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First-order melting of the vortex lattice in an anisotropic superconductor in a magnetic field with arbitrary direction

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Abstract. We calculate the angular dependence of the transition line of the first-order melting in strong type-II superconductors using an angle-dependent nonperturbative model for the critical behaviour in three-dimensional anisotropic superconductors and a self-consistent Hartree treatment of correlations along the direction in which fluctuations occur. The results are in good agreement with experiments performed on untwinned single crystals of $YBa_2Cu_3O_{7-\delta}$.

1. Introduction

The behaviour of vortices in high-temperature superconductors (HTSCs) has been widely discussed in many recent papers. The growing interest in the study of vortex behaviour in these materials stems from the richness and complexity of the new physics of the vortex state as well as the considerable possibilities for technological applications.

For conventional superconductors the Abrikosov mean-field theory predicts the formation of a vortex lattice in the mixed state which undergoes a second-order phase transition at the upper critical field $H_{c2}(T)$. In HTSCs however, thermal fluctuations occur over a broad temperature–field interval with the consequence that new transition lines appear. These lines were experimentally observed and attributed to first-order melting of the flux lattice. Many experimental studies of untwinned and twinned single crystals in the presence of moderate magnetic fields [1–7] have shown that the melting line in the mixed state of HTSCs corresponds to a first-order transition.

Safar *et al* [2, 3] have reported current–voltage measurements made on clean, untwinned $YBa_2Cu_3O_{7-\delta}$ single crystals; they found that for applied magnetic fields below a certain value ($\sim$10 T) the melting transition in the vortex lattice is hysteretic in both temperature and magnetic field, whereas for applied magnetic fields above that value the phase boundary (characterizing the first-order melting transition) sharply changes slope, giving way to a second-order transition.

Kwok *et al* [4, 5] have reported experimental results of AC resistivity measurements made on untwinned and twinned single crystals of $YBa_2Cu_3O_{7-\delta}$ which show a transition line attributable to melting for an untwinned single crystal in the presence of applied magnetic fields both parallel and perpendicular to the direction of anisotropy of the crystal (the c-axis). For twinned crystals it was shown that the magnitude of the sharp drop in the magnetoresistivity associated with the first-order vortex melting transition is reduced but not

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destroyed by the presence of a few twin boundaries. On the other hand, when a sufficient number of point defects are present in an untwinned crystal, the first-order melting transition is replaced by a second-order transition at lower temperature. Similar results were obtained by Ghumlouch *et al* [6] from the observation of vortex lattice melting in both untwinned and twinned single crystals of $YBa_2Cu_3O_{7-\delta}$ by means of Seebeck-effect measurements which do not require a transport current.

More recently Welp *et al* [7] have observed discontinuous jumps of the magnetization in an untwinned single crystal of $YBa_2Cu_3O_{7-\delta}$, whose location in the H–T phase diagram coincides with the location of the resistivity drops measured for the same sample. These results demonstrate the existence of a first-order melting transition of the flux line lattice, since the discontinuity in the magnetization is one of the defining characteristics of a magnetic first-order transition.

Tesanovic *et al* [8–11] have developed a nonperturbative theory of critical behaviour for anisotropic superconductors for both two- and three-dimensional (2D and 3D) systems in the presence of strong magnetic fields applied in the direction parallel to the c-axis (perpendicular to the ab-planes), describing the critical behaviour by means of an interacting particle system with long-ranged multiple-body forces (a dense vortex plasma). The superconducting transition corresponds to the liquid–solid transition in the dense vortex plasma (DVP). This theory uses a nonperturbative approach to the Ginzburg–Landau (GL) free-energy functional in which the order parameter is expanded in terms of the lowest Landau levels (LLL). The scale invariance of the DVP leads to a universal character of the vortex melting line at which the superconducting transition occurs.

