Decoupling and melting in a layered superconductor

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We report results for a 3D simulation of a layered superconductor. There are two significant temperatures. The first corresponds to melting of the vortex lattice in the $a$-$b$ plane ($T_{ab}$) and the second to decoupling of the layers ($T_{dc}$) with $T_{ab} \leq T_{dc}$. The decoupling is found to be a first order transition with an associated entropy of $\sim 0.25 - 0.4k_B$/pancake. The melting has no obvious thermodynamic signature, and could be a crossover. The width of the intermediate regime $T_{ab} < T < T_{dc}$, decreases with increasing anisotropy such that for the more anisotropic system we cannot distinguish the melting and decoupling temperatures.

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The phase diagram for high temperature superconductors is known to be complicated by the enhanced thermal fluctuations and the large anisotropy due to the layered structure of the crystals. Most measurements to date have been transport and thus indirect, making it difficult to ascertain the order of phase transitions and whether they are artifacts of the measuring current. However, Zeldov et al. have recently presented direct thermodynamic evidence of a first order transition in Bi-2212 using local magnetization techniques. Subsequently first order transitions have also been reported in the magnetization data of YBaCuO$_{7-\delta}$ by Liang et al. and Welp et al. and in the specific heat data of Schilling et al. The anisotropic nature of these materials is such that we could expect to lose the groundstate at different temperatures in the $a$-$b$ plane (corresponding to the Cu-O layers) and the $c$-axis along which the external magnetic field is applied. If we assume a vortex lattice at low temperatures (where it is common to think of a vortex in these layered systems as pancakes in the $a$-$b$ planes connected via Josephson vortices) then the transition corresponding to loss of order in the `a-$b$' plane is an `a-$b$ plane melting' transition. The loss of order only along the $c$-axis is a `decoupling' transition. The predicted field-temperature dependences are similar for these two transitions such that although the Zeldov et al. data fits the decoupling scenario marginally better it is not decisive. It is of course possible that the two transitions occur simultaneously.

In this letter we investigate the $a$-$b$ melting and decoupling transitions within a layered pancake model. We study the transition as a function of fixed magnetic field, $B$ (density of vortices), which is always perpendicular to the layers (along the $c$-axis), and vary the temperature. We can also alter the effective anisotropy of our system by changing the strength of the coupling between the layers. In order to be able to study the loss of the vortex lattice order we let the vortex position vary continuously. An underlying discrete lattice may lead to spurious phases. An essential difference from previous simulations is the manner in which we allow the correlation along the $c$-axis to vary with temperature by allowing the vortices to cross, or in ‘pancake’ language to interchange neighbours in adjacent planes, when it is energetically favorable. It is this decoupling of the layers which leads to an entropy jump of magnitude comparable to that seen experimentally. It is important to note that the simulation does not include free vortex loops in the $a$-$b$ plane. It has been suggested that these loops are a requirement for seeing the large entropy jumps that are measured experimentally.

We find that we can lose the correlation in the $a$-$b$ plane and along the $c$-axis at different temperatures, with the width of the intermediate regime determined by the anisotropy of the system. In the more anisotropic case melting and decoupling occur over a temperature range smaller than our resolution. However, in the less anisotropic case the $a$-$b$ order is lost at a lower temperature than the $c$-axis order. There is a large entropy jump which occurs concurrently with the loss of order in the $c$-direction, $0.2 - 0.4k_B$/pancake. There is no obvious thermodynamic signal associated with the loss of order in the $a$-$b$ direction, such that it may be a crossover. In terms of the pancakes this means that by raising the temperature the system changes from a 3D vortex-line lattice to a 3D line-liquid to a 2D pancake-liquid or gas, with the existence of the intermediate regime being dependent on the anisotropy.

