Monte Carlo Search for the Flux-Lattice-Melting Transition in Two-Dimensional Superconductors

J. A. O'Neill and M. A. Moore
Department of Theoretical Physics, University of Manchester, Manchester, M13 9PL, United Kingdom
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A Monte Carlo simulation of the vortices in a two-dimensional type-II superconductor shows that the correlation length, which measures the range over which triangular lattice ordering of the vortices exists, diverges to infinity in the zero-temperature limit, just as predicted by a scaling argument based on phase fluctuations. No evidence is found for the formation of a vortex-lattice phase at a finite temperature.

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It is widely believed that in a thin film of a type-II superconductor, the vortices present in a magnetic field will form a triangular lattice below a nonzero transition temperature T_M. The melting of this vortex- or flux-lattice phase has been investigated theoretically by Huberman and Doniach [1] and also by Fisher [2], who argued that the melting mechanism was that of dislocation unbinding. Monte Carlo studies [3–5] on various approximations to the full Landau-Ginzburg partition function have been claimed to be consistent with the existence of a flux-lattice phase, as have experimental studies [6].

We shall present here the results of a Monte Carlo simulation which are in complete disagreement with the existence of an Abrikosov flux-lattice phase at finite temperatures, but which are in full agreement with the proposals previously made by one of us [7,8] (see also [9]). It was argued in [8] that the lower critical dimension of the Abrikosov flux lattice was four, because phase changes induced by thermal excitation of the elastic shear modes of the lattice destroyed superconducting phase coherence below four dimensions (the lower critical dimension fell to three in the commonly employed approximation of keeping the vector potential **A** fixed [8]). It seems natural to conclude that the absence of long-range phase coherence would result in the nonexistence of the flux-lattice phase in two- and three-dimensional systems. It was noted that in three-dimensional systems the length scale over which order is lost is very large, of the order of millimeters, so this effect of thermal fluctuations is probably undetectable experimentally [8]. It was suggested, however, that the consequences of the phase fluctuations in two-dimensional systems should be readily seen, and our Monte Carlo simulations in two dimensions bear this out and provide strong evidence that no flux-lattice phase exists at finite temperatures. These simulations show that as the temperature is lowered, the correlation length, which measures the range over which triangular lattice ordering of the vortices exists, diverges to infinity in the zero-temperature limit.

The starting point of the calculation is the Landau-Ginzburg free-energy functional of the complex order parameter $\psi(\mathbf{r})$ in a fixed vector potential $\mathbf{A}(\mathbf{r})$,

$$F[\psi(\mathbf{r})]/k_B T_c = \int d^3r \{\alpha(T)|\psi|^2 + \beta|\psi|^4/2 + |\mathbf{D}\psi|^2/2\mu\} . \tag{1}$$

As usual μ, β, and $\alpha(T)$ are phenomenological parameters [11], T_c is the mean-field, zero-field transition temperature, and $\mathbf{D} = -i\hbar\nabla - 2e\mathbf{A}$. For thin films it is a very good approximation to ignore fluctuations in the vector potential **A** since the length scale associated with changes in the magnetic field is of order λ^2/d, where λ is the bulk penetration depth and d is the film thickness [10]. This length scale can become of macroscopic size for very thin films. Even if this is not the case, we do not believe that using the approximation that **A** is fixed and nonfluctuating changes the essential physics in two dimensions [8]. This approximation also has the virtue of having been extensively used by other authors [3,11,12] and comparison with their results provided useful checks on our Monte Carlo procedure.

The crucial improvement in the simulation reported here is that our two-dimensional system is the surface of a sphere rather than a plane as in other Monte Carlo work (e.g., [3]). This cuts down finite-size effects dramatically as has also been observed in similar numerical studies of the quantum Hall effect [13]. At the center of the sphere one places a monopole which produces a radial magnetic field B so that at the surface $B4\pi R^2 = N\Phi_0$, where R is the radius of the sphere, N is the number of vortices, and Φ_0 is the flux quantum. The vector potential can be chosen to be $A^r = 0$, $A^\theta = 0$, and $A^\phi = BR\tan(\theta/2)$ in the usual spherical polar coordinates. The thermodynamic limit is obtained by taking the limit $N \to \infty$, $R \to \infty$, with B fixed.