Herbut and Tesanovic [12] have calculated the transition line of the first-order melting of the vortex lattice in a 3D type-II superconductor in the presence of moderate magnetic fields along the c-axis by using the results from the density functional theory of vortex melting in two dimensions [13] and a self-consistent Hartree treatment of correlations along the c-axis. In the calculation of the melting line carried out in reference [12] the Lindemann criterion is not used, in contrast with preceding work [14, 15].

In a recent study [16] the nonperturbative Tesanovic theory for the critical behaviour of 3D anisotropic superconductors has been generalized for an arbitrary direction of the applied magnetic field. In this paper we use this generalized form of the Tesanovic's theory to obtain the angular dependence of the melting line in a 3D anisotropic superconductor.

In section 2 the angle-dependent forms of the GL free energy and the coupling constant are presented. Section 3 displays the calculation of the angular dependence for the melting line. Finally in section 4 the main results of the work are discussed and compared with experiment.

2. Angular dependence of the free energy

For a strongly type-II anisotropic 3D superconductor with fluctuations of the magnetic field neglected (the GL parameter $\kappa \gg 1$), in the presence of an applied magnetic field with arbitrary direction, the partition function can be written in the form

$$Z = \int \mathrm{D}\Psi\ \mathrm{D}\Psi^*\ \exp\left(-\frac{F_{GL}}{k_B T}\right) \tag{1}$$

with F_{GL} being the GL free energy given [8] by

$$F_{GL} = \int \mathrm{d}^3 r\ \left[\alpha(T)|\Psi(\boldsymbol{r})|^2 + \frac{\beta}{2}\,|\Psi(\boldsymbol{r})|^4 + \sum_\mu \gamma_\mu \left|\left(\partial_\mu + \frac{2e\mathrm{i}}{c}A_\mu\right)\Psi(\boldsymbol{r})\right|^2\right] \tag{2}$$

where $\alpha(T)$, β and γ_μ are the usual GL coefficients and μ runs over the three directions x, y and z. If we consider the above free energy in the subspace spanned by the LLL it is possible to rewrite the problem in a more suitable form.

We expand Ψ in terms of the LLL and choose the gauge [16]

$$\boldsymbol{A} = \frac{B}{2}(z\sin\theta - y\cos\theta, x\cos\theta, -x\sin\theta) \tag{3}$$

to describe the microscopic magnetic field $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$ which forms an angle θ with the z-direction (c-axis). By introducing the following coordinate transformation:

$$\begin{bmatrix} y_1 \\ z_1 \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \varepsilon\sin\theta & \varepsilon^{-1}\cos\theta \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix} \tag{4}$$

and also carrying out the changes $\sqrt{\delta}x \to \bar{x}$, $y/\sqrt{\delta} \to \bar{y}$ and $z_1 \to \bar{z}$, the GL free energy in the LLL subspace is transformed to

$$\frac{F_{GL}}{k_B T} = \frac{\epsilon}{k_B T\delta^2}\int \mathrm{d}^2\bar{r}\ \mathrm{d}\bar{z}\ \left[\bar{\alpha}(T,H,\theta)\,|\Psi|^2 + \frac{\beta}{2}\,|\Psi|^4 + \gamma_{\bar{z}}\,|\partial_{\bar{z}}\Psi|^2\right] \tag{5}$$

where $\bar{\alpha}(T,H,\theta) = \alpha(T)[1 - H/H_{c2}(T,\theta)]$, $\epsilon^2 = m_{ab}/m_c$ is the mass anisotropy ratio, $\delta^2 = \cos^2\theta + \epsilon^2\sin^2\theta$ is the angle-dependent anisotropy parameter and $\gamma_{\bar{z}} = \delta^2\gamma_c/\epsilon^2$. For an explicit evaluation of the free energy, the integral and derivative along the $\bar{z}$-axis may be defined on a set of intervals of size Λ and then at the end of the calculation the limit $\Lambda \to 0$ is to be taken. However, it is necessary to define a cut-off length of the order of the correlation length, because the exact free energy is actually divergent in the $\Lambda \to 0$ limit [10]. In a first approximation we assume $\Lambda = \xi_{\bar{z}}$ as that cut-off length and use a suitable rescaling for the fields and lengths, obtaining the free energy in the form [16]

