Thermodynamics of the first–order vortex lattice melting transition in YBa$_2$Cu$_3$O$_{7−δ}$

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Using the London approximation within the high field scaling regime, we calculate the jump in the specific heat $\Delta c$ at the first–order melting transition of the vortex lattice in YBa$_2$Cu$_3$O$_{7−δ}$. This has recently been measured [A. Schilling et al., Phys. Rev. Lett. 78, 4833 (1997)] and reported to be at least 100 times higher than expected from the fluctuations of field induced vortices alone. We demonstrate how the correct treatment of the temperature dependence of the model parameters, which are singular at the mean–field $B_2$ line, leads to good agreement between the predictions of the London model and the size of the experimental jump. In addition, we consider the changes in the slopes of the magnetization $\Delta(\partial M/\partial T)$ and $\Delta(\partial M/\partial H)$ at the transition. Using continuum anisotropic scaling theory we demonstrate the consistency of measurements at different angles of the magnetic field with respect to the crystal c-axis.

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I. INTRODUCTION

In a recent paper$^1$ we calculated the size of the jumps in the entropy and magnetization at the vortex–lattice melting transition within the London model. We have shown that, by correctly treating the temperature dependence of the model parameters, and knowing the volume of the relevant fluctuation degrees of freedom, good agreement is obtained with the experimental results in both YBa$_2$Cu$_3$O$_{7−δ}$ (YBCO) and Bi$_2$Sr$_2$Ca$_2$Cu$_2$O$_{8}$ (BiSCCO) superconductors. The analysis contains only one unknown number, which can be taken from numerical simulations. The importance of these results is that they settle a controversy of recent years: it had been thought that the observed jumps of order 1 $k_B$ per vortex per layer$^2$ are incompatible with a simple melting scenario based on fluctuations of field induced vortices alone. Our analysis has demonstrated that there is no incompatibility because the temperature dependence of the model parameters reflects the underlying microscopic degrees of freedom. This allows the correct size of jumps to be found without having to explicitly include extra fluctuations.

Another characteristic of the melting transition is the jump in the specific heat capacity $\Delta c = T \Delta (\partial s/\partial T) = -T \Delta (\partial^2 g/\partial T^2)$, where $g$ is the Gibbs free energy density. There have been careful measurements of this in YBCO$^3$ and in Ref.$^4$ it was claimed that the step in the specific heat is at least one hundred times too large to be explained by the extra fluctuations of the translational degrees of freedom in the vortex liquid. The main purpose of this paper is to explain the size of the specific heat step using the London model, following the same approach of Ref.$^4$. We emphasize that at the relevant melting fields in the YBCO system, the penetration depth $\lambda(T)$ is much larger than the distance between vortices $a_0 \sim (\Phi_0/B)^{1/2}$ ($B$ is the magnetic induction, or flux density, and $\Phi_0$ is the flux quantum). In this regime the London model has simple scaling properties, which may be used to find the exact form of the jumps at the transition.

In the next section we calculate the heat capacity within the London model, and compare our estimated jump at the transition with the experimental values. In Sec.$^5$ we consider the jumps in the magnetization slopes $\Delta(\partial M/\partial T) = -\Delta (\partial^2 g/\partial H \partial T)$ and $\Delta(\partial M/\partial H) = -\Delta (\partial^2 g/\partial H^2)$ and find results consistent with experimental values given by Welp et al.$^6$

We also take the opportunity to compare the jumps in the entropy and the specific heat between a system at constant external field (the experimental scenario) and a system at constant vortex density (the case for most simulations). Finally in Sec.$^7$ we consider the effects of rotating the magnetic field away from the c-axis, as has been done in recent specific heat measurements.$^8$

II. THE HEAT CAPACITY IN THE LONDON MODEL

We first consider an isotropic superconductor in the mixed state. Within the London approximation, the magnitude of the superconducting order parameter is taken to be constant, except within the vortex cores, which are assumed to be much smaller than the distance between vortices. These assumptions will hold at low enough fields below the upper critical field $H_{c2}$. The free energy of the system can then be expressed as a sum over pairwise interactions between vortex segments.$^5$ i.e.
\[ F_L(\{r_\mu\}) = \frac{\varepsilon_0}{2} \sum_{\mu\nu} \int dr_\mu \cdot dr_\nu e^{-|\mathbf{r}_\mu - \mathbf{r}_\nu|/\lambda}. \]  

Disregarding the small distance cut-off, \( \xi \), there are two length scales in this problem: the London screening length \( \lambda \) and the average distance between vortices \( a_0 \).

The energy scale per unit length \( \varepsilon_0 \) is equal to \( (\Phi_0/4\pi\lambda)^2 \). It is simple to include a uniaxial anisotropy into the model when the effective mass in the field direction is different from the other two perpendicular directions: For a ratio of \( m_\text{ab}/m_c = \varepsilon^2 \), the lengths in the field direction are scaled by \( \varepsilon \).