The order parameter $\psi(\theta,\phi)$ can be expanded in terms of the angle-dependent factors of the eigenstates of the operator $\mathbf{D}^2/2\mu$. The form of these has been studied in [14]. Those spanning the lowest "Landau" level are the orthonormal set

$$\psi_m(\theta,\phi) = g_m \sin^m(\theta/2)\cos^{N-m}(\theta/2)e^{im\phi} , \tag{2}$$

with $m = 0, 1, \ldots, N$, $g_m = [(N+1)!/4\pi R^2 m!(N-m)!]^{1/2}$, and all have the eigenvalue $eB\hbar/\mu$. The usual approximation will be made of keeping only states in the lowest level [3,11,12]. We have shown that the use of this approximation does not alter the argument why phase fluctuations will destroy the order in two dimensions [8].

With ψ restricted to the eigenstates of the lowest level, one can write

$$\psi(\theta,\phi)=Q\sum_{m=0}^{N} v_m\psi_m(\theta,\phi)\,, \tag{3}$$

with $Q=(\Phi_0/\beta dB)^{1/4}$. The free energy becomes in terms of the (complex) expansion coefficients v_m

$$F\{v_m\}/k_BT_c=\alpha_T\sum_{m=0}^{N} v_m v_m^* + \sum_{m,p,n,r=0}^{N} W(m+p,m,n)v_m v_p v_n^* v_r^* \delta_{m+p,n+r}\,, \tag{4}$$

and $\alpha_T=dQ^2\alpha_H$ with $\alpha_H=\alpha+eB\hbar/\mu$. Here

$$W(m+p,m,n)=\frac{2(N+1)^2}{N(2N+1)}\frac{f(m+p,m,n)f(2N-m-p,N-m,N-n)}{f(2N,N,N)}\,, \tag{5}$$

with $f(x,y,z)=x!/[y!z!(x-y)!(x-z)!]^{1/2}2^{x+2}$.

The partition function now becomes (up to a multiplicative factor) the $2(N+1)$-dimensional integral

$$Z=\int\prod_{m=0}^{N} d^2v_m\, e^{-F\{v_m\}/k_BT_c}\,. \tag{6}$$

Notice that all the dependence on the physical parameters is contained within the dimensionless parameter α_T. Low temperatures correspond to large negative values of α_T. Mean-field behavior is recovered in the limit α_T goes to minus infinity, which corresponds to zero temperature. In this limit fluctuations about the mean-field solution become negligible.

It is useful to reexpress the expansion of Eq. (3) in terms of spinor variables. Up to an overall (complex) amplitude

$$\psi(\theta,\phi)\sim\prod_{i=1}^{N}(vu_i-uv_i)\,, \tag{7}$$

where $u=\cos(\theta/2)e^{-i\phi/2}$ and $v=\sin(\theta/2)e^{i\phi/2}$. When $u=u_i$ and $v=v_i$, $\psi=0$, so u_i,v_i specify the position of the ith vortex, defined as a zero of ψ. For given $\{v_m\}$, the values of θ_i and ϕ_i are obtained for $i=1,\ldots,N$, by solving for the complex zeros of the polynomial $\sum_{m=0}^{N} v_m g_m z^m$, where $z=v/u=\tan(\theta/2)e^{i\phi}$.

