Freezing transition of the vortex liquid in anisotropic superconductors

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We study the solid-liquid transition of a model of pancake vortices in laminar superconductors using a density functional theory of freezing. The physical properties of the system along the melting line are discussed in detail. We show that there is a very good agreement with experimental data in the shape and position of the first order transition in the phase diagram and in the magnitude and temperature dependence of the magnetic induction jump at the transition. We analyze the validity of the Lindemann melting criterion and the Hansen-Verlet freezing criterion. Both criteria are shown to be good to predict the phase diagram in the region where a first order phase transition is experimentally observed.

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I. INTRODUCTION

The thermodynamics and dynamical properties of vortex matter in high temperature superconductors have received the interest of a large experimental and theoretical community. One of the most salient findings, already predicted in 1985, is the first order melting transition of the vortex lattice. Large thermal fluctuation in a high $T_c$ material induce the melting transition first observed in transport measurements and confirmed by a number of equilibrium properties like direct measurements of the magnetization jump and latent heat.

It is now well accepted that in clean Bi$_2$Sr$_2$CaCu$_2$O$_8$ (BSSCO) and untwined YBa$_2$Cu$_3$O$_{7}$ (YBCO) samples the melting of the vortex lattice for an external magnetic field parallel to the $c$-axis of the samples is first order and that the superconducting coherence is lost simultaneously in all directions at the melting temperature. Despite of the great amount of work devoted to the subject, the nature of the melting transition of the vortex lattice is still controversial.

The first theories for melting of the vortex lattice were based on the Lindemann criterion and describe a situation in which the vortex lattice melts into a liquid of entangled vortex lines. However the behavior of the entropy change at the melting transition suggest that at the first order transition a simultaneous loss of the triangular crystal structure and a decoupling of the planes take place. In this last scenario, the liquid would be a liquid of pancake vortices. Many authors have analyzed the experimental results obtaining good fittings with this picture. The precise nature of the transition and the structure of the liquid phase at the melting line is still an open problem.

More recently, some striking regularities -weak universalities- observed in the transport properties at the melting temperature were interpreted in terms of the Hansen-Verlet freezing criterion. This criterion, that has been proved to work very well in the case of classical liquids, states that the liquid freezes when the first peak of the structure factor $S(k)$ reaches a critical value. However, for the case of vortex matter, the validity of this criterion has not been analyzed.

In this context it is interesting to revisit the density functional theory for vortices in the highly anisotropic high $T_c$ superconductors. This theory describes interacting pancake vortices in layered superconductors. The interactions are of electromagnetic nature, Josephson interactions involving charge transfer are neglected, and consequently it is a good starting point to describe highly anisotropic systems. However, as we discuss below, it may be also appropriate to describe even the less anisotropic high $T_c$ cuprates. The theory allows to calculate the melting temperature, thermodynamic properties at the melting line as well as the validity of the phenomenological criteria for melting and freezing.

In what follows we present the model for the inter-vortex interaction and the method for the calculus of the melting line. We present the results for the phase diagram and compare them with experimental data. We analyze the validity of the Lindemann and Hansen and Verlet criteria for melting and freezing.

II. DESCRIPTION OF THE MODEL

Our starting point is the functional density theory for pancake vortices in a layered superconductor in a magnetic field perpendicular to the layers. In a layered system in the limit of infinite effective mass perpendicular to the layers (zero Josephson coupling) the pancake vortices can be treated as point-like classical particles restricted to move in the planes. The vortex-vortex interaction is given by a three-dimensional (3D) anisotropic pair potential which in Fourier space is given by:

$$\beta V(k) = \frac{\Gamma \lambda^2 (k_z^2 + (4/d^2) \sin^2(k_z d/2))}{k_z^2 [1 + \lambda^2 k_z^2 + 4 (\lambda^2/d^2) \sin^2(k_z d/2)]}$$ (1)
here, $k = (k_x, k_y)$ is the wave vector, $\lambda$ is the planar London penetration depth and $\Gamma = \beta d \Phi_0^2/4\pi^2$ is a dimensionless strength parameter where $\Phi_0$ is the flux quantum, $d$ is the distance between planes and $\beta = (k_BT)^{-1}$ is the inverse temperature.

