Theory for superconductivity in a magnetic field: A local approximation approach

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(Dated: February 1, 2008)

We present a microscopic theory for superconductivity in a magnetic field based on a local approximation approach. We derive an expression for free energy density $F$ as a function of temperature $T$ and vector potential $a$, and two basic equations of the theory: the first is an implicit solution for energy gap parameter amplitude $|\Delta_k|$ as a function of wave vector $k$, temperature $T$ and vector potential $a$, and the second is a London-like relation between electrical current density $j$ and vector potential $a$, with an “effective superconducting electron density” $n_a$ that is both $T$- and $a$-dependent. The two equations allow determination of spatial variations of $a$ and $|\Delta_k|$ in a superconductor for given temperature $T$, applied magnetic field $H_a$ and sample geometry. The theory shows the existence of a “partly-paired state,” in which paired electrons (having $|\Delta_k| > 0$) and de-paired electrons (having $|\Delta_k| = 0$) co-exist. Such a “partly-paired state” exists even at $T=0$ when $H_a$ is above a threshold for a given sample, rise to a non-vanishing Knight shift at $T = 0$ for $H_a$ above the threshold. We expect the theory to be valid for highly-local superconductors for all temperatures and magnetic fields below the superconducting transition. In the low-field limit, the theory reduces to the local-limit result of BCS. As examples, we apply the theory to the case of a semi-infinite superconductor in an applied magnetic field $H_a$ parallel to the surface of the superconductor and the case of an isolated vortex in an infinite superconductor, and determine, in each case, spatial variations of quantities such as $a$ and $|\Delta_k|$. We also calculate magnetic field penetration depth $\lambda(T, H_a)$ and lower critical magnetic field $H_{c1}(T)$. The ratio $H_{c1}(T)/H_c(T)$ (where $H_c$ is the thermodynamic critical magnetic field) is found to be only weakly $T$-dependent for low temperatures and nearly $T$-independent for intermediate and high temperatures, and quantitatively not very different from that of the Ginzburg-Landau theory for Ginzburg-Landau parameter $\kappa \gg 1$.

PACS numbers: 74.20.-z, 74.20.Fg

I. INTRODUCTION

Currently accepted microscopic theories for superconductivity in a magnetic field include the microscopic derivation of the Meissner effect in the BCS theory and the microscopic derivation of the phenomenological Ginzburg-Landau equations by Gorkov from the BCS theory. However, the BCS derivation of the Meissner effect is based on a linear-response approach (i.e., an externally applied magnetic field is treated as a weak perturbation), and thus, is valid only in the low-field limit. The Gorkov derivation of the Ginzburg-Landau equations is based on the assumption that energy gap function $\Delta(x)$ is a small quantity, and thus, is valid only for temperatures just below critical temperature $T_c$. Various extensions of the Gorkov theory also rely heavily on the assumption of $\Delta(x)$ being small, or the assumption of magnetic field being weak.

It is desirable to have a microscopic theory for superconductivity in a magnetic field that is valid under more general conditions. As an effort along this line, we present in this paper a theory based on a local approximation approach. The theory allows microscopic description of the suppression of superconductivity by an externally applied magnetic field. The theory is expected to be valid for highly-local superconductors (the high-temperature copper-oxide superconductors are examples of highly-local superconductors, for which Ginzburg-Landau parameter $\kappa \gg 1$) for all temperatures and magnetic fields below the superconducting transition (except, perhaps, in the high-field limit when the effect of spin paramagnetism, which is neglected in the present work, may become important). In the low-field limit, the theory reduces to the local-limit result of BCS.

In Sec. II we present the details of the theory, and derive an expression for free energy density $F$ as a function of temperature $T$ and vector potential $a$, and two basic equations of the theory: the first is an implicit solution for energy gap parameter amplitude $|\Delta_k|$ as a function of wave vector $k$, temperature $T$ and vector potential $a$, and the second is a relation between electrical current density $j$ and vector potential $a$. We also analyze solutions for $|\Delta_k (T, a)|$. In Sec. III as examples, we apply the theory to the case of a semi-infinite superconductor in an applied magnetic field $H_a$ parallel to the surface of the superconductor and the case of an isolated vortex in an infinite superconductor, and determine, in each case, spatial variations of quantities such as $a$ and $|\Delta_k|$. We also calculate magnetic field penetration depth $\lambda(T, H_a)$ and lower critical magnetic field $H_{c1}(T)$. A brief summary is given in Sec. IV.

II. THEORY

We consider a superconductor in an applied magnetic field. Our starting point is the same BCS pairing Hamiltonian:

$$\hat{H} = \sum_{k\sigma} (\epsilon_k - \epsilon_F) c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{kk'} V_{kk'} c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger} c_{-k'\downarrow} c_{k'\uparrow}, \quad (1)$$
where \( \epsilon_k \) is the normal state single-electron energy, \( \epsilon_F \) the Fermi energy, \( V_{kk'} \) the pairing interaction matrix element, and \( c_k^\dagger \) and \( c_k \) are the Fermi operators of an electronic state of wave vector \( k \) and spin \( \sigma \) in the normal state. Single-electron energy \( \epsilon_k \) and its corresponding single-electron wave function \( \phi_k(x) \) satisfy the Schrödinger equation

\[
H(x)\phi_k(x) = \epsilon_k \phi_k(x)
\]

with single-electron Hamiltonian

\[
H(x) = \frac{1}{2m} \left[ -i\hbar \nabla + e \mathbf{a}(x) \right]^2 + U(x),
\]

where \( \mathbf{a}(x) \) is the vector potential, and \( U(x) \) a periodic scalar potential.

