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Structure of Vortex Lines in Pure Superconductors*

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A method is given for solving the Bogoliubov equations for quasiparticle excitations in superconductors in the WKBJ approximation. It is applied to calculate the excitation spectrum and the scattering states of an isolated vortex line in a type-II superconductor. The pair potential and magnetic field in the vicinity of the core are determined by a variational method. For values of the Ginzburg-Landau parameter κ near 1, the energy so calculated is about 10% too high and the critical κ for type-II superconductivity about 25% too high, indicating that the variational functions used are only approximately of the correct form. The energy of the bound states depends on the magnetic quantum number like a Landau energy; the effective magnetic field is of the order of the upper critical field H_{c2} for all values of κ.

I. INTRODUCTION

THERE is considerable interest in the theory of superconductors in which the pair potential $\Delta(\mathbf{r})$ and the magnetic field $\mathbf{h}(\mathbf{r})$ vary in space or time or both. These problems include vortex lines in type-II superconductors, surface superconductivity, the intermediate state in type-I superconductors, and various problems associated with fluctuations. Considerable progress has been made in treating such problems for temperatures near T_c, or in type-II superconductors for magnetic fields near H_{c2}, where Δ is small and can be used as an expansion parameter.[1] Gor'kov[2] showed in this way that the phenomenological Ginzburg-Landau (GL) equations follow from microscopic theory and are valid near T_c. Extensions of these equations to include higher-order terms and time dependence have been given.[3] However, it has been necessary in these derivations to assume that quantities such as $\Delta(\mathbf{r})$ vary slowly over a coherence distance ξ. This limits the validity to temperatures near T_c or to fields near H_{c2}.

In this paper we show how the WKBJ approximation can be adapted to the Bogoliubov equations for quasiparticle excitations, and we apply it to derive the excitation spectrum and the scattering states of an isolated vortex line in a pure superconductor. By a variational method, we derive an approximately self-consistent solution for $\Delta(\mathbf{r})$ and $\mathbf{h}(\mathbf{r})$ and the energy of the line. This allows a calculation of the lower critical field H_{c1} for all values of the GL parameter κ and for all temperatures. It is believed that the method used here will be useful in other problems.

The most complete calculation of the structure of a vortex line based on a generalized GL theory is that of Neumann and Tewordt,[4] who used a free-energy functional which includes terms to the fourth order in Δ. They calculated $\Delta(\mathbf{r})$, $\mathbf{h}(\mathbf{r})$, and H_{c1} as functions of the GL parameter κ and the temperature T [to first order in $(T_c-T)/T_c$] both for pure superconductors and for various values of the mean free path.

Various calculations making use of Green's-function techniques have been made to extend the GL theory of vortex structure for fields near H_{c2} to arbitrary temperatures. An expression for $\kappa_1(T)\equiv H_{c2}/\sqrt{2}H_c$ was first derived by Gor'kov[5] by a variational method. More complete calculations for κ_1 have been given by Maki and Tsuzuki,[6] Helfand and Werthamer,[7] and Eilen-

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[1] For a review of the theory of type-II superconductors, see A. L. Fetter and P. C. Hohenberg, in *A Treatise on Superconductivity*, edited by R. D. Parks (Marcel Dekker, Inc., New York, 1969), Chap. 15.

[2] L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. **36**, 1918 (1959) [English transl.: Soviet Phys.—JETP **9**, 1364 (1959)].

[3] For a review of the GL theory and its extensions, see N. R. Werthamer, in *A Treatise on Superconductivity*, edited by R. D. Parks (Marcel Dekker, Inc., New York, 1969), Chap. 6.

[4] L. Neumann and L. Tewordt, Z. Physik **189**, 55 (1966).

[5] L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. **34**, 735 (1958) [English transl.: Soviet Phys.—JETP **7**, 505 (1958)].

[6] K. Maki and T. Tsuzuki, Phys. Rev. **139**, A868 (1965).

[7] E. Helfand and N. R. Werthamer, Phys. Rev. Letters **13**, 686 (1964); Phys. Rev. **147**, 288 (1966).

berger.[8] The latter has also given calculations of the GL parameter $\kappa_2(T)$ (relating to the magnetization near H_{c2}) for both pure superconductors and for arbitrary values of a scattering mean free path. Leadon and Suhl[9] have made an approximate calculation of the density of states for vortex lines in pure superconductors that is valid when effects of the magnetic field are small, corresponding to large values of κ. The space average of the density of states in the vortex state has been calculated by Brandt, Pesch, and Tewordt.[10] This theory avoids an expansion in powers of Δ and therefore can be used for all energies and the whole range of fields between H_{c2} and H_{c1}. Brandt[11] has used this method to improve the calculation of κ_2 in the pure superconductor near $T=0°$K.

An alternative to the Green's-function methods for treating nonhomogeneous superconductors is the generalized pairing scheme introduced by Bogoliubov.[12,13] The latter method can be used, and is equivalent to the Green's-function method, when effects associated with the finite quasiparticle lifetime can be neglected. In the nonhomogeneous case, the Green's functions $G(\mathbf{r},\mathbf{r}')$ depend on two space points, $\mathbf{r}$ and $\mathbf{r}'$, and this often makes the equations very difficult to solve. On the other hand, since the Bogoliubov functions $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ in the general pairing scheme depend on a single space point, they are easier to deal with.

The equations for u_n and v_n are difficult to solve exactly, but they can be simplified considerably by use of the WKBJ approximation. This approximation requires that $\Delta(\mathbf{r})$ and $h(\mathbf{r})$ vary slowly over atomic distances, which should be nearly always true. Slow variation over a coherence distance is not required. The method is an extension of one used by Mathews[14] for application to the normal-superconducting boundary in the intermediate state.

The WKBJ approximation has been used in past work to get information about vortex lines. Caroli, de Gennes, and Matricon[15] calculated the spectrum of bound states with $E<\Delta_\infty$ in the vortex core. We follow their procedure, in which the functions u_n and v_n are described in cylindrical coordinates (z,r,θ) with the z axis along the axis of the vortex line. For a vortex line with one quantum of flux, the magnetic quantum numbers of the paired states are $(\mu-\frac{1}{2})\uparrow$, $(-\mu-\frac{1}{2})\downarrow$, where μ is half an odd integer. There is generally only a single bound state for each μ, and the quasiparticle energy $E(\mu)$ is positive for μ positive and negative for μ negative. We show that this implies that at $T=0°$K, orbitals of positive μ are unoccupied, those of negative μ occupied. This gives a circulation in the core in the same direction as that of the paired states outside of the core. We also consider the scattering states with $E>\Delta_\infty$, and show that they are superpositions of a particlelike and a holelike excitation of the same energy E.

In their calculations, Caroli *et al.* omitted effects of the magnetic field except as a cutoff in the limit where the penetration depth λ is large compared with the core radius, of the order of the coherence distance ξ. This implies that the GL parameter $\kappa\gg1$. The magnetic field has a large effect on the bound-state energy when $\kappa\sim1$. As pointed out by Hansen[16] and by Tewordt,[17] the effect of the magnetic field can be interpreted as giving a Landau energy of order $\mu e\hbar h(0)/2mc$, where $h(0)$ is the field in the core. This Landau energy is also positive for μ positive, the same sign as arising from the pair potential.

We show that when effects of both pair potential and magnetic field are included, the bound-state energy for μ small is of order $\mu e\hbar H_{c2}/2mc$. This result may account for different predictions in regard to the Hall effect in pure type-II superconductors between Bardeen and Stephen[18] on the one hand and Nozières and Vinen[19] on the other. On the basis of general considerations and analogy with vortex lines in a fluid, the latter two suggested that in the absence of scattering, a vortex line in a type-II superconductor should drift with the electron fluid, which would imply a Hall angle equal to that in the normal metal for a field $H=H_{c2}$. The local model used by Bardeen and Stephen might well give a similar result if the effective field for the Hall effect includes the effect of the pair potential on the bound-state energies.

In previous work, Cleary[20] has extended the calculation of Caroli *et al.* to determine the phase shifts of the scattering states with $E>\Delta_\infty$. From these, he could calculate the scattering of quasiparticles by vortex lines and thus the ultrasonic attenuation in a pure type-II superconductor. Ultrasonic attenuation in type-II alloys has been considered by Galaiko and Fal'ko.[21]

In all of these earlier calculations, the dependence of $\Delta(r)$ on the radial distance r from the axis was assumed or estimated from the GL theory rather than derived

[8] G. Eilenberger, Z. Physik **190**, 142 (1966); Phys. Rev. **153**, 584 (1967).

[9] R. Leadon and H. Suhl, Phys. Rev. **165**, 596 (1968).

[10] U. Brandt, W. Pesch, and L. Tewordt, Z. Physik **201**, 209 (1967); U. Brandt, Phys. Letters **27A**, 645 (1968).

[11] U. Brandt (unpublished).

[12] N. N. Bogoliubov, V. V. Tolmachev, and D. V. Shirkov, *A New Method in the Theory of Superconductivity* (Consultants Bureau Enterprises, Inc., New York, 1959).

[13] The Bogoliubov equations have been used extensively by de Gennes and collaborators. See P.-G. de Gennes, *Superconductivity in Metals and Alloys* (W. A. Benjamin, Inc., New York, 1966).

[14] W. N. Mathews, Jr., Ph.D. thesis, University of Illinois, Urbana, Ill., 1966 (unpublished).

[15] C. Caroli, P.-G. de Gennes, and J. Matricon, Phys. Letters **9**, 307 (1964); C. Caroli and J. Matricon, Phvsik Kondensienten Materie **3**, 380 (1965).

[16] E. B. Hansen, Phys. Letters **27A**, 576 (1968).

[17] L. Tewordt, in *Proceedings of the Advanced Summer Institute on Superconductivity, Montreal, 1968* (Gordon and Breach, Science Publishers, Inc., New York, 1969). The explicit calculation will be given in Ref. 27.

[18] J. Bardeen and M. J. Stephen, Phys. Rev. **140**, A1197 (1965).

[19] P. Nozières and W. F. Vinen, Phil. Mag. **14**, 667 (1966); W. F. Vinen and A. C. Warren, Proc. Phys. Soc. (London) **91**, 409 (1967).

[20] R. M. Cleary, Phys. Rev. **175**, 587 (1968); and to be published.