Following the pioneering work of Ramakrishnan and Yussouff (RY) and the extensions made to describe the vortex matter [2, 3], the functional describing the free energy difference between the solid and liquid phases is given by:

$$\frac{\Delta \Omega}{k_B T} = \sum_n \int d^2 r \left\{ \rho_n(r_\perp) \left[ \frac{\ln \left( \rho_n(r_\perp) / \rho_T \right)}{\rho_T} - 1 \right] + \rho_T \right\}$$

$$- \frac{1}{2} \sum_{n,n'} \int d^2 r_\perp d^2 r'_\perp c_{\ell n-n'}(j' | j - r_\perp |) \times$$

$$\left[ \rho_n(r_\perp) - \rho_T \right] [\rho_{n'}(r'_\perp) - \rho_T].$$

(2)

here, $r \equiv (r_\perp, n d)$ where $r_\perp$ is the in-plane coordinate and $n$ is an integer (the plane index). The quantity $\rho_n(r_\perp) = \sum_i \delta(r_\perp - r_{i,\perp}^n)$ is the vortex density with $r_{i,\perp}^n$ the 2D coordinate of the $i$-th particle at plane $n$. $\rho_T$ is the mean areal density of the liquid and $c_{\ell n-n'}(j' | j - r_\perp |)$ is the direct correlation function in the liquid phase. The first integral in the right hand side of Eq. (2) describes the non-interacting contribution to the free energy, the second integral incorporates the effect of the interactions up to second order in the difference $(\rho_n(r_\perp) - \rho_T)$. To evaluate this energy difference it is necessary to calculate the direct correlation function of the liquid defined below.

The pair distribution function is defined as:

$$g(r, r') = \frac{\rho_{n,n'}(r_\perp, r'_\perp)}{\rho_n(r_\perp) \rho_{n'}(r'_\perp)}.$$

(3)

where:

$$\rho_{n,n'}(r_\perp, r'_\perp) = \langle \sum_i \delta(r_\perp - r_{i,\perp}^n) \delta(r'_\perp - r'_{i,\perp}^{n'}) \rangle.$$

(4)

Here $\rho_{n,n'}(r_\perp, r'_\perp)$ is the probability density of finding two particles at $r = (r_\perp, n d)$ and $r' = (r'_\perp, n' d)$ respectively. Due to the symmetry of the liquid $g(r, r') = g(n-n')(r_\perp - r'_\perp)$.

The direct correlation function $c_n(r_\perp)$ is defined by means of Ornstein-Zernike equation [2, 3]

$$h_n(r_\perp) = c_n(r_\perp) + \rho_T \sum_{n'} \int d^2 r'_\perp c_{\ell n-n'}(j' | j - r'_\perp |) h_{n'}(r'_\perp).$$

(5)

where $h_n(r_\perp) = g_n(r_\perp) - 1$ is the pair correlation function.

This integral equation for the direct correlation function $c_n(r_\perp)$ can be solved in the hiperated chain approximation, and inserting the solution in Eq. (2), the free energy difference between the solid and liquid phase is given only as a functional of the density $\rho_n(r_\perp)$. At this point, we can expand the density in a set of trial reciprocal-lattice vectors:

$$\rho_n(r_\perp) / \rho_T = 1 + \eta + \sum_{G \neq 0} \rho_G e^{iG \cdot r}$$

(6)

The quantities $\eta$ and $\rho_G$ may be viewed as dimensionless order parameters, $\eta$ is the fractional density difference between the liquid and the solid phases and the $\rho_G$ are the Fourier components of the density in the solid phase. Minimizing the free energy (6) with respect to these parameters, we obtain the following equation:

$$1 + \eta + \sum_{G \neq 0} \rho_G e^{iG \cdot r} = \exp(\rho_T \epsilon_0 \eta + \rho_T \sum_{G \neq 0} \rho_G \epsilon_G e^{iG \cdot r})$$

(7)

where $\epsilon_G$ is the Fourier transform of the direct correlation function and $\epsilon_0 \equiv \epsilon_G = 0$.

