High-$T_c$ Superconductors in Applied Magnetic Fields Parallel to the CuO Planes: First Order Transition with Slow Onset of Resistivity

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The three dimensional uniformly frustrated XY model is used as a model of a high temperature superconductor in an applied magnetic field parallel to the CuO-planes. Through Monte Carlo simulations with anisotropy $\eta^2 = 10$ on large lattices we find evidence for a first order transition. Earlier simulations and theoretical treatments are discussed and the experimentally found smooth onset of resistivity is suggested to be due to a large potential barrier against vortex line motion above $T_c$ present for perfect alignment of the applied field.

The behavior of cuprate superconductors in applied magnetic fields has been, and continue to be, a very active area of research. The most studied geometry is with the applied field perpendicular to the CuO-planes. In that case, for clean samples, a first order transition associated with the melting of the Abrikosov lattice is by now well established both through calorimetric measurements \[1\] and measurements of the jump in the magnetic induction \[2\]. Also, a number of transport measurements are consistent with a first order transition.

The geometry with the applied field \textit{parallel} to the planes, has not been that thoroughly examined. It has, however, been found that the sharp increase in resistivity associated with the first order melting transition vanishes for perfect alignment of the field, and that the temperature-dependence of the resistivity is consistent with a continuous transition \[3\]. This remarkable finding naturally rises the question of the possibility of a continuous vortex line lattice melting, and the commonly accepted theoretical picture is that the system undergoes a continuous transition analogous to the nematic to smectic transformation in liquid crystals \[4\]. A more recent experiment \[5\] suggests that the transition from a vortex liquid to a vortex solid phase takes place in two steps, with an intermediate ‘possible smectic’ phase.

In the first Monte Carlo study of this model \[6\], the authors examined a model with anisotropy $\eta^2 = 100$ (see below), and argue that the behavior of both the helicity modulus and the specific heat suggest a continuous transition. However, a comparison between their Fig. 2 and corresponding data for a 2D XY model of the same size shows a remarkable similarity, suggesting that it is the individual layers that dominate the behavior of this three-dimensional system. This makes it difficult to draw any conclusions based on these results.

In this Letter we report on a study of a similar system, but with anisotropy $\eta^2 = 10$. The smaller value for the anisotropy is chosen with the hope to get a more clearly visible signal from the transition. The behavior of the system is clearly dependent on the system size. Only for very large systems does it become clear that the melting transition is first order instead of continuous. We also discuss problems with the suggested smectic phase and suggest a simple mechanism behind the apparently continuous onset of resistivity at the transition. The suggested scenario is directly open for experimental verification.

For the study of superconductors in applied magnetic fields we make use of the uniformly frustrated anisotropic 3D XY model, with the Hamiltonian

$$\mathcal{H} = -\sum_{i,\mu} J_{\mu} \cos(\theta_{i+\mu} - \theta_i - A_{i\mu}), \quad (1)$$

where the sums are over the lattice points $i$ and $\mu = \hat{x}, \hat{y}, \hat{z}$. To include a magnetic field in the $y$-direction we choose $A_{i\mu} = (2\pi/\phi_0) f_i^{\hat{y}+\mu} A \cdot d\mathbf{l}$ such that

$$\frac{1}{2\pi} \mathbf{D} \times A_{i\mu} = f^\hat{y},$$

where $\mathbf{D}$ is the discrete difference operator. We use equal couplings in the $x$-$y$ planes, $J_x = J_y = J_{xy}$, but a different coupling, $J_z$, between the planes. The anisotropy is given by the parameter

$$\eta = \sqrt{\frac{J_{xy}}{J_z}} = \frac{\lambda_z}{\lambda_{xy} \xi_{xy}}, \quad (2)$$

where the relation to the physical parameters, the penetration lengths $\lambda_{\mu}$ in the different directions, the interplane distance $d$ and the bare vortex core size in the planes $\xi_{xy}$, is given by the second equality. A derivation and justification of Eqs. (1) and (2) may be found in Ref. \[7\].

To examine the behavior of this system we have simulated Eq. (1) with periodic boundary conditions, $f = 1/24$, and several values for the anisotropy and system sizes. The results reported here are for $\eta^2 = 10$ and $L_x = 48$, and $L_y = 64, 96, 108, 192$, and 384. We measure several different quantities. The superconducting coherence in the different directions as examined through the helicity moduli $\Upsilon_x$, $\Upsilon_z$, and $\Upsilon_y \equiv \Upsilon_y \Upsilon_z$. To study the melting of the vortex lattice we measure the structure...
factor $S(k_1)$ where $k_1$ is a wave vector perpendicular to the field and monitor $\Delta S = |S(K) - S(R_z[K])|$ where $K$ is a reciprocal lattice vector of the ordered vortex lattice, and $R_z$ reflects $K$ through the $z$ axis, and we average over the three smallest non-zero values of $K$. Our Monte Carlo simulations consist, for the larger systems, typically of $10^5$ passes through the lattice for equilibration followed by $1 \times 10^6$ through $4 \times 10^6$ passes for calculating averages. The runs on the smaller systems were typically somewhat shorter.

