First-Order Melting Transition of an Abrikosov Vortex Lattice

R. E. Hetzel,[1],[a] A. Sudbø,[2] and D. A. Huse[2]
[1]*Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544*
[2]*AT&T Bell Laboratories, Murray Hill, New Jersey 07974*
(Received 6 April 1992)

We report results of extensive Monte Carlo simulations of a three-dimensional model system containing the essential physics required to describe the melting of an unpinned Abrikosov lattice in an extreme type-II superconductor. A *first-order* phase transition is found. At the field which we have studied, corresponding very roughly to a field of 10 T along the c axis in $YBa_2Cu_3O_7$, the latent heat of melting is $\simeq 0.3 k_B T$ per vortex per layer.

PACS numbers: 74.60.Ec, 74.60.Ge

In a classic paper, Alekseĭ Abrikosov demonstrated that a magnetic field starts to penetrate a type-II superconductor in the form of a *lattice of flux lines* when the applied magnetic field reaches a critical value from below [1]. The statistical mechanics of such vortex or flux-line lattices (FLLs) in extreme type-II, anisotropic superconductors has been of considerable recent interest and a source of much controversy. That the three-dimensional vortex *lattice* melts into a vortex *liquid* over a *large part* of the (H,T) phase diagram in high-T_c superconductors, due to their anisotropy and large operating temperatures, was proposed based on experimental results [2] and theoretical considerations [3]. In the same context, it was emphasized [4,5] that the FLL in very anisotropic and extreme type-II superconductors is intrinsically soft due to *both* the quasi-two-dimensionality of these compounds *and*, very importantly, the long range of vortex-vortex interactions. The Fourier modes $\tilde{V}(\mathbf{k})$ of the vortex interaction are essentially Lorentzians in the wave number $\mathbf{k}$, and the width of these Lorentzians is controlled by the anisotropy of the compounds and the value of the Ginzburg-Landau parameter $\kappa=\lambda/\xi$ [6], where λ is the magnetic penetration depth and ξ is the superconducting coherence length.

From the results of Refs. [4–6] it is clear that the response of the FLL to *nonuniform perturbations* with $\mathbf{k}\neq 0$, such as thermal fluctuations (with dominant Fourier modes at the *boundary* of the Brillouin zone of the reciprocal FLL), *softens rapidly* with increasing κ and mass anisotropy. Hence, a vortex lattice in a high-T_c superconductor is expected to be very susceptible to thermal fluctuations. Estimates for its melting temperature $T_M(B)$ based on a Lindemann criterion [2–5] indeed predict that the FLL in high-T_c superconductors should be melted over a substantial region of the (B,T) phase diagram; however, the experimental evidence for a melting transition remains controversial. The Lindemann estimates do not address the question of the *character* of such FLL melting. It has so far not been satisfactorily resolved whether the melting transition of the *three-dimensional* (3D) FLL is continuous or first order, although a numerical renormalization-group analysis demonstrated that the melting *is* first order for $d=6-\epsilon$; it was furthermore *indicated* that this could be so even for $d=3$ [7].

In this paper, we address the issue of the nature of the proposed melting transition of the 3D FLL within the simplified framework of a lattice superconductor model using Monte Carlo simulations. Such an approach has the advantage of allowing a systematic analysis of the phase transition of the model. The model system we consider is given by the uniformly frustrated 3D XY model [8], defined by the Hamiltonian

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

where the sum is over nearest-neighbor pairs of sites. Screening is neglected in this model, which should describe well a relatively dense vortex system ($H\gg H_{c1}$) in a very hard ($\kappa\gg 1$) superconductor. Hence, the softening of the FLL due to long-range interactions is well captured by the model. The above given model may be viewed as the simplest lattice version of a type-II superconductor, derivable from a Lawrence-Doniach model [9] when not only the z coordinate, but also the x-y plane has been discretized.

