Vortex fluctuations in layered superconductors and thin films

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We determine the free energy of a vortex line within the Ginzburg-Landau formalism. Besides the usual translational modes we also take account of self-fluctuations of the order parameter in the calculation of the vortex free energy. The latter are due to the internal structure of a vortex line and lead to an observable downward renormalization of the lower critical-field line $H_{c_1}(T)$ in strongly layered superconductors. In thin films the self-fluctuations of the vortex lead to a reduction in the power-law exponent of the current-voltage characteristic. We argue that in a three-dimensional system the spontaneous creation of vortex lines cannot occur.

I. INTRODUCTION

Fluctuation effects in superconductors have been the subject of many past and recent investigations.[1–7] Whereas in conventional superconductors fluctuations play only a minor role, the situation is different in the high-temperature superconductors where thermal fluctuations are relevant deep into the phase diagram well below the mean-field transition at $H_{c_2}(T)$.[8] As usual we have to distinguish between the critical fluctuations close to the mean-field transition (Ginzburg region) and the Gaussian fluctuations outside of this regime. The width of the critical regime depends on the magnetic field and on the dimensionality of the system (see below) and is of the order of 1 K wide in the oxides. The fluctuation contributions to the thermodynamic as well as to various transport properties have been analyzed both experimentally[9–11] and theoretically[5–7] and good agreement has been obtained in their scaling behavior. Even outside the critical region fluctuations play a crucial role in the high-T_c's leading to novel phenomena such as the melting of the Abrikosov lattice.[12,13] Here we are interested in the effects fluctuations have on an individual vortex line outside of the critical region.

An immediate consequence of fluctuations is the lowering of the free energy of a vortex line due to its motional degrees of freedom. In two dimensions this effect leads to the well-known Kosterlitz-Thouless transition[14] above which the quasi-long-range order of the Berezinskii phase[15] is lost due to the spontaneous creation of free vortices. At the transition, the entropy term in the free energy arising from the translational fluctuations, $-T\ln(L^2/\xi^2)$, exactly cancels the vortex self-energy $d\varepsilon_l$. Here L is the system size, d the film thickness, ξ is the coherence length, and $\varepsilon_l = (\Phi_0/4\pi\lambda)^2\ln(L/\xi)$ is the line energy of the vortex excitation. In a three-dimensional system the system size L has to be replaced by some appropriate cutoff length due to the screening and both the line energy as well as the entropy term are reduced. Still, as the line energy vanishes on approaching the transition, the free energy of the vortex line drops to zero at some point T_s within the superconducting region, and the question of a possible spontaneous creation of vortex lines arises. Recently the latter has been proposed to occur by Bulaevskii, Ledvij, and Kogan,[16] with a temperature T_s sufficiently below the mean-field transition to be observable in strongly layered high-temperature superconductors. The study of Bulaevskii *et al.* has been formulated within the continuum elastic theory of the vortex system which inherently limits the fluctuation spectrum to the translation modes. In the present paper we give a complete description of the problem in terms of the more fundamental Ginzburg-Landau (GL) theory.

Within the GL formulation the vortex line is a structured object with a spacially dependent order parameter. Fluctuations of the order parameter around the mean-field vortex solution (we call them self-fluctuations) then lead to an additional contribution to the vortex free energy. In fact, these self-fluctuation corrections always dominate over the translational fluctuations, leading to an even larger reduction of the vortex free energy than the one obtained by Bulaevskii *et al.* In spite of this very encouraging result, we conclude from our analysis that no spontaneous creation of vortex lines can take place in a three-dimensional system.

The effects described below in the main body of the paper are observable in the case of strongly layered materials such as the Bi- or Tl-based compounds. In a first step (Sec. II) we derive a suitable expression for the free energy of a flux line in terms of the fluctuation spectra

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of the homogeneous (no vortex) and of the inhomogeneous (one vortex) system. In Sec. III we determine the relevant eigenvalues and calculate the free energy of the vortex line. It is convenient to combine the self-fluctuation term with the mean-field line energy into a new renormalized line energy $\varepsilon_l^R(T)$. The latter goes to zero at a new fluctuation-corrected transition temperature $T_{c0} < T_0$ which we calculate explicitly in Sec. IV. We then discuss our results in Sec. V, the downward bending of the lower critical field line $H_{c_1}(T)$ on approaching the transition in a layered superconductor and the downward renormalization of the characteristic power-law exponent in the current-voltage characteristic of a thin film. Furthermore, we discuss the absence of the spontaneous vortex creation in three dimensions (3D). We compare our results with recent experimental measurements of the lower critical field line $H_{c_1}(T)$ by Brawner *et al.*[17] on a $Bi_2Sr_2CaCu_2O_8$ (BSCCO) single crystal and discuss their findings in the light of the present theoretical analysis. Finally we conclude in Sec. VI.

II. THERMODYNAMICS OF VORTEX FLUCTUATIONS

Our starting point is the Ginzburg-Landau functional in the Lawrence-Doniach[18] form describing the free energy of a layered superconductor:

$$\mathcal{F}[\Delta_n] = \frac{\varepsilon_0 d}{2\pi} \sum_{n=1}^{N} \int d^2r \Big[-|\Delta_n|^2 + \frac{1}{2}|\Delta_n|^4 + |\nabla\Delta_n|^2 + \frac{\gamma}{2}|\Delta_{n+1} - \Delta_n|^2 \Big], \tag{1}$$

