Two-Dimensional Vortex Lattice Melting

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Abstract

We report on a Monte-Carlo study of two-dimensional Ginzburg-Landau superconductors in a magnetic field which finds clear evidence for a first-order phase transition characterized by broken translational symmetry of the superfluid density. 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. We estimate the latent heat per vortex of the melting transition to be $\sim 0.38k_B T_M$ where $T_M$ is the melting temperature.
In mean-field theory type II Ginzburg-Landau superconductors in a magnetic field have an unusual second-order phase transition. In the low-temperature ($T < T_{c}^{MF}$) 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 $T_{c}^{MF}$ 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 $T_{c}^{MF}$.

For $D$ dimensional superconductors fluctuations in a magnetic field at temperatures well above $T_{c}^{MF}$, where different channels are independent, are like those of a $D - 2$ dimensional system [3] at zero magnetic field suggesting that the mean-field phase transition to the Abrikosov state will be destroyed by fluctuations for $D < 4$. High-temperature perturbative expansions [4,5], even when evaluated to high-order where coupling between different channels becomes important, show no evidence of a transition for $D = 3$ or $D = 2$ between the high-temperature fluid state and Abrikosov’s vortex-lattice state. The results of Monte-Carlo simulations for $D = 2$ have been controversial. Tešanović and Xing [6] and Kato and Nagaosa [7] find evidence for a phase transition at a temperature below $T_{c}^{MF}$ while O’Neill and Moore [8] have concluded that the Abrikosov phase transition is suppressed by thermal fluctuations. In this letter we present [9] the results of a Monte-Carlo simulation for $D = 2$ in which we find unambiguous evidence for a first-order phase transition.

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

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

($F \equiv \int d^2\vec{r} f[\Psi(\vec{r})]$.) The quadratic terms in Eq. (1) are minimized by order-parameters
which correspond to a lowest Landau level (LLL) wavefunction for the Cooper pairs. It follows that the mean-field theory superconducting instability occurs at $T_{c}^{MF}$ ($\alpha H(T_{c}^{MF}) = 0; \alpha = \alpha + \hbar eB/m^* )$ 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 wavefunctions.

In this work we adopt the LLL approximation in which we assume that fluctuations in higher Landau level channels can be neglected \[6,10\] and consider only the two dimensional limit where variations of the order parameter along the $\hat{z}$ 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 \[3,12\] to develop many useful insights.) This limit applies to films thinner than a coherence length and to layered systems when the inter-layer coupling can be neglected. We choose the Landau gauge ($\vec{A} = (0, Bx, 0)$) and apply quasi-periodic 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 $\vec{A}$.) The order parameter $\Psi(\vec{r})$ can then be expanded in the form,

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

(2)

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

$$\chi_{SF_D}(\vec{k}) \equiv \frac{1}{L_x L_y} \int d^2\vec{r} \int d^2\vec{r}' \langle |\psi(\vec{r})|^2 |\psi(\vec{r}')|^2 \rangle \exp[i\vec{k} \cdot (\vec{r} - \vec{r}')]$$

(3)

We evaluate $\chi_{SF_D}(\vec{k})$ by expressing it in terms of

$$\Delta(\vec{k}) \equiv \frac{1}{N_\phi} \sum_{j_1,j_2} \delta_{j_2-j_1-n_y} \exp[-ik_x(X_{j_1} + X_{j_2})/2]$$

(4)

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

$$
\chi_{SF D}(\vec{k}) = \frac{N^2_\phi}{L_x L_y} \left( \frac{\alpha_H \pi \ell^2 L_z}{\beta} \right)^2 \exp[-k^2 \ell^2/2] (|\Delta(\vec{k})|^2)
$$

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

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

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

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

$$
\lim_{|\vec{k}| \to \infty} \chi_{SF D}(\vec{k}) = \frac{\Delta_0^2 \alpha_H L_z}{2\beta} \exp[-k^2 \ell^2/2] \tag{7}
$$

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

$$
\int \frac{f[\Psi]}{k_B T} d\vec{r} = \frac{E_\beta(\beta, \Delta_0)}{k_B T} = N_\phi g^2 [\text{sgn}(\alpha_H) \Delta_0 + \frac{\beta [\tilde{\Delta}] \Delta_0^2}{4}] \tag{8}
$$

where

$$
\beta [\tilde{\Delta}] \equiv \sum_{\vec{k}} |\tilde{\Delta}(\vec{k})|^2 \exp[-k^2 \ell^2/2]. \tag{9}
$$
and $g \equiv \alpha_H(\pi \ell^2 L_z/\beta K_B T)^{1/2}$. $\beta[\tilde{\Delta}]$ has its minimum value in the Abrikosov state and increases as the vortex positions become less correlated. It is readily verified that in the uncorrelated vortex fluid $\beta[\tilde{\Delta}] = 2$ while for the triangular lattice Abrikosov state $\beta[\tilde{\Delta}] = \beta_A \sim 1.159595$. (This relatively weak variation in $\beta$ was exploited recently [12] by Tešanović et al.) We regard $\beta[\tilde{\Delta}]$ and $\Delta_0$ as the 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 $\Delta_0$ by

$$S_{\beta}(\beta, \Delta_0) \equiv k_B \ln(W(\beta, \Delta_0))$$

where

$$W(\beta, \Delta_0) \equiv (|a_H|\pi \ell^2 L_z)^{N_\phi} \prod_j \int dCjdC_j \delta(\beta - \beta[\tilde{\Delta}])\delta(\Delta_0 - \sum_j C_jC_j)$$