To reproduce the London theory at zero temperature, the in-plane and out-of-plane coupling constants in the model are given by $J_{xy,z}=\Phi_0^2 a/16\pi^3\lambda_{xy,z}^2$, the magnetic penetration lengths in the x-y plane and along the z axis are given by λ_{xy} and λ_z, respectively, and $\Phi_0=2.07\times 10^{-7}\,\mathrm{G\,cm^2}$ is the flux quantum. The lattice constant a serves as a measure of the coherence length ξ. The phases ϕ_i represent the local phase of the superconducting order parameter, and $A_{ij}\equiv(2e/\hbar c)\int_i^j d\mathbf{l}\cdot\mathbf{A}(\mathbf{l})$, with $\mathbf{A}$ being a vector potential giving the induction in the superconductor, $\mathbf{B}=\nabla\times\mathbf{A}$. We consider the phases ϕ_i as distributed on a *stacked triangular* lattice (coordination number 8) which serves as our numerical mesh. The z coordinate represents the c axis, while the x-y plane represents the a-b plane in compounds such as Y-Ba-Cu-O and Bi-Sr-Ca-Cu-O. When $\mathbf{B}\|\hat{\mathbf{c}}$, the vortex ground state in a uniaxially anisotropic superconductor is an *equilateral* hexagonal vortex lattice, determining the choice of discretization of the x-y plane.

An important simplification inherent in the model Eq.

(1) is the complete neglect of fluctuations in the induction $\mathbf{B}=\nabla\times\mathbf{A}$, which we take to be oriented perpendicular to the x-y layers of our stacked triangular lattice, and furthermore *uniform*. This is well justified in extreme type-II superconductors $\kappa\gg 1$ and at not too low average inductions: The intervortex distance $a_0\approx(\Phi_0/B)^{1/2}$ should be much smaller than the magnetic penetration depth λ, and much larger than the mean-field coherence length in order to justify the neglect of screening effects and of *amplitude* fluctuations of the order parameter. Within Ginzburg-Landau theory, the lower and upper critical fields are given by $H_{c1}\approx\Phi_0/4\pi\lambda^2$ and $H_{c2}=\Phi_0/2\pi\xi^2$, respectively, with $H_{c2}/H_{c1}\approx 2\kappa^2\gg 1$ by assumption. Hence, there exists a wide field range where the model of Eq. (1) adequately describes the relevant physics of the vortex fluctuations believed to be primarily responsible for melting the FLL [3–5]. It is, however, clear that the vortex-vortex interaction at and beyond distances of order λ is *overestimated* by the logarithmic potential resulting from Eq. (1), due to the neglect of screening. This should not seriously affect the melting transition for $a_0\ll 1$. Throughout the simulations, the filling is preserved, corresponding to satisfying the constraint $\nabla\times\mathbf{A}=\mathbf{B}$, which is simple, due to the assumption of uniformity in $\mathbf{B}$.

In general, the J_{ij} may be anisotropic, and in the limit $J_z/J_{xy}\ll 1$, we expect the physics to be essentially two dimensional (2D). The melting transition for the strictly 2D model was investigated by Huberman and Doniach, and also Fisher [10], and argued to be of the Kosterlitz-Thouless type. Of more recent interest has been the issue of the possible melting of a 3D system of vortex *lines*. The model in Eq. (1) with $J_z/J_{xy}\simeq 1$ is expected to describe an ensemble of vortices strongly correlated along the z direction, *and hence forming a collection of linelike objects*, motivating our choice of *isotropic* couplings.

A recently developed technique [11] is used to unambiguously identify first-order phase transitions on purely numerical grounds, and which has been used extensively in studying the 2D and 3D q-state Potts models. To our knowledge, this is the first time a similar analysis has been attempted for studying the *nature of a melting transition*. We briefly recapitulate the essentials of the theory. The probability distribution of the total energy E is given by

