Two-Phase Region of the Vortex-Solid Melting Transition: 3D $XY$ Theory

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In clean enough samples of the high-$T_c$ oxide materials, the phase transition into the superconducting state occurs along a first order line in the $H$-$T$ plane. This means that a two-phase region occurs in the $B$-$T$ plane, in which the liquid and solid vortex phases coexist. We discuss the thermodynamics of this two-phase region, developing formulae relating experimental quantities of interest. We then apply the 3D $XY$ scaling theory to the problem, obtaining detailed predictions for the boundaries of the coexistence region. By using published data, we are able to predict the width of the two-phase region, and determine the physical parameters involved in the 3D $XY$ description.

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The phase transition into the superconducting state in the high-$T_c$ oxide materials is a topic of great current interest. It is well known that the mean-field description of the superconducting transition must be modified to incorporate strong fluctuation effects. In the presence of magnetic fields, the resulting transition has been described as the melting of a vortex-solid into a vortex-liquid, and is predicted to be first order in very clean samples. This prediction is borne out both in experiments and simulations. Important thermodynamic support for the first order scenario has been provided by Schilling et al., who verify that the Clausius-Clapeyron equation is satisfied.

In contrast, the zero field transition ($H = 0, T = T_c$) is continuous, and belongs to the universality class of the 3D $XY$ model. The discontinuities of the entropy density ($\Delta s$) and magnetization ($\Delta M$) therefore both go to zero approaching this critical point. The observed range of the critical fluctuations extends over large portions of the phase diagram in both clean and disordered samples. The 3D $XY$ theory provides a rigorous framework for analyzing the first order transition, and thus places strict constraints on its interpretation. Experimental data supporting this description have been obtained by Liang et al.

As illustrated in Fig. 1, the first order transition occurs along a line $H_m(T)$ in the $H$-$T$ plane. However, in the $B$-$T$ plane, the first order line becomes an area of two-phase coexistence. This area is analogous to the region of liquid-solid coexistence in the $T$-$\rho$ (temperature-density) plane of a substance such as water. When $B$ (the average magnetic field) and $T$ are such that the superconductor is in the two-phase region, the system separates into two phases, each with its own value of $B$. It is a point of general and fundamental interest to understand the distinction between the $H$-$T$ and $B$-$T$ planes; as we shall explain, some nontrivial signatures of the first order transition can be inferred by keeping this distinction in mind.

The purpose of this paper is to use 3D $XY$ scaling to discuss the two-phase region. We start by giving a general thermodynamic analysis, emphasizing the $H_{ex}$-$T$ plane, where $H_{ex}$ is the externally applied magnetic field. This allows us to obtain relations between the different experimental quantities of interest, thus providing important consistency checks for experimental investigations. We then apply the 3D $XY$ scaling theory to make more specific predictions concerning the coexistence region. Background effects are carefully included, in terms of the background inverse permeability $\Omega$. We evaluate the important parameters of the scaling theory using published data; this allows us to make definite predictions about the size of the coexistence region for several systems.

General Theory. We consider the coexistence of two phases: the vortex-liquid (L) and the vortex-solid (S). (These names are used only for convenience; the particular nature of the two phases plays no role in the analysis.) We assume that each phase is characterized by a distinct free energy density, denoted as $f_L(B,T)$ and $f_S(B,T)$. The conjugate fields $H_\alpha(B,T)$ are defined in the usual way:

$$H_\alpha(B,T) = 4\pi \partial f_\alpha/\partial B,$$  \hspace{1cm} (1)

where $\alpha = L$ or $S$. The curves bounding the two-phase region in the $B$-$T$ plane are denoted by $B_L(T)$ and $B_S(T)$, as in Fig. 1. The fundamental equations describing coexistence along the line $H_m(T)$ are then

$$H_L(B_L(T), T) = H_S(B_S(T), T) \equiv H_m(T),$$  \hspace{1cm} (2)

$$f_S(B_S(T), T) - f_L(B_L(T), T) = H_m(T)[B_S(T) - B_L(T)]/4\pi.$$  \hspace{1cm} (3)

The first equation requires that $H$ be the same in the two phases at a given temperature, while the second equation requires that the magnetic Gibbs free energies be the same at that temperature. Eqs. (2) and (3) can be solved simultaneously to determine the two unknowns, $B_S(T)$ and $B_L(T)$.