(10)

With this definition the free energy, $\beta$ and $\Delta_0$ at any value of $g$ can be determined by minimizing

$$F_{\beta}(\beta, \Delta_0) \equiv E_{\beta}(\beta, \Delta_0) - TS(\beta, \Delta_0)$$

(11)

with respect to $\beta$ and $\Delta_0$. ($F_{\beta}$ 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 [13] including $E_{\beta}$, $\Delta_0$, $\beta[\tilde{\Delta}]$, and $|\tilde{\Delta}(\vec{k})|^2$ as a function of both $g$ and $N_\phi$. Finite system shapes have been chosen to accommodate perfect triangular lattices. For all simulations the order parameter was initialized to the Abrikosov lattice value and the first $10^4$ Monte Carlo steps were discarded. Some typical results for $\langle |\tilde{\Delta}(\vec{k})|^2 \rangle$ at $T < T_c^{MF}$ are shown in Fig. (1). At $g^2 = 30$ the vortex fluid has developed strong correlations. For $N_\phi = 120$, $N_\phi \langle |\tilde{\Delta}(\vec{G})|^2 \rangle \sim 3$ which is three times larger than for the high-temperature uncorrelated flux-fluid but still $\sim 40$ times smaller than its mean field value. For $g^2 = 50$, $\langle |\tilde{\Delta}(\vec{G})|^2 \rangle$ has increased to more than half its mean field value. The insets in Fig. (1) show the dependence of $|\tilde{\Delta}(\vec{G})|^2$ on system size for these two values of $g^2$. For $g^2 = 30$, $\langle |\tilde{\Delta}(\vec{G})|^2 \rangle \sim N_\phi^{-1.0}$ as expected in the fluid state while for $g^2 = 50$, $\langle |\tilde{\Delta}(\vec{G})|^2 \rangle \sim N_\phi^{-0.13}$, consistent with the quasi-long-range order expected in the Abrikosov state. Fig. (2) shows that for a given system size
\langle |\hat{\Delta}(\vec{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 determine the order of the phase transition we have examined the dependence of the energy distribution function [13,14] on system size for \( g^2 \sim 43 \) and \( N_\phi = 80, 100, 120, 144, 168 \). 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 \( 8 \times 10^6 \). For \( N_\phi > 100 \) a double peak structure indicative of a first-order phase transition is clearly visible. For each \( N_\phi \) the adjusted [13,14] 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 at \( g^2 = g_M^2 = 43.5 \pm 1.0 \). By comparing the separations between the peak positions we estimate that the latent heat per flux quantum associated with the transition is \( \sim 0.01 k_B T g_M^2 / \beta_A \sim 0.38 k_B T \). In Fig. (3b) we compares the \( \langle |\hat{\Delta}(\vec{G})|^2 \rangle \) distribution from values of the order parameter with high-energies with that from low-energies for \( N_\phi = 168 \). For high-energy configurations the \( \langle |\hat{\Delta}(\vec{G})|^2 \rangle \) is \( \sim 5.0 N_\phi^{-1} \) while for the low-energy configurations the distribution is peaked at \( \sim 0.5 \) demonstrating that the phase transition occurs between a high-energy strongly correlated vortex fluid state and a low-energy Abrikosov state.

In Fig. (4a) we show distribution functions for \( \beta(\hat{\Delta}) \) at several fixed values of \( \Delta_0 \) and in Fig. (4b) we show distribution functions for \( \Delta_0 \) at several fixed values of \( \beta(\hat{\Delta}) \) for \( \beta(\hat{\Delta}) \) and \( \Delta_0 \) near the values at which the phase transition takes place. The \( \beta(\hat{\Delta}) \) 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 \( \partial S_\beta / \partial \beta = K_B^{-1} N_\phi g^2 \Delta_0^2 / 4 \). The double peak structure apparent in the \( \beta(\hat{\Delta}) \) distribution demonstrates that the phase transition is driven by the \( S_\beta \) 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 \( \Delta_0 \) 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 magnitude of
the superconducting order parameter.

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FIGURES

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

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

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 ratio of the peak heights to the intermediate minimum grows with system size but for the sizes we are able to study does not yet show the $\exp[c N_\phi^{1/2}]$ behavior expected at large $N_\phi$. 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 $|\tilde{\Delta}(\vec{G})|^2$.

FIG. 4. Distribution functions of (a) $\beta[\tilde{\Delta}]$ for several values of $\Delta_0$ and of (b) $\Delta_0$ for several values of $\beta[\tilde{\Delta}]$. 

10