Two-Dimensional Vortex Lattice Melting

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We report on a Monte Carlo study of two-dimensional Ginzburg-Landau superconductors in a magnetic field. We find evidence suggestive of a first-order phase transition between a low-temperature state characterized by power-law positional correlations in the superfluid density and a high-temperature vortex-fluid state. A key aspect of our study is the introduction of a quantity proportional to the Fourier transform of the superfluid density which can be sampled efficiently in Landau gauge Monte Carlo simulations and which satisfies a useful sum rule.

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In mean-field theory type II Ginzburg-Landau superconductors in a magnetic field have an unusual second-order phase transition. In the low-temperature ($T < T_c^{\rm MF}$) phase discovered by Abrikosov [1] the zeros of the superconducting order parameter (vortices) form a lattice and the system exhibits both broken translational symmetry and off-diagonal long-range order (ODLRO). Unusual aspects of the transition are related to the Cooper-pair Landau level structure [2] which causes the mean-field instability of the disordered phase to occur simultaneously at $T_c^{\rm MF}$ in a macroscopic number of channels. However, the nature of this phase transition is qualitatively altered by thermal fluctuations. Interest in the effect of thermal fluctuations on the thermodynamic properties of type II superconductors has increased since the discovery of high-temperature superconductors which have an unusually short coherence length so that fluctuation effects are important over a relatively wide temperature interval surrounding $T_c^{\rm MF}$.

For D-dimensional superconductors fluctuations in a magnetic field at temperatures well above $T_c^{\rm MF}$, where different channels are independent, are like those of a $(D-2)$-dimensional system [3] at zero magnetic field; fluctuations become important for $D < 6$ and if coupling between channels could be neglected, the mean-field phase transition to the Abrikosov state would be destroyed by fluctuations for $D < 4$. Brézin *et al.* [4] have shown that to leading order in $6 - D$ fluctuations drive the Abrikosov transition first order and suggest that this result is probably correct for $D = 3$. Indeed Hetzel *et al.* [5] have found evidence from Monte Carlo calculations that the transition is first order for $D = 3$ at least when fluctuation effects are strong enough to shift the transition point into the simpler London regime which applies for $T/T_c^{\rm MF} \ll 1$. However, high-temperature perturbative expansions [6,7], even when evaluated to high order where coupling between different channels becomes important, show no evidence of a transition for $D = 3$ or $D = 2$. The results of Monte Carlo simulations for $D = 2$ have been controversial. Tešanović and Xing [8] and Kato and Nagaosa [9] find evidence for a phase transition at a temperature below $T_c^{\rm MF}$ while O'Neill and Moore [10] have concluded that the Abrikosov phase transition is entirely suppressed by thermal fluctuations. In this Letter we present [11] the results of a Monte Carlo simulation for $D = 2$ in which we find clear evidence of a phase transition and behavior suggestive of a first-order transition.

The free energy density of a Ginzburg-Landau superconductor is given by

$$f[\Psi] = \alpha(T)|\Psi|^2 + \frac{\beta}{2}|\Psi|^4 + \frac{1}{2m^*}|(-i\hbar\nabla - 2e\mathbf{A})\Psi|^2. \tag{1}$$

($F \equiv L_z \int d^2\mathbf{r}\, f[\Psi(\mathbf{r})]$, where L_z is the film thickness.) The quadratic terms in Eq. (1) are minimized by order parameters which correspond to a lowest Landau level (LLL) wave function for the Cooper pairs. It follows that the mean-field theory superconducting instability occurs at $T_c^{\rm MF}$ [$\alpha_H(T_c^{\rm MF}) = 0, \alpha_H = \alpha + \hbar eB/m^*$] for all Cooper pair states which are in the LLL but only at much lower temperatures for channels corresponding to higher Landau level Cooper pair wave functions. In this work we adopt the LLL approximation in which we assume that fluctuations in higher Landau level channels can be neglected [6,8,10] (see below) and consider only the two-dimensional limit where variations of the order parameter along the $\hat{\mathbf{z}}$ direction can be neglected. In the LLL approximation the order parameter is defined up to an overall scale factor by its zeros, i.e., by the positions of the vortices. (This property has been used by Tešanović and collaborators [8,12] to develop many useful insights.) This limit applies to films thinner than a coherence length and to layered systems when the interlayer coupling can be neglected. We choose the Landau gauge [$\mathbf{A} = (0, Bx, 0)$] and apply quasiperiodic boundary conditions to the order parameter inside a finite system with lengths L_x and L_y. (For thin films, especially those formed of strongly type II materials, it is a good approximation to ignore fluctuations in the vector potential $\mathbf{A}$.) The order parameter $\Psi(\mathbf{r})$ can then be expanded in the form