For the geometry with the field perpendicular to the CuO layers it has been found that the vortex lattice melting transition is best examined by starting with a disordered system and slowly lowering the temperature until the system finds an ordered configuration with a vortex lattice [3]. However it turns out that the choice of $L_\parallel$ – the extension of the system in the field direction – is crucial in order to succeed with this cooling into an ordered state and obtain the correct transition behavior. With a too large value of $L_\parallel$ it becomes very difficult – or due to limited computer resources even impossible – to cool into a lattice. With a too small $L_\parallel$ the simulations incorrectly give at hand that there are two separate transitions with the vortex lattice melting taking place at the lower temperature followed by the vanishing of $\Upsilon_\parallel$ at a higher temperature. The proper choice of the length $L_\parallel$ depends on the parameters of the model, $f$ and $\eta$. In the first simulations with clear evidence of a first order transition, with $\eta^2 = 10$ and $f = 1/25$, this length was chosen as $L_\parallel = 40$ [4], but for isotropic systems, $\eta^2 = 1$ and $f = 1/20$, the evidence of a sharp transition was only found for $L_\parallel = 128$ [5] or $L_\parallel = 120$ [6].

Guided by the experience with fields perpendicular to the CuO planes we therefore first tried slowly cooling the system, but we never succeeded cooling into a lattice. We therefore instead started the simulations with an artificially prepared initial configuration with a perfect vortex lattice and slowly increased the temperature. In this way we obtained results similar to Fig. 1 of Ref. [7]. The vortex lattice melting as probed by $\Delta S(K)$ is shown together with $\Upsilon_\parallel$ in Fig. 2 for $L_\parallel = 48$, 96, 192, and 384.

FIG. 1. The melting of the ground state vortex lattice for $L_x = L_y = 48$ and several different values for $L_\parallel$. Shown is the structure factor together with $\Upsilon_\parallel$. Only for $L_\parallel \geq 192$ does it become clear that there is a single transition with simultaneous vanishing of both $\Delta S(K)$ and $\Upsilon_\parallel$.

This data shows that one needs at least $L_\parallel \approx 192$ for obtaining evidence that the vanishing of $\Upsilon_\parallel$ goes together with the melting of the vortex lattice. The similarity with data from Ref. [5] for the field perpendicular to the planes strongly suggests a first order transition also for this case with the field parallel to the planes.

From these simulations for $\eta^2 = 10$ we can of course not immediately draw any conclusions regarding the character of the transition for larger $\eta$. Still, we will argue below that both the simulation results presented in Ref. [5] and the experimentally found smooth onset of the resistivity are consistent with first order transitions. Since we also find problems with the continuous melting scenario, we suggest that the transition actually is first order for all finite values of the anisotropy.

Turning to the simulation results for $\eta^2 = 100$ [7], we first note that the choice $L_\parallel = 40$, or 80, in the light of Fig. 1 is not large enough for giving the correct behavior. But it also seems that their results are dominated by the behavior of the (weakly coupled) two-dimensional layers in the $x$-$y$ plane. To understand the relation to the 2D XY model we note that it is possible to choose a gauge with $A_{xy} = A_{iy} = 0$, and the frustration included in the $A_{iz}$. Considered in this way, the system consists of some stacked unfrustrated 2D XY planes with a weak inter-plane coupling that at some points between the planes is ferromagnetic ($A_{iz} = 0$), at some points is antiferromagnetic ($A_{iz} = \pi$), and otherwise is something in between.

Fig. 2 of Ref. [7] shows that the specific heat in the three dimensional model has a peak around $T = 1.05$. The maximum value of the plotted quantity is $24 \times C \approx 36$. The result was found to be about the same for all three different system sizes in the figure, of which the smallest was $48 \times 40 \times 48$. To compare with the specific heat for a single 2D layer, we have made simulations with $L = 44$ which is chosen to have close to the same area as $48 \times 40$. Recall that the peak of the specific heat in the 2D model is a non-singular feature well separated from the Kosterlitz-Thouless temperature $T_{KT} \approx 0.892$ [11].

Our results for $24 \times C$ for the 2D system are shown in Fig. 3. The similarity to the data of Hu and Tachiki (inset of their Fig. 2) is striking. Not only the shape of the curves is the same but also the position and the height of the maximum: at $T \approx 1.05$ we find the value $\approx 36.6$ which is the same as – or possibly slightly higher than – the data in their Fig. 2. We therefore conclude that the data for $\eta^2 = 100$ of Ref. [7] is dominated by 2D fluctuations. The absence of any sharp features in this data should therefore not be taken as evidence for a continuous transition in the 3D model.