Due to the small compressibility of the system the fractional density change is small ($\eta \ll 1$), and as a first approximation can be neglected in the first term of (6). Note that the product $\epsilon_0 \eta$ is not necessarily small and the first term in the exponential of the right hand side of (6) has to be retained. Transforming Fourier Eq. (6) we obtain after some algebra a set of coupled equations for the $\rho_G$:

$$\rho_G = \frac{\sum_n \int_{A_\perp} d^2 r_\perp e^{-iG \cdot r} \rho_T \sum_{G \neq 0} \rho_G \epsilon_G e^{iG \cdot r}}{\sum_n \int_{A_\perp} d^2 r_\perp \exp(\rho_T \sum_{G \neq 0} \rho_G \epsilon_G e^{iG \cdot r})}.$$

(8)

Here $A_\perp$ is the area of the in-plane unit cell. Given the Fourier components $\epsilon_G$ of the direct correlation function, these equations can be solved for $\{\rho_G\}$. Before presenting the numerical results, the following points deserve a comment:

i) A uniform liquid is always a solution of $\{\rho_G = 0\}$. As the $\epsilon_G$ increase, non-uniform solutions may suddenly appear (with $\epsilon_G \sim 0.5$) and correspond to the solid phase with a spatially periodic density.

ii) At the transition the free energy difference $\Delta \Omega$ defined in (2) is equal to zero. To calculate the transition line in the $B-T$ phase diagram, we have to calculate the direct correlation function as a function of the magnetic induction and temperature and use it as an input in the RY density functional theory. The transition is obtained when a set of order parameters $\{\rho_G \neq 0\}$ given by (8) satisfy the condition $\Delta \Omega = 0$.

iii) As discussed in previous works, the numerical calculation can be simplified by noting that in the liquid phase, the Fourier transform $\epsilon_G$ of the direct correlation function rapidly decay with increasing $|G|$, it is then a good approximation to truncate the series $\sum_{G \neq 0} \rho_G \epsilon_G e^{iG \cdot r}$ in (8) and take only a few terms with $\epsilon_G \neq 0$. The number of terms retained defines the number of self consistent order parameters $\{\rho_G\}$ included in the theory. In what follows we consider only two order
parameters corresponding to the first two peaks of the in-plane direct correlation function as first suggested by Ramakrishnan \cite{11} for a 2D system.

\textit{iv) With the resulting set of order parameters that characterize the solid phase at the melting point in the limit }\eta < 1\text{, the fractional density change can be estimated. However in the RY approximation used here the results for }\eta \text{ are not accurate, in particular it is easy to show that }\eta > 0\text{ in contradiction to what is expected for the case of vortices. Rather than improving the estimate of }\eta \text{ by including higher order terms in the functional }\Delta \Omega \text{ of Eq. (2)-which are given by not available three particle correlation functions- we estimate the entropy change at the transition and calculate }\eta \text{ by means of the Clausius-Clapeyron relation. The higher order corrections to }\Delta \Omega \text{ are not strongly coupled to the order parameters }\{\rho_0\}\text{ and the present approximation is known to give accurate results when the crystal structure of the solid phase is given.}

\section{III. CORRELATION FUNCTIONS}

In this section we present results for the pair correlations in the liquid phase, we use the hiperminated chain approximation (HNC) which is well described in the literature. For the sake of completeness we only give here the basic formulas of classical liquids theory relevant for our case.

The pair correlation function can be written in the form:

\begin{equation}
 g_n(r_\perp) = e^{[g_n(r_\perp)-1-\beta n_n(r_\perp)-\eta_\perp(r_\perp)+B_n(r_\perp)]},
\end{equation}

where \(B_n(r_\perp)\) is known as the bridge function and its closed expression is not known for an arbitrary potential. In the HNC approximation we have \(B_n(r_\perp) = 0\) which is an excellent approximation for long ranged soft potentials as the one we are dealing with. In the HNC approximation Eq. (8) can be rewritten in the following form:

\begin{equation}
 c_n(r_\perp) = e^{-\beta V_n(r_\perp)+Y_n(r_\perp)-1-Y_n(r_\perp)},
\end{equation}

where \(Y_n(r_\perp) = h_n(r_\perp)-c_n(r_\perp)\). This equation together with the Ornstein Zernike relation (Eq. (3)) are the basic equations that allows to evaluate the pair correlation functions. The asymptotic behavior of the direct correlation function as \(r_\perp \to \infty\) and \(n \to \infty\) is known to be \(c_n(r_\perp) = -V_n(r_\perp)/k_B T\). For the numerical calculation it is then convenient to divide the correlation functions in short and long ranged contributions according to:

\begin{equation}
 c_n(r_\perp) = c_{nS}(r_\perp) + c_{nL}(r_\perp),
\end{equation}

with

\begin{equation}
 c_{nL}(r_\perp) = -\beta V_n(r_\perp)
\end{equation}

and

\begin{equation}
 Y_n(r_\perp) = Y_{nS}(r_\perp) + Y_{nL}(r_\perp),
\end{equation}