$$\Psi(\mathbf{r}) = \left(\frac{|\alpha_H|\pi\ell^2 L_z}{\beta}\right)^{1/2} \sum_j C_j \left(\sum_s (L_y L_z)^{-1/2}(\pi\ell^2)^{-1/4} \exp(iyX_{j,s}/\ell^2)\exp[-(x - X_{j,s})^2/4\ell^2]\right). \tag{2}$$

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In Eq. (2) $X_{j,s} = j2\pi\ell^2/L_y + sL_x$, $\ell^2 = \hbar c/2eB$, and s runs over all integers and j runs from 1 to $N_\phi = L_xL_y/2\pi\ell^2$ which must be chosen to be an integer.

A central role in our study is played by the superfluid-density spatial correlation function, whose Fourier transform is defined by

$$\chi_{\rm SFD}(\mathbf{k}) \equiv \frac{1}{L_xL_y}\int d^2\mathbf{r}\int d^2\mathbf{r}'\langle|\psi(\mathbf{r})|^2|\psi(\mathbf{r}')|^2\rangle \times \exp[i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')]. \quad (3)$$

We evaluate $\chi_{\rm SFD}(\mathbf{k})$ by expressing it in terms of

$$\Delta(\mathbf{k}) \equiv \frac{1}{N_\phi}\sum_{j_1j_2}\bar{C}_{j_1}C_{j_2}\delta_{j_2-j_1-n_y} \times \exp[-ik_x(X_{j_1}+X_{j_2})/2], \quad (4)$$

where for a finite system $\mathbf{k} = 2\pi(n_x/L_x, n_y/L_y)$, $\delta_j = 1$ if j is a multiple of N_ϕ and is zero otherwise, and $X_j \equiv X_{j,0}$. [Note that $\Delta_0 \equiv \Delta(\mathbf{k}=0)$ is proportional to the integrated superfluid density.] $\Delta(\mathbf{k})$ is conveniently sampled in our Landau gauge Monte Carlo simulations and

$$\chi_{\rm SFD}(\mathbf{k}) = \frac{N_\phi^2}{L_xL_y}\left(\frac{\alpha_H\pi\ell^2L_z}{\beta}\right)^2\exp[-k^2\ell^2/2]\langle|\Delta(\mathbf{k})|^2\rangle. \quad (5)$$

Moreover $\Delta(\mathbf{k})$ satisfies the following sum rule for each configuration of the Ginzburg-Landau system,

$$\frac{1}{N_\phi}\sum_{\mathbf{k}}[|\tilde{\Delta}(\mathbf{k})|^2 - 1/N_\phi] = 0, \quad (6)$$

where $\tilde{\Delta}(\mathbf{k}) \equiv \Delta(\mathbf{k})/\Delta_0$. Note that $\tilde{\Delta}(\mathbf{k})$ depends only on the distribution of $|\Psi(\mathbf{r})|^2$ and not on its overall magnitude. Equation (6) reflects the LLL restrictions on the superfluid density distribution. [For a finite system, both n_x and n_y in the sum over $\mathbf{k}$ in Eq. (6) range over any N_ϕ consecutive values.]