with $\Delta_n(\mathbf{r}) = \Psi_n(\mathbf{r})/\Psi_\infty$, the normalized order parameter of the nth layer. Here, the distances $\mathbf{r}$ within the layers are measured in units of ξ, the planar coherence length. The energy scale is determined by $\varepsilon_0 = (\Phi_0/4\pi\lambda)^2$, where λ is the London penetration depth for the planar currents. The coupling between the layers is described by the parameter $\gamma = 2\xi_c^2/d^2 = 2\xi^2/\Lambda^2$, with d the interlayer distance and ξ_c the coherence length in the z direction. The Josephson length Λ is given by the relation $\Lambda = d\,(\xi/\xi_c)$. Contributions from the electromagnetic field are neglected since we consider the strong type-II limit with a large Ginzburg-Landau parameter $\kappa = \lambda/\xi \gg 1$. The temperature dependence of the main energy scale is given by $\varepsilon_0(\tau) = \varepsilon_0(0)\,\tau$, with $\tau = 1 - T/T_0$, and T_0 is the bare transition temperature. Whereas the mean-field line energy of a vortex perpendicular to the layers is given by the expression $\varepsilon_l = \varepsilon_0 \ln\kappa$, its exact thermodynamic free energy has to be determined from the definition

$$F = -T \ln\left(\frac{\mathcal{Z}_v}{\mathcal{Z}_0}\right), \tag{2}$$

where the partition functions $\mathcal{Z}_v$ and $\mathcal{Z}_0$ correspond to the situations with and without a flux line present. Both partition functions can be calculated from the functional integral representation

$$\mathcal{Z} = \int \prod_{n=1}^{N} (\mathcal{D}\Delta_n) \exp\left(-\frac{\mathcal{F}[\Delta_n]}{T}\right) \tag{3}$$

and making use of the corresponding free energy functional. Away from the immediate vicinity of the phase transition we can assume only small fluctuations in the order parameter and use a Gaussian approximation in the calculation of the free energy (2). For the vortex free state the order parameter takes the form

$$\Delta_n = 1 + a_n(\mathbf{r}) + ib_n(\mathbf{r}), \tag{4}$$

with a_n and b_n describing the (small) fluctuations in the modulus and in the phase. In the presence of a vortex we write instead

$$\Delta_n = \Delta_v(r)e^{i\phi} + [a_n(\mathbf{r}) + ib_n(\mathbf{r})]e^{i\phi}, \tag{5}$$

where ϕ is the azimuthal angle, i.e., $\mathbf{r} = (r,\phi)$. The first term in Eq. (5) is the equilibrium solution for a vortex going to zero on a scale $r < 1$. On intermediate distances the order parameter is suppressed due to the flow of screening currents:

$$\Delta_v^2(r) = 1 - 1/r^2 \quad \text{for} \quad 1 < r < \lambda/\xi. \tag{6}$$

Substituting the ansatz (5) into the Lawrence-Doniach functional (1) and dropping higher-order terms we obtain

$$\mathcal{F}_v = \mathcal{F}_0 + \varepsilon_0 L_z \ln\kappa + \delta\mathcal{F}_0 + \delta\mathcal{F}_v. \tag{7}$$

Here, the first two terms are the mean-field energies for the homogeneous state ($\mathcal{F}_0$) and for the vortex line ($\varepsilon_l L_z = \varepsilon_0 L_z \ln\kappa$; L_z denotes the sample size along the z axis), whereas the last two terms describe the fluctuation contributions

$$\delta\mathcal{F}_0 = \frac{\varepsilon_0 d}{2\pi} \sum_n \int d^2r \left\{ 2a_n^2 + (\nabla a_n)^2 + (\nabla b_n)^2 + \frac{\gamma}{2}(a_{n+1} - a_n)^2 + \frac{\gamma}{2}(b_{n+1} - b_n)^2 \right\} \tag{8}$$

and

$$\delta\mathcal{F}_v = \frac{\varepsilon_0 d}{2\pi} \sum_n \int d^2r \left\{ \left(3\Delta_v^2 - 3 + \frac{1}{r^2}\right) a_n^2 + \left(\Delta_v^2 - 1 + \frac{1}{r^2}\right) b_n^2 + \frac{2}{r^2}\left(a_n \frac{\partial b_n}{\partial\phi} - b_n \frac{\partial a_n}{\partial\phi}\right) \right\}. \tag{9}$$

For the vortex free state the total free energy involves only the terms $\mathcal{F}_0 + \delta\mathcal{F}_0$. In a next step let us formally diagonalize the two fluctuation contributions $\delta\mathcal{F}_0$ and $\delta\mathcal{F}_0 + \delta\mathcal{F}_v$ ($g = a$ or $g = b$):

$$\frac{\delta}{\delta g}\delta\mathcal{F}_0 = \mu^{(1,2)} g \tag{10a}$$

and

$$\frac{\delta}{\delta g}\{\delta\mathcal{F}_0+\delta\mathcal{F}_v\}=M^{(1,2)}g, \tag{10b}$$

where we have introduced the eigenvalues $\mu^{(1,2)}$ and $M^{(1,2)}$ for the fluctuation modes of the homogeneous and of the inhomogeneous state. The superscript refers to the amplitude (1) and to the phase dominated (2) mode, respectively. Using the eigenmode representation for the fluctuation energies we can rewrite the ratio of partition functions into the form[19]

$$\frac{\mathcal{Z}_v}{\mathcal{Z}_0}=\exp\left[-\frac{\varepsilon_l L_z}{T}\right]\frac{\prod\sqrt{\mu}}{\prod\sqrt{M}}. \tag{11}$$

The products have to be taken over all the eigenvalues of the fluctuation modes. From the definition (2) of the vortex free energy we then conclude that the vortex fluctuations will change the free energy to deviate from the mean-field result $\varepsilon_l L_z$. In the next section we will estimate the magnitude of this effect.