The multidimensional integral of Eq. (6) was evaluated by a Metropolis Monte Carlo algorithm. An initial configuration of the complex coefficients $\{v_m\}$ was chosen at random and a coefficient picked out randomly. Its value was altered by a random complex distance such that the magnitude of the change in the coefficient was less than ϵ. ϵ was chosen so that, on average, half of all attempted changes were accepted. Next, we calculated $\Delta F/k_BT_c$, the change in the free energy associated with the proposed alteration of the one coefficient. If ΔF were negative then the change in the coefficient was accepted; otherwise a random number was generated between 0 and 1 and the coefficient was changed only if $\exp(-\Delta F/k_BT_c)$ was greater than this random number. Notice that changing the coefficient simultaneously moves all the vortices. Defining a Monte Carlo step as $N+1$ attempted moves, it was found that 10^4 Monte Carlo steps were required for $N=40$, 60, and 80 down to $\alpha_T=-10$ (2×10^4 and 3×10^4 steps were required for very low temperatures, i.e., $-7\lesssim\alpha_T<-10$). At low temperatures the relaxation times become very long, and this prevented us from going below $\alpha_T=-10$. The first 10^3 steps were discarded at all temperatures. Thermal averages were as usual computed by replacing them by "time averages."

To check our program, we calculate the entropy S per vortex, defined by

$$S=-\frac{1}{N}\frac{\partial\mathcal{F}}{\partial T}=\frac{S_0}{N}\sum_{m=0}^{N}\langle v_m v_m^*\rangle\,, \tag{8}$$

where $S_0=d\alpha_H' Q^2k_BT_c$, and we shall take α_H' $(=\partial\alpha_H/\partial T)$ to be temperature independent. For $N=40$, 60, and 80, the entropy per vortex was found to be N independent down to $\alpha_T=-10$.

Ruggeri and Thouless [11] and Fujita, Hikami, and Brézin [12] have obtained series expansions for the specific heat in powers of the coupling constant β. The latest series extend to eleven terms [12]. We obtained an estimate for the specific heat by numerically differentiating our entropy S with respect to α_T, and normalized it to the mean-field prediction for the discontinuity in the specific heat ΔC. Figure 1 shows that our Monte

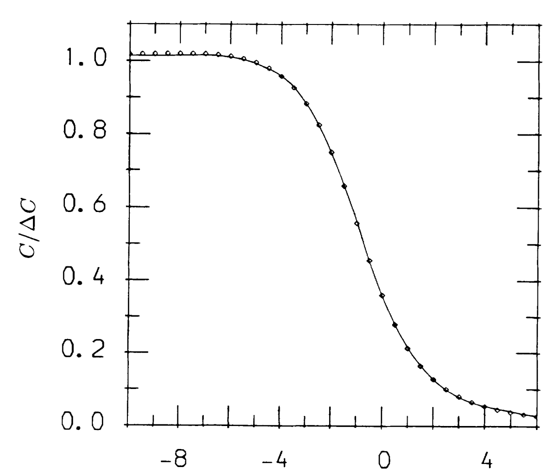

FIG. 1. Specific heat as a function of α_T for $N=80$, calculated by numerical differentiation of our Monte Carlo estimate of the entropy, normalized to the mean-field jump ΔC at the transition (continuous line). The results of the [5,5] Padé-Borel approximant derived from the series of [12] are shown as $\diamond$.

Carlo estimates for $C/\Delta C$ are in very good agreement with the [5,5] Padé-Borel approximant deduced from the series, provided the approximant is constructed to give $C/\Delta C \to 1$ as $\alpha_T \to -\infty$. We believe the generally good agreement checks our program and the utility of studying vortices on the surface of the sphere. (Our studies of the specific heat on the plane showed that there finite-size effects were large.)

We next examined the growth of crystalline order as α_T is decreased. The vortex density at the point (θ,ϕ) on the surface of the sphere is defined as

$$\rho(\theta,\phi)=\sum_{i=1}^{N}\delta(\theta-\theta_i)\delta(\phi-\phi_i)/R^2\sin\theta . \tag{9}$$

We construct the "harmonic" transform of the vortex density

$$\rho_l^m = R^2\int_0^{2\pi}d\phi\int_0^{\pi}d\theta\sin\theta\,\rho(\theta,\phi)Y_l^{m*}(\theta,\phi)/R = (1/R)\sum_{i=1}^{N}Y_l^{m*}(\theta_i,\phi_i) . \tag{10}$$

