PHYSICAL REVIEW B VOLUME 51, NUMBER 17 1 MAY 1995-I

Undulating vortices in layered superconductors

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(Received 11 October 1994)

We present the detailed structure of vortices normal to the layers in layered superconductors, assuming only that the order parameter varies continuously between the layers. The magnetic field along the c axis undulates due to the reduced screening between the layers. The radial magnetic field also undulates, becoming zero on the layers, as well as midway between them.

Recent works[1] have proposed that the nonzero order parameter between the layers should be taken into account in the phenomenological description of layered superconductors, and they have incorporated explicit spatial variations of the order parameter in the z direction, normal to the layers. This was achieved by adopting z-dependent coefficients in the phenomenological Ginzburg-Landau (GL) free-energy functional, such that the superconductivity be maximal on the layers. The corresponding upper critical fields were determined, as were some new physics resulting from these new models.

Clearly, the particulars depend on the choice of these spatially varying coefficients. However the structure of the vortices should not depend on these particulars, but rather on the periodicity of the spatially varying order parameter. We describe in detail the structure of these vortices in this paper, making no assumption about the particular form of the z-dependent coefficients in the GL free energy.

Indeed, we make a reasonable ansatz for the order parameter between the layers, for vortices normal to the layers, and we then solve the field equations for the magnetic fields analytically. Our solution depends only on the periodicity of the order parameter along the z axis, and not on the detailed form of the GL free energy. We find that the magnetic field h_z along the z axis undulates. Its value at the core is greater on the layers than in between them, while its value away from the core is least on the layers. This happens because the total magnetic flux passing through a given slice normal to the z axis is constant. Thus, in slices of reduced order parameter (and hence reduced screening) there will be more magnetic flux away from the core, and less magnetic flux at the core. This means that the magnetic field h_z at the core undulates, acquiring its maximum value on the layers.

As for the radial magnetic field h_ρ along the layers, which must be zero at the core in order to be well defined there, it also presents undulations. It is zero on the layers, and it undulates in the space between two neighboring layers, flipping direction midway between them.

The above-mentioned behavior of h_z and h_ρ is independent of the precise form of the free energy, and it depends only on the periodicity of the order parameter along the c axis. In other words, it results from the undulation of the order parameter along the c axis.

Such an undulation will result typically from a GL Gibbs free-energy functional of the form

$$\int\int\int dx\, dy\, dz \left[a(z,T)|\Psi|^2+\beta|\Psi|^4/2 + \frac{\hbar^2}{2m}|\Pi_\parallel\Psi|^2+\frac{\hbar^2}{2M}|\Pi_z\Psi|^2 + \mathbf{h}^2/8\pi-\mathbf{hH}/4\pi \right] . \tag{1}$$

Here $\Psi(x,y,z)$ is the order parameter, $\nabla_\parallel\Psi$ is the gradient of Ψ along the layers, z is the direction normal to the layers, $\mathbf{A}$ is the vector potential, $\mathbf{h}$ is the magnetic field, and $\Pi=-i\nabla-(2e/\hbar c)\mathbf{A}$. In the absence of magnetic fields, and for $M\to\infty$, we would have $|\Psi|^2=-a(z,T)/\beta$. Hence $|\Psi|^2$ follows the periodicity of $a(z,T)$, which follows the periodicity of the layered structure.

We can write the GL Gibbs free energy in dimensionless form, by measuring x,y,z in units of the distance d between the layers, $\mathbf{A}$ in units of $\hbar c/2ed$, $\mathbf{H}$ and $\mathbf{h}$ in units of $\hbar c/2ed^2$, Ψ in units of $\sqrt{\alpha/\beta}$, and the free energy in units of $d^3\alpha^2/\beta$, where α is a positive constant with the dimensions of $a(z,T)$. This constant is taken out of $a(z,T)$, so as to render it dimensionless. In other words, $a(z,T)/\alpha=\alpha(z,T)$ where $\alpha(z,T)$ is dimensionless. Note that the constant α may be a function of T, but not of z.