For most experimental situations, it is the external field $H_{ex}$ which is directly under control. For an ellip-
soidal sample with demagnetizing factor \( n \), \( H_{\text{ex}} \) is related to \( B \) and \( H \) by

\[
H_{\text{ex}} = nB + (1 - n)H = B + 4\pi(n - 1)M,
\]

when the field is applied along a symmetry axis of the ellipsoid \([1]\).

We will now consider the two most common experimental procedures for collecting data: (i) varying \( H_{\text{ex}} \) while keeping \( T \) fixed, (ii) varying \( T \) while keeping \( H_{\text{ex}} \) fixed. It will be seen that the distinction between these two cases is nontrivial.

The first results are evident from Eqs. (2) and (4) \([12]\):

\[
\Delta H_{\text{ex}}|_T = n\Delta B|_T = 4\pi n\Delta M|_T.
\]

Here, the operator \( \Delta \) is defined as the value measured on the liquid side minus the value measured on the solid side of the transition. The notation of Eq. (3) also signifies that the difference is measured at constant \( T \) in this case. Note that the discontinuity \( \Delta B|_T \) occurs because fields in the range \( B_s(T) < B < B_L(T) \) are not stable. However, the discontinuity \( \Delta H_{\text{ex}} \) reflects only the boundaries of the two-phase region; there are no unattainable values of \( H_{\text{ex}} \).

We now discuss the constant-\( H_{\text{ex}} \) path across the coexistence region. Eq. (4) shows that a discontinuity \( \Delta B|_{H_{\text{ex}}} \) causes corresponding discontinuities in \( \Delta H|_{H_{\text{ex}}} \) and \( \Delta M|_{H_{\text{ex}}} \). According to Eq. (3), if \( H \) changes values in the coexistence region, then it must follow the line \( H_m(T) \). Since the discontinuities \( \Delta B \) and \( \Delta H \) are much smaller than \( B \) and \( H \) respectively (except when \( T \approx T_c \)), we see that

\[
\Delta H|_{H_{\text{ex}}} / \Delta T|_{H_{\text{ex}}} \approx \partial H_m / \partial T.
\]

The following relations are thus obtained at constant \( H_{\text{ex}} \):

\[
\Delta B|_{H_{\text{ex}}} = (1 - 1/n)\Delta H|_{H_{\text{ex}}} = 4\pi(1 - n)\Delta M|_{H_{\text{ex}}} \\
\simeq (1 - 1/n)(\partial H_m / \partial T)\Delta T|_{H_{\text{ex}}}.
\]

In the final equation, \( H \) may be replaced by \( H_{\text{ex}} \) using the approximate relation \([1 + (n - 1)(1 - \Omega)]H \simeq \Omega H_{\text{ex}} \), where the inverse background permeability \( \Omega \) is defined below, and satisfies \( \Omega \approx 1 \). Corrections to this approximation are of order \( M/H_{\text{ex}} \), and are therefore extremely small for typical YBa\(_2\)Cu\(_3\)O\(_{7-\delta} \) (YBCO) samples, but become more noticeable in Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_8 \) (BSCCO).

Equations (3) and (4) are related through the following geometrical statement:

\[
\Delta H_{\text{ex}}|_T / \Delta T|_{H_{\text{ex}}} \approx -\partial H_{\text{ex}m}/ \partial T. \tag{7}
\]

This equation is important in its own right, since it is not affected by the sample geometry.

Using the above results, we may obtain various relations of interest. For example, we find \([1 + (n - 1)(1 - \Omega)]\Delta M|_{H_{\text{ex}}} \approx \Omega \Delta M|_T \), with corrections of order \( M/H_{\text{ex}} \). When \( \Omega = 1 \), this equation reduces to \( \Delta M|_{H_{\text{ex}}} \approx \Delta M|_T \), which is independent of sample geometry. Similarly for \( \Omega = 1 \), we find \( \Delta (B - H_{\text{ex}})|_T \approx \Delta B|_{H_{\text{ex}}} \), which is also geometry-independent. Finally, we state the Clausius-Clapeyron equation appropriate for this transition:

\[
4\pi \Delta s|_T / \Delta B|_T = -\partial H_{\text{ex}m}/ \partial T. \tag{8}
\]

Equations (3)-(8) form a set of thermodynamic relations between quantities of interest for the first order transition.