[21] V. P. Galaiko and I. I. Fal'ko, Zh. Eksperim. i Teor. Fiz. **52**, 976 (1967) [English transl.: Soviet Phys.—JETP **25**, 646 (1967)].

self-consistently. This is also true of the magnetic field variation. Our calculation is the first attempt to derive $\Delta(r)$ and $h(r)$ self-consistently from the solution of the Bogoliubov equations. Actually, we do not do this directly, but make use of a variational expression for the free energy. This expression, derived from one of Eilenberger,[22] involves the eigenvalues E_n of the Bogoliubov equations, but not the functions u_n and v_n. If the E_n are calculated for given variational functions $\Delta(r)$ and $h(r)$, the free energy is a minimum for the $\Delta(r)$ and $h(r)$ that satisfy the correct self-consistent equations.

An estimate of H_{c1} as a function of κ in pure superconductors at $T=0°$K can be made from exact calculations for limiting cases and the results of the GL theory. Our variational solution lies above this estimated curve, indicating some improvement is possible in the variational functions used.

In Sec. II we give an outline of the Bogoliubov equations and some properties of their solutions. We also give the variational expression for the free energy based on the eigenvalues of these equations. Section III describes a convenient method for solution by the WKBJ approximation, a method that can be used in other problems as well as that of the vortex line. The application to the vortex line is given in Sec. IV with the basic equations to be solved for bound states and scattering states. To illustrate the method and to show qualitatively what the solutions are like, we apply it to the simple case of a step pair potential, with $\Delta(r)=0$ for $r<r_c$ and $\Delta(r)=\Delta_\infty$ for $r>r_c$. Bound states are discussed in Sec. V and scattering states in Sec. VI. These results are applied to a discussion of the current density in Sec. VII. In Sec. VIII we return to the problem of calculating the free energy of a vortex line from the eigenvalues for the bound states and the phase shifts for the scattering states. Numerical calculations made with use of digital computers are described in Sec. IX. One-parameter families of trial functions were used for $\Delta(r)$ and for $h(r)$, and the values chosen to make the energy a minimum. Conclusions and possible extensions of the theory are described briefly in Sec. IX.

II. VARIATIONAL METHOD

In this section we give a brief outline of the Bogoliubov equations[12,13] and derive a variational expression for the free energy in terms of the eigenvalues of these equations. Expressed in the Nambu spinor notation,[23] the wave field operators are given in terms of the quasiparticle operators $\gamma_{n\uparrow}$ and $\gamma_{n\downarrow}$ by

$$\begin{pmatrix}\psi_\uparrow(\mathbf{r},t)\\ \psi_\downarrow^\dagger(\mathbf{r},t)\end{pmatrix} =\sum_n\left[\gamma_{n\uparrow}e^{-iE_nt}\begin{pmatrix}u_n(\mathbf{r})\\ v_n(\mathbf{r})\end{pmatrix}-\gamma_{n\downarrow}^\dagger e^{iE_nt}\begin{pmatrix}v_n^*(\mathbf{r})\\ -u_n^*(\mathbf{r})\end{pmatrix}\right], \quad (2.1)$$

[22] G. Eilenberger, Z. Physik **184**, 427 (1965); **190**, 142 (1966).
[23] Y. Nambu, Phys. Rev. **117**, 648 (1960).

where $E_n>0$ is the energy of a quasiparticle excitation relative to the Fermi energy E_F. In this and the following section, we take units such that $\hbar=1$. The ground state Ψ_0 is the vacuum for quasiparticle excitations:

$$\gamma_{n\uparrow}\Psi_0=\gamma_{n\downarrow}\Psi_0=0. \quad (2.2)$$

The functions $u_n(r)$ and $v_n(r)$ are to be determined from the solutions of the Bogoliubov equations:

$$E_nu_n(\mathbf{r})=[(1/2m)(-i\nabla-(e/c)\mathbf{A}(\mathbf{r}))^2-E_F+U(\mathbf{r})]u_n(\mathbf{r})+\Delta(\mathbf{r})v_n(\mathbf{r}), \quad (2.3a)$$

$$E_nv_n(\mathbf{r})=-(1/2m)(i\nabla-(e/c)\mathbf{A}(\mathbf{r}))^2-E_F+U(\mathbf{r})]v_n(\mathbf{r})+\Delta^*(\mathbf{r})u_n(\mathbf{r}). \quad (2.3b)$$

The functions u_n and v_n satisfy the orthogonality relations

$$\int[u_n^*(\mathbf{r})u_m(\mathbf{r})+v_n^*(\mathbf{r})v_m(\mathbf{r})]d^3r=\delta_{nm}, \quad (2.3c)$$

$$\int[u_n(\mathbf{r})v_m(\mathbf{r})-v_n(\mathbf{r})u_m(\mathbf{r})]d^3r=0 \quad (2.3d)$$

and the completeness relations

$$\sum_n[u_n(\mathbf{r})u_n^*(\mathbf{r}')+v_n^*(\mathbf{r})v_n(\mathbf{r}')]=\delta(\mathbf{r}-\mathbf{r}'), \quad (2.4a)$$

$$\sum_n[u_n(\mathbf{r})v_n^*(\mathbf{r}')-v_n^*(\mathbf{r})u_n(\mathbf{r}')]=0. \quad (2.4b)$$

The quasiparticle operators given explicitly in terms of the wave field operators are

$$\gamma_{n\uparrow}=\int[\psi_\uparrow(\mathbf{r})u_n^*(\mathbf{r})+\psi_\downarrow^\dagger(\mathbf{r})v_n^*(\mathbf{r})]d^3r, \quad (2.5a)$$

$$\gamma_{n\downarrow}^\dagger=\int[-\psi_\uparrow(\mathbf{r})v_n(\mathbf{r})+\psi_\downarrow^\dagger(\mathbf{r})u_n(\mathbf{r})]d^3r. \quad (2.5b)$$

There are solutions of the Bogoliubov equations corresponding to both positive and negative values of E_n. If u_n, v_n corresponds to $E_n>0$, another solution is v_n^*, $-u_n^*$ with eigenvalue $-E_n$. An operator which gives a negative energy should be regarded as a destruction operator for an excitation. Thus (2.5a) is a destruction operator obtained from the creation operator (2.5b) by the transformation $(u_n,v_n)\to(v_n^*,-u_n^*)$. A complete set of functions is obtained from the set (u_n,v_n) going with positive eigenvalues, $E_n>0$.

The pair potential $\Delta(\mathbf{r})$ and the vector potential $\mathbf{A}(\mathbf{r})$ describing the magnetic field are to be determined self-consistently. The pair potential is given by

$$\Delta(\mathbf{r})=V\sum_n u_n(\mathbf{r})v_n^*(\mathbf{r})[1-2f(E_n)], \quad (2.6)$$

where V is the attractive interaction constant defined by BCS. The vector potential can be obtained from

Maxwell's equations with the current density given by

$$J(\mathbf{r})=(e\hbar/2mi)\sum_n \{f(E_n)u_n^*[\nabla-(ie/\hbar c)\mathbf{A}]u_n +[1-f(E_n)]v_n[\nabla-(ie/\hbar c)\mathbf{A}]v_n^*-\text{c.c.}\}. \quad (2.7)$$

A straightforward solution of the Bogoliubov equations would involve choosing tentative forms for $\Delta(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$, solving the equations, recalculating $\Delta(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$ with use of (2.6) and (2.7), and then repeating the procedure until a self-consistent solution is obtained. This would be prohibitively difficult.

The thermal Green's functions $G_\omega(\mathbf{r},\mathbf{r}')$ may be expressed in the quasiparticle approximation in terms of the solutions of the Bogoliubov equations[24]

$$G_{\omega 11}(\mathbf{r},\mathbf{r}')=G_{\omega 22}^*(\mathbf{r},\mathbf{r}') =\sum_n\left(\frac{u_n(\mathbf{r})u_n^*(\mathbf{r}')}{i\omega-E_n}+\frac{v_n(\mathbf{r})v_n^*(\mathbf{r}')}{i\omega+E_n}\right), \quad (2.8)$$

where $\omega=\pi\nu/\beta$ and ν is an odd integer.

Eilenberger[22] has shown that the problem of getting a self-consistent solution can be avoided by use of a variational principal for the free energy. He showed that if the thermal Green's function $G_\omega(\mathbf{r},\mathbf{r}')$ is determined for a given $\Delta(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$ from the solution of the Gor'kov equations, the free energy in an external field H_a,

$$G_S=\int\left(\frac{1}{V}|\Delta(\mathbf{r})|^2+\beta^{-1}\sum_{\nu=-\infty}^{\infty}\int_{\omega}^{\infty\,\mathrm{sgn}\,\omega}d\omega'\,T_r \times[i\tau_3 G_{\omega'}(\mathbf{r},\mathbf{r})]+\frac{1}{8\pi}[\mathbf{h}(\mathbf{r})-H_a]^2\right)d^3r, \quad (2.9)$$

is a minimum when $\Delta(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$ satisfy the proper self-consistent equations. Here $\beta^{-1}=k_BT$.

By use of (2.8), one can express G_S simply in terms of the eigenvalues of the Bogoliubov equations:

$$G_S=-2\beta^{-1}\sum_n \ln(2\cosh\tfrac{1}{2}\beta E_n) +\int\left(\frac{|\Delta(\mathbf{r})|^2}{V}+\frac{1}{8\pi}[\mathbf{h}(\mathbf{r})-H_a]^2\right)d^3r. \quad (2.10)$$

The factor of 2 accounts for the two spin states for each E_n.

The expression (2.10) is a generalization of that used by BCS[25] for the case of $\Delta=$const. The sum over n is just what would be obtained for the free energy for an assembly of independent fermions with energies E_n. As in the Hartree-Fock approximation, this counts the interaction energy twice. The next term $\int[|\Delta(\mathbf{r})|^2/V]d^3r$, the negative of the interaction energy, corrects for this double counting. The last term is the magnetic energy.

One may choose variational forms for $\Delta(\mathbf{r})$ and $\mathbf{h}(\mathbf{r})$ involving some parameters, and solve the Bogoliubov equations to get the eigenvalues. The best values for the parameters are those that make G_S a minimum. Note that only the eigenvalues occur in (2.10); the functions u_n and v_n are not required.

In order to get rapid convergence for E_n large it is best to calculate the difference in free energy between superconducting and normal states, or between superconducting states with and without a vortex line present. The states involved are then close to the Fermi surface, since it is only these that are affected by the normal-superconducting transition.