In the vortex-fluid state $\chi_{\rm SFD}(\mathbf{k})$ should be a smooth function of wave vector and if the sum over $\mathbf{k}$ in Eq. (6) is to converge we must have $\lim_{|k|\to\infty}|\tilde{\Delta}(\mathbf{k})|^2 \to N_\phi^{-1}$ and hence that

$$\lim_{|k|\to\infty}\chi_{\rm SFD}(\mathbf{k}) = \frac{\Delta_0^2\alpha_HL_z}{2\beta}\exp[-k^2\ell^2/2]. \quad (7)$$

It is readily verified [13] that Eq. (7) is satisfied for all $\mathbf{k}\neq 0$ when $T \gg T_c^{\rm MF}$ and the vortex fluid is completely uncorrelated. On the other hand, in a vortex-lattice state $\Delta(\mathbf{k}) = \Delta_0\delta_{\mathbf{k},\mathbf{G}}$, where $\mathbf{G}$ is a reciprocal lattice vector. To see that Eq. (6) is satisfied in this case note that there are N_ϕ wave vectors per Brillouin zone in the Abrikosov state. Equation (6) tells us that averages of $|\tilde{\Delta}(\mathbf{k})|^2$ over large areas of reciprocal space yield N_ϕ^{-1} irrespective of the degree of correlation among the vortices. $N_\phi\langle|\tilde{\Delta}(\mathbf{k})|^2\rangle - 1$ provides a very convenient measure of the degree of vortex correlation in a system.

We can express the Ginzburg-Landau free energy in terms of $|\Delta(\mathbf{k})|^2$ as follows

$$\int\frac{f[\Psi]}{k_BT}d\mathbf{r} \equiv \frac{E_\beta(\beta,\Delta_0)}{k_BT} = N_\phi g^2\left(\mathrm{sgn}(\alpha_{\rm H})\Delta_0 + \frac{\beta[\tilde{\Delta}]\Delta_0^2}{4}\right), \quad (8)$$

where

$$\beta[\tilde{\Delta}] \equiv \sum_{\mathbf{k}}|\tilde{\Delta}(\mathbf{k})|^2\exp\left(-\frac{k^2l^2}{2}\right) \quad (9)$$

and $g \equiv \alpha_H(\pi\ell^2L_z/\beta K_BT)^{1/2}$. $\beta[\tilde{\Delta}]$ has its minimum value in the Abrikosov state and increases as the vortex positions become less correlated. It is easy to show that in the uncorrelated vortex fluid $\beta[\tilde{\Delta}] = 2$ while for the triangular lattice Abrikosov state $\beta[\tilde{\Delta}] = \beta_A \sim 1.159\,595$. (This relatively weak variation in β was exploited recently [12] by Tešanović *et al.*) We regard $\beta[\tilde{\Delta}]$ and Δ_0 as two intensive thermodynamic variables which characterize the state of the LLL Ginzburg-Landau system. We can define an entropy which measures the function-space volume associated with a given $\beta[\tilde{\Delta}]$ and Δ_0 by $S_\beta(\beta,\Delta_0) \equiv k_B\ln[W(\beta,\Delta_0)]$, where

$$W(\beta,\Delta_0) \equiv \left(\frac{|\alpha_H|\pi\ell^2L_z}{\beta}\right)^{N_\phi}\prod_j\int d\bar{C}_j\,dC_j\,\delta(\beta-\beta[\tilde{\Delta}])\delta\left(\Delta_0-\sum_j\bar{C}_jC_j\right). \quad (10)$$

With this definition the free energy, β and Δ_0 at any value of g can be determined by minimizing

$$F_\beta(\beta,\Delta_0) \equiv E_\beta(\beta,\Delta_0) - TS(\beta,\Delta_0) \quad (11)$$

with respect to β and Δ_0. (F_β is extensive so fluctuations become negligible in the thermodynamic limit.) We will use Eq. (11) to interpret the Monte Carlo results discussed below.