$$P(E;T,L)=Z^{-1}(T,L)\mathcal{D}(E,L)\exp(-E/k_BT)\,, \qquad (2)$$

where Z is the partition function, $\mathcal{D}(E,L)$ is the density of states with energy E, and L is the linear dimension of the system. Provided that the system is maintained close to its first-order phase transition, $P(E;T,L)$ will have a characteristic double-peak structure corresponding to a high-temperature *disordered* state with a peak in the distribution at E_0, and a low-temperature *ordered* state with a peak in the distribution at E_1. These two peaks in the distribution will be separated by a *minimum* in $P(E;T,L)$ at an energy E_m. The two peaks in $P(E;T,L)$ will be of equal height at a temperature $T_c(L)$, which we denote as a pseudo critical temperature approaching the true critical temperature of the system as $L\rightarrow\infty$. To observe and measure the double-peak structure in $P(E;T,L)$ it is crucial to be near $T_c(L)$, in order for the system to be able to spontaneously flip back and forth between the ordered and the disordered states. In our simulations, we determine $T_c(L)$ approximately by a temperature sweep of the system; $T_c(L)$ is near the temperature at which the maximum in the specific heat occurs. At the temperature $T_c(L)$, we then have

$$[F(E_m;T_c(L),L)-F(E_0;T_c(L),L)]/k_BT_c(L)=\Delta F(L)\,, \qquad (3)$$

where $F(E;T,L)\equiv -k_BT\ln[P(E;T,L)]$, and $k_BT_c(L)\times\Delta F(L)$ is a free-energy barrier that must be crossed to go between ordered and disordered states. To obtain proper equilibrium, it appears necessary to allow the system to run long enough to flip an appreciable number of times (≥ 10) back and forth between the two states. The crucial test for determining whether or not the transition is first order, is that ΔF *should be proportional to the cross-sectional area of the system for large* L: $\Delta F=aL^{d-1}+O(L^{d-2})$, where d is the dimensionality of the system (in our case $d=3$), and a is proportional to the surface tension of the interface between the two phases.

The Monte Carlo simulations have been performed using a single-spin update Metropolis algorithm. A field of $f=\frac{1}{6}=Ba^2\sqrt{3}/4\Phi_0$ vortices per plaquette in each lattice layer was used, and the simulations were performed on a stacked triangular lattice, rather than a simple cubic lattice. This discretization is fully compatible with an ideal hexagonal Abrikosov lattice, which can thus form in the low-temperature phase *without any amount of frustration*. This point is important, since it is the phase transition of a vortex system in the *continuum* that we are ultimately interested in studying. Our choice of numerical mesh is in this respect preferable to the simple cubic numerical lattice, where the hexagonal Abrikosov lattice *is* frustrated. In the simulations reported here, the couplings are all taken to be equal, $J_{xy}=J_z=1$, and periodic boundary conditions are used in *all* directions. Moreover, we only consider samples such that $L_x=L_y=L_z=L$, and $N_{\text{spin}}=L^3$, to hold fixed possible geometric effects in the finite-size scaling analysis.

For the actual production runs on the 3D model, the initial phase differences on each bond corresponding to the ideal ground state, shown in Fig. 1, are loaded onto the lattice. (The numbers on the links correspond to the gauge-invariant phase differences $\phi_i-\phi_j-A_{ij}$ on each bond in units of $\pi/9$.) An alternative would be to use a fixed vector potential appropriate for a field $f=\frac{1}{6}$ to set up random starting configurations. The role of the vector

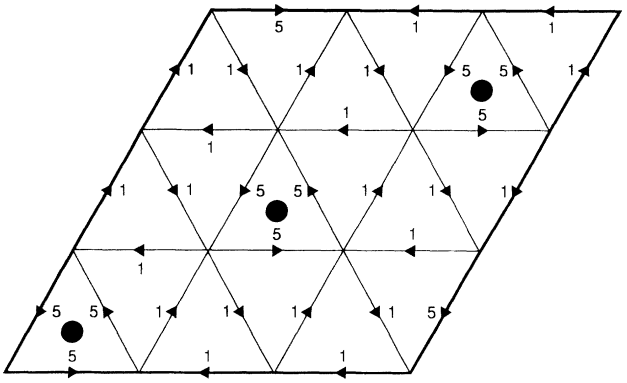

FIG. 1. A unit cell of the vortex ground state of one layer of our stacked triangular lattice at a field of $f=Ba^2\sqrt{3}/4\Phi_0=\frac{1}{6}$. The dots represent the vortices, the numbers on the links correspond to the gauge-invariant phase differences $\phi_i-\phi_j-A_{ij}$ in units of $\pi/9$, and the arrows on the links show the direction of current flow. In the ground state all layers have the same phase-difference pattern.