The experiments of interest are carried out at constant external field \( H \). For the case of large field melting, as in YBCO, the magnetization is small and \( B \approx H \). In this regime we have \( a_0 \ll \lambda \) and the London free energy takes a simple scaling form,

\[ F_L(\{r_\mu\}) \approx \varepsilon_0 a_0 f_L(\{s_\mu\}), \]  

where \( s_\mu = (x_\mu, y_\mu, z_\mu/\varepsilon)/a_0 \) are dimensionless position vectors and \( f_L(\{s_\mu\}) \) is a dimensionless functional independent of \( \lambda \). The thermodynamic properties of the system are determined by the partition function, \( Z = \text{Tr} \exp(-\varepsilon_0 a_0 f_L(\{s_\mu\}))/T) \). Notice that one may think of \( \tau = T/\varepsilon_0 a_0 \) as an effective dimensionless temperature. From the standard thermodynamic relations, \( F = -T \ln Z \), \( S = -(\partial F/\partial T)_B \), and \( E = F + TS \), the entropy is

\[ S = -\frac{F}{T} + \left\langle \frac{\langle F \rangle}{T} \right\rangle - \left\langle \frac{\partial F}{\partial T} \right\rangle. \]  

The contribution \( S_0 = (\langle F \rangle - F)/T \) may be thought of as the configurational entropy of the coarse grained model, while the last term in (3) represents additional contributions from the underlying microscopic degrees of freedom that appear in the temperature dependence of the model parameters.

In the London model we must include the temperature dependence of the energy scale \( \varepsilon_0(T) \) which we show in Ref. 10 to be important for an adequate determination of the jump in the entropy at the melting transition. Using the scaling of Eq. (2), the entropy jump is

\[ \Delta S = \left(1 - \frac{T}{\varepsilon_0} \frac{d\varepsilon_0}{dT}\right) \Delta S_0 \approx \frac{(1 + t^2)}{(1 - t^2)} \Delta S_0, \]  

where the transition occurs at \( \tau = \tau_m \approx 0.088 \). Eq. (4) shows that the jump in configurational entropy is a constant per elementary degree of freedom: \( \Delta S_0 = 0.17 V/V_\text{eff} \), where \( V_\text{eff} = \varepsilon_0 a_0 \Phi_0 / B \approx \varepsilon_0^3 \). The scaling factor \((1 + t^2)/(1 - t^2)\) in (4) then leads to a constant jump in entropy per vortex per superconducting layer. In Ref. 3 this was found to be \( \Delta S_0 \approx 0.4k_B \) when YBCO parameters were used, consistent with the experimental result measured in Ref. 3.

The main point of this paper is to apply similar considerations to the heat capacity. This can be defined for changes at constant field \( H \) or at constant flux density \( B \). In the incompressible limit (which coincides with \( \lambda/a_0 \to \infty \)) these will be the same, and

\[ C_H = C_B = T \left( \frac{\partial S}{\partial T} \right)_B = \left( \frac{\partial E}{\partial T} \right)_B. \]  

(In the next section we will consider the difference...
\[ C_{H} - C_{B} \] for a compressible system, and show that the difference between the jump in specific heat at constant \( B \) and at constant \( H \) is negligible on the YBCO melting line.) We again use the results of Ref. [10] (shown here in Fig. [1]) but this time to determine the jump in the heat capacity.

Let us first assume that \( \varepsilon_0 \) is independent of temperature. Using (3), the heat capacity at constant density takes the form,

\[ C_{B0} = \frac{\partial}{\partial T} \langle f_L \rangle = \frac{\langle f_L^2 \rangle - \langle f_L \rangle^2}{\tau^2}. \tag{7} \]

Note that this “bare” heat capacity is simply a measure of the amplitude of energy fluctuations, which can be expected to jump at the transition from solid to liquid. It turns out that the first form is more accurate to use, once many temperatures have been sampled in the simulations. The change in slopes in Fig. [1] gives the result

\[ \Delta C_{B0} \approx 0.38N \lambda_z/\varepsilon_0. \tag{8} \]

This is interpreted as a jump in heat capacity of 0.38 \( k_B \) per vortex degree of freedom (defined above). As Schilling et al. point out, this result is far too small to account for the jump in specific heat observed in their experiment. However, we have neglected the additional terms arising from the temperature dependent parameters, which we have seen give dominant contributions to the entropy jump close to \( T_c \). For a general temperature dependence of the energy scale \( \varepsilon_0(T) \), we find that the heat capacity is,

\[ C_{B} = -\frac{T^2}{\varepsilon_0} \frac{d^2 \varepsilon_0}{d T^2} \frac{\langle f_L \rangle}{\tau} + \left(1 - \frac{T}{\varepsilon_0} \frac{d\varepsilon_0}{dT}\right)^2 C_{B0}. \tag{9} \]

Note that we need both results (3) and (4) to find the jump in \( C_B \), although as \( T_c \) is approached and \( \varepsilon_0 \rightarrow 0 \), the last term in (3) dominates.

In the following, we consider a more complex dependence for the energy scale of the vortex system \( \varepsilon_0(T) \) than was used in Ref. [10] and include a correction that accounts for the suppression in the superconducting density as the mean-field \( B_{c2} \) line is approached. This \( B_{c2} \) correction is important for a quantitative fit to London theory of the melting line of YBCO at fields above 1–2 T. While the agreement for the entropy jump was found in Ref. [6] between the prediction of the uncorrected London theory and the experimental values, we will see that the specific heat jump determined from (3) is more sensitive to the exact form of the melting line. This is because the terms arising from the internal temperature dependence of \( \varepsilon_0(T) \) are more strongly diverging in this case than for the entropy jump in Eq. (3).