III. SOLUTION OF BOGOLIUBOV EQUATIONS BY WKBJ METHOD

An approximate solution corresponding to the WKBJ method may be obtained by writing the solution in the form

$$\begin{pmatrix}u_n\\ v_n\end{pmatrix}=\begin{pmatrix}e^{i\eta/2}\\ e^{-i\eta/2}\end{pmatrix}e^{iS}, \quad (3.1)$$

where it is assumed that η is slowly varying over atomic distances and ∇S is a wave vector close to the Fermi surface. We keep terms of order $(\nabla S)^2$ or $\nabla S\cdot\mathbf{A}$ and $\nabla S\cdot\nabla\eta$, but neglect terms in $(\nabla\eta)^2$ and $(\nabla\mathbf{A})^2$. For simplicity, we choose the gauge such that $\Delta(\mathbf{r})$ is real. Substitution of (3.1) into the Bogoliubov equations then gives

$$E_n=(1/2m)[-i\nabla^2S+(\nabla S)^2+(e^2/c^2)\mathbf{A}^2+\nabla S\cdot\nabla\eta -(2e/c)\nabla S\cdot\mathbf{A}]-E_F+\Delta(\mathbf{r})e^{-i\eta}, \quad (3.2a)$$

$$E_n=-(1/2m)[-i\nabla^2S+(\nabla S)^2+(e^2/c^2)\mathbf{A}^2-\nabla S\cdot\nabla\eta +(2e/c)\nabla S\cdot\mathbf{A}]+E_F+\Delta(\mathbf{r})e^{i\eta}. \quad (3.2b)$$

These equations are satisfied if ∇S and η are solutions of

$$(1/2m)\nabla S\cdot\nabla\eta+\Delta(\mathbf{r})\cos\eta=E_n+(e/mc)\mathbf{A}\cdot\nabla S, \quad (3.3a)$$

$$(1/2m)[-i\nabla^2S+(\nabla S)^2+(e^2/c^2)\mathbf{A}^2]-E_F =i\Delta(\mathbf{r})\sin\eta. \quad (3.3b)$$

In (3.3a), to a sufficient approximation we may take ∇S to be a wave vector in the direction of ∇S but on the Fermi surface. The departure from the Fermi surface is then given by the second equation. In general, both S and η are complex.

It is usually possible to choose a gauge such that the term in A^2 is negligible. For the isotropic case we may write S in the form

$$S(r)=\mathbf{k}_F\cdot\mathbf{r}+\xi(\mathbf{r}), \quad (3.4)$$

where ξ is small and $\nabla^2\xi$ and $(\nabla\xi)^2$ may be neglected. Equation (3.3b) then becomes

$$m^{-1}(k_F\cdot\nabla\xi)=i\Delta(r)\sin\eta. \quad (3.5)$$

[24] See, e.g., J. R. Schrieffer, *Theory of Superconductivity* (W. A. Benjamin, Inc., New York, 1964), Chap. 7.

[25] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

By a change in normalization, one may regard the WKBJ solutions as corresponding to slowly varying $\tilde{u}(\mathbf{r})$ and $\tilde{v}(\mathbf{r})$:

$$\begin{pmatrix} u_n \\ v_n \end{pmatrix} = (2\cos\eta)^{1/2} \begin{pmatrix} \tilde{u}(\mathbf{r}) \\ \tilde{v}(\mathbf{r}) \end{pmatrix} e^{i\tilde{S}}. \tag{3.6}$$

Here $\tilde{u}(\mathbf{r})$ and $\tilde{v}(\mathbf{r})$ are defined in the usual way, but in terms of a slowly varying energy $\tilde{E}(\mathbf{r})$ and complex $\tilde{\epsilon}(\mathbf{r})$ and $\tilde{\Delta}(\mathbf{r})$:

$$\tilde{u}(\mathbf{r})^2 = 1 - \tilde{v}(\mathbf{r})^2 = \tfrac{1}{2}(1+\tilde{\epsilon}/\tilde{E}). \tag{3.7}$$

This solution is identical with (3.1) with the following definitions:

$$\tilde{E} = E(\hbar^2 e/mc)\mathbf{A}\cdot\nabla S, \tag{3.8}$$

$$\tilde{E}/\tilde{\Delta} = \cos\eta, \tag{3.9}$$

$$\tilde{S} = -\tfrac{1}{2}i\ln(2\cos\eta) + S, \tag{3.10}$$

$$\tilde{\epsilon} = i\tilde{E}\tan\eta. \tag{3.11}$$

Note that

$$\tilde{E}^2 = \tilde{\epsilon}^2 + \tilde{\Delta}^2. \tag{3.12}$$

This method was used by Mathews[14] for a discussion of the normal-superconducting boundary in the intermediate state. It is useful in that it gives a physical interpretation of the variable η. However, the functions in the form (3.1) are somewhat simpler and we shall use them in the subsequent discussion.

IV. BOGOLIUBOV EQUATIONS FOR VORTEX LINE

We consider a vortex line of unit strength along the z axis of cylindrical coordinates r, θ, and z. Our notation is similar to that used by de Gennes.[13] In a gauge for which $\Delta(r)$ is a real, the magnetic field is described by a vector potential

$$A_\theta(r) = \hbar c/2er + A_\theta'(r), \tag{4.1}$$

where $A_\theta' \to 0$ as r goes to zero. For e positive and r small compared with the penetration depth λ,

$$A_\theta' = -\tfrac{1}{2}rh_0, \quad r \ll \lambda \tag{4.2}$$

where $h_0 = -h_z(0)$ is the magnetic field in the $-z$ direction on the axis of the vortex line. When $r \gg \lambda$, so that $h_z \to 0$, $A_\theta(r) \to 0$.

The solutions of the Bogoliubov equations in the gauge, where $\Delta(r) = |\Delta(r)|e^{-i\theta}$ may be expressed in spinor notation as

$$\begin{pmatrix} u_n \\ v_n \end{pmatrix} = \hat{f} e^{ik_z z} e^{i\mu\theta} e^{-i\sigma_z \theta/2}, \tag{4.3}$$

where 2μ is an odd integer and

$$\hat{f} = \begin{pmatrix} f_+(r) \\ f_-(r) \end{pmatrix}.$$

The paired states u_n, v_n^* have angular momenta $\mu - \frac{1}{2}$, $-\mu - \frac{1}{2}$, with a net of -1 per pair. With use of the Pauli matrices σ_x, σ_y, and σ_z the equation for $\hat{f}$ may be written in the form

$$\sigma_z \frac{\hbar^2}{2m}\left[-\frac{d^2\hat{f}}{dr^2} - \frac{1}{r}\frac{d\hat{f}}{dr} + \left(\mu - \frac{\sigma_z e r}{\hbar c} A_\theta\right)^2 \frac{\hat{f}}{r^2} - k_\rho^2 \hat{f}\right] + \sigma_x \Delta(r)\hat{f} = E\hat{f}, \tag{4.4}$$

where $k_z^2 + k_\rho^2 = k_F^2$. Here A_θ is defined by (4.1).

When $A_\theta(r) \equiv 0$ and $\Delta(r) \equiv \Delta_\infty$, one finds the exact solutions

$$f = \frac{\text{const}}{\sqrt{2}} \times \begin{pmatrix} [1 \pm (E^2 - \Delta_\infty^2)^{1/2}/E]^{1/2} \\ [1 \mp (E^2 - \Delta_\infty^2)^{1/2}/E]^{1/2} \end{pmatrix} \times H_\mu^{(1),(2)}\left[\left(k_\rho^2 \pm \frac{2m}{\hbar^2}(E^2 - \Delta_\infty^2)^{1/2}\right)^{1/2} r\right], \tag{4.5}$$

where $H_\mu^{(1),(2)}$ are the Hankel functions of the first and second kind. For $E < \Delta_\infty$, there are two independent exponentially decaying solutions; for $E > \Delta_\infty$, there are four independent solutions. An asymptotic form for the Hankel functions corresponding to the WKBJ approximation is

$$H_\mu^{(1),(2)} \sim \exp\left(\pm i \int_{r_t}^{r} \beta(r')dr'\right) \Big/ (r^2 - r_t^2)^{1/4}, \tag{4.6}$$

where $r_t = \mu/k_\rho$ is the radial distance to the turning point, and where we have

$$\beta(r) = (k/r)(r^2 - r_t^2)^{1/2}. \tag{4.7}$$

Another limiting case which applies at the core of the vortex line is $A_\theta' = 0$ and $\Delta = 0$, for which the appropriate solutions are the Bessel functions $J_{\mu \pm 1/2}(kr)$:

$$f_\pm \approx A_\pm J_{\mu \mp 1/2}[(k_\rho \pm q)r], \tag{4.8}$$

where $q = mE/\hbar^2 k_\rho$. The energy is above the Fermi surface for q positive, below for q negative.

Following Caroli *et al.*,[15] we express the solutions of (4.4) in the form

$$\hat{f}(r) = \hat{g}(r) H_\mu^{(1)}(k_\rho r) + \text{c.c.}, \tag{4.9}$$

where $\hat{g}(r)$ is a slowly varying function.

One may neglect terms in d^2g/dr^2 in comparison with those of order $k_\rho dg/dr$. These terms are of order $(\xi k_\rho)^{-1}$ or Δ/E_F, where ξ is the coherence distance. To the same order, we may neglect terms in A_θ^2. The equation for $\hat{g}$ then becomes

$$(-i\hbar^2/m)\sigma_z \beta_\rho(r)(d\hat{g}/dr) + \Delta(r)\sigma_x \hat{g} = [E + (\mu e\hbar/mcr)A_\theta]\hat{g}, \tag{4.10}$$

where $\beta_\rho(r)$ is $\beta(r)$ for $k = k_\rho$.

In order that the solutions be well behaved at the origin, $\hat{g}(r)$ must be real at the turning point, $r = r_t$, so that the Hankel functions add to become ordinary Bessel functions.