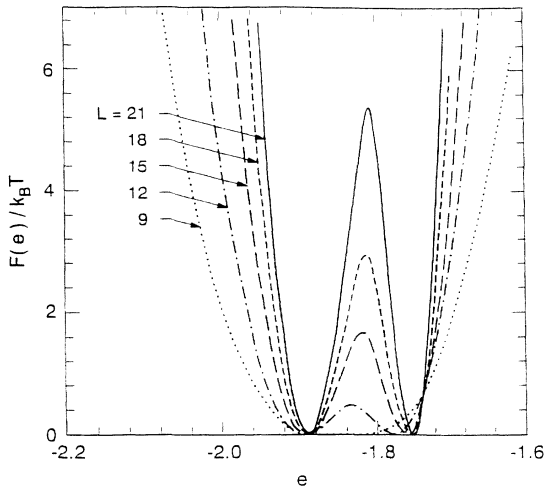

FIG. 2. $F(e;T_c(L),L)/k_BT_c(L)=-\ln P(e;T_c(L),L)$ is shown for various system sizes $N=L^3$, $L=9,12,15,18,21$, where $e=E/N_{\rm spin}$ is the energy per site, and $T_c(L)$ denotes the pseudo critical temperature of a system of size L. Each curve has individually been shifted by a constant so that its minimum is at $F=0$. Note the rapid increase with increasing L in the free energy barrier $\Delta F(L)$ between the ordered and disordered states. The results are obtained for a field of $f=Ba^2\sqrt{3}/4\Phi_0=\frac{1}{6}$, and the melting transition occurs at $T_c\simeq 1.175$ at all L.

potential would then be to fix the induction **B** at the start of the simulations. An example would be the use of the Landau gauge $\mathbf{A}=Bx\hat{\mathbf{y}}$, in which case the smallest x-y layer one can consider without introducing frustration of the ground state from simply periodic boundary conditions would be of size $L_x\times L_y=18\times 18$. This also appears to be the case for the symmetric gauge $\mathbf{A}=(\mathbf{B}\times\mathbf{r})/2$. The prospect of having to do simulations on a system where the L_i are multiple integers of 18 would essentially eliminate the possibility of performing a finite-size scaling analysis along the lines of Ref. [11]. Our procedure produces periodic boundary conditions that are fully compatible with the vortex-lattice ground state, provided that $L_x=L_y=3N$; $N=1,2,\ldots$ for the particular case where $f=\frac{1}{6}$. The 3D system can then be heated and cooled through the phase transition, while guaranteeing that a regular hexagonal Abrikosov lattice will form in the low-temperature phase, without frustration from boundary conditions. For the gauge-invariant phase differences that are loaded onto the 3D lattice, no reference is ever made to a specific vector potential, nor to the individual phases ϕ_i. The Monte Carlo moves are carried out on the phase differences themselves, and the *simulations are therefore performed in a manifestly gauge-invariant manner.*

The vortices are located from information about the phases in the standard way: The gauge-invariant phase *differences* in Eq. (1) are summed around each of the triangular plaquettes in each 2D layer $\sum_\Delta[\phi_i-\phi_j-A_{ij}]=2\pi(n-f)$, where f is the filling and n is the number of vortices inside the plaquette. For the case of $f=\frac{1}{6}$, the vortex positions *in the ground state* are shown in Fig. 1. The next two fillings that are compatible with the stacked triangular lattice, and hence will allow an unfrustrated hexagonal Abrikosov lattice to form, are $f=\frac{1}{8}$ and $f=\frac{1}{14}$. To consider the phase transition at a filling substantially different from $f=\frac{1}{6}$, the filling $f=\frac{1}{14}$ would be interesting. However, we have so far been unsuccessful in our limited attempts to equilibrate the system at $f=\frac{1}{14}$.