III. CALCULATION OF THE VORTEX FREE ENERGY

The eigenvalue problem (10) for the fluctuation modes is most easily tackled by going over to a Fourier representation both for the planar coordinate $[\mathbf{q}=(q_x,q_y)]$ as well as along the z axis:

$$\Delta_n(\mathbf{r})=\frac{d}{L_z}\sum_{k=-\pi}^{\pi}\Delta_k(\mathbf{r})e^{ikn}=\int_{-\pi}^{\pi}\frac{dk}{2\pi}\Delta_k(\mathbf{r})e^{ikn}. \tag{12}$$

The homogeneous problem then is trivially solved and the two eigenvalues are given by [see Eqs. (8) and (10a)]

$$\mu^{(1)}_{\mathbf{q}k}=2+\mu^{(2)}_{\mathbf{q}k}\quad\text{and}\quad\mu^{(2)}_{\mathbf{q}k}=q^2+\gamma\left[1-\cos(k)\right], \tag{13}$$

with $\mu^{(1)}$ corresponding to the (massive) moduluslike and $\mu^{(2)}$ to the (massless) phaselike mode. The corresponding eigenvalues for the vortex state are determined by the (real-space) equations

$$-\nabla^2 a_k+2a_k+\left(\frac{1}{r^2}-3+3\Delta_v^2\right)a_k+\frac{2}{r^2}\frac{\partial b_k}{\partial\phi}=\left[M-\gamma(1-\cos k)\right]a_k \tag{14a}$$

and

$$-\nabla^2 b_k+\left(\frac{1}{r^2}-1+\Delta_v^2\right)b_k-\frac{2}{r^2}\frac{\partial a_k}{\partial\phi}=\left[M-\gamma(1-\cos k)\right]b_k. \tag{14b}$$

Again, this system of equations has two different solutions describing amplitude and phase modes. The problem to be solved is essentially a scattering problem for a two-component wave function scattered off a centrally symmetric potential. The spectrum involves "bound" as well as "scattering" states, whereby the latter ones give the dominant contribution to the partition function in (2). The asymptotic ($r\gg 1$) form of the moduluslike eigenfunctions is given by

$$a_1(\mathbf{r})=e^{i\mathbf{q}\cdot\mathbf{r}}\quad\text{and}\quad b_1(\mathbf{r})=\frac{i(\mathbf{q}\times\mathbf{r})_z}{r^2}e^{i\mathbf{q}\cdot\mathbf{r}}, \tag{15a}$$

whereas the phaselike eigenfunctions behave like

$$b_2(\mathbf{r})=e^{i\mathbf{q}\cdot\mathbf{r}}\quad\text{and}\quad a_2(\mathbf{r})=\frac{i(\mathbf{q}\times\mathbf{r})_z}{r^2}e^{i\mathbf{q}\cdot\mathbf{r}}. \tag{15b}$$

Projecting the eigenvalue equations (14a) and (14b) onto the "incoming" plane wave $\exp(i\mathbf{q}\cdot\mathbf{r})$ and using the normalization condition $\int d^2r\,a_1e^{-i\mathbf{q}\cdot\mathbf{r}}=\int d^2r\,b_2e^{-i\mathbf{q}\cdot\mathbf{r}}=L_xL_y$, we can derive the following relations for the desired eigenvalues:

$$M^{(1)}_{\mathbf{q},k}-\mu^{(1)}_{\mathbf{q},k}=\int\frac{d^2r}{L_xL_y}e^{-i\mathbf{q}\cdot\mathbf{r}}\left\{\left(\frac{1}{r^2}-3+3\Delta_v^2\right)a_1+\frac{2}{r^2}\frac{\partial b_1}{\partial\phi}\right\} \tag{16a}$$

and

$$M^{(2)}_{\mathbf{q},k}-\mu^{(2)}_{\mathbf{q},k}=\int\frac{d^2r}{L_xL_y}e^{-i\mathbf{q}\cdot\mathbf{r}}\left\{\left(\frac{1}{r^2}-1+\Delta_v^2\right)b_2-\frac{2}{r^2}\frac{\partial a_2}{\partial\phi}\right\}. \tag{16b}$$

The main contribution to the above integrals comes from the interval $1<r<\lambda/\xi$ which gives rise to a logarithmic divergence. Using the dependence (6) for the order parameter Δ_v as well as the asymptotic forms (15) for the eigenfunctions, the integrations in (16) can be performed explicitly and we obtain the results

$$M^{(1)}_{\mathbf{q},k}=\mu^{(1)}_{\mathbf{q},k}+2\pi\frac{q^2-2}{L_xL_y}\ln\kappa \tag{17a}$$

and

$$M^{(2)}_{\mathbf{q},k}=\mu^{(2)}_{\mathbf{q},k}-2\pi\frac{q^2}{L_xL_y}\ln\kappa \tag{17b}$$

for the eigenvalues of the amplitude and phase fluctuation modes in the vortex state. In addition to these *self-fluctuation* modes we also have to take into account the planar *translational* vortex modes, $\nabla[\Delta_v(\mathbf{r})\exp(i\phi)]$. For these modes, only the relative positions of the vortex cores in the different layers are important. Consequently, the left-hand side of the equations (14) is zero and the eigenvalues are determined by the finite coupling between the layers

$$M^x_k=M^y_k=\gamma(1-\cos k). \tag{18}$$

We can now calculate the desired ratio of partition functions as given in (11). Making use of the results (13), (17), and (18) for the eigenvalues μ and M we obtain

$$\frac{\mathcal{Z}_v}{\mathcal{Z}_0} = \exp\left(-\frac{\varepsilon_l L_z}{T}\right) \zeta_{\rm tr}\, \zeta_{\rm self}, \tag{19}$$

with the translational part $\zeta_{\rm tr}$ given by

$$\zeta_{\rm tr} = \prod_k \left[M_k^{(x)} M_k^{(y)}\right]^{-1/2} \tag{20}$$

and the self-fluctuation part, after expanding the square root, by

$$\zeta_{\rm self} = \prod_{k\mathbf{q}} \left[1 + \frac{2\pi}{L_x L_y} \ln\kappa \, \frac{q^2 + \mu^{(2)}}{\mu^{(1)}\mu^{(2)}}\right]. \tag{21}$$