Then, if we define the dimensionless constants $\Gamma^2=M/m$, $\nu=\hbar^2/2M\alpha d^2$, $\Lambda^2=mc^2\beta/16\pi e^2\alpha$, and

$$\kappa=\beta(\hbar c/2ed^2)^2/4\pi\alpha^2=2\nu\Gamma^2\Lambda^2/d^2 ,$$

the GL Gibbs free energy takes the dimensionless form

$$\int\int\int dx\, dy\, dz[\alpha(z,T)|\Psi|^2+|\Psi|^4/2 +\nu\Gamma^2|\Pi_\parallel\Psi|^2+\nu|\Pi_z\Psi|^2 +\kappa(\mathbf{h}^2-2\mathbf{hH})/2] , \tag{2}$$

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where $\Pi=-i\nabla-\mathbf{A}$. The length Λ corresponds to the penetration depth in the standard GL theory, while ν corresponds to ξ_z^2/d^2, where ξ_z is the coherence length along the z axis. However this correspondence should not be considered as an identification with the quantities of the standard GL theory, except in the limit that $\alpha(z,T)=-1$, when the free energy does become the standard GL one.

The field equations that minimize the above Gibbs free energy are

$$\kappa(\nabla\times\mathbf{h})_{\parallel}=\nu\Gamma^2\Psi^*\Pi_{\parallel}\Psi+\text{c.c.}\ , \tag{3}$$

$$\kappa(\nabla\times\mathbf{h})_z=\nu\Psi^*\Pi_z\Psi+\text{c.c.} \tag{4}$$

We shall examine the case of a single vortex in an applied magnetic field $H\hat{z}$ along the z axis. In that case, we shall have, in terms of cylindrical coordinates, $\Psi=\psi(\rho,z)e^{i\phi}$ and

$$\mathbf{A}=A(\rho,z)\hat{\phi}\ , \tag{5}$$

$$\mathbf{h}=-\hat{\rho}\frac{\partial A}{\partial z}+\hat{z}\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho A)\ . \tag{6}$$

Equation (4) is identically satisfied, while Eq. (3) becomes

$$\frac{\partial^2 A}{\partial z^2}+\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho A=\frac{d^2}{\Lambda^2}\psi^2(\rho,z)[A-1/\rho]\ . \tag{7}$$

If we define the quantity $Q=1-\rho A$, then

$$\frac{\partial^2 Q}{\partial z^2}+\rho\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial Q}{\partial\rho}=\frac{d^2}{\Lambda^2}\psi^2 Q\ . \tag{8}$$

We see that $A=(1-Q)/\rho$. Since A must not be singular at the origin, we expect that

$$Q\to 1\quad\text{as }\rho\to 0\ . \tag{9}$$

We also require that the order parameter be continuous along the z axis, in which case Eq. (7) indicates that A and $\partial A/\partial z$ must be continuous. Otherwise $\partial^2 A/\partial z^2$ would involve δ functions, and ψ would not be continuous.

Our approach then will be to make a reasonable periodic ansatz for the order parameter, and then solve Eq. (8) to find the magnetic fields, subject to the boundary condition that Q and $\partial Q/\partial z$ be continuous along the z axis, and $Q\to 1$ as $\rho\to 0$.

We expect that ψ will be maximal on the layers, and that it is independent of ρ away from the origin. We also expect that ψ is zero at the origin. These requirements are independent of the details of $\alpha(z,T)$, and are valid for any vortex in a layered structure.

We adopt thus the ansatz:

$$\Psi=\psi(\rho,z)e^{i\phi}=a_0 e^{i\phi}\frac{\rho}{R}\cosh[\gamma(z-n-1/2)]\ , \tag{10}$$

as long as $n\le z\le n+1$, with $R=\sqrt{\rho^2+b^2}$. Here the layers are located at $z=n$ and $z=n+1$. We shall think of γ as a given parameter that is determined by $\alpha(z,T)$, while a_0 and b will be variational parameters. This ansatz can describe the usual case of a uniform superconductor $[\gamma=0,\alpha(z,T)=-1]$, as well as the case of a well layered structure (large γ), and its ψ is manifestly continuous along the z axis.