This quantity is analogous to the Fourier transform $\rho_{\mathbf{k}}$ of the vortex density on the plane, $(1/\sqrt{N})\sum_{i=1}^{N}e^{i\mathbf{k}\cdot\mathbf{r}_i}$. We define the rotationally averaged "structure factor"

$$S_l=\overline{\langle\rho_l^m\rho_l^{m*}\rangle}$$

via

$$S_l=\frac{1}{R^2}\frac{1}{2l+1}\sum_{m=-l}^{l}\sum_{i,j=1}^{N}\langle Y_l^m(\theta_i,\phi_i)Y_l^{m*}(\theta_j,\phi_j)\rangle = \frac{1}{2N\pi}\sum_{i,j=1}^{N}\langle P_l(\mathbf{n}_i\cdot\mathbf{n}_j)\rangle , \tag{11}$$

where $\mathbf{n}_i=(\sin\theta_i\cos\phi_i,\sin\theta_i\sin\phi_i,\cos\theta_i)$, P_l is a Legendre polynomial, and R is measured in units of the magnetic length $P^{1/2}$, where $2\pi P=\phi_0/B=(\sqrt{3}a^2/2$, a is the spacing between vortices in the vortex lattice). l/R is equivalent to $|\mathbf{k}|$ on the plane.

Figure 2 shows plots of S_l vs l/R for $l\geq 1$ for $N=40$, 60, and 80 at $\alpha_T=-6$ and for $N=80$ at $\alpha_T=+6$. In the high-temperature example, $\alpha_T=+6$, there is a broad rounded peak in S_l characteristic of the fluid flux. As the temperature is lowered (i.e., as α_T becomes more and more negative) peaks in S_l appear where $l/R=|\mathbf{G}|$, where $\mathbf{G}$ are reciprocal-lattice vectors of the infinite triangular lattice, and the peaks grow in height and shrink in width. We have plotted in Fig. 3 the peak height S_{peak} associated with the smallest value of $|\mathbf{G}|$ vs α_T^2 and a good straight line is found for $-10<\alpha_T<-3$. For most of this region the error bars on the peak heights (obtained by averaging over several runs) are small, and have been omitted for clarity. Below $\alpha_T\sim -8$, long relaxation time effects become very important and the $N=60$ and 80 error bars begin to grow very large. The number of Monte Carlo steps was increased to 2×10^4 steps for $N=60$ and to 3×10^4 steps for $N=80$ for $-10<\alpha_T<-8$.

It will now be shown that it follows from simple zero-temperature scaling arguments that S_{peak} should indeed vary as α_T^2 for large negative values of α_T. The correlation length ξ associated with triangular lattice ordering will diverge to infinity only at $T=0$ (i.e., for $\alpha_T=-\infty$ in our notation), on the assumption that there is no transition at finite temperature to a vortex lattice state. From general phase-transition arguments, $S_{\text{peak}}\sim\xi^{2-\eta}$ where for a zero-temperature transition it is always the case that $2-\eta=d$ provided the ground state is nondegenerate, so $\eta=0$ in two dimensions [15].

We next develop a zero-temperature scaling argument

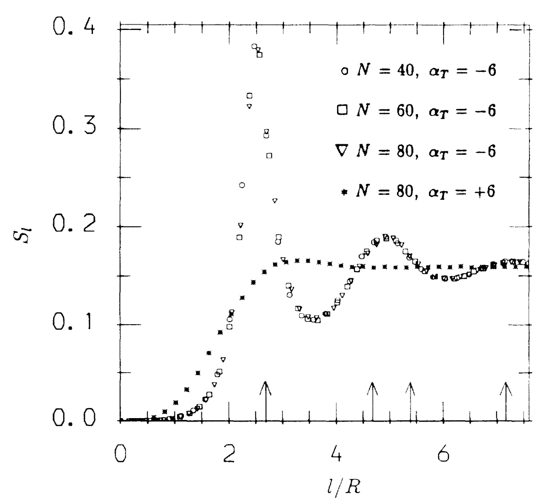

FIG. 2. Structure factor S_l vs l/R for $N=40$, 60, and 80 at $\alpha_T=-6$ and for $N=80$ at $\alpha_T=+6$. The arrows on the abscissa denote the positions of the reciprocal-lattice vectors $|\mathbf{G}|$ of the triangular lattice.