The thermodynamic free energy of the vortex then is given by

$$F = \varepsilon_l L_z + F_{\rm tr} + F_{\rm self}, \tag{22}$$

with $F_{\rm tr} = -T\ln\zeta_{\rm tr}$ and $F_{\rm self} = -T\ln\zeta_{\rm self}$. The contribution from the translational modes is particularly simple for the 2D case, where $F_{\rm tr} = -T\ln(L_x L_y/\xi^2)$ is determined by the freedom to place the vortex at any point within the plane. It is this part of the free energy which drives the Berezinskii-Kosterlitz-Thouless transition in a two-dimensional system. Going over to a system of coupled layers the freedom of placing an individual pancake vortex is restricted due to the interaction between the vortices in different layers. For a very weak coupling the Josephson interaction can be neglected with respect to the electromagnetic one and the cutoff in the logarithm is given the screening length λ. On the other hand, for a dominant Josephson coupling the cutoff is determined by the Josephson length $\Lambda = d\,(\xi/\xi_c)$. As a result, we can use the interpolation formula

$$F_{\rm tr} = -\frac{TL_z}{d} \ln\left(\frac{1}{\xi^2/\Lambda^2 + \xi^2/\lambda^2}\right), \tag{23}$$

representing the competition between the Josephson length and the London penetration depth for the in-plane currents. The result (23) applies to a long vortex. For the case of a short vortex segment ($L_z \simeq d$) the electromagnetic restoring force cannot build up and the cutoff in the logarithm is always given by the Josephson length Λ. In the limit of vanishing interplanar coupling we have $\Lambda \to \infty$ and the cutoff is given by the size of the sample such that (23) goes over into the result for a film.

Second, let us turn to the self-fluctuation part:

$$F_{\rm self} = -\frac{2\pi T L_z}{d} \ln\frac{\lambda}{\xi} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \int \frac{d^2q}{(2\pi)^2} \frac{q^2 + \mu^{(2)}}{\mu^{(1)}\mu^{(2)}}. \tag{24}$$

For the quasi-2D strongly layered superconductor with $\xi_c < d$ we can neglect the coupling term $\propto \gamma$ in the eigenvalues $\mu^{(1,2)}$. The integrand of (24) is well behaved at $q = 0$ and the interesting quantity is the large q cutoff. The smallest scale for the fluctuations is given by $\xi(0)$ and accounting for our convention to measure lengths in units of $\xi(T)$ we obtain for the large wavevector cutoff the value $q \simeq \xi(T)/\xi(0) = \tau^{-1/2}$. Performing the integration in (24) we obtain for the self-fluctuation part the expression

$$F_{\rm self} = -\frac{L_z T}{d} \ln\kappa \, \ln\frac{1}{\tau}, \tag{25}$$

which exhibits a nontrivial temperature dependence under the logarithm. The result (25) is correct to logarithmic accuracy. Collecting terms we can write the free energy of a vortex line into the form

$$F = L_z \varepsilon_l^R(\tau) + F_{\rm tr} \tag{26}$$

with the renormalized line energy ε_l^R given to logarithmic accuracy by

$$\varepsilon_l^R(\tau) = \varepsilon_0^R(\tau)\ln\kappa, \tag{27a}$$

$$\varepsilon_0^R(\tau) = \varepsilon_0(\tau) - \frac{T}{d}\ln\left(\frac{1}{\tau}\right), \quad \xi_c < d. \tag{27b}$$

Note that we have split the free energy into a renormalized line energy which accounts for all of the internal structure of the vortex (including self-fluctuations of the order parameter) and a contribution arising solely from the translational degrees of freedom in the problem. The second term in (26) has been found before by Nelson and Seung[20] and in the work of Bulaevskii, Meshkov, and Feinberg.[21] It corresponds to the entropic contribution to the free energy driving the Berezinskii-Kosterlitz-Thouless transition in a two-dimensional system. However, the result (27) shows that in addition to this translational term, the short-wavelength self-fluctuations [on length scales $\sim \xi(0)$] lead to a downward renormalization of the line energy of the vortex. This contribution is due to the nontrivial internal structure of the vortex line and usually represents the *dominating* term. For a structureless (pointlike) object the corresponding term is absent.

The Gaussian approximation used in the above derivation is equivalent to the one-loop perturbation expansion for calculating the free energy.[22] In this approximation, the logarithmic term in Eq. (27) is a perturbative correction implying the condition $T/\varepsilon_0 d \ll 1$. Within the present approximation the line energy extrapolates to zero at a temperature τ_R given by the implicit equation

$$\tau_R = 1 - \frac{T_R}{T_0} \approx \frac{T_0}{\varepsilon_0(0)d} \ln\left[\frac{1}{\tau_R}\right]. \tag{28}$$

The fluctuation corrections to the line energy become large at reduced temperatures $\tau \gtrsim \tau_R$, well outside the regime of critical fluctuations, and thus our approximation is applicable over a large temperature range. For a 2D superconductor the extent of the Ginzburg region is given by

$$\tau_G = 1 - \frac{T_G}{T_0} \approx \frac{T_0}{\varepsilon_0(0)d} < \tau_R. \tag{29}$$

Using parameters typical for the quasi-2D BSCCO compound [$T_0 \approx 100$ K, $d \approx 15$ Å, $\lambda(0) \approx 1000$ Å, resulting in $\varepsilon_0(0)d \approx 3000$ K], we obtain the estimates $\tau_G \approx 0.033$

and $\tau_R \approx 0.083$.