In the limit \( B \approx B_{c2} \), the system is described by Ginzburg-Landau (GL) theory, with an order parameter \( \psi \) restricted to the lowest Landau level.\[10\]

The GL free energy takes the form \[ F_{GL} = \int d^3 r \left[ -\alpha|\psi|^2 + \beta|\psi|^4 + \gamma|\partial\psi/\partial z|^2 \right], \] where \( \alpha(T,B) = \alpha_0(1 - b) \) and \( b = B/B_{c2}(T) \) (see for example Ref. [12]). Notice the dimensional reduction in the derivative term; there is a diverging GL coherence length in the field direction only.\[13\] The only length scale remaining in the two perpendicular directions is the magnetic length \( a_0 \). The order parameter scale is \( |\psi_0|^2 = \alpha/2\beta \) and the condensation energy scale is \( 2|\psi_0|^2 = \alpha^2/\beta \). For this reason, the shear modulus has the behavior \( c_{66} \sim (1 - b)^2 \) (as calculated by Labusch\[14\]). However, the tilt modulus at short wavelengths (equal to the superfluid density in the \( z \)-direction) has a linear dependence \( c_{44} \sim (1 - b) \).

(The correct thermodynamic limit of a constant order parameter scale is \( 2\beta \)) to an isotropic one by scaling all \( c_{44} \) with \( 1/\lambda \) and anisotropy \( \varepsilon \).

Our intention is to use an effective pairwise interaction in (3) that gives the London model at low fields, but with the correct elastic moduli in the high field limit. We take the scale of interactions to be \( \varepsilon_0(T) = \varepsilon_0(T)(1-b)^2 \). This then accounts for the suppression of the order parameter around both vortex segments in an interaction term. To account for the increasing stiffness in the field direction we scale the effective anisotropy \( \varepsilon \) as \( \varepsilon = (1 - b)^{-1/2} \). Using these effective parameters in the London model we find \( c_{66} \propto (1 - b)^2 \), in agreement with the results of GL theory at intermediate fields that have recently been calculated\[15\] and \( c_{44} \propto (1 - b) \). A similar extrapolation technique was used twenty years ago by Brandt\[15\] converting the effective London system (with energy scale \( \varepsilon_0 \) and anisotropy \( \varepsilon \)) to an isotropic one by scaling all lengths in the field direction, as in Eq. (3), gives the overall energy scale factor,

\[ \varepsilon_0^{\text{eff}} = \left( \varepsilon_0 \right)^{1/2} \left( \frac{\varepsilon_0}{\varepsilon_0^{\text{iso}}} \right)^{1/2} = \varepsilon_0(1 - b)^{3/2} \]

FIG. 2. London scaling fits to the melting line observed in Ref. 3 (circles) with (full line) and without (dashed line) \( H_{c2} \) corrections. The \( H_{c2} \) line we used is shown as the dotted line. The parameters used are given in the text.
with $\varepsilon_{00} = (\Phi_0/4\pi\lambda_0)^2$. In the last line we have assumed the form $B_{c2}(T) = B_{c2}(0)(1 - t^2)$ and written $\tilde{b} = B/B_{c2}(0)$.

We now compare our results to the measurements of Schilling et al. and concentrate on the case where the field is directed perpendicular to the CuO$_2$ layers. In the scaling regime, the melting line is described by a fixed value of $\tau = \tau_m$, i.e. $T_m = g\varepsilon_0(B)\varepsilon_{\text{eff}}(T_m, B)$. In Fig. 2 we show our fit to the experimental melting line, where we find a value of $g \approx 0.21$ (this corresponds to a Lindemann number of $c_L = 0.24$ when the melting line from the Lindemann criterion is written in the standard form of $T_m \approx 2\sqrt{\pi c_L \varepsilon_0 a_0}$). To obtain this fit we took the physical values: $T_c = 93$ K, $\varepsilon = 1/8$, $dH_{c2}/dT|_{T=T_c} = 1.8$ TK$^{-1}$, $\lambda_0 = 1300$ Å. In Fig. 2 we also show our fit without including $B_{c2}$ corrections, which leads to a value of $g = 0.13$, or $c_L = 0.19$.

With (10) the formula for the entropy jump in (8) now becomes,

$$\Delta S = \frac{[1 - \tilde{b} + (2\tilde{b} - t^2)t^2]}{(1 - t^2 - \tilde{b})(1 - t^2)} \Delta S_0. \quad (11)$$

Note that the factor on the RHS now diverges at the $B_{c2}$ line rather than at $T_c$. In Fig. 2 we compare our predictions for the entropy jump per vortex per layer, calculated with and without $B_{c2}$ corrections, to the experimental values of Ref. 3. Interestingly, there is little difference between the two approaches in this temperature regime.