Using the Metropolis algorithm we have determined distribution functions for several quantities [14] including E_β, Δ_0, $\beta[\tilde{\Delta}]$, and $|\tilde{\Delta}(\mathbf{k})|^2$ as a function of both g and N_ϕ. Finite system shapes have been chosen to accommodate perfect triangular lattices. ($\frac{L_y}{L_x} = \frac{2}{\sqrt{3}}\frac{N_y}{N_x}$, where $N_\phi = N_x \times N_y$.) For all simulations the order parameter was initialized to the Abrikosov lattice value and the first 10^4 Monte Carlo steps were discarded. (We have compared the results from different stages of our Monte Carlo runs to make sure our systems were well equilibrated.) Some typical results for $\langle|\tilde{\Delta}(\mathbf{k})|^2\rangle$ at $T < T_c^{\rm MF}$ are shown in Fig. 1. At $g^2 = 30$ the vortex fluid has developed strong correlations. For $N_\phi = 120$, $N_\phi\langle|\tilde{\Delta}(\mathbf{G})|^2\rangle \sim 3$ which is 3 times larger than for the high-temperature uncorrelated flux fluid but still ~ 40 times smaller than

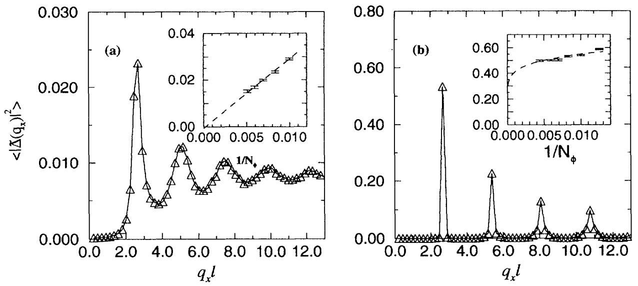

FIG. 1. $\langle|\tilde{\Delta}(q_x)|^2\rangle$ at $g^2 = 30$ (a) and $g^2 = 50$ (b) for a finite system with $N_\phi = 120$. ($q_y = 0$ and $T < T_c^{\rm MF}$.) The insets show the dependences of $\langle|\tilde{\Delta}(\mathbf{G})|^2\rangle$ on system size at these g^2 values. The dashed line in the inset of (a) is proportional to $N_\phi^{-1.0}$ while that in the inset of (b) is proportional to $N_\phi^{-0.13}$. ($\mathbf{G}$ is a member of the first shell of reciprocal lattice vectors of the Abrikosov lattice.) These averages were obtained from (1–2)$\times 10^6$ Monte Carlo steps.

its mean-field value. For $g^2 = 50$, $\langle|\tilde{\Delta}(\mathbf{G})|^2\rangle$ has increased to more than half its mean field value. The insets in Fig. 1 show the dependence of $|\tilde{\Delta}(\mathbf{G})|^2$ on system size for these two values of g^2. For $g^2 = 30$, $\langle|\tilde{\Delta}(\mathbf{G})|^2\rangle \sim N_\phi^{-1.0}$ as expected in the fluid state while for $g^2 = 50$, $\langle|\tilde{\Delta}(\mathbf{G})|^2\rangle \sim N_\phi^{-0.13}$, consistent with the quasi-long-range order expected in the Abrikosov state. Figure 2 shows that for a given system size $\langle|\tilde{\Delta}(\mathbf{G})|^2\rangle$ increases relatively abruptly at $g^2 \sim 42.5$ suggesting the occurrence of a phase transition.

To examine this possibility and to attempt a determination of the order of the phase transition we have examined the dependence of the E_β distribution function [15,16] on system size for $g^2 \sim 43$ and $N_\phi = N_x \times N_y = 10 \times 8, 10 \times 10, 12 \times 10, 12 \times 12$, and 14×12. The results are shown in Fig. 3. For each system size the number of Monte Carlo steps required to determine these distribution functions accurately exceeded 8×10^6. For $N_\phi > 100$ a double peak structure is clearly visible which provides unambiguous evidence of a phase transition. This structure becomes more pronounced with increasing system size suggesting the occurrence of a first-order phase transition. However, for the system sizes we are able to study the free energy barrier between the two states does not yet show the $N_\phi^{1/2}$ behavior which would be expected at large N_ϕ in the case of a first-order transition. (In each of these Monte Carlo runs the number of flips between high and low energy states of the system exceeded 30.) For each N_ϕ the adjusted [15,16] distribution function at the value of g^2 where the peaks have equal height is plotted. By extrapolating these values of g^2 to $N_\phi = \infty$ as shown in the inset we estimate that a first-order phase transition occurs [17] at $g^2 = g_M^2 = 43.5 \pm 1.0$. (This can be compared with previous estimates $g_M^2 \sim 50.0$ by Tešanović and Xing [8] and $g_M^2 \approx 49.0$ by Kato and Nagaosa [9]). In Fig. 3(b) we compare the $\langle|\tilde{\Delta}(\mathbf{G})|^2\rangle$ distribution from values of the order parameter with high energies with that from low energies for $N_\phi = 168$. For high-energy configurations the $\langle|\tilde{\Delta}(\mathbf{G})|^2\rangle$ is $\sim 5.0 N_\phi^{-1}$ while for the low-energy configurations the distribution is peaked at ~ 0.5 demonstrating that the phase transition occurs between a high-energy strongly correlated vortex-fluid state and a low-energy Abrikosov state. The magnetization discontinuity and latent heat associated with the phase transition depend on material parameters and are [14] typically $\sim 10^{-5}\Phi_0/\lambda_{ab}^2$ and $\sim 0.6 k_B N_\phi T_M^2(-dH_{c2}^{\rm MF}/dT)/(H_{c2}^{\rm MF} - H)$, respectively.