Closer to the transition temperature one has to go beyond the Gaussian approximation and the inclusion of higher-order corrections then is expected to lead to a renormalization of the expression under the logarithm in (27). The exact result for the line energy $\varepsilon_l^R(T)$ turns to zero at some fluctuation-corrected transition temperature $T_{c0} < T_0$, $\varepsilon_l^R(T_{c0}) = 0$. Again, the fluctuation-induced shift $\delta T_0 = T_0 - T_{c0}$ of the transition temperature is large,[2,4] $\delta T_0 > \tau_G T_0$, and thus can be calculated within our approach. We will give a brief derivation of the renormalized transition temperature T_{c0} in the next section. Before doing so, let us compare our result (27) for the quasi-2D case with the corresponding results for the intermediate layered case, where $\xi_c(0) < d < \xi_c$, and for the continuous (anisotropic) case with $d < \xi_c(0)$.

For an intermediate layering, as it is the case in the Y-based cuprates, the long-wavelength cutoff in (24) is given by the coupling term $\gamma(1-\cos k)$ instead of the mass term and the result for the renormalized line energy is

$$\varepsilon_l^R(\tau) = \left\{\varepsilon_0(\tau) - \frac{T}{d}\ln\left[\frac{d^2}{\xi_c^2(0)}\right]\right\}\ln\kappa, \quad \xi_c(0) < d < \xi_c. \tag{30}$$

Finally, for the continuous anisotropic situation we can expand the cosine and go over to a three-dimensional momentum space integration with the result

$$\varepsilon_l^R(\tau) = \left[\varepsilon_0(\tau) - \frac{T}{\pi\xi_c(0)}\right]\ln\kappa, \quad d < \xi_c(0). \tag{31}$$

In contrast to the quasi-2D result (27) the line energy renormalization involves only a trivial shift *independent of temperature* for the intermediate layered and for the continuous (anisotropic) 3D cases. Hence, the downward renormalization of the line energy should be observable in strongly layered quasi-2D materials such as the Bi- or Tl-based compounds, whereas no such effect is expected to be observable in the intermediate layered Y-based material.

IV. SHIFT OF THE TRANSITION TEMPERATURE

For a field theoretical calculation of the renormalized transition temperature T_{c0} it is convenient to approach the transition temperature from above. We rewrite the Ginzburg-Landau functional (1) in the form $\mathcal{F} = \mathcal{F}_0 + \mathcal{F}_{\rm int}$, where

$$\frac{\mathcal{F}_0}{T} = \frac{1}{2}\sum_n \int d^2r \times \left\{-\tau\Psi_{1n}^2 - \tau\Psi_{2n}^2 + (\nabla\Psi_{1n})^2 + (\nabla\Psi_{2n})^2 + \frac{\xi_c(0)^2}{d^2}\left[(\Psi_{1\,n+1} - \Psi_{1n})^2 + (\Psi_{2\,n+1} - \Psi_{2n})^2\right]\right\} \tag{32}$$

and

$$\frac{\mathcal{F}_{\rm int}}{T} = \frac{\pi T}{4\varepsilon_0(0)d}\sum_n \int d^2r\,\left(\Psi_{1n}^2 + \Psi_{2n}^2\right)^2, \tag{33}$$

with $\Psi_n = \Psi_{1n} + i\Psi_{2n}$. The above form is equivalent to (1) if we measure planar distances in units of $\xi(0)$ and use the normalization $\Psi_n^2 = [|\varepsilon_0|d/\pi T]\Delta_n^2$ for the order parameter. Defining averages as usual,

$$\langle X\rangle = \int \prod_n (D\Psi_{1n})\,(D\Psi_{2n})\;X\,\exp\left(-\mathcal{F}/T\right), \tag{34}$$

with X a function of Ψ_{1n} and Ψ_{2n}, we can construct the two-point correlation functions[22] $G_k^{(1,2)}(\mathbf{q})$, in Fourier representation

$$\langle\Psi_{1,2\,k}(\mathbf{q})\Psi_{1,2\,k'}(\mathbf{q}')\rangle = (2\pi)^3\delta(k+k')\,\delta^2(\mathbf{q}+\mathbf{q}')\,G_k^{(1,2)}(\mathbf{q}). \tag{35}$$

The free propagator takes the form

$$G_{0\,k}^{(1,2)}(\mathbf{q}) = \left[q^2 - \tau + \frac{2\xi_c(0)^2}{d^2}(1-\cos k)\right]^{-1}. \tag{36}$$

Fluctuations are treated by the usual perturbative expansion in $\mathcal{F}_{\rm int}$.[22] Note that the coupling constant is $\sim T/\varepsilon_0(0)d$, which is small in the same sense as previously discussed in connection with the result (27) for the renormalized line energy. Within the most simple Hartree-type approximation we can immediately write down the Dyson equation for the propagator in the form

$$G_k^{(1)}(\mathbf{q}) = G_{0\,k}^{(1)}(\mathbf{q}) + G_{0\,k}^{(1)}(\mathbf{q})\Sigma(\tau)G_k^{(1)}(\mathbf{q}), \tag{37}$$

with the self-energy $\Sigma(\tau)$ given by

$$\Sigma(\tau) = -\frac{\pi T}{\varepsilon_0(0)d}\int\frac{dk'}{2\pi}\int\frac{d^2q'}{(2\pi)^2} \times\left[3G_{0\,k'}^{(1)}(\mathbf{q}') + G_{0\,k'}^{(2)}(\mathbf{q}')\right]. \tag{38}$$