3D XY Scaling Theory. The main features of 3D XY scaling can be derived from a single ansatz for the free energy density \([13,14]\). The new assumption for the coexistence region is that the liquid and solid free energies densities independently satisfy this scaling. This means that we may write the free energies in the following form, using \( t \equiv |T - T_c| / T_c \):

\[
f_L(B, T) = f_{KL}t^{2\nu} \phi_L(B - 2\nu / H_{KL}) + f_0(T) + \Omega B^2 / 8\pi \\
f_S(B, T) = f_{KS}t^{2\nu} \phi_S(B - 2\nu / H_{KS}) + f_0(T) + \Omega B^2 / 8\pi.
\]

Note the following points:

1. The exponent \( \nu \approx 0.67 \) is the correlation length exponent for the 3D XY model. The central assumption of the scaling ansatz is that the magnetic field \( B \) scales as an inverse length squared \([14] \). \( B \) and \( T \) then enter the scaling function only in the combination \( B - 2\nu/\nu \).

2. The parameters \( f_{KL}, f_{KS}, H_{KL}, \) and \( H_{KS} \) are material dependent and thus nonuniversal. \( f_k \)'s have dimensions of free energy density, while \( H_k \)'s have dimensions of magnetic field. Below, we show that \( f_{KL} = f_{KS} \).

3. The term \( f_0(T) + \Omega B^2 / 8\pi \) approximates the smooth background contribution to the free energy density near the zero field transition. The quantities \( f_0(T) \) and \( \Omega(T) \) are nonuniversal and contain no singularities near \( T \approx T_c \). The inverse background permeability \( \Omega(T) \)
is only weakly temperature dependent in many cases, and satisfies $\Omega \approx 1$. We assume that the background terms have the same form in both the solid and liquid phases.

(4) The two scaling functions $\phi_S$ and $\phi_L$ are distinct and universal. However, the two phases should become indistinguishable when $B = 0$. Thus, we expect the following equality to hold:

$$f_{KL} \phi_L(0) = f_{KS} \phi_S(0).$$  \hspace{1cm} (9)

(5) The conjugate fields are obtained from Eq. (8):

$$H_\alpha(B, T) = \Omega B + (4\pi f_{K\alpha}/H_{K\alpha})t^\alpha' \phi'_\alpha(Bt^{-2\nu}/H_{K\alpha})$$

where $\alpha = L$ or $S$. We now use Eqs. (2) and (3) to determine the coexistence boundary lines $B_S(T)$ and $B_L(T)$. This is accomplished by noting that all terms in the free energy involving $\phi_\alpha$ explicitly (the superconductivity terms) are small compared to the remaining background terms. (This assumption breaks down very near the zero field transition, where a more careful treatment is required) The following explicit solutions are obtained:

$$B_L(T) = B^* t^{2\nu} + bt^\nu,$$

$$B_S(T) = B^* t^{2\nu} - bt^\nu.$$  

According to our assumptions, $B^* \gg b$ here, while the apparent negative value of $B_S(T)$ (when $T \approx T_c$) is unphysical. The field-like parameters $B^*$ and $b$ are determined from the following equations:

$$f_{KS}\phi_S(B^*/H_{KS}) = f_{KL} \phi_L(B^*/H_{KL}),$$

$$b = (2\pi/\Omega)[f_{KS}/H_{KS})\phi'_S(B^*/H_{KS}) - (f_{KL}/H_{KL})\phi'_L(B^*/H_{KL})].$$

The width of the coexistence region in the $B$-$T$ plane can now be computed along the constant-$T$ path:

$$\Delta B|_T \equiv B_L(T) - B_S(T) = 2bt^\nu.$$  \hspace{1cm} (10)

Similarly, along a constant-$B$ path, the temperature width of the coexistence region is given by leading order by

$$\Delta T|_B = (T_c b/\nu B^*)(B/B^*)^{(1/2\nu) - 1/2}.$$  \hspace{1cm} (11)

Using Eqs. (6)-9, these discontinuities can be related to other quantities of interest. For example, the magnetization discontinuity $\Delta M|_T$ is found to scale in the same way as the magnetization in the 3D XY theory, as first pointed out by Liang et al.