$$\frac{F_{GL}}{k_B T} = \int \mathrm{d}^2\bar{r}\ \mathrm{d}\bar{z}\ \left[g(T,H,\theta)|\Psi|^2 + |g(T,H,\theta)||\partial_{\bar{z}}\Psi|^2 + \frac{1}{4}|\Psi|^4\right] \tag{6}$$

where the coupling constant $g(T,H,\theta)$ is defined by

$$g(T,H,\theta) = \frac{\sqrt{\epsilon}}{\delta}\left(\frac{\pi l^2\xi_{\bar{z}}}{\beta k_B T}\right)^{1/2}\bar{\alpha}(T,H,\theta) = \left(\frac{\pi l^2\xi_\theta}{\beta k_B T}\right)^{1/2}\bar{\alpha}(T,H,\theta) \tag{7}$$

where $\xi_{\bar{z}} = (\delta/\epsilon)(\gamma_c/|\bar{\alpha}(T,H,\theta)|)^{1/2}$ and $\xi_\theta(T,H)$ is the correlation length along the direction of the field at an angle θ with respect to the c-axis, given by

$$\xi_\theta(T,H) = \frac{1}{\delta}\left(\frac{\gamma_c}{|\bar{\alpha}(T,H,\theta)|}\right)^{1/2}. \tag{8}$$

Equation (8) is the generalized form of the temperature- and field-dependent correlation length defined in reference [8]. This equation has the limits $\xi_c(T,H)$ and $\xi_{ab}(T,H)$ for the angles $\theta = 0$ and $\theta = \pi/2$ respectively. The properties of the DVP are determined by the value of the coupling constant. The value $g(T,H,\theta) = 0$ corresponds to the mean-field-theory upper critical field $H_{c2}(T,\theta)$, whereas the solid–liquid transition may be obtained from the melting value $g(T,H,\theta) = g_M < 0$. In the particular case where $\theta = 0$, the coupling constant is reduced to that obtained by Tesanovic for the case of a magnetic field applied along the c-axis of the crystal [8].

3. Angular dependence of the melting line

In order to obtain an explicit expression for the melting line, we take $\alpha(T)$, β and γ_c from equation (5) as phenomenological parameters and introduce the rescaling $\psi \to (4\pi l^2 \beta d/k_B T\delta)^{-1/4}\psi$, $\bar{r} \to \sqrt{2\pi} l \bar{r}$ and $\bar{z} \to (\delta d/\epsilon)\bar{z}$, where l is the magnetic length for charge $2e$ and d is typically the spacing between the pairs of CuO_2 planes. Thereby the GL free energy becomes

$$\frac{F_{GL}}{k_B T} = \int d^2\bar{r}\; d\bar{z}\; \left[g_\alpha |\Psi|^2 + g_\gamma |\partial_{\bar{z}}\Psi|^2 + \frac{1}{4}|\Psi|^4 \right] \tag{9}$$

in which $g_\alpha = (\pi l^2 d/\beta k_B T\delta)^{1/2}\bar{\alpha}(T, H, \theta)$ and $g_\gamma = (\pi l^2 d/\beta k_B T\delta)^{1/2}(\gamma_c/d^2)$.

The transition line in the H–T phase diagram is obtained by using the correlation length $\xi_{\bar{z}}$ calculated from a self-consistent Hartree treatment [12] of equation (9):

$$\xi_{\bar{z}} = \left(\frac{g_\gamma}{g_\alpha + \langle |\Psi|^2 \rangle /4} \right)^{1/2} \tag{10}$$

where the thermal average is determined by

$$\langle |\Psi|^2 \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{dk}{g_\gamma k^2 + g_\alpha + \langle |\Psi|^2 \rangle /4}. \tag{11}$$

