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Melting of the vortex lattice in high-T_c superconductors

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The precise measurements of vortex melting point towards a need to develop a quantitative theoretical description of thermal fluctuations in vortex matter. To tackle the difficult problem of melting, the description of both the solid and the liquid phase should reach the precision level well below 1%. Such a theory in the framework of the Ginzburg-Landau approach is presented. The melting line location is determined, and magnetization and specific-heat jumps along it are calculated. We find that the magnetization in the liquid is larger than that in the solid by 1.8% regardless of the melting temperature, while the specific-heat jump is about 6% and slowly decreases with temperature. The magnetization curves agree with experimental results on Y-Ba-Cu-O and Monte Carlo simulations.

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A magnetic field generates an array of vortices in type-II superconductors. The vortices strongly interact with each other forming highly correlated configurations such as the vortex lattice. In high-T_c cuprates at relatively high temperatures, vortices move and vibrate due to thermal fluctuations to the extent that the lattice can melt becoming a "vortex liquid."[1] Several recent remarkable experiments clearly determined that the vortex lattice melting in high-T_c superconductors is a first-order phase transition with magnetization jumps[2] and spikes in specific heat.[3] The magnetization and entropy jumps were measured using diverse techniques such as local Hall probes, superconducting quantum interference device,[4,5] torque magnetometry,[6,7] and integration of the specific-heat spike.[3] Related investigations indicate that, in addition to the spike, there is also a jump in specific heat.[3,8] In spite of those precise measurements of vortex melting, a quantitative theoretical description of vortex melting is still lacking. We present such a theory in the framework of the Ginzburg-Landau approach in this work.

Thermal fluctuations in vortex matter have attracted great attention since the high-Tc superconductors were discovered over a decade ago. In highly anisotropic superconductors like Bi-Sr-Ca-Cu-O near the melting point vortices are quite well separated and the system can be approximated by an array of pointlike objects.[1] In less anisotropic ones like Y-Ba-Cu-O, near the melting point the vortices overlap and one has to use the Ginzburg-Landau (GL) model. The model is defined by the following free energy:

$$F=\int d^3x\frac{\hbar^2}{2m_{ab}}|\mathbf{D}\psi|^2+\frac{\hbar^2}{2m_c}|\partial_z\psi|^2-a(T)|\psi|^2+\frac{b'}{2}|\psi|^4+\frac{(\mathbf{B}-\mathbf{H})^2}{8\pi}, \qquad (1)$$

where $\mathbf{A}=(By,0)$ describes magnetic field (considered constant and nonfluctuating, see below) in Landau gauge and covariant derivative is defined by $\mathbf{D}\equiv\boldsymbol{\nabla}-i(2\pi/\Phi_0)\mathbf{A},\Phi_0\equiv(hc/e^*)(e^*=2e)$. When $\kappa=\lambda/\xi$ is large (greater than 10), where λ magnetic penetration depth and ξ coherence length, the magnetic field can be considered constant and nonfluctuating (an excellent approximation in the region studied). Statistical physics is described by the statistical sum $Z=\int D\psi D\bar{\psi}\exp(-F/T)$. It accurately describes thermal fluctuations in the range of relatively large magnetic fields ($H\gg H_{c1}=100$ G in Y-Ba-Cu-O) and temperatures near T_c (70–110 K in Y-Ba-Cu-O). Near T_c, $a(T)$ can be approximated bt $\alpha T_c(1-t)$. In this paper, we will consider only high κ and temperatures near T_c. The model is, however, highly nontrivial even within the lowest Landau-level (LLL) approximation. In this approximation, which is valid when the magnetic field is high, only lowest Landau-level mode is retained and the free energy simplifies (after rescaling):[9]

$$f=\frac{1}{4\pi\sqrt{2}}\int d^3x\left[\frac{1}{2}|\partial_z\psi|^2+a_T|\psi|^2+\frac{1}{2}|\psi|^4\right]. \qquad (2)$$

The simplified model has only one parameter, the dimensionless scaled temperature $a_T=-(b\omega/4\pi\sqrt{2})^{-2/3}a_h$, where $\omega=\sqrt{2Gi}\pi^2t, a_h=(1-t-b)/2, t=T/T_c, b=B/H_{c2}$. The dimensionless Ginzburg number Gi characterizing the importance of thermal fluctuations is $\frac{1}{2}(8\pi\kappa^2\xi T_c\gamma/\Phi_0^2)^2$, and the anisotropy parameter γ is $\sqrt{m_c/m_{ab}}$.