In the $H$-$T$ plane, the phase transition is given by

$$H_m(T) = \Omega B^* t^{2\nu} + [\Omega b + (4\pi f_{KL}/H_{KL})\phi'_L(B^*/H_{KL})]t^\nu,$$

where the $t^\nu$ term is again much smaller than the $t^{2\nu}$ term. The coexistence boundaries in the $H_{ex}$-$T$ plane can then easily be computed using Eq. (4). The entropy discontinuity can be calculated to leading order from Eq. (8). For simplicity, we give the result in terms of $B$:

$$\Delta s|_T = (bB^* \Omega \nu/\pi T_c)(B/B^*)^{(3\nu-1)/2\nu}.$$  \hspace{1cm} (12)

Finally, we show that the material parameters $f_{KS}$ and $f_{KL}$ must be equal. Eq. (6) can first be rewritten as $f_{KL}/f_{KS} = \phi_{KS}(0)/\phi_{KL}(0)$. Since the scaling functions $\phi_{KS}$ and $\phi_{KL}$ are universal, the ratio $\phi_{KS}(0)/\phi_{KL}(0)$ must also be universal. $f_{KL}$ and $f_{KS}$ are therefore related by a universal proportionality constant, which can be absorbed into either $\phi_{KS}$ or $\phi_{KL}$. Therefore $f_{KL} = f_{KS}$.

Comparison with Experiments. We now use published data to obtain preliminary estimates for the 3D XY field parameters $B^*$ and $b$, and thus the width of the coexistence region, for several systems. Additionally, we check the thermodynamic relations (3-6). In order to apply our analysis to real physical situations, it is necessary to assume a particular sample geometry. In accordance with the discussion above, we approximate the differences between ellipsoidal geometries and more realistic plate-like geometries, which are more difficult to treat exactly (23). Although geometrical effects of this type may partially account for the inconsistencies discussed below, we believe that some of the discrepancies may be too large to be attributable to geometry alone. We also make the approximation that $\Omega = 1$.

The first experiments we shall consider, in very pure, optimally-doped YBCO single crystals, typically involve bulk magnetization or specific heat data obtained at constant $T$ or $H_{ex}$. In Ref. (3), Liang et al. observe a discontinuity in $M$ which is well described by the 3D XY theory throughout the studied field range, 5-40 kG. (For simplicity, the different fields are all specified here in units of Gauss.) Using the results above, and assuming $n \approx 0.93$ as appropriate for this sample, we find that $B^* \approx 1.0 \times 10^6$ G and $b \approx 0.66$ G. To take a particular example then, the width of the coexistence region should be equal to $\Delta T|_{H_{ex}} \approx 4 \times 10^{-5}$ K when $H_{ex} = 40$ kG. We have also obtained estimates for $B^*$ and $b$ from two other published magnetization studies of YBCO, with results nearly identical to those given above (3-6). These values may therefore be characteristic of optimally-doped YBCO (6).

According to the estimates given above, the coexistence region may be difficult to resolve along the temperature axis, due to its narrow width. However in the experiments of Schilling et al. (7), estimates for $\Delta H_{ex}|_T$ and $\Delta M|_T$ can be obtained simultaneously, thus allowing Eq. (10) to be tested. The following results are observed when $T = 85$ K: $4\pi \Delta M|_T \approx 0.2$ G and $\Delta H_{ex}|_T \approx 1500$ G. (Similar results are obtained in Ref. (4). Note that the quantity $\Delta T$ studied in Ref. (3) is unrelated
to the quantity $\Delta T\big|_{H_{\text{ex}}}$ discussed above.) According to Eq. (7), the observed value of $\Delta H_{\text{ex}}|_{T}$ is too large by a factor of 7500. On the other hand, Schilling et al. have shown that the Clausius-Clapeyron equation is obeyed in this system. It seems likely therefore that the former discrepancy does not signal the failure of the thermodynamic relations; instead, it may only reflect sample dependent effects, which may be generically identified as “broadening.” Further experiments are required to resolve this issue. In any event, the predicted width of the coexistence region in YBCO appears to be much narrower than the typical experimental resolution. Observed jumps in the different measured quantities should therefore be treated as true discontinuities.