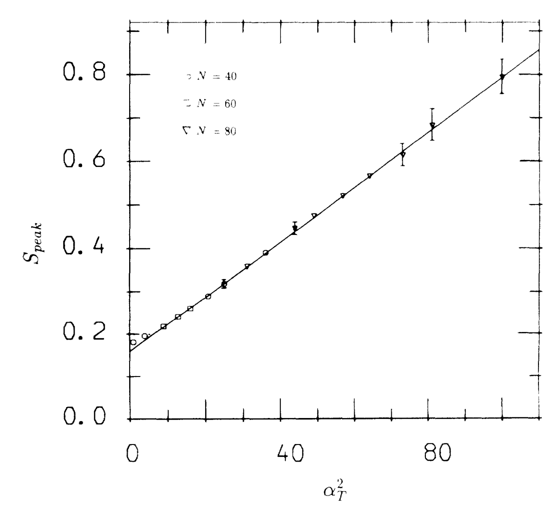

FIG. 3. Peak height S_{peak} vs α_T^2 for various system sizes (○=40, □=60, and ∇=80), which give the biggest value and, hence, the best estimate of the true peak height.

for the dependence of the correlation length ξ on α_T. In [7,8], it was shown that shear motions of the lattice induce phase variations. The effective free energy of the Goldstone mode associated with phase fluctuations is given in two dimensions by [7]

$$F_{\text{eff}}/k_B T_c = \frac{1}{2} \int d^2 r\, c_{66} P^2 (\nabla_\perp^2 \Omega)^2 , \qquad (12)$$

where c_{66} is the mean-field shear modulus of the lattice (of order α_T^2 [7]), Ω is the phase of the order parameter (in Ref. [8], a gauge invariant prescription for defining Ω was given), and $\nabla_\perp^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2$. If there is a phase change of order 2π over a region of linear extent ξ, then the free-energy cost (divided by $k_B T_c$) is of order $c_{66} P^2 \xi^{-2}$. When this quantity is of order 1, phase coherence on the length scale ξ exists, which implies that the phase coherence length $\xi \sim |\alpha_T| a$. Thus, provided the correlation length for phase fluctuations and for the length over which triangle lattice ordering exists are the same (and for most phase transitions, including zero-temperature transitions, there is only one correlation length) we would predict that $S_{\text{peak}} \sim \alpha_T^2$ as $\alpha_T \to -\infty$. The data of Fig. 3 support this identification of length scales.

Above $\alpha_T = -3$, the data for the peak height are larger than predicted by the α_T^2 formula, but this is readily understood since as $\alpha_T \to 0$, ξ will remain finite rather than vanish like $|\alpha_T|$. In other words, $\alpha_T > -3$ is outside the zero-temperature scaling regime. By comparison with Fig. 1, we can see that most of the data in Fig. 3 are in the temperature regime where the specific heat has reached its low-temperature limiting form.

A full analysis of the structure factor as a function of α_T and N, and also of the specific heat, will be published elsewhere [16].

It might be argued that a phase transition could still take place at temperatures much lower than those we were able to investigate. Indeed, in [3] it is claimed that the melting temperature was (in our units) for α_T between -10 and -12. Unfortunately, insufficient detail is given in [3] to judge how this conclusion was reached. Unless care is taken, long relaxation time effects can easily be mistaken for a phase transition. We are confident that no such transition exists since it seems improbable that the data in the range $-3 \geq \alpha_T \geq -10$ would be described by zero-temperature scaling if there were a finite-temperature phase transition.

In conclusion, we have provided strong numerical evidence that no Abrikosov flux-lattice phase exists in two dimensions and that the mechanism of its destruction is the phase fluctuations associated with the shear modes of the lattice.

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