The equation for $G^{(2)}$ is analogous and $G^{(1)} = G^{(2)}$. For the self-energy we thus can write

$$\Sigma(\tau) = -\frac{4\pi T}{\varepsilon_0(0)d}\int_{-\pi}^{\pi}\frac{u\kappa}{2\pi}\int\frac{d^2q}{(2\pi)^2} \times\frac{1}{q^2 - \tau - \Sigma + 2[\xi_c(0)/d]^2[1-\cos k]}. \tag{39}$$

The physical transition temperature T_{c0} is determined by the condition $\Sigma + \tau = 0$. For the strongly layered quasi-2D situation the lower cutoff $\sim [\xi_c(0)/d]^2$ is smaller than the width τ_G of the Ginzburg region. On the other hand, the condition $\Sigma + \tau = 0$ should be understood to be accurate only up to the width of the critical regime. We then choose τ_G as the lower cutoff in the quasi-2D case, $\Sigma + \tau \simeq -\tau_G$. The upper limit of integration is given by $q \approx 1$ [corresponding to fluctuations of wavelength $\xi(0)$] and we obtain the result

$$\tau_{c0} = 1 - T_{c0}/T_0 \approx \frac{T_0}{\varepsilon_0(0)d} \ln\left(\frac{1}{\tau_G}\right), \quad \xi_c < d, \qquad (40)$$

for the shift in the transition temperature. This shift is larger than the width τ_G of the Ginzburg region and thus our use of the simple Hartree approximation is consistent. Using parameters for BSCCO we obtain an estimate $\tau_{c0} \approx 0.113$ for the shift in the transition temperature.

For the intermediate layered case with $\xi_c(0) < d < \xi_c$ the lower cutoff in (39) is provided by the coupling into the third dimension and we obtain

$$\tau_{c0} = 1 - T_{c0}/T_0 \approx \frac{T_0}{\varepsilon_0(0)d} \ln\left[\frac{d^2}{\xi_c(0)^2}\right], \quad \xi_c(0) < d < \xi_c. \qquad (41)$$

Finally, for a 3D material the result for the renormalization of the transition temperature takes the form

$$\tau_{c0} = 1 - T_{c0}/T_0 \approx \frac{1}{\pi} \frac{T_0}{\varepsilon_0(0)\xi_c(0)}, \quad d < \xi_c(0). \qquad (42)$$

Comparing these results for the T_0 shift with the results for the temperature where the renormalized vortex line energy is expected to vanish, we observe that for the two cases of intermediate layering and for a continuous 3D material the shifted transition temperature coincides with the zero in the renormalized line energy, $\varepsilon_l^R(T_{c0}) = 0$, see Eqs. (30) and (31). For the quasi-2D case the same result holds.

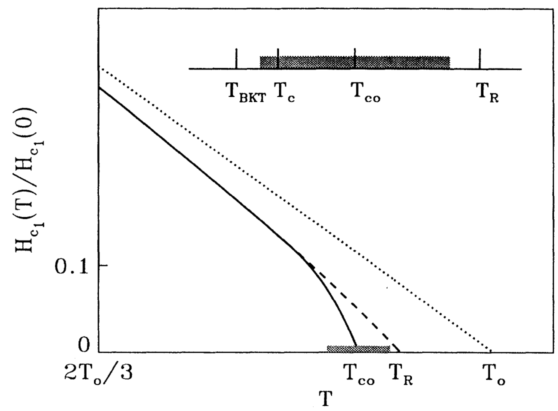

FIG. 1. Temperature dependence of the lower critical field $H_{c_1}(T)$ for the case of a strongly layered quasi-2D material. The dotted line is the linear extrapolation of $H_{c_1}(T)$ defining the bare transition temperature T_0. Fluctuations lead to a downward renormalization of $H_{c_1}(T)$. Within the Gaussian approximation the lower critical field extrapolates to zero at T_R. The regime where the Gaussian approximation applies is limited to temperatures well outside the Ginzburg regime of critical fluctuations (shaded area). Within the region where fluctuations become large (beyond Gaussian) the lower critical field line rapidly decreases and drops to zero close to the fluctuation-corrected transition temperature T_{c0}. Above the Berezinskii-Kosterlitz-Thouless transition at $T_{\rm BKT}$ a gas of confined vortex-antivortex pairs appears. Its presence prohibits the spontaneous creation of vortex lines in the system. At the three-dimensional ordering temperature T_c the pairs dissociate and long-range order is lost. The relative arrangement of the various temperatures is illustrated in the inset.

V. DISCUSSION

To begin with let us consider the quasi-2D situation where the interlayer coupling is still appreciably strong such that $\Lambda < \lambda$. For this case the translational contribution to the vortex free energy is given by the expression $F_{\rm tr} = -T(L_z/d) \ln(\Lambda^2/\xi^2)$, see (23). This formula is valid for a vortex of any length $d < L_z < \infty$ directed along the c axis. In contrast, the total free self-energy of a vortex line as given by the first term in Eq. (26) only applies to a vortex of infinite length L_z. For a finite vortex segment of length L_z (e.g., the vertical part of a vortex loop of extent L_z along the c axis) the total free energy can be written as

$$F = L_z \left[\varepsilon_0^R(T) \ln \frac{l(L_z)}{\xi} - \frac{T}{d} \ln \frac{\Lambda^2}{\xi^2}\right]. \qquad (43)$$

The upper cutoff $l(L_z)$ in the logarithm depends on the length L_z of the segment with the two limits at d and at infinity given by $l(d) = \Lambda$ and by $l(\infty) = \lambda$.[8] The lower critical field H_{c_1} is determined by Eq. (43) with $L_z = \infty$ and we obtain

$$H_{c_1} = \frac{4\pi}{\Phi_0} \left[\varepsilon_l^R(T) - \frac{T}{d} \ln \frac{\Lambda^2}{\xi^2}\right]. \qquad (44)$$