It is convenient to divide by $\Delta(\infty)=\Delta_\infty$ and change variable from r to x, defined by

$$x=(2m\Delta_\infty/\hbar^2k_\rho)(r^2-r_t^2)^{1/2}; \tag{4.11}$$

we also define

$$\Lambda=E/\Delta_\infty, \tag{4.12}$$

$$F(x)=(\mu e\hbar/mcr\Delta_\infty)A_\theta(r),$$
$$\delta(x)=\Delta(r)/\Delta_\infty. \tag{4.13}$$

The equation for $\hat{g}(x)$ then becomes

$$-2i\sigma_z(d\hat{g}/dx)+\delta(x)\sigma_x\hat{g}=[\Lambda+F(x)]\hat{g}. \tag{4.14}$$

To solve this equation, we express g in the form

$$\hat{g}=A\begin{pmatrix} e^{i\eta/2} \\ e^{-i\eta/2}\end{pmatrix}e^{i\xi}, \tag{4.15}$$

where A is a normalization factor and η and ξ are in general complex functions of r. Substituting in (4.14), we find that

$$\left(\frac{d\eta}{dx}+2\frac{d\xi}{dx}\right)e^{i\eta/2}+\delta(x)e^{-i\eta/2}=[\Lambda+F(x)]e^{i\eta/2}, \tag{4.16a}$$

$$\left(\frac{d\eta}{dx}-2\frac{d\xi}{dx}\right)e^{-i\eta/2}+\delta(x)e^{i\eta/2}=[\Lambda+F(x)]e^{-i\eta/2}. \tag{4.16b}$$

Multiplying by $e^{\mp i\eta/2}$ and adding and subtracting the resulting equations, we find that

$$(d\eta/dx)+\delta(x)\cos\eta=\Lambda+F(x), \tag{4.17}$$

$$2(d\xi/dx)=i\delta(x)\sin\eta. \tag{4.18}$$

These equations are to be solved subject to appropriate boundary conditions, which determine the eigenvalues Λ. As x (or r) $\rightarrow\infty$, $F(x)\rightarrow 0$, $\delta(x)\rightarrow 1$, and $\eta\rightarrow\eta_\infty$, where $\cos\eta_\infty=\Lambda=E/\Delta_\infty$. Then (4.9), together with (4.15), goes over into (4.5). For the bound states in the core, $|E|<\Delta_\infty$, η is real, and ξ a pure imaginary. The decaying solution for $x\rightarrow\infty$ requires that η_∞ be between 0 and π so that $\sin\eta_\infty$ is positive. In order that $g(x)$ be real at the turning point, we must have $\eta=0$ or $\pi(\text{mod}2\pi)$ at $x=0$. These conditions determine the eigenvalue E for given μ and k_ρ.

When $E>\Delta_\infty$, η and ξ are complex. They may be expressed as $\eta=\eta_1-i\eta_2$ and $\xi=\xi_1-i\xi_2$, where η_1 and ξ_1 are the real parts and η_2 and ξ_2 are the negatives of the imaginary parts. Separating the real and imaginary parts, we have

$$(d\eta_1/dx)+\delta(x)\cos\eta_1\cosh\eta_2=\Lambda+F(x), \tag{4.19}$$

$$d\eta_2/dx=\delta(x)\sin\eta_1\sinh\eta_2, \tag{4.20}$$

$$2d\xi_1/dx=\delta(x)\cos\eta_1\sinh\eta_2, \tag{4.21}$$

$$2d\xi_2/dx=-\delta(x)\sin\eta_1\cosh\eta_2. \tag{4.22}$$

Note that there are two solutions that differ in the sign of η_2. These correspond to the two signs in the solutions (4.5). When η_2 changes sign, ξ_1 also changes sign but η_1 and ξ_2 remain the same. These two degenerate solutions may be written in the form

$$\hat{g}_\pm=A\begin{pmatrix}\exp(\frac{1}{2}i\eta_1\pm\frac{1}{2}|\eta_2|\pm i\xi_1+\xi_2) \\ \exp(-\frac{1}{2}i\eta_1\mp\frac{1}{2}|\eta_2|\pm i\xi_1+\xi_2)\end{pmatrix}. \tag{4.23}$$

When x is large, we have $\eta_2\rightarrow\eta_{2\infty}$, such that $\cosh\eta_{2\infty}=E/\Delta_\infty$, and $\eta_1\rightarrow 0$. It is also convenient to normalize so that $\xi_2\rightarrow 0$ as $x\rightarrow\infty$.

The solutions that satisfy the boundary condition that $\hat{g}$ be real at $x=0$ are appropriate linear combinations of $\hat{g}_+$ and $\hat{g}_-$. Let us take $\hat{g}=\hat{g}_++C\hat{g}_-$:

$$\hat{g}=\begin{bmatrix}\exp(\frac{1}{2}i\eta_1+\frac{1}{2}\eta_2+i\xi_1)+C\exp(\frac{1}{2}i\eta_1-\frac{1}{2}\eta_2-i\xi_1) \\ \exp(-\frac{1}{2}\eta_1-\frac{1}{2}\eta_2+i\xi_1) \\ \qquad +C\exp(-\frac{1}{2}i\eta_1+\frac{1}{2}\eta_2-i\xi_1)\end{bmatrix}e^{\xi_2}. \tag{4.24}$$

The condition that $\hat{g}$ be real at $x=0$ is obtained by setting the imaginary parts equal to zero. This gives

$$\sin[\xi_1(0)+\tfrac{1}{2}\eta_1(0)]$$
$$=C\exp[-\eta_2(0)]\sin[\xi_1(0)-\tfrac{1}{2}\eta_1(0)], \tag{4.25a}$$

$$\sin[\xi_1(0)-\tfrac{1}{2}\eta_1(0)]$$
$$=C\exp[\eta_2(0)]\sin[\xi_1(0)+\tfrac{1}{2}\eta_1(0)]. \tag{4.25b}$$

These equations are consistent if $C^2=1$ or $C=\pm 1$. The values $\eta_1(0)$ and $\eta_2(0)$ are determined from the solutions of (4.17) that satisfy the boundary conditions $\eta_1\rightarrow 0$ and $\eta_2\rightarrow\eta_{2\infty}$ as $x\rightarrow\infty$. One may regard (4.25) as determining the phase $\xi_1^\pm(0)$ at $x=0$:

$$\frac{\sin[\xi_1^\pm(0)+\frac{1}{2}\eta_1(0)]}{\sin[\xi_1^\pm(0)-\frac{1}{2}\eta_1(0)]}=\pm e^{-\eta_2(0)}. \tag{4.26}$$

The two solutions corresponding to $C=\pm 1$ give the appropriate linear combinations. These solutions are equivalent to those used by Cleary.[20]

It may be noted that the positive signs (η_2 positive) in (4.23) correspond to quasiparticle states with energies above the Fermi surface and the negative signs (η_2 negative) to holes of a corresponding energy below the Fermi surface. Note that if A is chosen so that $|u(\infty)|^2+|v(\infty)|^2=1$, we have

$$|u(\infty)|^2=A^2e^{\eta_{2\infty}}=\tfrac{1}{2}(1+\epsilon/E), \tag{4.27a}$$

$$|v(\infty)|^2=A^2e^{-\eta_{2\infty}}=\tfrac{1}{2}(1-\epsilon/E), \tag{4.27b}$$

where

$$\epsilon=2\Delta_\infty d\xi_1/dx=\Delta_\infty\sinh\eta_{2\infty} \tag{4.28}$$

is the normal-state energy relative to the Fermi surface. Positive η_2 corresponds to positive ϵ, negative η_2 to negative ϵ. The solutions that satisfy the boundary conditions are the linear combinations (4.24).

V. SOLUTIONS FOR STEP PAIR POTENTIAL: BOUND STATES

In order to indicate the qualitative nature of the solutions without undue mathematical complexity, we shall discuss the simple case of a step pair potential for the vortex core with $\delta(r)=0$ for $r<r_c$ and $\delta(r)=1$ for $r>r_c$, where r_c is the radius of the core of the order of the coherence distance $\xi_0=\hbar v_F/\pi\Delta_\infty$. We may express x for a given μ in terms of dimensionless parameters $b_c=2m\Delta_\infty r_c/\hbar^2k_\rho$, of the order of unity if $r_c\sim\xi_0$, and $\mu_c=k_\rho r_c$, the value of μ which gives the turning point at $r=r_c$. In terms of b_c and μ_c, we have

$$x=b_c[(r/r_c)^2-(\mu/\mu_c)^2]^{1/2}. \qquad (5.1)$$

Note that the value of x corresponding to $r=r_c$ is

$$x_c=x(r_c)=b_c[1-(\mu/\mu_c)^2]^{1/2}. \qquad (5.2)$$

We may express μ in terms of a parameter b defined by

$$b=(\mu/\mu_c)b_c. \qquad (5.3)$$

We then have

$$r=(r_c/b_c)(x^2+b^2)^{1/2}. \qquad (5.4)$$

If we omit the term in $A_\theta(r)$ from the magnetic field [i.e., set A_θ' in (4.1) equal to zero], we have in reduced variables

$$F(x)=b/(x^2+b^2). \qquad (5.5)$$

We may take the penetration depth λ into account in a rough way by setting $F(x)=0$ for $r>\lambda$ or $x>x_\lambda$, where x_λ is the value of x corresponding to $r=\lambda$. Although this is nonphysical, it should give qualitatively correct results if $\lambda\gg r_c$. Note that $F(x)$ is an odd function of b and thus of μ.

We shall first discuss the bound states with $|E|<\Delta_\infty$ and then the scattering states for $|E|>\Delta_\infty$.

For the bound states, η is real. Following Caroli *et al.*, it is convenient to introduce a new variable $\psi=\eta-\frac{1}{2}\pi$, so that for η between 0 and π, ψ lies between $-\frac{1}{2}\pi$ and $\frac{1}{2}\pi$. Equation (4.17) becomes

$$d\psi/dx-\delta(x)\sin\psi=\Lambda+F(x). \qquad (5.6)$$

If there is a solution ψ, Λ for a given b, there is a second solution of opposite sign, $-\psi$, $-\Lambda$, $-b$. We will consider only those with positive Λ. With $F(x)$ given by (5.5), we have for a step potential

$$d\psi/dx=\Lambda+F(x),\quad x<x_c. \qquad (5.7)$$

The solution that satisfies the boundary condition that η be equal to a multiple of π at $x=0$ is

$$\psi=-\pi(n+\tfrac{1}{2})+\tan^{-1}(x/b)+\Lambda x,\quad x<x_c \qquad (5.8)$$

where n is an integer.