We now turn to the main results of our simulations (obtained at $f=\frac{1}{6}$), displayed in Fig. 2, which shows $F(e;T_c(L),L)/k_BT_c(L)=-\ln P(e;T_c(L),L)$ for various system sizes, where $e=E/N_{\rm spin}$ is the energy per lattice site. Note the marked increase in the barrier $\Delta F(L)$ between the ordered and disordered state with increasing L. For the system sizes we have been able to access, $\Delta F(L)$ is fitted by

$$\Delta F(L)=aL^{d-1}-bL^{d-2}, \tag{4}$$

with $a=0.028$ and $b=0.301$. We have used $L=12$, 15, 18, and 21 to obtain this fit, and emphasize that the numbers are valid for *isotropic couplings* $J_z/J_{xy}=1$. At least 10^6 Monte Carlo sweeps over the lattice are necessary to get good statistics for the system sizes $L=18,21$, while 5×10^5 suffice for $L=12,15$. Note that the double-minimum structure in $F(e;T_c(L),L)$ has vanished at $L=9$. The large value of the coefficient b distinguishes our results from those of the 3D q-state Potts model [11], and is responsible for the vanishing of $\Delta F(L)$ between $L=12$ and $L=9$. Formally, the L^{d-2} term in our case corresponds to a line energy, but what it means physically is at present unclear.

The energy versus temperature is shown in Fig. 3 for a

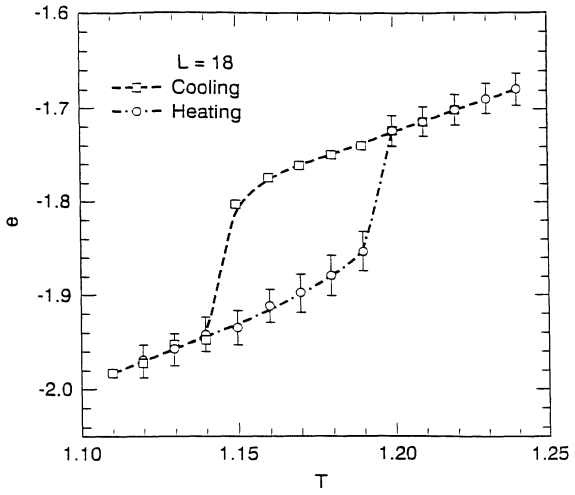

FIG. 3. Energy per site $e=E/N_{\text{spin}}$ as a function of temperature T, as measured upon rapidly heating and cooling. At each temperature the system has been run for only 4000 Monte Carlo sweeps. Note the strong hysteresis effect, indicative of the first-order melting transition.

rapid heating and cooling run for $L=18$; note the hysteresis effect similar to the one found in Monte Carlo studies of flux-flow resistance in a 2D frustrated Josephson junction array [12], but considerably more pronounced in our case. The change in entropy $\Delta S=\Delta E/T$ of the transition that we measure from Figs. 2 or 3 is $\Delta S\simeq 0.3k_B$ per vortex per layer. Our model with $J_z=J_{xy}$ has an essentially isotropic coherence length in lattice units of the stacked triangular lattice grid. In Y-Ba-Cu-O, the coherence length is anisotropic by a factor of 6–8, the layer spacing is $\simeq 12$ Å, and hence our in-layer grid spacing corresponds to 80 Å in Y-Ba-Cu-O. This means that the vortices are $\simeq 140$ Å apart, and our magnetic field of $f=\frac{1}{6}=Ba^2\sqrt{3}/4\Phi_0$ corresponds very roughly to $B\approx 10$ T. The simplifications in the model Eq. (1) could cause our prediction for the jump in the entropy to be off by an appreciable amount. However, as an order of magnitude estimate it should be useful as an indication of what sensitivity is needed for an experiment to detect ΔS or the jump ΔM in the magnetization M at this melting transition. Note that, neglecting demagnetization effects, ΔS and ΔM are related by the Clausius-Clapeyron equation [13], $dT_M/dH_{\text{appl}}=\Delta M/\Delta S$, where H_{appl} is the applied magnetic field. However, the usual demagnetization factor, depending on the sample geometry, will *reduce* M and ΔM from this value.