Substituting (11) into (3) leads to

$$\Delta C_B = \frac{[1 - \tilde{b} + t^2(2\tilde{b} - t^2)t^2]}{[(1 - t^2)(1 - t^2 - \tilde{b})]^2} \Delta C_{B0} + \frac{t^2[2(1 - t^2)^3 - \tilde{b}(1 - t^2)^3 - \tilde{b}^2(1 + 2t^2)]}{[(1 - t^2)(1 - t^2 - \tilde{b})]^2} \Delta \langle f_L \rangle. \quad (12)$$

The result for $\Delta C_B$ in (12) combined with (5) and (6) tells us the jump in the heat capacity per degree of freedom (i.e., per volume $V_{\text{eff}}$), which diverges as $T_c$ is approached. Indeed, we find that over the region of temperatures where measurements have been performed, the heat capacity jump is of order $100$ k$\text{g}$ per vortex degree of freedom. Because the melting field falls to zero, the volume of a degree of freedom also diverges in this limit, such that the heat capacity jump in a physical sample of fixed volume drops to zero, $\Delta C_B \propto (1 - t^2)$, on approaching $T_c$. In Ref. 3 the results for the jump in heat capacity are expressed for a fixed volume. The specific heat is defined as the heat capacity in a mole of YBCO which fills a volume $V_{\text{mol}} = 1.05 \times 10^{-4}$ m$^3$ (this is the volume of 602 x 10$^{23}$ unit cells). We therefore convert to the specific heat jump $\Delta C_B = (V_{\text{mol}}/V)\Delta C_B$ and make use of the fit to the melting line of Fig. 2 in Eq. (3), $\Delta C_{B0} \approx 0.38V/V_{\text{eff}} \propto B_{c2}^{3/2}(T)$.

![FIG. 3. The calculated entropy jump per vortex per layer (solid line). For comparison the results when $B_{c2}$ corrections are not included are also shown (dashed line). Both curves are within the error bars of the experimental values from Ref. 3.](image)

Our result for the specific heat jump per molar volume is shown in Fig. 4 along with the experimentally measured points. This shows that we can explain the size of the specific heat jump within about 50% accuracy. We should not expect a much better agreement as we extrapolate the London approximation into a region where it will not be exact and also neglect the effects of disorder. In fact, the measurements of the magnetization jump in Ref. 3 show $\Delta B$ falling to zero at a temperature several Kelvin below $T_c$, and this is usually attributed to the effects of quenched disorder which may smooth the jumps at a first-order transition. There may be a similar explanation behind the non-monotonic behavior.
in the experimental value of $\Delta c$. Nevertheless, the important point here is that the size of the experimentally observed jumps in the specific heat are consistent with a model that only includes field induced vortices.

III. THE MAGNETIZATION AND ITS DERIVATIVES

The aim of this section is to use our results for the entropy and specific heat jumps from the previous section to calculate the jumps in the derivatives of $B$ (or in the magnetization $M = (B - H)/4\pi$) with respect to $H$ and $T$. We first introduce the Clausius-Clapeyron relation, and then describe the conditions under which the jump in entropy in a system at constant external field $H$ is the same as the entropy jump in a system of fixed flux density $B$. We need these conditions to hold in order to justify our application of the results of Section II, which we calculated at constant $B$, to the experimental results, which are measured at constant $H$. After ensuring that these conditions are fulfilled for the melting line of YBCO, we then calculate the jumps in the thermal compressibility $\Delta(\partial B/\partial T)_H$ and in the susceptibility $\Delta(\partial B/\partial H)_T$. Finally we will be in a position to describe the conditions for the specific heat jump to be approximately the same in a constant $B$ system compared to that in a constant $H$ system, and then verify that these conditions are also satisfied.

At the first-order transition of a system at constant field $H$, the continuity of the Gibbs free energy $G = F - (BH/4\pi)V$ leads to the Clausius-Clapeyron equation

$$\Delta s = \frac{1}{4\pi} \frac{dH_m}{dT} \Delta B,$$

relating the jump in flux density $\Delta B$ to the melting line $H_m(T)$ and the jump in the entropy density $\Delta s$. In the previous section we calculated the jumps in entropy and heat capacity for a transition at fixed $B$, using the scaling form of the London model [see Eq. (4)]. An important difference between the melting transition at constant $B$ and at constant $H$ is that in the former, coexistence occurs over a finite temperature region, see Fig. 5. The entropy jumps at constant $H$ and constant $B$ will not be the same: We must take into account the different values of $B$ on either side of the constant $H$ transition, $\Delta B|_H = B'(H,T_m) - B'(H,T_m)$, and also the width in temperature of the constant $B$ transition, $\Delta T|_B = T_m'(B) - T_m'(B)$ [the symbol $s$ denotes the solid (lattice) phase, while the symbol $f$ is for the fluid (liquid) phase]. The entropy jump at constant $B$ is defined as $s^f(B,T_m') - s^s(B,T_m')$ as shown in Fig. 6, which to first order in $\Delta T$ is

$$\Delta s|_B = s^f(B,T_m') - s^s(B,T_m') + \frac{c_f}{T_m'} \Delta T|_B.$$

We can now relate the entropy jump at fixed $H$ to that at fixed $B$,
\[ \Delta s_{t} = s^{\ell}(H_{m}, T) - s^{s}(H_{m}, T) \]
\[ = s^{\ell}(B_{m}^{s}, T) - s^{s}(B_{m}^{s}, T) + \left( \frac{\partial s^{\ell}}{\partial B} \right) \Delta B_{t} \]
\[ = \Delta s_{B_{m}} + \frac{1}{4\pi} \left( \frac{\partial H^{s}}{\partial B} \right)_{T} \left( \frac{\partial B^{s}}{\partial T} \right)_{H} \Delta B_{t} - \frac{c_{B}}{T} \Delta T_{t} \]

where in the last line we have used the Maxwell relation
\[ \left( \frac{\partial s}{\partial B} \right)_{T} = -\frac{1}{4\pi} \left( \frac{\partial H}{\partial T} \right)_{B} = \frac{1}{4\pi} \left( \frac{\partial H}{\partial B} \right)_{T} \left( \frac{\partial B}{\partial T} \right)_{H} . \]