We may assume that for $x=x_c$, $|\psi|<\frac{1}{2}\pi$. Since $\Lambda<1$, the only possible solution is for $n=0$ unless $x_c>\pi$. When $n=0$, b must be positive unless $x_c>\frac{1}{2}\pi$. Thus when $r_c\sim\xi_0$, so that $x_c\sim1$, there is normally only a single bound state for a given μ, and for positive energy, μ must be positive. This corresponds with the conclusion of Caroli *et al.*[15]

To determine the eigenvalue Λ, we need to match (5.8) with the solutions for $x>x_c$. Explicit solutions can be obtained only for certain limiting cases. If ψ is small for $x>x_c$ so that we may replace $\sin\psi$ by ψ, we have

$$d\psi/dx-\psi=\Lambda+F(x),\quad x_c<x<x_\lambda \qquad (5.9)$$

and for $x>x_\lambda$, we have $F(x)=0$ and $\psi=-\Lambda$. The solution of (5.9) satisfying the boundary condition at $x=x_\lambda$ is

$$\psi=-\Lambda-\int_x^{x_\lambda}e^{(x-x')}F(x')dx',\quad x_c<x<x_\lambda. \qquad (5.10)$$

The condition that the solutions (5.10) and (5.8) join at $x=x_c$ determines Λ:

$$-n\pi-\tan^{-1}(b/x_c)+\Lambda x_c=-\Lambda-\int_{x_c}^{x_\lambda}e^{(x_c-x')}F(x')dx', \qquad (5.11)$$

or, for $n=0$,

$$\Lambda=\frac{E}{\Delta_\infty}=\frac{1}{1+x_c}\left(\tan^{-1}\frac{b}{x_c}-\int_{x_c}^{x_\lambda}e^{(x_c-x')}F(x')dx'\right). \qquad (5.12)$$

An expression valid for $x_\lambda\gg x_c$ and $b\ll x_c$ is

$$E=\frac{2m\mu\Delta_\infty^2e^{x_c}}{\hbar^2k_\rho^2(1+x_c)}\int_{x_c}^{\infty}\frac{e^{-x}}{x}dx. \qquad (5.13)$$

This expression can in fact be obtained[26] directly by joining Bessel's-function solutions of (4.4) appropriate for $r<r_c$ with Hankel-function solutions valid for $r>r_c$ at the core boundary $r=r_c$.

More generally, we may write $\psi=\psi_0+\psi_1$, where ψ_1 is assumed small and $\Lambda=-\sin\psi_0$. The equation for ψ_1 for $x>x_c$ is

$$d\psi_1/dx-\psi_1\cos\psi_0=F(x), \qquad (5.14)$$

or

$$\psi_1(x)=-\int_x^{x_\lambda}e^{(x-x')\cos\psi_0}F(x')dx'. \qquad (5.15)$$

The matching condition at $x=x_c$ is

$$\psi_0+\psi_1(x_c)=-\tan^{-1}(b/x_c)-x_c\sin\psi_0. \qquad (5.16)$$

This equation for ψ_0 is valid only if ψ_1 is indeed small. This will be the case not only when b/x_c is small so that ψ_0 is small, but also when $b>b_c$ and when ψ_0 is close to $-\frac{1}{2}\pi$. In this latter case, the boundary condition is that $\eta=0$ at $x=0$, or $\psi=-\frac{1}{2}\pi$ at $x=0$. The equation for ψ_0 is then

$$\psi_0=-\tfrac{1}{2}\pi+\int_0^{x_\lambda}e^{(x_c-x')\cos\psi_0}F(x')dx'. \qquad (5.17)$$

[26] R. Kümmel, dissertation, Universität Frankfurt, 1968 (unpublished).

This equation is valid when the integral $-\psi_1(0)$ is small. In the limit where $\cos\psi_0$ is so small that the exponential is close to unity throughout the range of integration, the integral can be carried out explicitly to give

$$\psi_0 = -\tfrac{1}{2}\pi + \tan^{-1}(x_\lambda/b), \tag{5.18}$$

$$E = -\Delta_\infty \sin\psi_0 \simeq \Delta_\infty[1 - \tfrac{1}{2}(x_\lambda^2/b^2)]. \tag{5.19}$$

These solutions are equivalent to those of Caroli *et al.*[15] in the appropriate limits. A qualitative plot of E as a function of μ is given in Fig. 1. As we have mentioned, there is normally only one bound state for each μ and spin orientation and for these E is positive for μ positive and negative for μ negative. The positive-energy excitations may be regarded as a linear combination of equal weights of a particle in $\mu - \frac{1}{2}$ above the Fermi sea and hole in $-(\mu + \frac{1}{2})$ below the sea, with μ positive. In the ground-state wave function of the system, the bound states of negative μ are completely filled and those for positive μ empty. As indicated in (2.7), the occupation at $T=0$ [corresponding to $f(E_n)=0$] is given by v_n^* with angular momentum $-(\mu+\frac{1}{2})$. These occupied states give a current in the core in the same direction as that of the general circulation outside of the core corresponding to the pairing $(\mu-\frac{1}{2})\uparrow$, $-(\mu+\frac{1}{2})\downarrow$. The bound states are unpaired in the sense that only the negative angular momentum is occupied in the ground state. Nevertheless, according to (2.6), they do contribute to the pair potential. The qualitative nature of the current distribution from the bound states is discussed in Sec. VII.

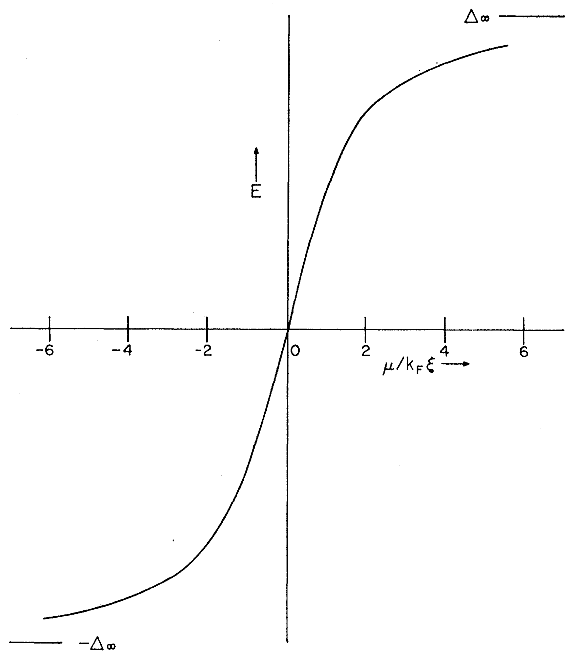

FIG. 1. Energy of bound states as a function of magnetic quantum number μ [schematic, after Caroli *et al.* (Ref. 15)].

VI. SCATTERING STATES FOR STEP PAIR POTENTIAL

We next consider the scattering states with $E > \Delta$. There are solutions for E positive for both signs of μ. Far from the core where $\Delta = \Delta_\infty$, there are two degenerate states (4.5) with $E = (\epsilon^2 + \Delta_\infty)^{1/2}$ corresponding to positive and negative values of ϵ, where ϵ is the energy in the normal state relative to the Fermi surface. One may regard the quasiparticle states with ϵ positive as particles above the Fermi surface and those with ϵ negative as holes below, although it should be remembered that in a superconductor there is no sharp change in the character of these states as the Fermi surface is crossed. As discussed in Sec. IV, the scattering states that satisfy the appropriate boundary conditions at the vortex core are linear combinations of the degenerate states for $\pm\epsilon$.

We again assume a step pair potential with $\delta(x)=0$ for $x<x_c$ and $\delta(x)=1$ for $x>x_c$, so that the basic equations are

$$d\eta/dx = \Lambda + F(x), \quad x < x_c \tag{6.1a}$$

$$d\eta/dx + \cos\eta = \Lambda + F(x), \quad x > x_c. \tag{6.1b}$$

Now $\Lambda > 1$ and $\eta = \eta_i - i\eta_2$ is complex. For $x_c \sim 1$, $\eta_1 < \frac{1}{2}\pi$. We first want to find the solution such that $\eta_1 \to 0$ and $\eta_2 \to \eta_{2\infty}$ as $x \to \infty$, where

$$\cosh\eta_{2\infty} = \Lambda. \tag{6.2}$$

Since the equation is nonlinear, analytic solutions can be given only for certain limiting cases. For $x<x_c$, we may integrate immediately to get

$$\eta = \eta^0 + \tan^{-1}(x/b) + \Lambda x, \quad x < x_c. \tag{6.3}$$

For $x > x_c$, we assume that we may write η in terms of real and imaginary parts as

$$\eta = \eta_1 - i(\eta_{2\infty} + y). \tag{6.4}$$

A limiting case for which analytic solutions are possible is that of small η_1 and y. Neglecting terms in η_1^2 and y^2, we have

$$d\eta_1/dx + y\sinh\eta_{2\infty} = F(x), \tag{6.5}$$

$$dy/dx = \eta_1 \sinh\eta_{2\infty}, \tag{6.6}$$

or

$$d^2y/dx^2 + \sinh^2\eta_{2\infty}\, y = F(x)\sinh\eta_{2\infty}. \tag{6.7}$$

The solution that satisfies the boundary conditions $y \to 0$ and $\eta_1 \to 0$ as $x \to \infty$ is

$$y = \int_x^{x_\lambda} \sin[\alpha(x'-x)]F(x')dx', \tag{6.8}$$

$$\eta_1 = -\int_x^{x_\lambda} \cos[\alpha(x'-x)]F(x')dx', \tag{6.9}$$

where $\alpha = \sinh\eta_{2\infty}$. This solution is valid only when y

and η_1 are indeed small. This will be the case if $F(x)$ is small, which occurs when μ is either large or small compared with μ_c, or in the limits $b \ll x_c$ or $b \gg 1$.

Matching the solutions at $x=x_c$ determines η_2^0. Note that η_2 is constant for $x<x_c$, so that

$$\eta_2^0=\eta_{2\infty}+y(x_c). \tag{6.10}$$

The value of η_1^0 is determined from

$$\eta_1^0+\tan^{-1}(x_c/b)+\Delta x_c=\eta_1(x_c). \tag{6.11}$$

To the same approximation, we have for $x>x_c$

$$2d\xi_2/dx=-\eta_1 \cosh\eta_{2\infty}=-(dy/dx)\coth\eta_{2\infty}. \tag{6.12}$$

The integral that gives $\xi_2 \to 0$ as $x \to \infty$ is

$$\xi_2=-\tfrac{1}{2}y \coth\eta_{2\infty}. \tag{6.13}$$

Note that ξ_2 is independent of the sign of $\eta_{2\infty}$, but does depend on the sign of μ. When μ and thus $F(x)$ is positive, ξ_2 is negative, and when μ is negative, ξ_2 is positive. Since the amplitude of the pair wave function in the core is proportional to $e^{\xi_2(x_c)}$, it is small for μ positive, large for μ negative.