The LLL GL model was studied by a variety of different nonperturbative analytical methods. Among them are the density functional,[10] $1/N$,[11] elasticity theory,[12] and others.[13] The model was also studied numerically in both three-dimensional[14] (3D) and 2D.[15,16] However, we will not discuss those approaches in this paper.

While applying the renormalization group (RG) on the one-loop level to this model, Brezin, Nelson, and Thiaville[17] found no fixed points of the (functional) RG equations and thus concluded that the transition to the solid phase is not continuous. The RG method therefore cannot provide a quantitative theory of the melting transition. Two perturbative approaches were developed and greatly improved recently to describe the solid phase and liquid phases, respectively. The perturbative approach on the liquid side was pioneered by Ruggeri and Thouless,[18] who developed an expansion in which all the "bubble" diagrams are resummed. Unfortunately, they found that the series are asymptotic and, although first few terms provide accurate results at very high temperatures, the series become inapplicable for a_T less than -2 which is quite far above the melting line (located around $a_T=-10$). We obtained recently an optimized Gaussian series[9] that is convergent rather than asymptotic with radius of convergence of $a_T\approx-5$, but still above the melting line.

On the solid side, Eilenberger[19] calculated the fluctuations spectrum around Abrikosov's mean-field solution. Maki and Takayama[20] noticed that the vortex lattice phonon modes are softer than those of the usual acoustic phonons in atomic crystals and this leads to infrared (IR) divergences in certain quantities. This was initially interpreted as the destruction of the vortex solid by thermal fluctuations and the perturbation theory was abandoned. However, the divergences resemble the "spurious" IR divergences in the critical phenomena theory. A recent analysis demonstrated that all these IR divergences cancel in physical quantities[21] and the series therefore are reliable. The two-loop calculation was performed, so that the LLL GL theory on the solid side is now precise enough even for the description of melting.

However, on the liquid side, a theory for $a_T\leqslant-5$ is required. Moreover this theory should be extremely precise since the internal energies of the solid and the liquid near melting differ by a few percents only. Developing such a theory requires a better qualitative understanding of the metastable phases of the model. It is clear that the overheated solid becomes unstable at some finite temperature. It is not clear, however, whether the overcooled liquid becomes unstable at some finite temperature (like water) or exists all the way down to $T=0$ as a metastable state. Despite its limited precision, the Gaussian (Hartree-Fock) variational calculation, is usually a very good guide to the qualitative features of the phase diagram. While such a calculation in the liquid was performed quite some time ago,[18] on the solid side a more complicated one sampling inhomogeneous states was performed recently.[9] The results are as follows. The solid state is the stable one below the melting temperature, becomes metastable at somewhat higher temperatures and is destabilized at $a_T\approx-5$. The liquid state becomes metastable below the melting temperature, however, in contrast to the solid, it does not loose metastability all the way down to $T=0$ and the excitation energy approaches zero.

Meanwhile, similar qualitative results have been obtained in a different field of physics. A variety of analytical and numerical methods[22] have indicated that liquid (gas) phase of the classical one-component Coulomb plasma also exists as a metastable state down to $T=0$ with energy gradually approaching that of the Madelung solid and the excitation energy diminishing. We speculate that the same phenomenon would appear to happen in any system of particles interacting via long-range repulsive forces. In fact the vortices in the London approximation resemble repelling particles with the force even more long range than the Coulomb. In light of this impetus to consider the above scenario in the vortex matter, we provide both theoretical and phenomenological evidence that the above picture is a valid one.