To equilibrate our system we use Langevin dynamics and periodic boundary conditions in all directions with the temperature introduced via a noise term. We neglect the additional temperature dependencies of the penetration depth and other length scales. We focus purely on the vortex lattice aspect of the melting – that is only vortex loops representing fluctuations in the positions of the flux lines are included. We believe that our model includes the essential symmetry and topology of the vortex system. The Gaussian form of the potentials are chosen for numerical viability. Previous work in 2D has demonstrated that the qualitative behaviour is unchanged between the Gaussian and realistic poten-
The pancakes in the planes have an in-plane repulsive interaction between them, in our case modeled by a Gaussian potential \( U^{ll}_{vv'} = A_v \exp(-r^2/\xi^2_v) \), where \( r \) is the in-plane distance between the vortices, \( \xi \) is the in-plane vortex range, and \( A_v = 1 \) is the (fixed) strength of the vortex potential.

Across the layers the interaction is more complicated. In order to allow the pancakes to change neighbours freely throughout the simulation we cannot define unbreakable ‘strings’ of pancakes. The ‘strings’ effectively prohibit vortex cutting and re-connecting a mechanism which is thought to be important in the vicinity of the melting temperature; and is needed for the loss of long range phase coherence as seen in the pseudo-transformer experiments [14]. It has been shown by Clem [12] that in order to model the electromagnetic interactions across the layers only pair-wise potentials are needed. However, Bulaevskii et al. [13] have shown that including the lowest order terms of the Josephson coupling makes three and four-body terms equally necessary. Hence we include both an attractive two body potential \( U^{ll}_{vv'}(r_{ij}, r_{i'j'}) = -A_t \exp(-r_{ij}^2/r^2_{ij}/r_{i'j'}^2/\xi^2_v) \) (all \( r \) are in-plane) and a repulsive 3-body potential which stabilizes the triangular lattice phase.

\[
U^{ll}_{vv'v''}(i, j, j') = A_{3b} e^{-\left((r_{ij}^2 - r_{ij'}^2) + (r_{i'j'}^2 - r_{i'j''}^2) + (r_{i''j''}^2 - r_{i''j''}^2)\right)/\xi^2_{3b}}. \tag{1}
\]

\( A_{3b} \) and \( \xi_{3b} \) are the amplitude and range of the three body potential. It acts by excluding three or more pancakes (two in one layer and a third in an adjacent layer) from finding their equilibrium location to be within a coherence length in the \( x-y \) plane.

We change the anisotropy of the system by varying the interlayer coupling parameter \( A_t \); thus we have used three sets of parameters in our simulations, \( A_t = 0.05 \), \( A_t = 0.2 \) and \( A_t = 0.5 \). The other parameters are: \( A_v = 1 \) and \( A_{3b} = A_t \), for the amplitudes of the potentials and \( \xi_v = 0.6 \), \( \xi_t = 0.3 \), \( \xi_{3b} = \sqrt{2}\xi_t \) for the ranges in the Gaussians.

In order to detect phase changes we measure a number of physical properties of the system. The most pronounced feature is seen in the specific heat/pancake which has a peak centred on \( T_{dc} \). The origin of the peak is identified to be a first order transition by applying the Lee-Kosterlitz energy binning technique [14].

The shear modulus, \( c_{66} \) has recently been measured experimentally [15] and can also be estimated numerically. It should vanish when the system becomes liquid in the \( a-b \) planes. It is measured by applying a shear wave across the system and then holding the system pinned in two channels whilst allowing the rest if the system to relax [15]. We obtain \( c_{66} \) via,

\[
\Delta U = \frac{1}{2} c_{66} \int \int (\frac{\partial u}{\partial x})^2. \tag{2}
\]

There are fluctuations in the data due to the finite temperature but the drop to zero of \( c_{66} \) is well defined.

Using the same technique we also measure the Josephson contribution to the tilt modulus, \( c_{44} \) which corresponds to shearing across the layers. Within our model there is no contribution of the magnetic field energy so that \( c_{44} \) should be finite for a line liquid but will be zero for a 2d pancake liquid.