VII. CURRENT DENSITY

The current density can be obtained from the general expression (2.7) with use of the WKBJ wave functions. We shall discuss here only a qualitative picture based on the solutions for the step potential. The only component of current for a stationary vortex is J_θ, given for $T=0$°K by

$$J_\theta=-\frac{2e\hbar}{m}\left[\sum_{E>\Delta_\infty,\ \text{all}\ \mu}|v_n|^2\left(\frac{\mu}{r}+\frac{eA_\theta(r)}{\hbar c}\right)+\sum_{E<\Delta_\infty,\ \mu>0}|v_n|^2\left(\frac{\mu}{r}+\frac{eA_\theta(r)}{\hbar c}\right)\right], \tag{7.1}$$

where $A_\theta(r)$ is defined by (4.1). The first sum is over the continuum of states for $E>\Delta_\infty$ and the second over the bound states; the factor of 2 in front of the entire expression accounts for the two spin orientations. The orbital states may be designated by $n=(k_z,k_\perp,\mu)$ for the unbound and by $n=(k_z,\mu)$ for the bound. We assume only one bound state for each μ, with $k_\perp=k_\rho$.

We shall first discuss the contribution to the current density from the bound states. The total probability density for a state k_z,μ with k_z in the interval dk_z is

$$\frac{dk_z}{2\pi}|v_n|^2=\frac{A^2dk_z}{2\pi[r^2-(\mu/k_\rho)^2]^{1/2}}. \tag{7.2}$$

Here A^2 is the normalization factor such that

$$A^2\int_{\mu/k_\rho}^{r_\omega}\frac{2\pi r dr}{[r^2-(\mu/k_\rho)^2]^{1/2}}=\tfrac{1}{2}, \tag{7.3}$$

where r_ω is the average extent of the wave function. This gives

$$A^2 \simeq (4\pi r_\omega)^{-1}. \tag{7.4}$$

The contribution of the bound states from summing over μ and k_z is

$$J_{\theta B}=-\frac{2e\hbar A^2}{2\pi m}\int_{-k_F}^{k_F}\int_0^{rk_\rho}\frac{\mu d\mu dk_z}{r[r^2-(\mu/k_\rho)^2]^{1/2}} \tag{7.5}$$

$$=-e\hbar n/mr_\omega, \tag{7.6}$$

where $n=k_F^3/3\pi^2$ is the density of electrons. Since r_ω may be expected to be of the order of the coherence distance ξ, we find that $J_{\theta B}$ is of the same order as the critical current density for depairing, $J_c=nev_c$, where v_c is given by $p_Fv_c=\Delta_\infty$.

In the bulk of the superconductor, where $F(x)=0$ and $\eta=\eta_\infty$, $|v_n|^2$ is independent of the sign of μ. The current density $J_{\theta P}$ from the paired states is given by the London value:

$$J_{\theta P}=-(ne^2/mc)A_\theta(r). \tag{7.7}$$

In the neighborhood of the core, $|v_n|^2$ is changed by a factor

$$f(\mu)=\frac{\cosh\eta_2}{\cosh\eta_{2\infty}}e^{2\xi_2}, \tag{7.8}$$

resulting from changes in η_2 and ξ_2 from their values deep in the superconductor. This expression neglects some relatively small terms from interference effects between the two solutions in (4.24). If we assume that $y=\eta_2-\eta_{2\infty}$ is small, the factor may be written

$$\begin{aligned}f(\mu)&=\exp(\ln\cosh\eta_2-\ln\cosh\eta_{2\infty}+2\xi_2)\\&=\exp[-y(\coth\eta_{2\infty}-\tanh\eta_{2\infty})].\end{aligned} \tag{7.9}$$

This factor depends on the sign of μ, being >1 when μ is negative and <1 when μ is positive. The effect is to give a positive contribution to J_θ from the terms

$$-(2e\hbar/mr)\sum_n |v_n|^2\mu. \tag{7.10}$$

This contribution tends to compensate the negative contributions from (7.7) and from the bound states in the region of the core.

When the GL constant κ is of the order of unity, most of the current circulating about the axis of the vortex line comes from the bound states in the core. When $\kappa \gg 1$, most of the current circulates outside of the core, and the density is given by the London value (7.7).

It is of interest to note that the energies of the bound states in the core are qualitatively like those of electrons in circular orbits centered on the axis in a magnetic field parallel with the axis. The pair potential acts like an effective magnetic field of the order of H_{c2}. Neglecting the true magnetic field, the energies for small μ may be expressed in the form

$$E=\mu h_p(e\hbar/2mc), \tag{7.11}$$

where h_p depends on k_z and is of the order of H_{c2}. The magnetic field contributes an additional energy $\mu h_{\text{core}}(e\hbar/2mc)$, where h_{core} is the magnetic field in the core, of the order of H_{c1}.[16,17] The total effective field would then be $h_{\text{eff}}=h_p+h_{\text{core}}$, again of the order of H_{c2}. Some estimates of $dE/d\mu$ for the bound states are given in Table II.

VIII. FREE ENERGY OF VORTEX LINE

The free-energy difference ΔG between the state with a single vortex line and the Meissner state in the same applied field, H_a, is calculated from the general expression in Eq. (2.10). ΔG is divided into five contributions.

The term involving the space integral of $|\Delta(\mathbf{r})|^2=\Delta^2(r)$ yields the contribution

$$\Delta G_i=2\pi LV^{-1}\int_0^\infty dr\, r[\Delta^2(r)-\Delta_\infty^2], \tag{8.1}$$

where L is the length of the vortex line, V is the coupling constant, and Δ_∞ is the BCS energy gap at temperature T.

The difference in the magnetic field energies can be split up into two parts. The first part is

$$\Delta G_m=\frac{L}{4}\int_0^\infty dr\, rh^2(r). \tag{8.2}$$

There is also a term proportional to the applied field H_a:

$$\Delta G_a=-LH_a\hbar c/4e; \tag{8.3}$$

we have used the fact that the total flux of the line is equal to $hc/2e$.

When the vortex line is introduced into a homogeneous superconductor in the Meissner state, the bound states are pulled down from the level $E=\Delta_\infty$; the corresponding change in the free energy is

$$\Delta G_b=-2\beta^{-1}\sum_{0\leq E_n\leq\Delta_\infty}\ln\left(\frac{\cosh(\frac{1}{2}\beta E_n)}{\cosh(\frac{1}{2}\beta\Delta_\infty)}\right). \tag{8.4}$$

Here n is specified by $k_z=k_F\cos\alpha$ $(0\leq\alpha\leq\pi)$ and μ. Instead of μ, it is more convenient to use the quantity b defined by

$$b=\mu\Delta_\infty/E_F\sin^2\alpha. \tag{8.5}$$

Converting the sums over k_z and μ into integrals over α and b, we obtain

$$\Delta G_b=\pi\xi^2LN(0)\Delta_\infty^2\tfrac{1}{2}\pi^2\int_0^\pi d\alpha\,\sin^3\alpha \times\int_0^\infty db(\tfrac{1}{2}\beta\Delta_\infty)^{-1}\ln\left(\frac{\cosh(\frac{1}{2}\beta\Delta_\infty)}{\cosh[\frac{1}{2}\beta\Delta_\infty\Lambda(b,\alpha)]}\right). \tag{8.6}$$

The quantity $N(0)=k_Fm/2\pi^2\hbar^2$ is the density of states, $\xi=\hbar^2k_F/\pi m\Delta_\infty$ is the temperature-dependent coherence length, and $\Lambda(b,\alpha)=E_n/\Delta_\infty$ is the eigenvalue of Eq. (4.17).

The insertion of the vortex line into the homogeneous superconductor also leads to phase shifts in the continuum states, and in turn to shifts in their energies. The WKBJ solution is given by Eqs. (4.9) and (4.24). The phase shift of this solution at large r, in comparison to the solution (4.5) of the reference state with $\Delta(r)\equiv\Delta_\infty$ and $A_\theta(r)\equiv0$, is defined by (note that $\eta_1\to0$ as $r\to\infty$)

$$\xi_1\xrightarrow[r,x\to\infty]{}\delta\xi_1^{(\pm)}+(m/\hbar^2k_\rho)(E^2-\Delta_\infty^2)^{1/2}r =\delta\xi_1^{(\pm)}+\tfrac{1}{2}x\sinh\eta_{2\infty}. \tag{8.7}$$

This asymptotic behavior of ξ_1, together with Eq. (4.21), leads to the following expression for the phase shift:

$$\delta\xi_1^{(\pm)}=\xi_1^{(\pm)}(0)+\frac{1}{2}\int_0^\infty dx' \times[\delta(x')\sinh\eta_2\cos\eta_1-\sinh\eta_{2\infty}]. \tag{8.8}$$

The quantity $\xi_1^{(\pm)}(0)$, where the argument refers to $x=0$, has to be determined from Eq. (4.26).

The resulting energy shift ΔE_n can be calculated most conveniently by enclosing the vortex line in a finite cylindrical volume of radius $R\gg\xi$ and requiring that the solution vanish at $r=R$. Comparing this boundary condition with the corresponding one for the reference state (4.5), one finds, with the help of Eq. (8.7), that

$$\Delta E_n=-\frac{\hbar^2k_\rho}{m}\frac{(E^2-\Delta_\infty^2)^{1/2}}{E}\frac{\delta\xi_1^{(\pm)}}{R}. \tag{8.9}$$

The total change in the free energy due to the modification of the continuum states by the vortex line is then

$$\Delta G_c=-\sum_{E_n\geq\Delta_\infty}\Delta E_n[1-2f(\beta E_n)]. \tag{8.10}$$

The function f is the Fermi function. The summation index n is specified by four quantities: k_z, μ, the radial wave number k given by

$$k^2=k_\rho^2\pm2m\hbar^{-2}(E^2-\Delta_\infty^2)^{1/2}, \tag{8.11}$$

and finally the sign in $\delta\xi_1^{(\pm)}$. Recall that the two signs in the latter quantity correspond to the two possible linear combinations of the particle like and the holelike excitations [$C=\pm1$ in Eq. (4.24)].