The limiting case of a uniform superconductor ($\gamma=0$) has been considered by Clem.[2] The solution for $\gamma=0$ is given in terms of modified Bessel functions:

$$Q_0=\frac{q_0 R K_1(q_0 R)}{q_0 b K_1(q_0 b)}\ , \tag{11}$$

where $q_0=da_0/\Lambda$.

In the general case we have to solve the equation

$$\frac{\partial^2 Q}{\partial z^2}+\rho\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial Q}{\partial\rho}=\frac{d^2a_0^2}{\Lambda^2}\frac{\rho^2 Q}{R^2}\cosh^2 t\ , \tag{12}$$

for $n\le z\le n+1$, where $t=\gamma(z-n-\frac{1}{2})$. Due to the periodicity and continuity of Q along z, we expect Q to be an even function of $z-n-\frac{1}{2}$. Hence $\partial Q/\partial z$ will be an odd function of $z-n-\frac{1}{2}$. Then the continuity of $\partial Q/\partial z$ will require that $\partial Q/\partial z=0$ at $z=n$ and $z=n+1$.

Outside the core, $R\to\rho$, and hence ψ becomes a function of z only. In that case Eq. (12) is separable. We can easily verify that the solution that will not diverge at infinity is $Q=Nq\rho K_1(q\rho)Q_1(z)$, where N is a constant of proportionality, and where

$$\frac{\partial^2 Q_1}{\partial z^2}+q^2Q_1=\frac{d^2a_0^2Q_1}{\Lambda^2}\cosh^2 t\ . \tag{13}$$

If $\Lambda\to\infty$, then Q_1 is proportional to $\cos q(z-n-\frac{1}{2})$. But $\partial Q_1/\partial z=0$ at $z=n$, so $q\to 0$ and $Q_1\to 1$ as $\Lambda\to\infty$.

Typically, $d\ll\Lambda$, so we shall assume that q^2 and $d^2a_0^2/\Lambda^2$ are small, and we shall neglect their higher powers. Then we can easily integrate Eq. (13) to obtain

$$Q_1=1+\frac{d^2a_0^2}{\Lambda^2}S(z)\ , \tag{14}$$

where

$$S(z)=\frac{\cosh 2t-1}{8\gamma^2}-\frac{\sinh\gamma}{4\gamma}(z-n-1/2)^2\ , \tag{15}$$

and where $q^2=(d^2a_0^2/\Lambda^2)(\gamma+\sinh\gamma)/2\gamma$. Indeed, as $\gamma\to 0$, $q\to q_0$ and $Q_1\to 1$, giving us thus the solution of Clem away from the core [see Eq. (11)]. Furthermore, Q_1 is indeed an even function of $z-n-\frac{1}{2}$, and $\partial Q_1/\partial z$ is zero at $z=n$ and $z=n+1$, as expected. Thus the solution of the general Eq. (12) away from the core, for small da_0/Λ, is

$$Q=Nq\rho K_1(q\rho)[1+d^2a_0^2S(z)/\Lambda^2]\ . \tag{16}$$

Actually, we can solve Eq. (13) even for large da_0/Λ, but in this case we have to assume that γ is large. We can then easily verify that for large γ, and any value of da_0/Λ, the solution Q_1 of Eq. (13) is proportional to $\exp[d^2a_0^2S(z)/\Lambda^2]$, so long as $q^2=(d^2a_0^2/\Lambda^2)(\gamma+\sinh\gamma)/2\gamma$. We note that this exponential gives indeed the expression of Eq. (14) when da_0/Λ is small.