Equation (15) shows that there are two terms that lead to corrections in the entropy jump at fixed B compared to fixed H. The physical explanation is that the latent heat at fixed H includes the magnetic work done to increase the flux density by \( \Delta B_{t} \), while at fixed B there is an extra heat increase due to the temperature increase across the transition \( \Delta T_{t} \). Our results for the entropy jump at constant B will only be valid at constant H, \( \Delta s_{t} \approx \Delta s_{B=H(t)} \), if the two conditions
\[ \frac{c_{B}}{T} \Delta T_{t} \ll \Delta s_{t} \]
\[ \frac{1}{4\pi} \left( \frac{\partial H}{\partial B} \right)_{T} \left( \frac{\partial B}{\partial T} \right)_{H} \Delta B_{t} \ll \Delta s_{t} \]

are fulfilled.

To apply the results of the previous section, we must check the above conditions for the case of vortex-lattice melting in YBCO. We first consider the term arising from the temperature increase across the constant B melting transition. By writing \( \Delta B_{t} \approx (d B_{m}/d T) \Delta T_{t} \) (see Fig. 2), and using the Clausius-Clapeyron relation (13), we can express the condition (17) in the form,
\[ \frac{c_{B}}{T} \Delta T_{t} \ll \frac{1}{4\pi} \left( \frac{d B_{m}}{d T} \right)^{2} . \]

Using the numerical results presented in the previous section, the total heat capacity at the YBCO melting transition is of order \( c_{B}/T \approx 10 \text{ Jm}^{-3}\text{K}^{-2} \). From Fig. 2 we have \( d H_{m}/d T \approx -0.7 \text{TK}^{-1} \) on the melting line of YBCO, which gives \( (d H_{m}/d T)^{2}/4\pi \approx 4 \times 10^{5} \text{ Jm}^{-3}\text{K}^{-2} \). Therefore this condition is well satisfied on the YBCO melting line. Finally, we consider the term involving the jump in flux density at the transition with fixed H. If we insert the Clausius-Clapeyron relation (13) into the RHS of condition (18) we find that the condition is equivalent to \( (\partial B^{s}/\partial T)_{H} \ll d H_{m}/d T \), which is to say that the thermal compressibility of the vortex system \( (\partial B^{s}/\partial T)_{H} = 4\pi(\partial M^{s}/\partial T)_{H} \) must be smaller than the slope of the melting line. This is satisfied as long as the magnetization (which is of order the lower critical field \( H_{c1} \)) is less than the melting field, \( H_{c1} \ll H_{m} \), which is the case for vortex lattice melting in YBCO. We have therefore confirmed in our regime of interest (the large field scaling limit) that the same entropy jump is found for a transition at constant H and at constant B. If we also take \( B_{m}(T) = H_{m}(T) \), we can calculate \( \Delta B \) in the scaling regime using the Clausius-Clapeyron relation (13). This reasoning was used in Ref. 6 and excellent agreement was found between the London model predictions and the measured values of \( \Delta B \) in YBCO by Welp et al.

We now calculate the jumps in the derivatives of the magnetization. Consider a quantity \( X(T, H) \) which is discontinuous at the melting field \( H_{m}(T) \) with a jump \( \Delta X(T) \). The total temperature derivative of the jump in \( X \) (defined along the melting line) is then
\[ \frac{d \Delta X}{dT} = \Delta \left( \frac{\partial X}{\partial T} \right)_{H} + \frac{d H_{m}}{dT} \Delta \left( \frac{\partial X}{\partial H} \right)_{T} . \]

Note that inserting \( X = G \), the Gibbs free energy which is continuous, simply gives the Clausius-Clapeyron equation. Applying (20) to the entropy jump by taking \( X = s \), and using the Maxwell relation \( 4\pi(\partial s/\partial H)_{T} = (\partial B/\partial T)_{H} \), we find
\[ \frac{1}{4\pi} \frac{d H_{m}}{dT} \Delta \left( \frac{\partial B}{\partial T} \right)_{H} = -\frac{\Delta c_{H}}{T} + \frac{d \Delta s}{dT} . \]

This allows us to find \( \Delta (\partial B/\partial T)_{H} \) once we know the corresponding discontinuities in the calorimetric quantities \( c_{H} \) and \( s \). In the SQUID measurements of the magnetization in Ref. 6, an experimental value is found at a field of \( H = 4.2T \) of \( \Delta (\partial B/\partial T)_{H} = 4\pi \Delta (\partial M/\partial T)_{H} \approx 0.2 \text{ GK}^{-1} \) (the accuracy is only of order 50%). We convert from magnetic energy units to calorimetric units using \( 1 \text{ erg cm}^{-3} = 0.1 \text{ J m}^{-3} = 0.011 \text{ mJ mol}^{-1} \) for YBCO. For the specific heat jump we take \( \Delta c_{H} \approx 1 \text{ mJ mol}^{-1}\text{K}^{-2} \) from Eq. 6. We calculate \( \Delta s = \Delta S/V \) from Eqs. (6) and (13), giving \( d \Delta s/d T = -0.35 \text{ mJ mol}^{-1}\text{K}^{-2} \) at a field of \( H_{m} = 4.2T \). Inserting these results into (21) along with the melting slope of \( d H_{m}/d T = -0.7 \text{TK}^{-1} \), we find \( \Delta (\partial B/\partial T)_{H} = 0.23 \text{ GK}^{-1} \) consistent with the experimental value at this field.