That the system is becoming thermally excited is readily seen by the onset of self-diffusion. The time dependence of the displacements \( r^2(t) \) of the pancakes indicates the nature of the diffusion. Independent pancakes or rigid rods of pancake stacks behave as \( r^2 \propto t \). Whereas diffusion of flexible unbreakable lines follow \( r^2 \propto t^{1/2} \).

In the clean system that we are studying an indicator of the in-plane melting is given by monitoring via a Voronoi construction the coordination number of the vortices which is six for the triangular lattice ground-state. We find that the appearance of vortices with coordination number other than six and the onset of diffusion match to the accuracy that we have sampled the temperature. Finally the structure factor is used to confirm the nature of the vortex phases present in the simulation.

We shall first consider the results for the larger interlayer coupling \( A_t = 0.5 \). We started from the groundstate Abrikosov lattice at \( T=0 \) with a system size chosen such that it would be commensurate with the lattice. We then slowly heated the system up and observed the physical quantities detailed above. We ran for system sizes with either 8x8 or 12x12 vortices in the \( a-b \) plane and up to 64 layers. At approximately \( T_{ab} \approx 0.084 \) we found that the diffusion coefficient ‘D’ abruptly became non-zero, see Fig. 6. We then continued to heat the system and studied the exponent \( \alpha \) of the diffusion \( R^2 \sim t^{\alpha} \). For all systems it was clear that the exponent was initially in the range \( 1/2 < \alpha < 1 \). For the system size 12x12x16 we found that \( \alpha \) linearly interpolates between \( \alpha = 1/2 \) at \( T = T_{ab} \) and \( \alpha = 1 \) at a higher temperature \( T_{dc} \). See Fig. 6. That is from the diffusion alone we have evidence of a liquid phase in which there are lines present although their coherence decreases (susceptibility to breaking increases) with temperature up to \( T_{dc} \), at which point the entire system becomes a 2D pancake liquid.

Using a Voronoi construction we measure the onset of miscordination of the vortices. We find that the appearance of vortices with other than six-fold symmetry coincides with the onset of diffusion, \( T_{ab} \) and the temperature at which this saturates coincides with that at which the diffusion exponent \( \alpha \) becomes equal to one, \( T_{dc} \) see Fig. 6. The melting in the \( a-b \) plane could be a KTHNY transition [13]. This requires a phase in which paired 5 and 7 fold coordinated vortices are present. However, the 5 and 7 fold vortices occur abruptly at \( T_{ab} \), and there is no sign of pairing at any temperature.

The specific heat has a peak centered around \( T_{dc} \), whose height increases with increasing system size, see Fig. 2. In order to calculate the entropy from the Lee-Kosterlitz
procedure it is necessary to have a sufficiently large system such that $L << \xi$, this occurs for a system size $8x8x32$. The resulting entropy is $\sim 0.25 k_B$/pancake.

In agreement with the above scenario the shear modulus, $c_{66}$, which measures the rigidity in the $a$-$b$ plane falls to zero in the vicinity of the lower temperature $T_{ab}$ and the tilt modulus, $c_{44}$, falls to zero around the temperature $T_{dc}$. It is expected that $c_{44}$ should be non-zero in a vortex line liquid. These results hold true for all system sizes $L \gg \xi$. This is in agreement with losing the $a$-$b$ plane order at $T_{ab}$ but still retaining some $c$-axis correlation up to $T_{dc}$.

We can also see that the $c$-axis coherence persists to the higher temperatures $T_{dc}$ by measuring the relative diffusion of the pancakes with respect to their neighbours in adjacent layers, the diffusive width. We find that the width of the pancake stacks becomes larger than $a_0/\sqrt{2}$ above $T_{dc}$ corresponding to disintegration of the stacks, see Fig. 3.