with

\begin{equation}
 Y_{nL}(r_\perp) = +\beta V_n(r_\perp).
\end{equation}

Due to the highly anisotropic nature of the pair potential, as a first approximation we take the short ranged contribution different from zero only for the in-plane correlations:

\begin{equation}
 c_{nS}(r_\perp) = \delta_{n,0} c_{0S}(r_\perp)
\end{equation}

and the problem reduces to calculate a single function \(c_{0S}(r_\perp)\) given by the following set of integral equations:

\begin{equation}
 c_{0S}(r_\perp) = \exp(Y_{0S}(r_\perp)) - 1 - Y_{0S}(r_\perp),
\end{equation}

\begin{equation}
 Y_{0S}(k_\perp) = \frac{d}{2\pi} \int_{-\pi}^{\pi} dk_\parallel e^{ik_\parallel a} \frac{c_{0S}(k_\parallel) - \beta V(k_\parallel)}{1 - \rho(k) c_{0S}(k_\parallel) - \beta V(k_\parallel)},
\end{equation}

the last equation is the Fourier transformed Ornstein-Zernike equation. This expression can be further simplified by an analytic integration due to the particular form of the pair potential.

Finally the out of plane short ranged correlation functions in a second order approximation are given by the following equation:

\begin{equation}
 Y_{nS}(k_\perp) = \frac{d}{2\pi} \int_{-\pi}^{\pi} dk_\parallel e^{-ik_\parallel a} \frac{c_{0S}(k_\parallel) - \beta V(k_\parallel)}{1 - \rho(k) c_{0S}(k_\parallel) - \beta V(k_\parallel)}.
\end{equation}

In Fig. 3 we present results for the pair distribution function where the lengths are in units of the characteristic distance \(a\) given by \(\pi a^2 \rho_0 = 1\). The first peak of the in plane pair distribution function occurs at a finite value of the \(r_\perp\) which is given by the mean inter-particle distance (\(\sim 2a\)). For the out of plane distribution function the maximum occurs at \(r_\perp = 0\) which shows the tendency of pancake vortices to form stacks. In Fig. 2 the behavior of \(h(r_\perp = 0, n \neq 0)\) is presented and shows an exponential decay as a function of \(n\). This behavior allows as to define a correlation length \(\Lambda\) through the following relation: \(h(r_\perp = 0, n) \propto \exp(-dn/\Lambda)\). In Fig. 3 we present the behavior of \(\Lambda\) as a function of the magnetic induction \(B\), that can be fitted with \(\Lambda \propto 1/\sqrt{B}\). Other authors had an excellent fit of their data in a smaller range of fields with a function of the form \(\Lambda = A_1 + A_2/B\).

It is important to note that the characteristic length \(\Lambda\) describes the long distance behavior of the correlation functions. The short distance behavior is given by \(h(r_\perp = 0, n)\) with small \(n\) which in general decays very fast. As can be seen in Fig. 3 \(h(r_\perp = 0, n = 1)\) is very
small ($\sim 10^{-2}$), and although its value depends on field and temperature, in the liquid phase, it always remains much smaller than 1.

As the temperature decreases the system develops stronger correlations. This is clearly observed in the structure factor, defined by:

$$S(k_\perp, k_z) = 1 + \rho \sum_n \int d^2r_\perp h_n(r_\perp) e^{i(k_\perp \cdot r_\perp + k_z nd)}.$$  

(19)

In Fig. 4 the structure factor is shown for two different temperatures, the lower the temperature, the higher the first peak in $S(k)$.

In the next section we use these results to calculate the melting line.

IV. PHASE DIAGRAM

We used the correlation functions calculated above as an input to the RY density-functional theory of freezing. In Fig. 4 we show the results obtained for the phase diagram with parameters corresponding to BSCCO but without temperature dependence: $\lambda(T) = \lambda(0) = 1500 \text{Å}, d = 15\text{Å}$ and $T_c = 90K$. To understand these results we resort to a simple model obtained by mapping the vortex system onto a 2-D boson system. In this model, the free energy of a system of vortices is given by:

$$F(r(z)) = \int_0^L dz \left\{ \sum_i \frac{1}{2} g \left( \frac{dr_i(z)}{dz} \right)^2 + \sum_{i<j} V(r_{ij}(z)) \right\},$$