We now use two further relations between these jumps which will allow the jump in the susceptibility, \( \Delta (\partial B/\partial H)_{T} \), to be calculated. The total derivative with respect to temperature of (13) may be written as
\[ \Delta c_{H} = -\frac{T}{4\pi} \left[ \frac{2}{d H_{m}/d T} \Delta \left( \frac{\partial B}{\partial T} \right) \right]_{H} + \left( \frac{d H_{m}}{dT} \right)^{2} \Delta \left( \frac{\partial B}{\partial T} \right)_{T} + \frac{d^{2} H_{m}}{dT^{2}} \Delta B . \]

This equation was used in Ref. 6 to successfully test the thermodynamic consistency of the observed specific heat jump with the magnetization measurements of Welp et al.
Combining this with (24) gives an equation for the jump in \((\partial B/\partial H)_T\) in terms of calorimetric quantities only,

\[
\frac{1}{4\pi} \left( \frac{dH_m}{dT} \right)^3 \Delta \left( \frac{\partial B}{\partial H} \right)_T = \frac{dH_m}{dT} \left( \frac{\Delta c_B}{T} - \frac{2 d\Delta s}{dT} \right) + \frac{d^2 H_m}{dT^2} \Delta s. \tag{23}
\]

Note that this may also be derived by inserting \(X = B\) in Eq. (20) and using the Clausius-Clapeyron relation. We find this jump along the melting line of YBCO to be of order \(\Delta(B/\partial H)_T \approx 10^{-5} \text{G/\text{Oe}}\), consistent with the assumption that \(B \approx H\). However, we must be careful about ignoring this term. For instance, in the scaling regime, and from experimental values in YBCO, the temperature derivative \(d(\Delta B)/dT = \Delta(B/\partial H)|_H + (dH_m/dT)\Delta(B/\partial H)|_T\) is negative but the jump \(\Delta(B/\partial H)|_H\) is positive and therefore smaller in magnitude than \((dH_m/dT)\Delta(B/\partial H)|_T\).

We now determine whether the jump in the heat capacity at constant \(H\), as measured in experiments on YBCO, may be approximated by the jump in heat capacity at constant \(B\), which was calculated in Section II. From (24) by expanding to first order in the jumps,

\[
c_H = T \left( \frac{\partial s}{\partial T} \right)_H = T \left( \frac{\partial s}{\partial T} \right)_B + T \left( \frac{\partial B}{\partial T} \right)_H \left( \frac{\partial s}{\partial B} \right)_T
\]

\[= c_B + \frac{T}{4\pi} \left( \frac{\partial H}{\partial B} \right)_T \left( \frac{\partial B}{\partial T} \right)_H^2, \tag{24}\]

where the last line again uses the Maxwell relation (16). With the same reasoning that lead to (13) and using the notation defined as Fig. 1, we have,

\[
\Delta c_B|_B = \Delta c_B|_H - \left( \frac{\partial c_B}{\partial B} \right)_T \Delta B|_H + \left( \frac{\partial c_B}{\partial T} \right)_B \Delta T|_B. \tag{25}\]

We can also find the jump in the difference \((c_H - c_B)\) from (24) by expanding to first order in the jumps,

\[
\Delta (c_H - c_B)|_B \approx \frac{T}{4\pi} \left[ -2 \left( \frac{\partial B}{\partial T} \right)_H \left( \frac{\partial B}{\partial H} \right)_T \right] + \frac{T}{4\pi} \left( \frac{\partial H}{\partial B} \right)_T \left( \frac{\partial B}{\partial T} \right)_H \left( \frac{\partial B}{\partial H} \right)_T \Delta \left( \frac{\partial B}{\partial H} \right)_T. \tag{26}\]

Our previous results show that the first term on the RHS is negative, while the second term is positive. Although the total \(c_H - c_B\) is rigorously positive for thermodynamic stability, the change in this quantity may be of either sign. Combining this equation (20) with (25) gives

\[
\Delta c_B = \Delta c_B|_H + \left( \frac{\partial c_B}{\partial H} \right)_T \Delta T|_B - \left( \frac{\partial c_B}{\partial T} \right)_B \Delta B|_H + \frac{T}{4\pi} \left( \frac{\partial B}{\partial T} \right)_T \left( \frac{\partial B}{\partial H} \right)_H \left( \frac{\partial B}{\partial T} \right)_T \Delta \left( \frac{\partial B}{\partial H} \right)_T. \tag{27}\]