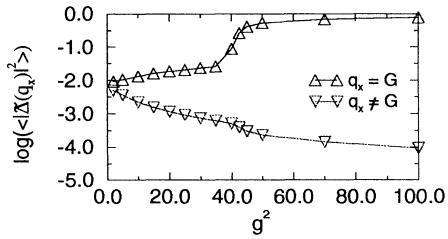

FIG. 2. Dependence of $\langle|\tilde{\Delta}(\mathbf{q})|^2\rangle$ on g^2 at $N_\phi = 120$ for $\mathbf{q} = \mathbf{G}$ and for $\mathbf{q} \neq \mathbf{G}$ where $\mathbf{G}$ is a reciprocal lattice vector of the Abrikosov lattice.

In Fig. 4(a) we show distribution functions for $\beta(\tilde{\Delta})$ at several fixed values of Δ_0 and in Fig. 4(b) we show distribution functions for Δ_0 at several fixed values of $\beta(\tilde{\Delta})$ for $\beta(\tilde{\Delta})$ and Δ_0 near the values at which the phase transition takes place. The $\beta(\tilde{\Delta})$ distribution function is proportional to $\exp[S_\beta(\beta,\Delta_0)/k_B - \beta N_\phi g^2 \Delta_0^2/4]$. [See Eq. (11). At extrema of the distribution $\partial S_\beta/\partial\beta = k_B N_\phi g^2 \Delta_0^2/4$.] The double peak structure apparent in

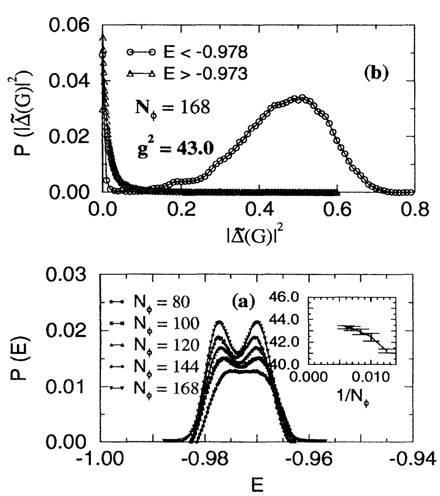

FIG. 3. (a) Landau-Ginzburg energy distribution function at the finite system phase transition point for various system sizes. Energies are in units of the mean-field condensation energy, $N_\phi k_B T g^2/\beta_A$. The inset shows the dependence of the g^2 at the phase transition on system size. (b) Low-energy and high-energy cuts of the distribution function for $|\tilde{\Delta}(\mathbf{G})|^2$.