Instead of the variables k_z, μ, and k (or E where $\Delta_\infty\leq E\leq\hbar\omega_D$), we introduce the dimensionless variables α, b, and $\Lambda=E/\Delta_\infty$, and convert the summations into integrations. Then Eq. (8.10) together with Eq. (8.9) yields

$$\Delta G_c = \pi\xi^2 L N(0)\Delta_\infty{}^2 \tfrac{1}{2}\pi \int_0^\pi d\alpha\, \sin^3\alpha \times \int_0^\infty db \int_1^{\hbar\omega_D/\Delta_\infty} d\Lambda\, \Sigma(\Lambda,b,\alpha)[1-2f(\beta\Delta_\infty\Lambda)]. \quad (8.12)$$

The quantity $\Sigma(\Lambda,b,\alpha)$ is equal to the sum of the four phase shifts for given Λ and α:

$$\Sigma(\Lambda,b,\alpha) = \delta\xi_1{}^{(+)}(b) + \delta\xi_1{}^{(-)}(b) + \delta\xi_1{}^{(+)}(-b) + \delta\xi_1{}^{(-)}(-b). \quad (8.13)$$

Inspired by the numerical results (see Sec. IX), Bergk[27] has shown, by means of a WKBJ solution of Eqs. (4.19) and (4.20), that for sufficiently large energies Λ, the sum of the phase shifts is inversely proportional to Λ:

$$\Sigma(\Lambda,b,\alpha) \xrightarrow[\Lambda\to\infty]{} C(b,\alpha)/\Lambda. \quad (8.14)$$

From his explicit expression for $C(b,\alpha)$, one can derive the relation

$$\frac{\pi}{2}\int_0^\pi d\alpha\, \sin^3\alpha \int_0^\infty db\, C(b,\alpha) = 2(\Delta_\infty\xi)^{-2}\int_0^\infty dr\, r[\Delta_\infty{}^2 - \Delta^2(r)]. \quad (8.15)$$

Equation (8.15), together with the BCS relation[25]

$$\frac{1}{N(0)V} = \int_1^{\hbar\omega_D/\Delta_\infty} \frac{d\Lambda}{(\Lambda^2-1)^{1/2}}[1-2f(\beta\Delta_\infty\Lambda)], \quad (8.16)$$

can be used to combine the expression for ΔG_c in Eq. (8.12) with that for ΔG_i in Eq. (8.1). The result is

$$\Delta G_{ci}\Delta G_c + \Delta G_i = \pi\xi^2 L N(0)\Delta_\infty{}^2 \tfrac{1}{2}\pi \int_0^\pi d\alpha\, \sin^3\alpha \int_0^\infty db\, K(b,\alpha), \quad (8.17)$$

where

$$K(b,\alpha) = \int_1^{\hbar\omega_D/\Delta_\infty} d\Lambda \left(\Sigma(\Lambda,b,\alpha) - \frac{C(b,\alpha)}{(\Lambda^2-1)^{1/2}}\right) \times [1-2f(\beta\Delta_\infty\Lambda)]. \quad (8.18)$$

One recognizes with the help of the asymptotic relation (8.14) that the two terms in large parentheses in the integrand of Eq. (8.18) almost cancel each other for large Λ. This ensures convergence of the Λ integral in the weak-coupling limit. Note that ΔG_{ci} is of order $N(0)V$ times ΔG_i, or ΔG_c.

[27] W. Bergk and L. Tewordt (to be published).

The final result for the free-energy difference between the vortex and the Meissner state is

$$\Delta G = \Delta G_m + \Delta G_a + \Delta G_b + \Delta G_{ci}, \quad (8.19)$$

where the contributions on the right-hand side are given by Eqs. (8.2), (8.3), (8.6), and (8.17).

IX. NUMERICAL RESULTS AND DISCUSSION

Instead of attempting to solve the Bogoliubov equations self-consistently, we have employed a variational method. The method consists simply of guessing forms (containing adjustable parameters) for the unknown functions $\Delta(r)$ and $h(r)$. The free-energy difference ΔG between the vortex and Meissner states is then calculated from Eq. (8.19), etc., and minimized with respect to these parameters.

The first function occurring in our differential equations (4.17)–(4.22) is $\delta(x) = \Delta(x) = \Delta(x)/\Delta_\infty$. A form for $\delta(r)$ which combines both the exponential approach to unity at $r \gg \xi$ and the linear behavior for $r \ll \xi$ found in the solution of the GL equations is

$$\delta(r) = \Delta(r)/\Delta_\infty = \tanh(dr/\xi), \quad (9.1)$$

where d is an adjustable parameter expected to be of order unity. For r greater than the turning point (i.e., $x \geq 0$), δ can be written as

$$\delta(x) = \tanh[a(x^2+b^2)^{1/2}], \quad (9.2)$$

where

$$a = \tfrac{1}{2}\pi d\, \sin\alpha. \quad (9.3)$$

The second function occurring in Eqs. (4.17) and (4.19) is $F(x)$ defined by Eq. (4.12); it can be written as

$$F(x) = bq(x)/(b^2+x^2), \quad (9.4)$$

where $q(r)$ is the net flux of the line outside a circle of radius r, measured in units $hc/2e$. We have chosen

$$q(r) = 1/\cosh(sr/\xi), \quad (9.5)$$

where s is an adjustable parameter expected to be of order $1/\kappa$. For $x \geq 0$,

$$q(x) = 1/\cosh[c(x^2+b^2)^{1/2}], \quad (9.6)$$

where

$$c = \tfrac{1}{2}\pi s\, \sin\alpha. \quad (9.7)$$

The field is related to the net flux q by

$$h(r) = -(\hbar c/2e)r^{-1}dq(r)/dr. \quad (9.8)$$

The form for q in Eq. (9.5) is such that $h(r)$ exhibits the same behavior as the GL solution for $r \gg \kappa\xi$ and $r \ll \kappa\xi$.

So far, the free-energy difference ΔG has been minimized only for zero temperature. At $T = 0°K$ the GL parameter κ for a pure superconductor and the thermodynamic critical field H_c are given by the relations

$$\kappa = 0.96\lambda_L/\xi_0, \qquad H_c{}^2 = 4\pi N(0)\Delta_\infty{}^2. \quad (9.9)$$

TABLE I. Numerical values of $N(a,c)$ [defined by Eq. (9.11)].

$c \backslash a/c$	1	2	4	20
0.25	0.870	0.738	0.631	0.647
0.5	0.573	0.467	0.462	0.471
1.0	0.319	0.304	0.310	0.321
2.0	0.190	0.192	0.197	0.202

With the help of these relations and our variational form for $h(r)$, we find that the general expression for ΔG in Eq. (8.19), taken at zero temperature, becomes

$$\Delta G=\pi\xi_0^2 LN(0)\Delta_\infty^2\left[0.691\kappa^2 s^2-3.789\kappa\left(\frac{H_a}{\sqrt{2}H_c}\right)+\tfrac{1}{2}\pi^2\int_0^\pi d\alpha\,\sin^3\alpha N(a,c)\right], \quad (9.10)$$

where

$$N(a,c)=\int_0^\infty db\{[1-\Lambda(b)]+\pi^{-1}K(b)\} \quad (9.11)$$

and

$$K(b)=-C(b)\ln 2+\int_1^\infty d\Lambda\{\Sigma(\Lambda,b)-C(b)\Lambda^{-1}\}. \quad (9.12)$$

The bound-state eigenvalues $\Lambda(b)$ and the sums of the phase shifts of the continuum states $\Sigma(\Lambda,b)$ depend, of course, on the parameters a and c in our variational forms for $\delta(x)$ and $q(x)$, and in turn on d, s, and α [see Eqs. (9.3) and (9.7)].

For the bound states, one determines by repeated integration of the differential equation (4.17) the value of $\Lambda(b)$ which makes the value of η at $x=0$ equal to $n\pi$, where $n=0, \pm 1, \pm 2$, etc. In Fig. 2, Λ is plotted versus b for different a and c and for $n=0$. For the continuum states, one integrates Eqs. (4.19) and (4.20) and calculates the sum of the phase shifts $\Sigma(\Lambda,b)$ from Eqs. (8.13) and (8.8).

One of the first results of the numerical calculations was that $\Sigma(\Lambda,b)\approx C(b)/\Lambda$ for $\Lambda\gg 1$; therefore the integral in Eq. (9.12) is rapidly convergent. In Fig. 3, we have plotted Σ versus Λ for different b and $a=2$ and $c=1$. Further, it was found that $C(b)$ satisfies the relation

$$\int_0^\infty db\,C(b)\approx\frac{1.0885}{a^2}. \quad (9.13)$$

With the help of this numerical relation we may calculate the left-hand side of Eq. (8.15). This should be equal to the right-hand side, which is easily calculated by inserting the $\Delta(r)$ of Eq. (9.1). Then one finds that Eq. (8.15) is satisfied to within 1 part in 10^3.

Before proceeding to minimize the free-energy difference ΔG [given by Eq. (9.10)], we remark that we are primarily interested in applying our results to pure type-II superconductors with κ values of order unity;

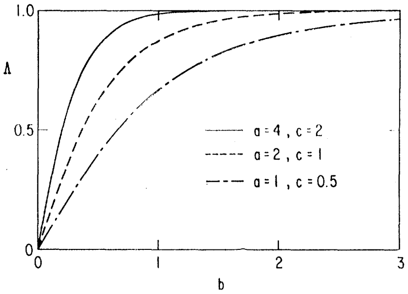

FIG. 2. Eigenvalue Λ of Eq. (4.17), as a function of b for three cases: $a=4$, $c=2$, $a=2$, $c=1$; and $a=1$, $c=0.5$.

hence we expect the value of s which minimizes the free energy also to be of order unity. Also, in the evaluation of the integral over α in Eq. (9.10), the region near $\alpha=\frac{1}{2}\pi$ is the most important. Calculated values of $N(a,c)$ for a range of values of a and c are given in Table I. The dependence of ΔG on d is rather small for $c=1$ and 2, corresponding to $\kappa\approx 1$; a flat minimum occurs for $a/c=d/s$ about 2 for $c=1$ and about 3 for $c=0.5$.