(20)

where $r_i(z)$ determines the position and shape of the i-th vortex, $g$ is the elastic energy and the last term describes the interaction between vortices, which is taken to be logarithmic, $r_{ij}(z)$ is the distance between vortices. In a solid phase, of lattice constant $a_0$, we can use an harmonic approximation for the pair interaction potential. Assuming a characteristic length $l$ which defines the correlation along the field direction, the free energy after a thermodynamic average can be approximated by:

$$F' = F/N \simeq \frac{<r^2>}{2} \left\{ \frac{g}{l} + kl \right\},$$

(21)

where $F'$ is the mean free energy per characteristic vortex segment of length $l$, $N$ is the number of independent segments in the sample, $<r^2>$ is the mean square displacement of the vortices and $k \propto e_0/a_0^2$ is the curvature of the logarithmic pair potential at the mean interparticle distance. Using the Lindemann melting criterion $<r^2> = a_L^2 a_0^2$, with $a_L \sim 0.1 - 0.3$ along the transition line and the equipartition theorem that states that $F' \sim k_BT$, the expression above reduces to:

$$k_BT_m = \frac{u_L^2 a_0^4}{2} \left( \frac{g}{l} + kl \right).$$

If the characteristic length $l$ is taken as the distance between planes which should be a good approximation at least in the high field regime we obtain:

$$k_BT_m \simeq \frac{u_L^2 e_0 d}{2} \left( 1 + \frac{g\Phi_0}{\Phi_0 B_m} \right).$$

(22)

If the inter-plane correlations were relevant at the melting point, the characteristic length $l$ should be obtained minimizing the free energy (21). In this case the melting line is given by:

$$k_BT_m = u_L^2 \sqrt{e_0} \left( \frac{\Phi_0}{B_m} \right)^{\frac{1}{2}}.$$  

(23)

The density functional data for the melting line were fitted with the following expression $T_m = T_{m2D} + A_1/B_m$ according to (22). This type of behavior is expected for a highly anisotropic system at high fields, when the liquid state at the melting temperature presents very short correlations along the $c$ axis. Although the fit is less accurate for small fields we never obtain a behavior of the type given by (23). This suggests that in our field and temperature range, the system simultaneously melts and the planes decouple to form a liquid of pancake vortices. The less accurate fit for the low field data could indicate that we are entering a cross-over to a line melting regime. In the limit of high fields the melting temperature goes asymptotically to the 2D melting temperature $T_{m2D}$. This is due to the fact that at high fields the inter-plane correlations become irrelevant and the system behaves as a collection of independent planes. The 2D melting temperature, obtained with a functional density theory in the RY approximation, is lower than expected from a Kosterlitz-Thouless dislocation unbinding theory. This is presumably due to the fact that the HNC approximation underestimates the correlations in the 2D case as was discussed by other authors.

In order to compare our results with the experimental data, we included the temperature dependence of the penetration length[20]: $\lambda(T) = \lambda(0)/[1 - (T/T_c)^4]^{1/2}$. In Fig. 5 we present our results with $\lambda(0) = 1500\text{Å}$ together with the experimental results of Zeldov et al. In the experimental data the first order transition ends at a critical point presumably due to point-like pinning centers, an effect not included in this functional density theory. In order to make this comparison, $\lambda(0)$ was used as a fitting parameter. A more realistic value of $\lambda(0)$ for BSCCO is $\sim 2000\text{Å}$. If the $\lambda(0)$ is increased, the melting line moves to lower fields due to the decrease of the intensity of the pancake-pancake interactions, this could be compensated by the inclusion of a small Josephson coupling between planes in a more realistic treatment.
V. ENTROPY AND MAGNETIC INDUCTION JUMP AT $T_M$

The entropy jump can be calculated as the temperature derivative of the free energy difference:

$$\Delta S = -\left( \frac{\partial \Delta \Omega}{\partial T} \right)_{V,H}$$

Using Ecs. 1 and 2 the free energy difference of Ec. 2 can be written as:

$$\frac{\Delta \Omega}{k_B T} = -\ln \left[ \int_{v_c}^{v_s} d^3 r \exp \left( \sum_G \rho_G c_G e^{iG \cdot r} \right) \right]$$

$$+ \frac{1}{2} \sum_G c_G \rho_G^2,$$

To evaluate the entropy jump we must calculate the temperature derivatives of the Fourier transforms of the liquid direct correlation functions $c_G$ at constant $H$ and $V$, that are not known. Following reference 4 this temperature derivatives can be estimated on the solid phase using the fluctuation-dissipation theorem in the classical limit. This procedure gives for the structure factor $S(G)$ a linear dependance on temperature. Using this result we obtain the following expression for the entropy jump:

$$\Delta s/k_B = 3[\rho_1^2(1 - c_1) + \rho_2^2(1 - c_2)],$$

in our two order parameter calculation.