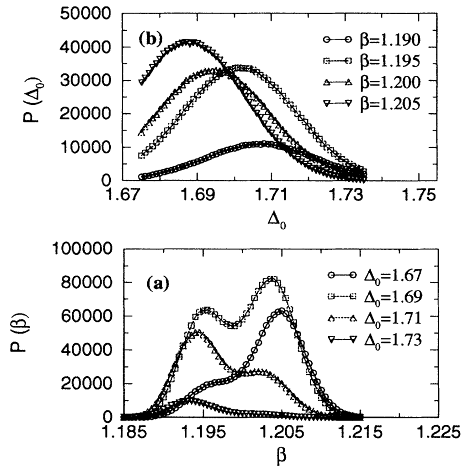

FIG. 4. Distribution functions of (a) $\beta[\tilde{\Delta}]$ for several values of Δ_0 and of (b) Δ_0 for several values of $\beta[\tilde{\Delta}]$.

the $\beta(\tilde{\Delta})$ distribution demonstrates that the phase transition is driven by the S_β term which describes the dependence of the volume in order parameter space on the degree of correlation in vortex positions. No similar double peak structure is seen in the Δ_0 distribution confirming that the phase transition is associated primarily with spatial correlations in vortex positions and hence in the superfluid density rather than with changes in the average magnitude of the superconducting order parameter.

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[1] A.A. Abrikosov, Zh. Eksp. Teor. Fiz. **32**, 1442 (1957).
[2] A.H. MacDonald, H. Akera, and M.R. Norman, Phys. Rev. B **45**, 10147 (1992).
[3] P.A. Lee and S.R. Shenoy, Phys. Rev. Lett. **28**, 1025 (1972).
[4] E. Brézin, D.R. Nelson, and A. Thiaville, Phys. Rev. B **31**, 7124 (1985).
[5] R.E. Hetzel, A. Sudba, and D.A. Huse, Phys. Rev. Lett. **69**, 518 (1992); see also A. Houghton, R.A. Pelcovits, and A. Sudbo, Phys. Rev. B **40**, 6763 (1989).
[6] D.J. Thouless, Phys. Rev. Lett. **34**, 946 (1975); G.J. Ruggeri and D.J. Thouless, J. Phys. F **6**, 2063 (1976).
[7] E. Brézin, A. Fujita, and S. Hikami, Phys. Rev. Lett. **65**, 1949 (1990); S. Hikami, A. Fujita, and A.I. Larkin, Phys. Rev. B **44**, 10400 (1991).
[8] Zlatko Tešanović and L. Xing, Phys. Rev. Lett. **67**, 2729 (1991).
[9] Yusuke Kato and Naoto Nagaosa, Phys. Rev. B **47**, 2932 (1993).
[10] J.A. O'Neill and M.A. Moore, Phys. Rev. Lett. **69**, 2582 (1992).
[11] Preliminary reports on these calculations have been presented previously: Jun Hu and A.H. MacDonald, Bull. Am. Phys. Soc. **38**, 635 (1993).
[12] Zlatko Tešanović, Lei Xing, Lev Bulaevskii, Quiang Li, and M. Suenga, Phys. Rev. Lett. **69**, 3563 (1992).
[13] For a discussion of the high-temperature perturbation expansion for $\chi_{\mathrm{SFD}}(\mathbf{k})$ see Jun Hu and A.H. MacDonald (to be published).
[14] We plan to publish further details of our results later. Jun Hu and A.H. MacDonald (to be published).
[15] J. Lee and J.M. Kosterlitz, Phys. Rev. Lett. **65**, 137 (1990).
[16] A.M. Ferrenberg and R.H. Swendsen, Phys. Rev. Lett. **61**, 2635 (1988).
[17] The LLL approximation is valid for $H/H_{c2} \geq 1/2$. For a system of decoupled layers $g^2 = \gamma(H/H_{c2})(1 - H/H_{c2})^2$, where $\gamma \equiv \Lambda(T)a_c/2\lambda_{ab}^2$, the fluctuation length $\Lambda(T) = \Phi_0^2/16\pi^2 T \sim 2 \times 10^8$ Å/K, and a_c is the layer separation. It follows that the LLL approximation will be approximately valid at the melting transition if $\gamma \geq g_M^2$. For typical superconductors this inequality is satisfied unless the transition occurs very close to the zero-field T_c, i.e., except for very small H. For high-temperature superconductors, particularly $Bi_2Sr_2CaCuO_8$, the LLL approximation may fail over a fairly wide range of temperature below the zero-field T_c.