Assuming the absence of singularities on the liquid branch allows to develop a sufficiently precise theory of the LLL GL model in a vortex liquid (even including an overcooled one) using the Borel-Pade[23] (BP) method at any temperature. After clarifying several issues that prevented its use and acceptance previously we then combine it with the recently developed LLL theory of solids[21] to calculate the melting line and the magnetization and specific-heat jumps along it. Early on, Ruggeri and Thouless[18] tried unsuccessfully to calculate the specific heat by using BP because their series was too short. Subsequent attempts to calculate the melting point by using BP also ran into problems. Hikami, Fujita, and Larkin[24] attempted to find the melting point by comparing the BP (liquid) energy with the one-loop solid energy and, in doing so, obtained the melting temperature $a_T^m=-7$. However, their one-loop solid energy was incorrect and, in any case, the two-loop correction is necessary. As demonstrated in the following, the BP energy combined with the correct two-loop solid energy computed recently not only gives $a_T^m=-9.5$, but also allows to obtain a wide range of quantitative predictions within the model.

Now we present the solution of the LLL GL model. The liquid LLL (scaled) effective free energy [of the scaled model defined in Eq. (2)] is written as $f_{liq}=4\varepsilon^{1/2}[1+g(x)]$. The function g can be expanded as $g(x)=\Sigma c_n x^n$, where the high-temperature small parameter $x=\frac{1}{2}\varepsilon^{-3/2}$ is defined as a solution of the Gaussian gap equation, $\varepsilon^{3/2}-a_T\varepsilon^{1/2}-4=0$ for the excitation energy . The coefficients can be found in Refs. 24 and 25. We will denote $g_k(x)$ by the $[k,k-1]$ BP transform of $g(x)$ (other BP approximants clearly violate the correct low-temperature asymptotics). The BP transform is defined as $\int_0^\infty g_k'(xt)\exp(-t)dt$ where g_k' is the $[k,k-1]$ Pade transform of $\Sigma_{n=1}^{2k-1}(c_n x^n/n!)$. For $k=4$ the liquid energy already converges. We used in this work $k=5$ to achieve the required precision ($\sim 0.1\%$). The liquid energy completely agrees with the optimized Gaussian expansion results[9] above its radius of convergence at $a_T=-5$. In addition similar results we obtained in the 2D GL model agree with existing Monte Carlo simulations.[15] The solid effective energy to two-loops is:[21]

$$f_{sol}=-\frac{a_T^2}{2\beta_A}+2.848|a_T|^{1/2}+\frac{2.4}{a_T}. \tag{3}$$

Comparing the solid energy to that of the liquid (inset in Fig. 1), reveals that $a_T^m=-9.5$. This is in accord with experimental results. As an example, in Fig. 2 we present the fitting of the melting line of fully oxidized $YBa_2Cu_3O_7$ (Ref. 7) that gives $T_c=88.2$, $H_{c2}=175.9$, $Gi=7.0\ 10^{-5}$, $\kappa=50$. Melting lines of optimally doped untwinned[3] $YBa_2Cu_3O_{7-\delta}$ and $DyBa_2Cu_3O_7$ (Ref. 26) are also fitted extremely well. For example, for $YBa_2Cu_3O_{7-\delta}$ in (Ref. 3), the melting line fitting gives $T_c=93.07$, $H_{c2}=167.53$, $Gi\ =\ 1.9\ 10^{-4}$, $\kappa=48.5$ (see also Ref. 27).