Having thus seen the behavior of Q away from the core, we now attack that full problem of solving the general Eq. (12), which is valid everywhere. We define

$$Q = NqRK_1(qR)f(\rho,z) \ , \tag{17}$$

where N is just a proportionality constant. Then Eq. (12) becomes

$$\frac{\partial^2 f}{\partial z^2} + \frac{q^2\rho^2}{R^2}f - \frac{2q^2K_0(qR)}{qRK_1(qR)}\rho\frac{\partial f}{\partial \rho} + \rho\frac{\partial}{\partial \rho}\frac{1}{\rho}\frac{\partial f}{\partial \rho} = \frac{d^2a_0^2\rho^2}{\Lambda^2R^2}\cosh^2 t f \ . \tag{18}$$

We try the solution

$$f(\rho,z) = 1 + \frac{d^2a_0^2}{\Lambda^2}\rho g(\rho,z) \ . \tag{19}$$

Then, assuming that $d^2a_0^2/\Lambda^2$ and q^2 are small, and dropping higher-order terms, we obtain from Eqs. (18) and (19) the equation

$$\frac{\partial^2 g}{\partial z^2} + \frac{\partial^2 g}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial g}{\partial \rho} - \frac{g}{\rho^2} = \frac{\rho}{R^2}\left[\cosh^2 t - \frac{q^2\Lambda^2}{d^2a_0^2}\right] . \tag{20}$$

We introduce Hankel transforms to solve this equation. We shall make use of the fact that $\int_0^\infty \rho J_1(q\rho)J_1(q'\rho)d\rho = q^{-1}\delta(q-q')$. So, if we define the Hankel transform $\tilde{g}(k,z) = \int_0^\infty \rho J_1(k\rho)g(\rho,z)d\rho$, we get

$$\frac{\partial^2 \tilde{g}}{\partial z^2} - k^2\tilde{g} = \left[\cosh^2 t - \frac{q^2\Lambda^2}{d^2a_0^2}\right] bK_1(kb) \ . \tag{21}$$

We recall that Q, and hence g and $\tilde{g}$, must be even in $z-n-\frac{1}{2}$, while $\partial Q/\partial z$, and hence $\partial g/\partial z$ and $\partial \tilde{g}/\partial z$, must be zero at $z=n$ and $z=n+1$. The function $\tilde{g}$ that satisfies Eq. (21), as well as these boundary conditions, is

$$\tilde{g} = bK_1(bk)\left[\frac{q^2\Lambda^2}{d^2a_0^2k^2} + \frac{2\gamma^2}{k^2(k^2-4\gamma^2)} + \frac{\cosh^2 t}{4\gamma^2-k^2} + \frac{\cosh k(z-n-1/2)}{k^2-4\gamma^2}\frac{\gamma\sinh\gamma}{k\sinh(k/2)}\right] . \tag{22}$$

The inverse Hankel transform then yields g:

$$g(\rho,z) = \int_0^\infty k\tilde{g}(k,z)J_1(k\rho)dk \ . \tag{23}$$

We note however that, as $k \to 0$,

$$\tilde{g} \to k^{-3}[q^2\Lambda^2/d^2a_0^2 - 1/2 - (2\gamma)^{-1}\sinh\gamma] \ .$$

So the integrand of Eq. (23) will diverge logarithmically at the origin, unless the coefficient of k^{-3} is zero. Hence

$$q^2 = \frac{d^2a_0^2}{\Lambda^2}(\gamma + \sinh\gamma)/2\gamma \ , \tag{24}$$

a relation that must be familiar by now.

Then the exact solution of Eq. (20) can be written in the form

$$g(\rho,z) = \int_0^\infty bkJ_1(k\rho)K_1(bk)\left[\frac{\sinh\gamma}{2\gamma k^2} + \frac{\cosh 2t}{8\gamma^2-2k^2} + \frac{\cosh k(z-n-1/2)}{k^2-4\gamma^2}\frac{\gamma\sinh\gamma}{k\sinh(k/2)}\right]dk \ . \tag{25}$$

We note that $g \to 0$ as $\gamma \to 0$, and $q \to da_0/\Lambda$, in which case we recover Clem's solution. Also $g \to 0$ as $\rho \to 0$, which means that the proportionality constant N of Eq. (17) must be equal to $[qbK_1(qb)]^{-1}$, in order to ensure that $Q \to 1$ as $\rho \to 0$. Thus Eqs. (17), (19), and (25) give the full solution for Q, from the origin out to infinity, as long as we keep terms of at most first order in $d^2a_0^2/\Lambda^2$.