The effect of anisotropy in the coupling constants J_z and J_{xy} is an interesting issue, which will be addressed in detail in a forthcoming paper. Suffice it to say that for anisotropies such that $J_{xy}/J_z\leq 16$, we find that the transition becomes *more strongly first order* as J_{xy}/J_z is increased from 1.

In conclusion, we have considered a lattice superconductor model representing the vortex-line lattice in an extreme type-II superconductor. Monte Carlo simulations, in conjunction with finite-size scaling analysis, unambiguously show that the vortex-line lattice undergoes a first-order melting transition, and produce an estimate for its latent heat.

The authors acknowledge useful communications with J. M. Kosterlitz and D. R. Nelson. R.E.H. acknowledges support from the Deutsche Forschungs-Gemeinschaft, and thanks R. N. Bhatt for the extensive use of computational facilities at Princeton University.

Note added.—After the bulk of this work was completed, we received a preprint from J. Lee and K. J. Strandburg, with similar simulations performed on the *2D hard-disk system.* For this system, $\Delta F(L)$ is considerably smaller than for the 3D Abrikosov lattice studied here. Experimental evidence for a first-order melting transition of the Abrikosov lattice in twin-free Y-Ba-Cu-O crystals, based on transport measurements, has now been reported in a preprint by H. Safar *et al.*

[a]Present address: Physikalisches Institut der Universität Würzburg, 8700 Würzburg Am Hubland, Germany.

[1] A. A. Abrikosov, Zh. Eksp. Teor. Fiz. **32**, 1442 (1957) [Sov. Phys. JETP **5**, 1174 (1957)].

[2] P. L. Gammel, L. F. Schneemeyer, J. V. Wasczczak, and D. J. Bishop, Phys. Rev. Lett. **61**, 1666 (1988).

[3] D. R. Nelson, Phys. Rev. Lett. **60**, 1973 (1988); D. R. Nelson and H. S. Seung, Phys. Rev. B **39**, 9153 (1989); D. S. Fisher, M. P. A. Fisher, and D. A. Huse, Phys. Rev. B **43**, 130 (1991).

[4] E. H. Brandt, Phys. Rev. Lett. **63**, 1106 (1989); A. Houghton, R. A. Pelcovits, and A. Sudbø, Phys. Rev. B **40**, 6763 (1989).

[5] M. V. Feigel'man, V. B. Geshkenbein, and A. I. Larkin, Physica (Amsterdam) **167C**, 177 (1990); L. I. Glazman and A.E. Koshelev, Phys. Rev. B **43**, 2835 (1991).

[6] A. Sudbø and E. H. Brandt, Phys. Rev. Lett. **66**, 1781 (1991).

[7] E. Brézin, D. R. Nelson, and A. Thiaville, Phys. Rev. B **31**, 7124 (1985).

[8] Ying-Hong Li and S. Teitel, Phys. Rev. Lett. **66**, 3301 (1991).

[9] W. E. Lawrence and S. Doniach, in *Proceedings of the Twelfth International Conference on Low Temperature Physics, Kyoto, Japan, 1971*, edited by E. Kanda (Keigaku, Tokyo, 1971), p. 316.

[10] B. A. Huberman and S. Doniach, Phys. Rev. Lett. **43**, 950 (1979); D. S. Fisher, Phys. Rev. B **22**, 1190 (1980).

[11] J. Lee and J. M. Kosterlitz, Phys. Rev. Lett. **65**, 137 (1990); Phys. Rev. B **43**, 1268 (1991); **43**, 3265 (1991).

[12] Ying-Hong Li and S. Teitel, Phys. Rev. Lett. **65**, 2595 (1990).

[13] A. Kapitulnik, in *Phenomenology and Applications of High Temperature Superconductors*, edited by K. Bedell and M. Inui (Addison-Wesley, Reading, MA, 1991).