The 3D Monte Carlo simulations[14] are not precise enough to provide an accurate melting point since the LLL scaling is violated. One gets different values of $a_T^m=-14.5$, -13.2,

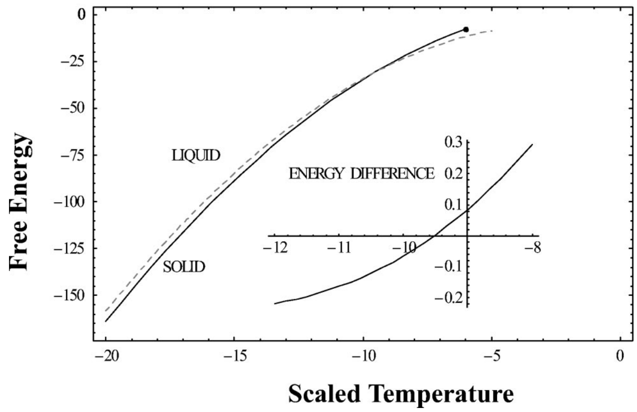

FIG. 1. Free energy of solid (line) and liquid (dashed line) as function of the scaled temperature. The solid line ends at a point (dot) indicating the loss of metastability. Inset shows a tiny difference between liquid and solid near the melting point.

-10.9 at magnetic fields 1, 2, 5 T, respectively. This violation is perhaps due to a small sample size (of order 100 vortices). The situation in 2D is better since the sample size is much larger. We performed similar calculation in the 2D LLL GL model and found that the melting point is $a_T^m = -13.2$. It is in good agreement with the MC simulations.[15] Phenomenologically the melting line can be located using Lindemann criterion or its more refined version using Debye-Waller factor.[28] The more refined criterion is required in the case of Y-Ba-Cu-O since vortices are not pointlike. Numerical investigation of the Yukawa gas[28] indicated that the Debye-Waller factor e^{-2W} (a ratio of the structure function at the second Bragg peak at melting to its value at $T=0$) is about 60%. We get using methods of Ref. 29 $e^{-2W}=0.59$ for $a_T^m=-9.5$.

The scaled magnetization is defined by $m(a_T) = -(d/da_T)f_{eff}(a_T)$. At the melting point $a_T^m=-9.5$ the

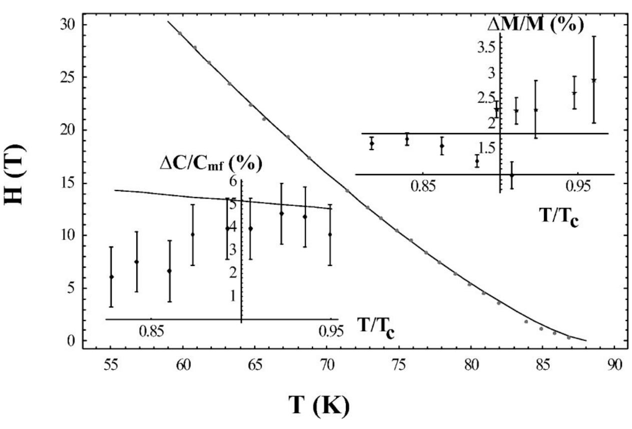

FIG. 2. Comparison of the experimental melting line for fully oxidized $YBa_2Cu_3O_7$ in Ref. 7 with our fitting. Inset on the right shows the relative universal magnetization jump of 1.8% (line) and experimental results for fully oxidized $YBa_2Cu_3O_7$ in Ref. 7 (rhombs) and optimally doped untwinned $YBa_2Cu_3O_{7-\delta}$ in Ref. 5 (stars). Inset on the left shows the relative nonuniversal specific-heat jump (line) and experimental results for optimally doped untwinned $YBa_2Cu_3O_{7-\delta}$ in Ref. 3.