It is difficult to evaluate the integral of Eq. (25) analytically. Thus we seek a reasonable approximation. We note that the expression $\rho S(z)/b^2$ is even in $z-n-\frac{1}{2}$, while its derivative with respect to z is indeed zero at $z=n$ and $z=n+1$. Furthermore, it satisfies Eq. (20) when $\rho \ll b$. So we are led to assume that

$$g(\rho,z) \approx \rho S(z)/R^2 \ , \tag{26}$$

and that

$$Q(\rho,z) \approx \frac{qRK_1(qR)}{qbK_1(qb)}\left[1 + \frac{d^2a_0^2}{\Lambda^2}\frac{\rho^2}{R^2}S(z)\right] , \tag{27}$$

where the quantity q is defined through Eq. (24). We note that if $\rho \gg b$ then we recover the solution away from the core of Eq. (16), while if $\rho \ll b$ the $g(\rho,z)$ of Eq. (26) reduces to $\rho S(z)/b^2$, which does satisfy Eq. (20). Furthermore, $Q \to 1$ as $\rho \to 0$, and Q and $\partial Q/\partial z$ are continu-

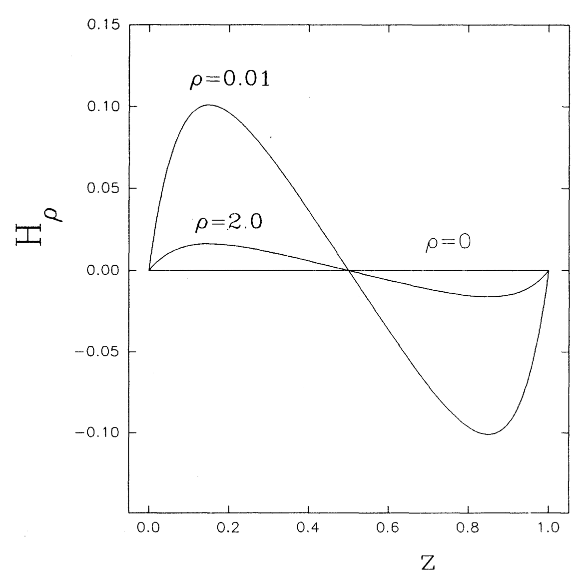

FIG. 1. The radial magnetic field h_ρ as a function of z, for various values of ρ. The numbers used were chosen for the sake of clarity.

ous along z, while $\partial Q/\partial z$ is zero at $z=n$ and $z=n+1$. Finally, for $\gamma\to 0$ it yields the Clem solution of Eq. (11).

In other words the assumption of Eq. (27) satisfies the equations away from the core and at the core, as well as all the appropriate boundary conditions. It is a very good approximation, for small $d^2a_0^2/\Lambda^2$, to the correct solution for the fields that corresponds to our original ansatz of Eq. (10) for the order parameter.

The corresponding radial magnetic field is

$$h_\rho=\frac{qRK_1(qR)}{qbK_1(qb)}\frac{d^2a_0^2}{\Lambda^2}\frac{\rho}{R^2}\left[\frac{\sinh 2t}{4\gamma}-\frac{\sinh\gamma}{2\gamma^2}t\right] . \tag{28}$$

We note that $h_\rho\to 0$ as $\rho\to 0$, and that $h_\rho=0$ at $z=n$, $z=n+\frac{1}{2}$ and $z=n+1$ (see Fig. 1). Since h_ρ is odd in $z-n-\frac{1}{2}$, there is no net radial flux between $z=n$ and $z=n+1$, and $\int_n^{n+1}2\pi\rho h_\rho dz=0$. Thus h_ρ undulates between neighboring layers, flipping its direction midway between them.