In Fig. 5 we present the density functional results for the entropy change. Its average value $\sim 0.3k_B$ is consistent with experimental data. With the entropy jump result and the Clausius-Clapeyron relation we can calculate the magnetic induction jump at the transition line:

$$\frac{\Delta B}{B_m} = \left( \frac{d\Phi_0}{4\pi \Delta s} \frac{dB_m}{dT} \right)^{-1},$$

where we have made the following approximation:

$$\frac{dH_m}{dT} \sim \frac{dB_m}{dT}.$$

The results for the relative magnetic induction jump are plotted in Fig. 5 with the Zeldov et al. experimental data digitized. The parameters used to obtain this data were the same as those used to calculate the phase diagram of Fig. 4. There is a very good agreement in the magnitude and temperature dependance with this direct experimental measurement.

VI. MELTING AND FREEZING CRITERIA

In this section we analyze the Lindemann melting criterion and the Hansen-Verlet freezing criterion for the vortex system. The Lindemann criteria states that the solid melts when the square root of the mean square displacement of the particles is an order of magnitude smaller than the lattice parameter i.e. $<u^2> / \rho_0^2 = u_L^2$, with $u_L \sim 0.1$. This criteria has been widely used to estimate the phase diagram and different properties of the system at the melting line. In general it is accepted that for the melting of vortex matter the Lindemann parameter is larger than for other classical 3D solids and its value is usually taken in the range 0.2 – 0.3.

We estimated the mean square displacement as:

$$<u^2> \sim \frac{1}{A_c} \int_{A_c} d^2 r \pi r^2 \rho_n(r)$$

the density at the melting line is obtained using (2) and the results for the Lindemann parameter are shown in Fig. 5. For low fields, numerical results show that $u_L \sim 0.2$ in good agreement with previous estimates, as the field is increased (the melting temperature decreases) the Lindemann parameter increases. This is due to the fact that, as discussed above, in the present model as the liquid develops the two plane coupling decreases and the transition becomes essentially 2D. For a 2D transition, the Lindemann parameter is larger than for a 3D one.

The Hansen-Verlet freezing criteria is the counterpart of the Lindemann criteria and states that a liquid freezes when the first peak of the structure factor reaches the value 2.85 in a 3D classical system and of the order of 5.5 for a 2D plasma. Having evaluated the structure factor at the melting transition within the functional density theory, we can show the validity of this criteria for the case of freezing of the vortex liquid. The results for $S(k_{\text{max}})$ are shown in Fig. 5 and as in the case of the Lindemann criteria the Hansen-Verlet criteria is valid for low fields with a value $S(k_{\text{max}}) \sim 6.5$, much larger than that obtained for isotropic 3D system. As the melting temperature decreases $S(k_{\text{max}})$ towards its two dimensional value. In our case the value of $S(k_{\text{max}})$ at small fields is larger than the 2D value due to the following reason: the idea behind the Hansen-Verlet criteria is that when the liquid develops correlations, that overcame some critical value, it freezes. At high temperatures the first peak in $S(k)$ dominates and is a good measure of the correlations, as the temperature decreases, the liquid develops stronger correlations for large $G$ and both the first and second peaks in $S(k)$ became relevant at the freezing point. Consequently, it is not necessary for $S(k_{\text{max}})$ to become too large to indicate that the liquid has developed critical correlations. This can be viewed as a relative increase of the order parameter $p_2$ with respect to $p_1$ at the transition as the melting temperature decreases. The results indicate that for low fields the ratio $\rho_1/\rho_2$ is larger than 4, while at high fields is of the order of 2.
VII. SUMMARY AND DISCUSSION

In this work we study the melting transition for the vortex system in layered superconductors using the RY functional density theory. Using reasonable set of parameters for BSCCO we obtained qualitative and quantitative agreement with the available experimental data.