We can group the corrections to \(\Delta c_B|_B\) into two contributions. The first correction term in (27) can be ignored compared to the total specific heat jump if \(\partial c_B/\partial T \Delta T|_B \ll \Delta c_B\). After some manipulations with the Clausius Clapeyron relation it may be written as

\[
\left( \frac{\partial c_B}{\partial T} \right)_B \Delta s \ll \frac{1}{4\pi} \left( \frac{dB_m}{dT} \right)^2 \Delta c_B, \tag{28}\]

which we find to be satisfied in the scaling regime from the simulation results. A second condition is found from the three remaining correction terms in (27) after dropping the term \(\propto \Delta T|_B\). Setting \(\partial(H/B)|_T = 1\) and using the identity \(\partial(c_B/B)|_T = -T(\partial(H/B)_T)(\partial^2 B/\partial T^2)_H\) [which also arises from the Maxwell relation (14)], gives

\[
\Delta c_H|_B - \Delta c_B|_B = -\frac{T}{4\pi} \left[ -2 \left( \frac{\partial B}{\partial T} \right)_H \left( \frac{\partial B}{\partial H} \right)_T \right] + \left( \frac{\partial c_B}{\partial T} \right)_B \left( \frac{\partial B}{\partial H} \right)_T \Delta \left( \frac{\partial B}{\partial H} \right)_T. \tag{29}\]

A direct comparison of this equation with the differentiated Clausius-Clapeyron relation (22) shows that we can take \(\Delta c_H|_B \approx \Delta c_B|_B\) as long as \(\partial H_m/dT \gg (\partial B/\partial T)_H\), which is the same condition we found for comparing the entropy jump at constant \(H\) versus constant \(B\), and which is valid as long as \(H_m \gg H_a\). Therefore, our calculation of \(\Delta c_B\) at constant \(B\) is justified in the application to vortex lattice melting in YBCO.

IV. DIFFERENT FIELD ANGLES

In Ref. 11 the heat capacity in YBCO was measured both with the magnetic field parallel to the \(c\)-axis, \(H \parallel c\), and parallel to the superconducting layers, \(H \perp c\). More recent experiments have been performed for a range of angles between these two limits. In the scaling regime, the effects of rotating the field may be simply understood using the anisotropic scaling rules of Blatter, Geshkenbein, and Larkin. The basis of these scaling rules is that \(\Delta(B/\partial H)_T \ll \Delta(B/\partial H)|_H\), which we find to be satisfied in the scaling regime from the simulation results. A second condition is found from the three remaining correction terms in (27) after dropping the term \(\propto \Delta T|_B\). Setting \(\partial(H/B)|_T = 1\) and using the identity \(\partial(c_B/B)|_T = -T(\partial(H/B)_T)(\partial^2 B/\partial T^2)_H\) [which also arises from the Maxwell relation (14)], gives

\[
\Delta c_H|_B - \Delta c_B|_B = -\frac{T}{4\pi} \left[ -2 \left( \frac{\partial B}{\partial T} \right)_H \left( \frac{\partial B}{\partial H} \right)_T \right] + \left( \frac{\partial c_B}{\partial T} \right)_B \left( \frac{\partial B}{\partial H} \right)_T \Delta \left( \frac{\partial B}{\partial H} \right)_T. \tag{29}\]

A direct comparison of this equation with the differentiated Clausius-Clapeyron relation (22) shows that we can take \(\Delta c_H|_B \approx \Delta c_B|_B\) as long as \(\partial H_m/dT \gg (\partial B/\partial T)_H\), which is the same condition we found for comparing the entropy jump at constant \(H\) versus constant \(B\), and which is valid as long as \(H_m \gg H_a\). Therefore, our calculation of \(\Delta c_B\) at constant \(B\) is justified in the application to vortex lattice melting in YBCO.
where $\tilde{Q}$ is the corresponding quantity in the isotropic superconductor (with $\lambda = \lambda_{ab}$), and $\varepsilon_0^2 = \varepsilon^2 \sin^2 \theta + \cos^2 \theta$. The factor $s_Q$ depends on the quantity $Q$. For the scalar quantities volume and energy it is independent of the angle, $s_Q = \varepsilon$, but for magnetic fields it is equal to $s_B = 1/\varepsilon_\theta$.

An initial consequence of (30) is that, at a fixed temperature, the magnetic field at which the system has the same physics scales as $H_X(\theta) = H_X/\varepsilon_\theta$. This implies that the melting line is raised to higher $\varepsilon$ values as the angle $\theta$ is increased,

$$H_m(T, \theta) = H_m(T, 0)/\varepsilon_\theta. \tag{31}$$

The same scaling form applies to the upper critical field $H_{c2}(T, \theta)$. These fields are lower for $H \parallel c$ than for $H \perp c$ by a factor $\varepsilon$. Furthermore, if we take the quantity $Q$ in (30) to be the energy, entropy or heat capacity of a fixed volume (e.g. the volume of the crystal) then after scaling the magnetic field as in (31) this quantity will be independent of the angle $\theta$. Therefore, if we write the entropy jump as a function of melting temperature, $\Delta s(T, \theta)$, the following relation holds,

$$\Delta s[T_m(H, \theta), 0] = \Delta s[T_m(\varepsilon_\theta H, 0), 0]. \tag{32}$$

We can also replace $s$ by $c$ in this equation. Therefore the measured jumps in the specific heat and in the entropy per molar volume, when plotted against the melting temperature, will be identical for the different angles. This prediction is fulfilled to within experimental error in recent measurements by Schilling[4].