As for the magnetic field along the z direction, it is equal to

$$h_z=\frac{q^2K_0(qR)}{qbK_1(qb)}+\frac{d^2a_0^2}{\Lambda^2}\frac{S(z)}{qbK_1(qb)}\times\left[\frac{\rho^2}{R^2}q^2K_0(qR)-qRK_1(qR)\frac{2b^2}{R^4}\right] . \tag{29}$$

Hence

$$h_z(\rho=0,z)=\frac{q^2K_0(qb)}{qbK_1(qb)}-\frac{2d^2a_0^2}{b^2\Lambda^2}S(z) . \tag{30}$$

Thus the value of the magnetic field h_z at the core is greatest on the layers. While the value of h_z far from the core is greatest at $z=n+\frac{1}{2}$ (see Fig. 2).

Indeed, the flux along z is $\int_0^\infty h_z\rho d\rho=1$, in units of $hc/2e$. Hence it is constant for every slice normal to the z axis. But there is less superconductivity between the layers, and thus h_z is screened less between the layers, than on the layers. Consequently h_z spreads out further towards infinity in the region between the layers, and it must lower its core value in that region, to compensate for this spreading of the magnetic flux.

Equations (10), (27), (28), and (29) are the main results of our paper. These results enable us to calculate the total energy for a single vortex in an externally applied field $H\hat{z}$. We need to note first that

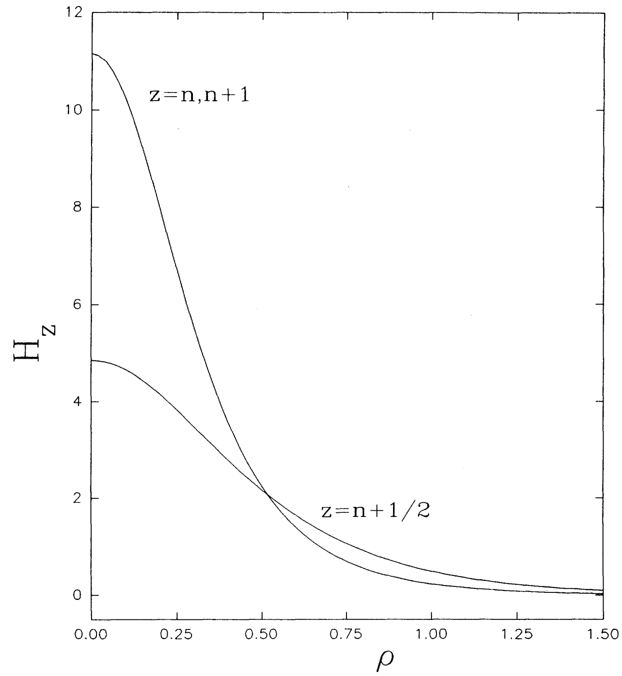

FIG. 2. The magnetic field h_z along the z axis at $z=n$ and $n+1$, and at $z=n+\frac{1}{2}$, as a function of ρ. The numbers used were chosen for the sake of clarity.

$$\frac{\partial^2Q}{\partial z^2}+\rho\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial Q}{\partial\rho}\approx\frac{d^2a_0^2}{\Lambda^2}\frac{\rho^2}{R^2}Q\left[\cosh^2t-\frac{8b^2}{R^4}S(z)\right] , \tag{31}$$

for the Q given by the ansatz of Eq. (27), having neglected terms of order $d^4a_0^4/\Lambda^4$. Furthermore, since we expect $\alpha(z,T)$ to be symmetric with respect to the layers, we shall assume that it is an even function of $z-n-\frac{1}{2}$. I.e., $\alpha(z,T)$ is really $\alpha(t,T)$. We can then calculate the total energy, after making use of Eq. (31). We obtain