The lower critical field line deviates from the usual mean-field result due to the nontrivial fluctuation correction in the renormalized line energy $\varepsilon_l^R(T)$, see (27). The temperature dependence of H_{c_1} close to the transition is illustrated in Fig. 1. The low-temperature linear extrapolation of the mean-field lower critical field line goes to zero at the bare transition temperature T_0. However, this large scale extrapolation may be difficult to observe in a real experiment as the linear approximation of the Ginzburg-Landau mean-field results itself breaks down at low temperatures $T \lesssim T_0/2$. Note that T_0 is only a parameter in the theory but has no real physical meaning in terms of a phase transition as the latter is shifted down to T_{c0}. The fluctuation-corrected H_{c_1} line *extrapolates to zero* at a temperature close to T_R where the renormalized line energy vanishes [we ignore here the small shift in the zero of the lower critical field (44) as compared with the zero of the line energy $\varepsilon_l^R(T)$ arising due to the translational fluctuations; this shift is smaller than the width of the critical region]. The lower critical field line exhibits a weak downward curvature which is mainly due to the contribution of the vortex self-fluctuations. The latter are large due to the appearance of the product of two logarithms, $-(4\pi T/\Phi_0 d) \ln\kappa \ln(1/\tau)$. In comparison, the translational fluctuations contribute only a small shift $-(4\pi T/\Phi_0 d) \ln(\Lambda^2/\xi^2)$. The actual zero of the lower critical field line is close to the fluctuation-corrected transition temperature T_{c0}. The expression for the shift $T_R - T_{c0}$ follows from Eqs. (28) and (40):

$$T_R - T_{c0} \approx \frac{T_0^2}{\varepsilon_0(0)d} \ln \frac{\tau_R}{\tau_G} > \tau_G T_0, \qquad (45)$$

and taking parameters appropriate for BSCCO we obtain the shift $T_R - T_{c0} \approx 3$ K between the extrapolated and the actual zero of the H_{c_1} line. Note that this shift is larger than the extent $\tau_G T_0$ of the critical fluctuation region.

In a next step, let us briefly discuss the thermodynamics of a layered superconductor. Starting out with an uncoupled system of superconducting layers (or a thin film) a low-temperature phase exists with (algebraic) quasi-long-range order (Berezinskii phase[15]). Thermal creation of vortex loops of minimal extent $L_z \approx d$ then destroys this phase at temperatures $T > T_{\rm BKT}$, where the Kosterlitz-Thouless temperature follows from the vanishing of the free energy (43):

$$T_{\rm BKT} = \frac{\varepsilon_0^R(T_{\rm BKT})d}{2}. \tag{46}$$

Solving for $T_{\rm BKT}$ we obtain

$$1 - \frac{T_{\rm BKT}}{T_{c0}} \approx \frac{2}{d}\left|\frac{d\varepsilon_0^R}{dT}\right|^{-1} < 2\tau_G, \tag{47}$$

where the derivative is taken at $T = T_{c0}$. For a finite Josephson coupling true long-range order exists at all temperatures below the 3D transition temperature T_c. The thermally created vortex loops above $T_{\rm BKT}$ then remain confined to lengths $\lesssim \Lambda$. The three-dimensional ordering temperature can be determined from the condition $\Lambda \approx \xi_{\rm BKT}(T_c)$,[8] where the BKT coherence length is given by[23]

$$\xi_{\rm BKT}(T) \approx \xi(T) \exp\left[\left(b\frac{T_{c0}-T}{T-T_{\rm BKT}}\right)^{1/2}\right]. \tag{48}$$

The parameter b is nonuniversal and typical values obtained in thin superconducting films are in the range[24,25] 2–16. The physical 3D ordering transition takes place at the temperature

$$1 - \frac{T_c}{T_{c0}} \approx \frac{2}{d}\left|\frac{d\varepsilon_0^R}{dT}\right|^{-1}\left[1 - \frac{b}{\ln^2(\Lambda/\xi)}\right]. \tag{49}$$

For temperatures $T > T_c$, the BKT-type resistivity starts to grow and for large temperatures $T > T_{c0}$ the resistivity goes over into the 2D Aslamazov-Larkin behavior.[26,27] The renormalization from T_0 down to T_{c0} is much larger than the distances $T_{c0} - T_c$ or $T_{c0} - T_{\rm BKT}$ from the fluctuation-corrected transition temperature T_{c0} to the 3D ordering temperature T_c or to the BKT temperature $T_{\rm BKT}$. The relative positions of the various temperatures are illustrated in Fig. 1.

Let us analyze the question of a possible spontaneous creation of vortex lines. As mentioned above, minimal loops of size $\delta z \approx d$ and $\delta r \approx \Lambda$ can be created at no cost for temperatures $T \geq T_{\rm BKT}$. Similarly, loops of size $\delta z \approx nd$, $\delta r \approx \Lambda$ could appear at temperatures $T \geq T_n$ where the free energy $F(L_z = nd)$ as given by (43) drops to zero. The sequence T_n approaches the value T_∞ where the vortex free energy and thus H_{c_1} vanishes. Unfortunately, the exact determination of T_∞ is impossible within the accuracy of the present (Gaussian) approximation. It is important to note that in the regime $T > T_{\rm BKT}$ the gas of small ($n = 1$) loops annihilates the large loops with $n > 1$. Hence, above $T_{\rm BKT}$ a gas of elementary loops consisting of bound vortex-antivortex pairs with radii $r < \Lambda$ exists. A vortex line embedded in this gas of elementary loops is unstable and bound to decay. Similarly, the creation of a long vortex line has to go through a nucleation process where the growing nucleus is again unstable due to the presence of the gas of elementary loops. At T_c the elementary pairs dissociate and the long-range order vanishes.

