_B$ are expected to be lower.

In summary, we have considered the frustrated XY model on a simple cubic lattice with a magnetic field applied in the [111] direction. At a uniform field corresponding to frustra-

tion $\mathbf{f}=(\frac{1}{3},\frac{1}{3},\frac{1}{3})$, we find a first-order melting transition at $T_m \approx 0.70$, and an entropy of melting of about $0.11k_B$ per superconducting grain, or equivalently, $0.19k_B$ per vortex per unit length. Both values are somewhat lower than those obtained by Hetzel et al. on a stacked triangular lattice at a lower magnetic field,[6] but are higher than the predictions of calculations for flux lattice melting carried out in the lowest Landau level approximation.

[1] For a recent comprehensive review of vortex behavior in high-T_c materials, see, e.g., G. Blatter et al., Rev. Mod. Phys. **66**, 1125 (1994).

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