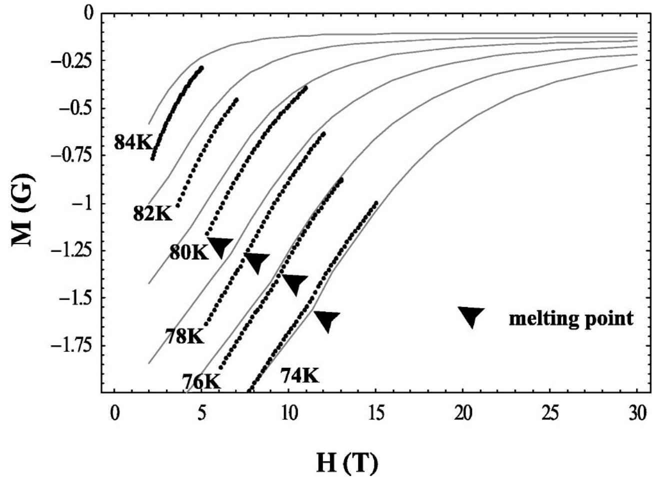

FIG. 3. Comparison of the theoretical magnetization curves (lines) of fully oxidized $YBa_2Cu_3O_7$ utilizing parameters obtained by fitting the melting line on Fig. 2 with torque magnetometry experimental results[7] (dots). Arrows indicate melting points while at low magnetic field the experimental data start from the point in which the magnetization is reversible indicating low disorder.

magnetization jump ratio defined by ΔM divided by the magnetization at the melting on the solid side is found to be equal to

$$\frac{\Delta M}{M_s} = \frac{\Delta m}{m_s} = 0.018. \tag{4}$$

This prediction is compared on Fig. 2 (the upper inset) with the experimental results on fully oxidized $YBa_2Cu_3O_7$ (Ref. 7, rhombs) and optimally doped $YBa_2Cu_3O_{7-\delta}$ (Ref. 5 stars).

These samples probably have the lowest amount of disorder that is not included in the calculations. From the model, we caculate the specific-heat jump ratio at the melting

$$\Delta c = 0.0075\left(\frac{2-2b+t}{t}\right)^2 - 0.20Gi^{1/3}(b-1-t)\left(\frac{b}{t^2}\right)^{2/3}. \tag{5}$$

It is compared on the lower inset on Fig. 2 with the experimental values of Ref. 3 (using the fitting parameters given above).

In addition to describing the melting, we present here an example of quantitative results that are obtained using the present approach—the magnetization curves. Our LLL magnetization curve coincides with the LLL Monte Carlo (MC) result of Ref. 14 (which is very accurate since the LLL scaling is obeyed) to the precision of MC. However in experiments away from the melting line higher Landau levels (HLL) are no longer negligible. Naively in vortex solid when the distance from the mean-field transition line is smaller than the inter-Landau-level gap, $1-t-b<2b$, one expects that the higher Landau modes can be neglected. More carefully examining the mean-field solution reveals that a weaker condition $1-t-b<12b$ should be used for a validity test of the LLL approximation[30] in vortex solids. In vortex liquid one has to go beyond the mean field to estimate the HLL contribution.[31] In 3D, Lawrie in Ref. 31, calculated the excitation energy in the framework of the Gaussian (Hartree-Fock) approximation. The excitation gap is 10 times smaller than inter Landau gap for fields in a wide range around melting line for fields larger than 0.1 T in Y-Ba-Cu-O. Therefore in the range of values of the interest in the present paper the LLL contribution should be dominant. Experimentally it is often claimed that one can establish the LLL scaling for fields above 3 T (see, for example, Ref. 32).

The theoretical expressions we use are the LLL contribution to the magnetization plus the corrections due to HLL calculated in Gaussian approximation. The results are compared on Fig. 3 with the experimental magnetization curves of Ref. 7. We use the parameters from the fitting of the melting curve (see Fig. 2) . The agreement is fair at higher fields, while at low magnetic fields the higher Landau-levels theory beyond Gaussian approximation is required. The LLL scaling has a limited validity away from melting line.

To summarize, the problem of the quantitative description of melting of the vortex lattice in the framework of the LLL Ginzburg-Landau approach is solved. The results for melting line, magnetization jump, and specific-heat jump are in good agreement with experiments and MC simulations. This is the first quantitative theory of the first-order melting of any kind to our knowledge. We believe that similar methods can be applied to other systems undergoing the first-order melting transition.

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