This scenario of a 3D vortex lattice melting to a 3D line liquid and then subsequently to a 2D pancake liquid is borne out by the structure factor, see Fig. 4. At temperatures below $T_{ab}$ we find rings of well defined spots in $k$-space consistent with a real space triangular lattice. For temperatures in the range $T_{ab} < T < T_{dc}$ we see a ring of intensity consistent with a liquid structure. The average height of the amplitude of the ring is a measure of the correlations along the $c$-axis. Finally, as the temperature becomes larger then $T_{dc}$ the amplitude of the ring decreases rapidly signaling that the stacks of pancakes evaporate and therefore the correlations along the $c$-axis are lost.

In order to see how the transitions changed when we increased the anisotropy (made the system more Bi-2212 like) the study was repeated with $A_f = 0.2$. The temperature scale at which the system started to break up was a little lower, around $T \simeq 0.062$. In this case the temperatures for melting and decoupling cannot be differentiated. Hence, there is no apparent intermediate regime where the diffusion is line-liquid like, the coordination reaches saturation over a very small temperature range and $c_{66}$ and $c_{44}$ seem to die off at approximately the same temperature. The peak in the specific heat is very sharp - with the small fluctuations in the temperature leading to large error bars on the peak height, hence direct evaluation of the entropy is inaccurate. However, the Lee-Kosterlitz energy plots yield an entropy of $\sim 0.4 k_B$/pancake for all system sizes greater than $8x8x8$. If this is the regime into which Bi-2212 falls it would appear that the system sublimates to a pancake gas $[13]$.

In this layered 3D simulation we include vortex crossing and allow the pancakes to move continuously in the $a$-$b$ plane. We find two significant temperatures for the loss of 3D lattice order. $T_{ab}$, at which the system melts in the $a$-$b$ plane and a second temperature $T_{dc}$, where the layers decouple. For the more anisotropic case the two temperatures coincide and we observe a first order transition with an entropy jump of the same order of magnitude as seen experimentally away from $T_c$. By making the system less anisotropic the two temperatures separated, with the entropy and first order nature remaining associated with the decoupling transition. It is important to note that these results have been obtained in the absence of $ab$-plane vortex loops, which have hitherto been claimed to be essential in producing the entropy jumps seen experimentally. We believe that our pancake model represents faithfully the physics of the vortex array degrees of freedom $[20]$.

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FIG. 1. The diffusion exponent $\alpha$ after the onset of diffusion and the fraction of five fold co-ordinated pancakes as a function of temperature. The inset show the onset of diffusion for the two different anisotropies studied. The more isotropic system starts to diffuse at a higher temperature.

FIG. 2. Specific heat peaks (per pancake) for different system sizes with interlayer coupling $A_l = 0.2$. The figure shows the specific heat for two system sizes. For the 8x8x32 the width of the peak has become narrower than our temperature resolution and the height of the peak has a large error bar, $\pm 20$ associated with it. The insert shows the Lee-Kosterlitz binning for $T=0.063$ for the 8x8x16 system. From this we estimate the entropy associated with the transition.

FIG. 3. Disappearance of the correlation along the c-axis as we increase the temperature for $A_l = 0.5$, $12 \times 12 \times 16$.

FIG. 4. The structure factor for the 8x8x8 $A_l = 0.5$ system. The top figure is for $T < T_{ab}$, the middle for $T_{ab} < T < T_{dc}$ and the bottom for $T > T_{dc}$. Figure available at http://th.ph.bham.ac.uk/nkw/res/sup1.ps
Temperature

Diffusion Exponent $\alpha$

$T_{ab}$

$T_{dc}$

5-fold co-ordinated pancakes

$2(t=15s)$

$A_l=0.2$

$A_l=0.5$

Temperature

$R^2(=15t)$

0.04 0.06 0.08 0.1

0.05 0.1 0.15 0.2

0.25 0.3
Diffusive width $R^2(t)$

Temperature

Diffusive width $R^2(t)$