Finally, let us concentrate on the weakly coupled case with $\Lambda > \lambda$. The translational free energy is given by the expression $F_{\rm tr} = 2(L_z/d)T \ln\kappa$ in the case of a long vortex, whereas for a short vortex ($L_z \simeq d$) we obtain $F_{\rm tr} = 2(L_z/d)T \ln(\Lambda/\xi)$ as the electromagnetic restoring force cannot build up. Similarly, the cutoff $l(L_z)$ is given by the screening length λ in the case of a long vortex, whereas $l(L_z \simeq d) \simeq \Lambda$. As a consequence, the two logarithms in (43) drop out and the temperatures T_n all collapse into the BKT temperature $T_{\rm BKT}$ above which the vortex lines dissociate. In superconducting films we further have to replace L_z by the film thickness d and the relevant screening length is $\lambda_{\rm eff} = 2\lambda^2/d$ (to avoid additional complications we always assume here that the spatial extent of the film is smaller than $\lambda_{\rm eff}$, as is usually the case[28]). The exponent $a(T)$ in the current-voltage characteristic[23–27] $V \sim I^{a(T)}$ is also renormalized by the self-fluctuations of the vortex. Below the BKT transition we have

$$a(T) = 1 + \frac{\nu_{XY} d\varepsilon_0^R(T)}{T} \tag{50}$$

and the downward renormalization of $a(T)$ due to the self-fluctuations competes with the XY-type renormalization $\nu_{XY} < 1$ close to $T_{\rm BKT}$. The result (50) also applies to layered superconductors in the large current limit where length scales $\lesssim \Lambda$ are probed.

In the light of the present theoretical considerations the experiments of Brawner *et al.*[17] are interpreted in the following way (see Figs. 1 and 2): In the strongly layered BSCCO compound the fluctuation corrections to the lower critical field line are large and show a nontrivial

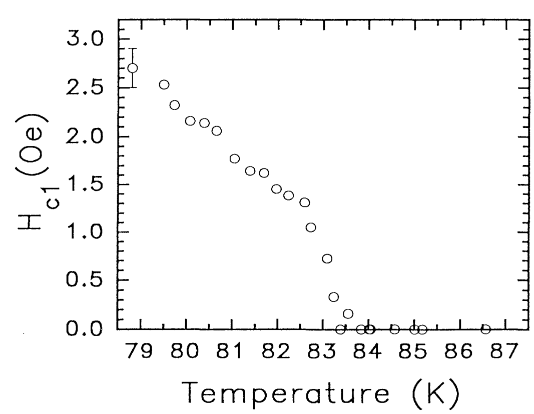

FIG. 2. Lower critical field line H_{c_1} versus temperature in a BSCCO single crystal as measured with a Hall probe technique by Brawner *et al.* (Ref. 17).

temperature dependence (see Fig. 2). Over an ~ 10 K range close to the transition the H_{c_1} line extrapolates to zero at a temperature ~ 86 K which we identify with our calculated extrapolated zero T_R, hence $T_R \approx 86$ K in the experiment of Ref. 17. Close to the renormalized transition temperature (but still outside the critical regime) fluctuations going beyond the Gaussian approximation lead to a further downward curvature of the H_{c_1} line such that its actual zero is close to T_{c0}. In the experiment the lower critical field goes to zero at a temperature ~ 83.5 K, hence we obtain $T_{c0} \approx 83.5$ K. The shift $T_R - T_{c0}$ between the extrapolated and the actual zero of the lower critical field line then is in good agreement with the above estimate for the Bi-based quasi-2D superconductor. The deviations of our lowest-order result for the $H_{c_1}(T)$ line from the actual curve are expected to become relevant within a region somewhat larger than the critical region $\tau_G T_0$. In the Y-Ba-Cu-O compound the H_{c_1} line only undergoes a parallel shift. The critical fluctuation region is small, $\lesssim 1$ K, and the downward bending of the lower critical field line is restricted to a narrow temperature interval, in agreement with the experimental observations of Brawner *et al.*[17]

VI. CONCLUSIONS

In this paper we have analyzed the influence which fluctuations have on the properties of an individual vortex line. In particular, we have determined the free energy of a vortex line within the Gaussian approximation. The fluctuation corrections to the line energy can be split into a term arising from the nontrivial vortex structure (self-fluctuations) and a second term arising from the translational degrees of freedom. The first term usually is the dominant one and leads to a downward renormalization of the line energy. The second term corresponds to the entropic contribution to the free energy which drives the BKT transition in 2D. Within the Gaussian approximation the renormalized line energy of the vortex extrapolates to zero at $T_R < T_0$, where T_0 is the bare mean-field transition temperature. Close to the transition fluctuations going beyond the Gaussian approximation lead to a further downward renormalization of ε_l^R such that the exact line energy vanishes at the fluctuation-corrected transition temperature $T_{c0} < T_R < T_0$. The shift in the transition temperature has been determined within the Hartree approximation and is larger than the width of the critical regime, $T_0 - T_{c0} > \tau_G T_0$. The difference between the extrapolated and the actual zero of the lower critical field line has been estimated to be $T_R - T_{c0} \approx 3$ K for the strongly layered BSCCO compound in good agreement with the experimental findings of Brawner *et al.*[17] For the case of intermediate and strong coupling between the layers ($d < \xi_c$) the lower critical field line only undergoes a constant shift and no pronounced effects are expected due to the fluctuations. Again this result agrees with the experimental findings on a Y-Ba-Cu-O superconductor.[17] The vanishing of the line energy below the transition allows for the appearance of a gas of confined ($r \lesssim \Lambda$) vortex-antivortex pairs within the temperature region $T_{\rm BKT} < T < T_c$. The presence of this gas of elementary loops prohibits the spontaneous creation of vortex lines. At the 3D ordering transition T_c the elementary pairs dissociate and long-range order is lost.

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