The phase boundary corresponding to the melting line of the vortex lattice is determined by the condition $g(T, H, \theta) = g_M$. In terms of g_α this condition takes the form

$$g_\alpha \xi_{\bar{z}}^{1/2} = g_M \tag{12}$$

with $\xi_{\bar{z}}$ measured in units of $\delta d/\epsilon$. In the 3D regime, $\xi_c > 1$ (in units of d), and therefore $\xi_{\bar{z}} > 1$ in this case. The value of g_M is assumed to be a universal number by Herbut and Tesanovic [12] which takes the value $g_M = -6.5$ [13] for both the 2D and 3D cases, as the vortex transition in 3D systems is driven by the same mechanism as in the 2D case, since the melting of the vortex lattice is effectively 2D in nature in both cases [12].

The explicit form of the melting line is reached by simultaneously solving equations (10), (11) and (12), to obtain

$$t + \delta h + \left(\frac{2c\kappa_{ab}^2 \xi_{ab}^2(0)}{\xi_c(0)\Lambda_T} \right)^{2/3} (\delta t h)^{2/3} = 1 \tag{13}$$

where $c^2 = g_M^4(\sqrt{1 + 1/(2g_M^2)} - 1)/2$, $\kappa_{ab} = \lambda_{ab}/\xi_{ab}$ is the GL parameter and $\Lambda_T = \phi_0^2/(16\pi^2 k_B T_{c0})$ with ϕ_0 being the flux quantum. The variables $t = T/T_{c0}$ and $h = H/H_{c2}^c(0)$ are, respectively, the temperature in units of the critical temperature at zero field and the magnetic field normalized to the upper critical field along the c-axis at $T = 0$. In the particular case where $\theta = 0$ (the applied magnetic field parallel to the c-axis), $\delta = 1$ and equation (13) reduces to that obtained by Herbut and Tesanovic [12]. One observes that equation (13) corresponds to an angular scaling function in the variables t and $h_\theta = H/H_{c2}(T, \theta) = \delta h$ for the first-order melting line in anisotropic 3D superconductors. In the next section the curves obtained from equation (13) are plotted for several orientations of the magnetic field and compared with experiments performed on $YBa_2Cu_3O_{7-\delta}$, since this material presents 3D scaling behaviour [17, 18].

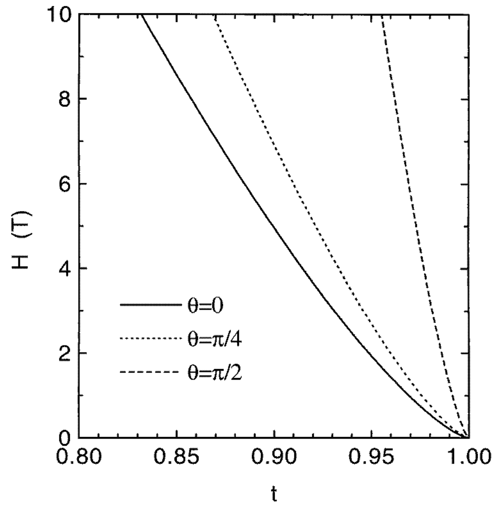

Figure 1. Melting lines of the vortex lattice calculated from equation (13) for three directions of the applied magnetic field. The same values as in reference [11] were used for the physical parameters.

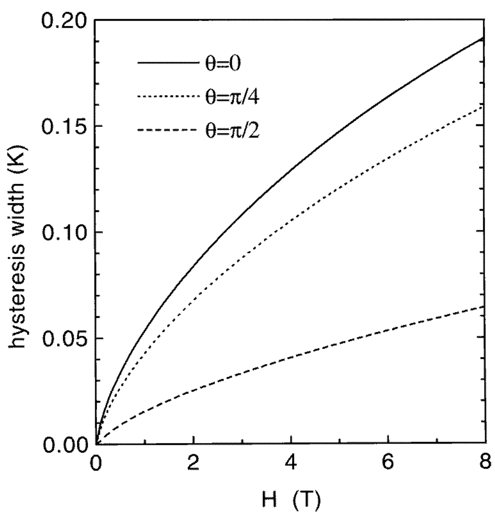

Figure 2. The field dependence of the temperature width of the hysteresis due to superheating of the low-temperature phase for three directions of the applied magnetic field. The solid line corresponds to the hysteresis width calculated in reference [11] for applied magnetic fields parallel to the *c*-axis. The hysteretic nature characterizing the first-order melting transitions is observed for all of the magnetic field directions.