In order to carry out the integration over α in (9.10), we have used empirical expressions for $N(a,c)$ that fit with reasonable approximation to the computed values. An empirical expression for the integral for the bound states that fits within $\sim 0.2\%$ for $c/a<1$ is

$$\int_0^\infty[1-\Lambda(b)]db=\frac{0.592}{c}+\left(\frac{1}{1.97c+3.04c^2}+0.001\frac{a}{c^3}\right)\times\left[\left(\frac{c}{a}\right)^{3/2}-0.825\right]. \quad (9.14)$$

The term $0.001(a/c^3)$ makes a negligible contribution except when c is small. An approximate expression for

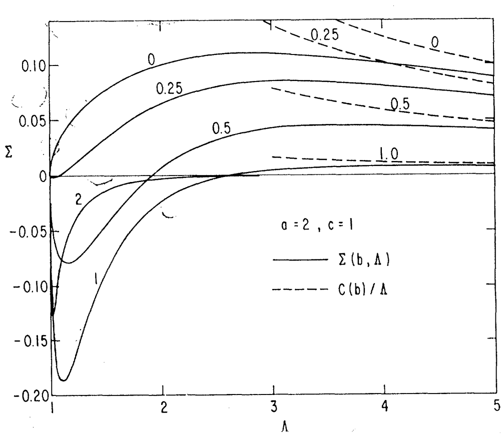

FIG. 3. Total phase shift $\Sigma(b,\Lambda)$, defined by Eq. (8.13), plotted against the energy Λ for the case $a=2$ and $c=1$; also plotted is $C(b)/\Lambda$, the asymptotic expression for Σ. The numbers beside the curves give the values of b.

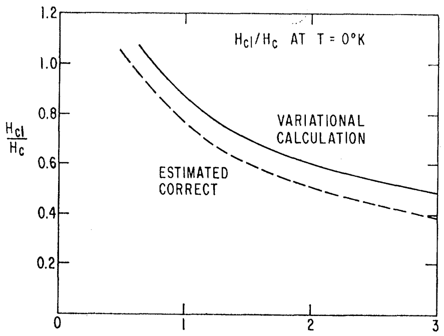

FIG. 4. Lower critical field H_{c1} at $T=0°$K as a function of κ. The solid line gives the results of the variational calculation; the dashed line gives an estimate of the correct behavior based on exact solutions for limiting cases.

the contribution from the scattering states is

$$\pi^{-1}\int_0^\infty K(b)db = -c^{-1}\{0.35(c/a)+0.08\}+0.11(c/a). \quad (9.15)$$

The sum of (9.14) and (9.15) gives $N(a,c)$. After integrating over α, one can find the value of $c/a=d/s$ that makes ΔG a minimum for a given s. The value of s for minimum free energy can then be determined as a function of κ.

A simpler procedure has also been used. For each c one can find the minimum in $N(a,c)$ as a function of the ratio a/c. These minimum values can be approximated by

$$N_m(c)\equiv N(a,c)_{\min}=1/(1.1+2.1c). \quad (9.16)$$

This latter expression is reasonably accurate for $c>0.25$, but does not have the correct limiting form for c very small. Use of (9.16) gives very nearly the same results for the integral over α and for ΔG as use of (9.14) and (9.15).

The integration over α may be regarded as replacing $\sin\alpha$ in $c=\frac{1}{2}\pi s\sin\alpha$ in the denominator of (9.16) by an average value nearly independent of s:

$$\langle c\rangle=\tfrac{1}{2}\pi s\langle\sin\alpha\rangle\approx 1.33s. \quad (9.17)$$

In this way we find

$$\pi^2\int_0^{\pi/2} N_m(c)\sin^3\alpha\, d\alpha\approx\frac{6}{1+2.6s}. \quad (9.18)$$

The value of s for a given κ is that which makes (9.10) a minimum, or approximately

$$1.381\kappa^2 s+\frac{\partial}{\partial s}\left(\frac{6}{1+2.6s}\right)=0. \quad (9.19)$$

TABLE II. Results of variational calculation for several values of κ.

κ	s	d	H_{c1}/H_c	$h(0)/H_c$	$(d\Lambda/db)_{b=0}$
0.74	1.2	~2.1	1.0	~1.4	~1.9
1.3	0.75	~1.5	0.75	~1.0	~1.5
3.0	0.35	~1.2	0.48	~0.48	~1.1

The lower critical field H_{c1} is the value of H_a that makes $\Delta G=0$. A plot of H_{c1}/H_c so calculated is given in Fig. 4. The critical value of κ for type-II superconductivity is that for which $H_{c1}=H_c$. We find that the variational calculation gives $\kappa_{\rm crit}=0.74$.

An estimate of the correct $H_{c1}(\kappa)$ at $T=0°$K can be obtained from the extended GL theory for very large κ and exact calculations for $H_{c2}(\kappa)$. For $\kappa=\kappa_{\rm crit}$,

$$H_{c1}=H_c=H_{c2} \quad (9.20)$$

and the exact theory[6,7] gives at $T=0°$K

$$H_{c2}/\sqrt{2}H_c=\kappa_1=1.25\kappa. \quad (9.21)$$

This gives $\kappa_{\rm crit}=1/1.25\sqrt{2}=0.56$. When κ is very large, one may write $H_{c1}/H_c=\ln\kappa_3/\sqrt{2}\kappa_3$ as in the GL theory, where $\kappa_3=1.15\kappa$ at $T=0°$K. Thus, $H_{c1}(\kappa)$ at $T=0°$K can be estimated by shifting the GL plot by a factor of 1/1.25 for $\kappa=\kappa_{\rm crit}$ and by a factor of 1/1.15 for κ large. Such an estimate is given by the dotted line in Fig. 4.

It is interesting that, as the temperature is decreased from T_c, the reduced lower critical field $H_{c1}(T)/H_c(T)$ for a given value of κ first increases above the GL value (this follows from the generalized GL theory in Ref. 4) and then decreases below it.

It can be seen that the values of $H_{c1}(\kappa)$ from our variational calculation are about 10% too large near $\kappa_{\rm crit}$ and about 20% too large for $\kappa\sim 3$. Since the dependence of the free energy on d is rather small for $\kappa\sim 1$, with a flat minimum, it is likely that it is the variational form for the magnetic field variaton $q(r)$, rather than that for $\Delta(r)$, that needs improvement. We are now trying some other forms for $q(r)$ and $\Delta(r)$ in an attempt to improve the results.

Some of the other quantities that can be estimated from the theory are given for several values of κ in Table II. In addition to $H_{c1}(\kappa)/H_c$, this table gives the approximate values of s and d for minimum free energy, the reduced magnetic field $h(0)/H_c$ on the axis of the vortex, and $(d\Lambda/db)_{b=0}$. The field on the axis is obtained from $h(0)/\sqrt{2}H_c=0.947\kappa s^2$. Since for $\kappa=\kappa_{\rm crit}$ we should have $h(0)=H_c$, the ratio $h(0)/H_c$ is too large near $\kappa=\kappa_{\rm crit}$, and it also seems to be too small near $\kappa\sim 3$. This may reflect an incorrect form from $q(r)$ and the need for an improved variational function.

As we have mentioned in Sec. VII, the dependence of the bound-state energy on the magnetic quantum number μ is of the order of that expected for a Landau energy in a field $H=H_{c2}$. The latter would give

$$E(\mu)=(e\hbar/2mc)\mu H_{c2}. \quad (9.22)$$

The value of H_{c2} at $T=0°K$ is given by

$$H_{c2}=0.66\hbar c/\xi_0^2, \tag{9.23}$$

where $\xi_0=\hbar v_F/\pi\Delta_\infty$ is the BCS coherence distance. This gives

$$E(\mu)=(1.63\Delta_\infty^2/E_F)\mu. \tag{9.24}$$

The dependence of the bound-state energy on μ near $\mu=0$ can be expressed in the form

$$\frac{dE_b}{d\mu}=\Delta_\infty\frac{d\Lambda}{db}\frac{db}{d\mu}=\frac{d\Lambda}{db}\frac{\Delta_\infty^2}{E_F\sin^2\alpha}. \tag{9.25}$$

As discussed in Sec. VII, we may define an effective magnetic field h_{eff} by writing the bound-state energy near $\mu=0$ in the form

$$E_b=(e\hbar/2mc)\mu h_{\text{eff}}; \tag{9.26}$$

comparing (9.22) and (9.26), we have

$$h_{\text{eff}}/H_{c2}=(d\Lambda/db)_{b=0}/1.63\langle\sin^2\alpha\rangle. \tag{9.27}$$

As can be seen from the values listed in Table II, this ratio is of the order of unity. Near $\kappa=\kappa_{\text{crit}}$, most of the dependence of the energy on μ comes from the magnetic field. When κ is large, the field in the core is small and most of the dependence comes from the pair potential.

It is suggested that h_{eff} is the appropriate field to use in calculating the motion of a vortex line in the local model. Bardeen and Stephen[18] showed that in a local model a vortex line should move at an angle relative to the direction transverse to the transport current equal to the Hall angle in the normal state for a magnetic field equal to that in the core. This means that near H_{c1}, the Hall angle should be equal to that in the normal metal in a field only slightly larger than H_{c1}. On the other hand, Nozières and Vinen[19] suggested that in a very pure metal, the velocity of the vortex line in a direction parallel to the transport current should be equal to the drift velocity of the electrons in the transport current. This corresponds to a Hall angle in the normal state in a field equal to H_{c2}. Recent experimental evidence [28,29] from Hall measurements on pure niobium in the mixed state is in accord with this view. If h_{eff} determines the Hall angle, as one might expect, the angle could indeed be that for a field H_{c2}. The anomalously large Hall angles found in some alloys might also be accounted for in this way.

The calculations of the free energy are being extended to finite temperatures by Cleary. From these, one can determine the specific heat from excitations in the vortex core. Cleary shows that near T_c one can expand the free energy (2.10) in a series in $\Delta(r)$ and obtain the GL expression. By changing the boundary conditions, calculations for a vortex lattice are also possible.

It is hoped that the WKBJ method can be extended to other problems, including time-dependent problems such as that involved in vortex motion. In addition to problems relating to vortices in type-II superconductors, the methods can be applied to a number of problems with plane boundaries in type-I superconductors, such as the calculation of the normal-superconducting boundary energy in the intermediate state and the proximity effect.

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