The functional density theory allows an estimation of the entropy jump at the transition and using the Clausius-Clapeyron relation we estimated the jump in magnetic induction. The same parameters used to fit the phase diagram, give results for the magnetic induction jump that are in quantitative agreement with the experimental results. Finally we analyzed the validity of the melting and freezing criteria and showed that in the region of interest - the low field region where the first order transitions occurs- the Lindemann and the Hansen-Verlet criteria are valid within an error of 10% which is typical for this type of criteria.

The model predicts the melting of the vortex lattice into a liquid of almost decoupled pancake vortices even in the low field region. In this sense we may interpret our results as a simultaneous decoupling and melting of the vortex lattice rather than a melting into a liquid of vortex lines. This picture may be appropriate for a highly anisotropic system like BSCCO. However, in a recent paper Kitazawa et al. successfully used a scaling suitable for simultaneous decoupling and melting not only for BSCCO but also for less anisotropic systems like YBCO. This scaling predicts that the melting line is given by:

\[ B_m = C \left( \frac{T}{T_m} - 1 \right) \]

where the prefactor depends on the anisotropy and interplane separation of the system. Both the experimental results of Zeldov et al. for BSCCO and our numerical results for low fields are in good agreement with this expression as shown in Fig. 10. In the figure we present results corresponding to a zero temperature penetration depth \( \lambda(0) = 1500 \text{Å} \) which gives very good agreement with the results of Zeldov et al. for the low field region where the first order transition is experimentally observed. As discussed in section IV, a more realistic value for \( \lambda(0) \) is 2000 Å, which gives a melting line laying below the experimental points. However, in any real system there is some Josephson coupling between the planes that should compensate the lowering of the electromagnetic coupling due to the increase of \( \lambda(0) \). In this sense, we take \( \lambda(0) \) as an effective parameter that measures the strength of the coupling between planes. A change in \( \lambda(0) \) does not change the temperature dependence of \( B_m \) for low fields, but only the coefficient \( C \) in Eq. (30).

If experimental results confirm the fact that even for less anisotropic system, the first order melting transition correspond to a simultaneous decoupling and melting of the vortex lattice, the present theory could be used to describe these systems provided that \( \lambda(0) \) or the interplane distance are chosen as effective parameters. In particular the validity of the melting and freezing criteria obtained for the highly anisotropic laminar BSCCO could be extended to other less anisotropic systems like YBCO.

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FIG. 1. HNC results for the pair distribution function $g(r_\perp, n = 0, 1, 2, \ldots)$ of the vortex liquid for $B = 3T$ and $T = 17K$. For $n = 0$, the first maxima as a function of $r_\perp$ is given by the mean particle spacing and for $n \neq 0$ is at $r_\perp = 0$.

FIG. 2. The pair correlation $h(r_\perp, n)$ at $r_\perp = 0$ as a function of $n$ for $B = 0.065T$ and $T = 31K$. The values can be fitted with an exponential decay, as shown in the inset with a log-normal scale.

FIG. 3. The c-axis correlation length as a function of the magnetic induction $B$ with $T = 31K$. The slope of the linear fit in the inset is $1/2$.

FIG. 4. Structure factor for $k_z = 0$. Note the increase in the structure as the temperature is lowered. The amplitude of the first peak is the quantity that we considered for the Hansen-Verlet criterion.
FIG. 5. Liquid-Solid transition line in the B-T phase diagram for the vortex system in BSCCO. The solid line is fit with $B = A_1/(T - T_{m}^{2D})$, where $A_1$ and $T_{m}^{2D}$ are variational parameters.

FIG. 6. Phase diagram of BSCCO. The open dots are the RY functional density results and the solid dots are direct measurements by Zeldov et al. In the experimental data there is a critical point where the first order transition ceases to exist, which is presumably caused by the presence point pinning centers in the sample.

FIG. 7. Entropy jump at the first order transition calculated with the RY functional density of freezing.

FIG. 8. Relative magnetic induction jump at the first order transition. The open dots were calculated using the Clausius-Clapeyron relation and the RY functional density theory of freezing. It is in very good agreement with the experimental results of Zeldov et al. (solid dots) in the magnitude and in the temperature dependence.
FIG. 9. Lindemann melting parameter and Hansen-Verlet freezing parameter as a function of $T_m$ for BSCCO calculated in the RY approximation. Both parameters are approximately constant in the region where the first order phase transition it is experimentally observed.

FIG. 10. $B_m$ as a function of $T_c/T - 1$. A test for sublimation. Calculations with different $\lambda(0)$ or $d$ give liquid-solid transition lines displaced parallel to each other giving the same effect of a different anisotropy.