Bulk measurements of magnetization discontinuities have also been performed in pure BSCCO single crystals. (For example, Ref. [12].) However, as our second example we consider the experiments of Zeldov et al., which involve small Hall sensors [3]. These devices are capable of measuring the local field $B$, thus avoiding many problems due to sample inhomogeneity. The following approximate information can be obtained from Ref. [3] for $T \approx 80 \, \text{K}$: $\Delta B|_{H_{\text{ex}}} \approx 0.4 \, \text{G}$, $\Delta T|_{H_{\text{ex}}} < 3 \, \text{mK}$, $\Delta(B - H_{\text{ex}})|_{T} \approx 0.4 \, \text{G}$, and $\partial H_{\text{ex}}/\partial T \approx -6 \, \text{G/K}$. The appropriate demagnetizing factor for this sample is $n \approx 0.71$. Using these estimates, the geometry-independent ($\Omega \approx 1$) relation $\Delta(B - H_{\text{ex}})|_{T} \approx \Delta B|_{H_{\text{ex}}}$ is well satisfied. The relation $\Delta(B - H_{\text{ex}})|_{T} = -(1 - 1/n)\Delta H_{\text{ex}}|_{T}$ is not quite satisfied; this small discrepancy may be attributable to geometric effects. However, relation [3] between $\Delta B|_{H_{\text{ex}}}$ and $\Delta T|_{H_{\text{ex}}}$ shows that the observed discontinuity $\Delta T|_{H_{\text{ex}}}$ is at least 50 times sharper than predicted. Similarly, if the estimates given above for $\Delta T|_{H_{\text{ex}}}$ and $\Delta H_{\text{ex}}|_{T}$ are taken as equalities, the geometry-independent result of Eq. (7) is violated by a factor of more than 20. To improve this situation, we would need to assume that $\Delta H_{\text{ex}}|_{T}$ was 20 times smaller than estimated. Unfortunately, such a modification leads to discrepancies in other thermodynamic relations.

The discrepancies observed in the local $B$ measurements of BSCCO are of a different nature than those in YBCO. In the latter case, the observed width of the two-phase region was much too large, a fact which can be attributed to broadening. In the BSCCO case, the observed two-phase region was much too narrow, a result which cannot be explained by any obvious thermodynamic arguments. However, it is instructive to continue with the present analysis to obtain the 3D XY parameters appropriate for BSCCO. According to Ref. [3], a reasonable estimate for $B^*$ is given by $B^* \approx 1000 \, \text{G}$. This result is not affected by the inconsistencies described above, and is corroborated by other experiments. Assuming the value given above for $\Delta(B - H_{\text{ex}})|_{T}$ to be the most reliable estimate of the discontinuities in BSCCO, we then obtain $b \approx 2.8 \, \text{G}$. From Ref. [12] (using low transverse fields, Fig. 10) we obtain a slightly different result of $b = 0.8 \, \text{G}$.

Conclusions. We conclude by discussing two points.

(1) The results given above for first order melting near the 3D XY critical point differ in several ways from earlier analyses aimed at fluid-like critical points [15]: (i) in the 3D XY scaling ansatz, it is the density-like variable ($B$), not the pressure-like variable ($H$), which appears naturally in the scaling functions; (ii) in contrast with the fluid system, neither of the scaling variables $B$ or $H$ are directly related to the superconducting order parameter; (iii) although a relation like $H_{k,\text{S}} = H_{k,\text{L}}$ occurs in fluid-like scaling theories, the same cannot be proven for the vortex-solid melting transition in the absence of a more microscopic theory.

(2) Our analysis should also apply to computer simulations aimed at understanding the first order transition [16]. Many of these simulations are performed by varying the temperature at fixed $B$. In this case, a two-phase region should be observed, with width $\Delta T|_{B}$. If the value of $B$ is small enough for 3D XY scaling to be valid, this width should be described by Eq. (11), and the entropy jump by Eq. (12).

In summary, we have presented both general and specific (3D XY) theories of the two-phase region for the vortex-solid melting transition. We find that in typical YBCO samples, the solid-liquid coexistence region may be too small to be observed experimentally. However, based upon available estimates for the discontinuity of $B$, the region should be easily detected in BSCCO using precision measurements. The observations of two-phase coexistence and thermodynamic self-consistency are both crucial for confirming the first order nature of the melting transition. The recent experiment of Schilling et al. provides a check of the self-consistency relations; in this case the Clausius-Clapeyron equation is well satisfied, although open questions remain, regarding other relations. It is hoped that future experiments may address this issue. Additionally, the scaling of the coexistence region provides information regarding the most fundamental fluctuations associated with superconductivity, which are governed by the 3D XY critical point.

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