To understand this result in more detail, we now consider the case of fixing the magnetic field, and comparing the jumps at different melting temperatures as the angle of the field is rotated. In this case, the field scales to a different value, $\tilde{H} = \varepsilon_\theta H$, in the isotropic system for different values of $\theta$. The melting temperature is,

$$T_m(H, \theta) = \varepsilon \tilde{T}_m(\varepsilon_\theta H). \tag{35}$$

This equation differs from (31) in that we need to know the full melting curve in the isotropic case to find the angular dependence of the melting temperature. Similarly, to determine the angular dependence of the entropy jump as a function of $H$ from (32), we need to know the full function $\Delta s(T, \theta = 0)$. We now consider the case of fixing the magnetic field, and comparing the jumps at different melting temperatures as the angle of the field is rotated. In this case, the field scales to a different value, $\tilde{H} = \varepsilon_\theta H$, in the isotropic system for different values of $\theta$. The melting temperature is,

$$T_m(H, \theta) = \varepsilon \tilde{T}_m(\varepsilon_\theta H). \tag{35}$$

If the jump in the entropy and the heat capacity were constant per vortex degree of freedom then this equation implies that the jumps would scale proportional to $\varepsilon_\theta^{-3/2}$, as is stated in Ref. 1. However, we showed in Section I that the temperature dependence of $\varepsilon_\theta(0)$ gives a non-trivial temperature dependence to the jumps per vortex degree of freedom. In the limiting case of no $B_{c2}$ corrections, the jump in entropy density is $\Delta s \propto (1/\varepsilon_{\text{def}})(1 - t^2)^{-1} \propto B_m \varepsilon_\theta$ and the jump in heat capacity is $\Delta c \propto (1/\varepsilon_{\text{def}})(1 - t^2)^{-2} \propto (B_m \varepsilon_\theta)^{1/2}$. This leads to the angular scaling

$$\Delta s(H, \theta) = \Delta s(H, 0) \varepsilon_\theta$$

$$\Delta c(H, \theta) = \Delta c(H, 0) \varepsilon_\theta^{1/2}. \tag{37}$$

For the general case when $B_{c2}$ corrections are included, there is no such simple form. However, the more general angular scaling of the jumps (32) still holds and it is straightforward to find $\Delta s(H, \theta)$ and $\Delta c(H, \theta)$ numerically.

V. CONCLUSIONS

We have not in this paper considered the case of the strongly layered high-$T_c$ superconductors such as Bi-SCCO, where the low melting field $B_m < \Phi_0/\lambda^2$ means that the scaling form of (3) does not apply. Still, in Ref. 3 we successfully determined the magnetization jump in BiSCCO using dimensional estimates, together with a Lindemann analysis of the melting line. The reason this works, while simple estimates for the entropy jump do not, is that the induction is a derivative of the Gibbs free
energy with respect to $H$ (rather than $T$ as for the entropy) and the $H$ dependence of the vortex parameters is much weaker than the $T$ dependence. The entropy jump for BiSCCO could then be found by combining our result for $\Delta B$ with the melting line and the Clausius–Clapeyron relation \cite{13}. It is not possible to simply follow this procedure to find $\Delta c$ using the relation \cite{12}, as the simple estimates will be incorrect for $\Delta(\partial B/\partial T)_H$. It is also interesting to consider whether the conditions for the calorimetric jumps to be the same in a constant $B$ system and in a constant $H$ system, derived in Sec. \ref{sec:conditions}, hold at these low fields. The melting field in BiSCCO is of the order of the bulk lower critical field $H_{c1}$, which is also the size of the magnetization: $H_m \sim H_{c1} \sim 4\pi M$. Therefore the slopes $dH_m/dT$ and $(\partial B/\partial T)_H$ will be of a similar size so that the condition \cite{13} is not fulfilled and the RHS of \cite{22} is not small. In experimental measurements on BiSCCO (at constant $H$) there will be a significant contribution to the entropy and specific heat jumps that is not present in a system of fixed flux density $B$.

To summarize, we have calculated the specific heat jump at the melting transition of the vortex lattice for YBCO, using the scaling form of the London model at high fields and numerical results from recent simulations. We find a jump with the same magnitude as the measured experimental values. We have used analogous relations to the Clausius–Clapeyron equation to find the jumps in the magnetization slopes, and these are also consistent with measured values for YBCO. A careful analysis was made to make sure that the jumps in the entropy and in the specific heat are the same for a system at constant $B$ and at constant $H$. We have constructed the relevant conditions and have verified that they are satisfied at the vortex–lattice melting line in YBCO. We have analyzed the changes to the jumps when the field angle is rotated with respect to the crystal and thereby explain the recently measured angular scaling of the entropy and specific heat jumps in YBCO \cite{26}. In conclusion, we find that the London model with temperature and field dependent parameters gives a consistent picture of the first–order transition observed in YBCO \cite{26}.

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\bibitem{20} The only other prediction we know of for the specific heat jump uses the LLL approximation with a scenario of a crossover due to growing length scales [S.-K. Chin and M.A. Moore, preprint, cond-mat/9709347]. A result of $\Delta c/T = 0.36$ mJ mole$^{-1}$K$^{-2}$ independent of melting temperature is found. This contrasts with our result which falls to zero as $T_c$ is approached, but which lies closer to the experimental values at lower temperatures.
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