4. Results and discussion

The present work analyses the angular dependence of the melting line using the GL theory within the LLL approximation. The main result is equation (13) which gives the transition line for an arbitrary direction of the magnetic field. Figure 1 shows the calculated melting lines for three different directions of the applied magnetic field. We use the same values as are used in reference [12] for the physical parameters. The solid line corresponds to the theoretical transition line calculated in reference [12] which is in good agreement with the experimental data of reference [3].

Herbut and Tesanovic [12] neglected the supercooling of the vortex liquid upon lowering the temperature and took only the superheating of the solid phase into account in order to calculate the thermodynamic hysteresis width in temperature as a function of the magnetic field in a 3D anisotropic superconductor by using the superheating condition $g_{SH} = -6.25$ as predicted by the density functional theory for the 2D vortex system [13]. The functional dependence of their calculated hysteresis width agrees with the observation from resistivity measurements [2, 3] but the result is roughly an order of magnitude larger, which they attribute to the effects of disorder and lack of equilibration in the experiment [12]. In order to obtain a qualitative picture of the hysteresis width for the different directions of the applied magnetic field, we use the same criterion as in reference [12] to estimate this width. Figure 2 displays the hysteresis width in temperature for several directions of the applied magnetic field which shows the hysteretic character of the transition for all of the directions of the applied magnetic field in the range of the fields studied.

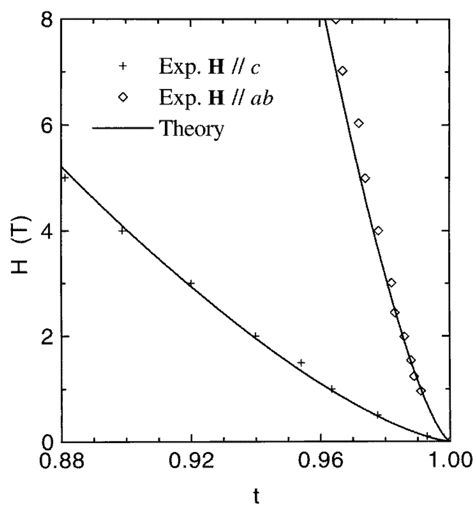

Figure 3. Theoretical melting lines for applied magnetic fields parallel and perpendicular to the c-axis (solid lines) compared with the experiments of reference [4]. The crosses and diamonds correspond to the experimental data of Kwok *et al* for magnetic fields parallel and perpendicular to the c-axis, respectively.

In figure 3 the calculated melting lines for applied magnetic fields in the directions parallel and perpendicular to the c-axis are compared with the experimental data from reference [4], showing a good agreement. For $g_M = -6.5$ we set $T_{c0} = 92.33$ K, $H_{c2}^{c}(0) = 166.7$ T and $\epsilon^{-1} = 7.7$ [4], the correlation length in the c-direction was assumed to be $\xi_c(0) = 3.0$ Å [12] and the best agreement with the experimental data is obtained for a GL parameter $\kappa = 50$, which is a reasonable value. For $\kappa = 55$ [4] the value of g_M must be renormalized to $g_M = -5.3$ in order to obtain good agreement with the experiments.

In conclusion, we have generalized the Herbut and Tesanovic calculation [12] for the first-order melting line for 3D anisotropic superconductors. The angular dependence of the melting line is obtained and compared with experimental data for fields parallel to the c-axis and parallel to the *ab*-planes, showing good agreement.

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