$$\sum_n\left[\pi\kappa\frac{d^2a_0^2}{2\Lambda^2}(\gamma+\sinh\gamma)/4\gamma+\pi\nu\gamma a_0^2(\sinh\gamma-\gamma)(2)^{-1}\left[L^2-b^2\ln\frac{L^2+b^2}{b^2}\right]\right.$$
$$+\frac{\pi a_0^4}{32\gamma}(6\gamma+8\sinh\gamma+\sinh 2\gamma)\left[L^2+b^2-2b^2\ln\frac{L^2+b^2}{b^2}\right]$$
$$\left.+\pi a_0^2I(T)\left[L^2-b^2\ln\frac{L^2+b^2}{b^2}\right]+\pi\kappa\frac{q^2K_0(qb)}{qbK_1(qb)}-2\pi\kappa H\right] , \tag{32}$$

where $I(T)=(2/\gamma)\int_0^{\gamma/2}\alpha(t,T)\cosh^2t\,dt$. Here we kept terms up to, and including, order $d^2a_0^2/\Lambda^2$, and we took qb to be quite small. Indeed, b is expected to be of the order of the coherence length. The integration over ρ has been performed from 0 to L, with $L\to\infty$.

Straightforward minimization of the energy gives

$$a_0^2=\frac{-I(T)-\nu\gamma(\sinh\gamma-\gamma)/2}{(6\gamma+8\sinh\gamma+\sinh 2\gamma)/16\gamma} \tag{33}$$

and

$$b^2=\nu\Gamma^2\left[1+\frac{\sinh\gamma}{\gamma}\right]\times[-I(T)-\nu\gamma(\sinh\gamma-\gamma)/2]^{-1} . \quad (34)$$

Minimization of the part in the energy that is proportional to L^2 will give γ. This γ will, of course, depend on $\alpha(t,T)$. For example, for $\gamma\to 0$ and $\alpha(z,T)\to -1$, we recover the Clem results $a_0^2=1$ and $b^2=2\nu\Gamma^2$, or, in dimensionful units, $b=\sqrt{2}\xi_{\parallel}$.[2] For the example used in one of the works of Ref. 1, $\alpha(z,T)=1-\alpha(T)\sum_n\delta(z-n)$, we find $b^2=[-1+\alpha(T)/2\sqrt{\nu}]^{-1}\nu\Gamma^2$, i.e., a coherence length that diverges at T_c, as it should.

At H_{c1} the minimized energy should be equal to the Meissner energy, i.e., the energy of the state with $\Psi=a_0\cosh\gamma(z-n-\frac{1}{2})$ and $\mathbf{A}=0$. This Meissner energy is the piece proportional to L^2. So we obtain

$$H_{c1}=\frac{q^2}{2}K_0(qb)+\frac{3q^2}{8} , \quad (35)$$

which reduces to the H_{c1} of Ref. 2 when $\gamma\to 0$, $a_0^2\to 1$, $b^2\to 2\nu\Gamma^2$.

We have thus managed to obtain the fully detailed structure of a single vortex normal to the layers, in any layered superconductor. Our analytic results, even though approximate, are quite general, and they depend on the details of the phenomenological description only through the parameter γ, that determines the extent of the layering of the structure. These results are given by the Eqs. (10), (27), (28), and (29). They describe fully the variation of the order parameter and of the magnetic fields h_z and h_ρ, which undulate between the layers. These undulations are weak when $d\ll\Lambda$. However they are expected to be ubiquitous. Indeed, our results, though derived perturbatively in the region $d\ll\Lambda$, will be qualitatively correct even away from this region, as discussed briefly after Eq. (16). Such will be the case in multilayers, where these undulations will be observable when d is a sizeable portion of Λ. We also note that these undulations will persist when we have many vortices, because they are simply the result of the variation of $\mathbf{A}$ along the z axis in a periodic fashion, a variation that is indeed present in a vortex lattice in a layered structure.

One of us (A.M.E.) thanks warmly the Department of Natural Sciences of the University of Cyprus for its hospitality and financial support during the completion of this work.

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