Why is the interplane coupling not more important?
An obvious but rough way to assess the importance of the coupling between two planes is to compare the total coupling with the temperature. The size of the planes should then be large enough if \( L_x \times L_y \times J_z \gg T \), which for our present values becomes 19.2 \( \gg 1.05 \). This would lead to the conclusion that the planes are large enough to make the interplane coupling very significant. The reason why this approach fails is the presence of the frustrating vector potential \( A_z \) that varies between 0 and 2\( \pi \). This means that the interplane couplings tend to cancel each other out, and we believe this to be the reason for the very 2D-like behavior found in the model.

In the theory by Balents and Nelson [4] the transition takes place in two steps with an intermediate smectic phase. The smectic phase is characterized by order in the \( \hat{z} \) direction (only certain layers occupied) but disordered in the \( \hat{x} \) direction. This disorder may, however, give rise to forces (as indicated by the arrow) that tend to move the vortex lines from the occupied layers and destroy the smectic order.

So far we have both discussed the validity of the claim of a continuous transition from simulations and some problems with the theory of continuous melting. We now turn to the experimentally found smooth onset of the resistivity [3] suggestive of a continuous transition. We will argue that this observation not is inconsistent with a first order melting transition.

A current through the system perpendicular to the applied field gives rise to a force on the vortex lines perpendicular to both the current and the field. If the vortex lines move in response to this force the system dissipates energy, which is experimentally seen as a resistivity in the sample. In the geometry of Ref. [3] with the current in the CuO planes and the applied field also parallel to these planes, dissipation is related to the motion of the vortex lines in the \( \hat{z} \) direction.

An interesting observation is that the mechanism for motion of vortex lines in the \( \hat{z} \) direction becomes qualitatively different for perfect alignment of the field with the CuO layers as compared to a tilted magnetic field. This is illustrated in Fig. 3. Panel a) shows the situation in the presence of a tilted magnetic field where the upward motion of a vortex line is linked to the vortices moving to the left in the figure. Panel b) shows the qualitatively different situation for fields perfectly aligned with the CuO planes. In this case the motion of a vortex line has to

\[ \langle u_z^2 \rangle \gg \langle u_x^2 \rangle \]
start with a ‘kink’ that then grows bigger until the whole line has crossed the plane. The crucial thing to note is that such a kink gives rise to a vortex anti-vortex pair in the x-y plane, and that this vortex pair separates as the vortex line gradually moves upward across the plane.

The energy barrier to be overcome for motion of the vortex lines in Fig. 4a is the pinning of individual vortices. In contrast, the energy barrier in Fig. 4b is the kink energy barrier – related to the vortex anti-vortex interaction in the plane – which may be quite large just above $T_c$. If we assume that the transition implies a change of this potential barrier from infinite to quite large, the first order transition should not be clearly seen in the resistivity. In a 2D system this potential barrier diverges as $T \to T_{KT}$, and as we expect $T_c \to T_{KT}$ as the anisotropy increases, and that the behavior is 2D-like above $T_c$, we believe that this assumption of a large potential barrier right above $T_c$ is a reasonable one at least for fairly large anisotropies.

![Figure 4](image-url)

FIG. 4. Motion of vortices and vortex lines. These figures illustrate the motion of vortex lines for a) a tilted magnetic field and b) perfect alignment. For perfect alignment of the field there is a vortex anti-vortex pair in the CuO plane, and together with the motion of an increasingly larger portion of the vortex line to the upper layer goes a separation of the vortices in the CuO plane.

With this mechanism for the transition the very strong dependence of the resistivity on the angle of the applied field follows naturally. Perfect alignment of the field corresponds to two-dimensional XY layers with only thermal vortex pairs and no free vortices in the low-temperature phase. But even a small non-zero angle of the field gives some additional free vortices, and the presence of them would lead to a qualitatively different behavior.

The existence of a first order melting transition should be possible to verify from measurements of e.g. the specific heat. This would be a direct experimental test of our proposed picture, since in the alternative scenario with a continuous transition into a smectic phase there should be no sharp anomaly in the specific heat. However, so far the experiments are inconclusive. In Ref. [3] the authors found features in the specific heat both for field parallel and perpendicular to the planes. The work was later extended to several different values of the angle of the field, including a parallel field, and it was found that the sizes of these features scaled with the angle in accordance with a simple scaling relation [4]. This seems to point to the existence of a first order melting transition, but not conclusively. As the authors point out [3,4], the reason for the apparent first order character could also be that the angular resolution was not sufficient to access the true perfect alignment region $|\theta| < 0.5^\circ$ [2]. A carefully designed experiment should make it possible to discriminate between the two different proposed pictures.

To conclude, we have found a single first order transition in the anisotropic 3D XY model with magnetic field applied parallel to the planes. The finding that very large system sizes are needed for obtaining the true behavior make us doubt the continuous transitions reported from simulations on smaller systems. Some weaknesses with the commonly accepted theory of continuous vortex lattice melting have been discussed and we suggest that the reason for the smooth onset of resistivity is a large potential barrier right above $T_c$ associated with the separation of vortex anti-vortex pairs which is linked to the motion of the vortex lines in the $\hat{z}$ direction.

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