In writing down Hamiltonian \( \hat{H} \), we have neglected, for simplicity, the effect of spin paramagnetism (which may be important for high fields).

We note that, if \( \epsilon_k \) and \( \phi_k(x) \) for \( \mathbf{a} \neq 0 \) are known, \( \hat{H} \) can be diagonalized in essentially the same way as for \( \mathbf{a} = 0 \) (i.e., by making the BCS pairing approximation, and then applying the Bogoliubov transformation). However, since \( \mathbf{a}(x) \) in the superconducting state is itself an unknown function, a simultaneous determination of \( \epsilon_k, \phi_k(x) \) and \( \mathbf{a}(x) \) does not seem possible. We therefore adopt a local approximation approach, which we describe next.

### A. Local Approximation Approach

We note that, in the superconducting state, vector potential \( \mathbf{a}(x) \) varies spatially with the length \( \lambda \), the magnetic field penetration depth, which is \( \sim 10^3 \text{Å} \). In contrast, single-electron wave function \( \phi_k(x) \) oscillates spatially with a much shorter length \( k_F^{-1} \sim 1 \text{Å} \) (here \( k_F \) is a Fermi wave vector) so that \( \mathbf{a}(x) \) can be considered locally constant over many wavelengths of \( \phi_k(x) \). Our approach is based on this observation, and can be outlined as consisting the following three steps.

**Step 1:** We focus on a small region around a local point, say \( \mathbf{x}' \). Dimension \( D \) of this small region satisfies \( d \ll D \ll \lambda \), where \( d \sim 1 \text{Å} \) is a crystal lattice constant of the superconductor. In this small region, we assume \( \mathbf{a}(x) = \mathbf{a}(x') \) is a constant, and solve the Schrödinger equation [Eq. (2)] to obtain \( \epsilon_k \) and \( \phi_k(x) \).

**Step 2:** Based on the obtained \( \epsilon_k \) and \( \phi_k(x) \) in the vicinity of \( x' \), we diagonalize Hamiltonian \( \hat{H} \), which now becomes a local quantity, because of its dependence upon \( \mathbf{a}(x') \) through \( \epsilon_k \) and \( \phi_k(x) \).

**Step 3:** Once Hamiltonian \( \hat{H} \) is diagonalized, we move on to derive an expression for local free energy density \( F \) and two basic equations of the theory. The equations allow determination of the spatial variations of vector potential \( \mathbf{a} \) and other quantities for given temperature, applied magnetic field and sample geometry.

Since the non-local effect (or coherence effect) \( \frac{1}{\lambda^2} \) in the superconducting state is not accounted for, we expect this approach to be valid only for highly-local superconductors for which magnetic field penetration depth \( \lambda \) is much larger than coherence length \( \xi \) (i.e., \( \lambda \gg \xi \)).

We explain the details of this approach in the following subsections.

### B. Determination of \( \epsilon_k \) and \( \phi_k(x) \)

As outlined above, we first focus on a small region around a local point, say \( \mathbf{x}' \). Dimension \( D \) of this small region satisfies \( d \ll D \ll \lambda \), where \( d \) is a crystal lattice constant of the superconductor, and \( \lambda \) is the magnetic field penetration depth. Since vector potential \( \mathbf{a}(x) \) varies spatially with the length \( \lambda \), which is \( \sim 10^3 \text{Å} \), whereas \( \phi_k(x) \) oscillates spatially with the length \( d \), which is \( \sim 1 \text{Å} \ll \lambda \), we can assume \( \mathbf{a}(x) = \mathbf{a}(x') \) is constant in this small region, and solve Eq. (2).

For a constant \( \mathbf{a}(x) = \mathbf{a}(x') \), it is not difficult to solve Eq. (2). For free electrons, for which scalar potential \( U(x) = \text{constant} \), solutions of Eq. (2) are easily obtained. Namely, for \( \mathbf{a} = 0 \), we have

\[
\epsilon_k^{(0)} = \frac{\hbar^2 k^2}{2m}
\]

and

\[
\phi_k^{(0)}(x) = e^{i\mathbf{k} \cdot \mathbf{x}}.
\]

and for \( \mathbf{a} \neq 0 \), we have

\[
\epsilon_k = \left( \frac{\hbar \mathbf{k} + e \mathbf{a}}{c} \right)^2 / 2m
\]

and

\[
\phi_k(x) = e^{i\mathbf{k} \cdot \mathbf{x}}.
\]

Here we have used \( \epsilon_k^{(0)} \) and \( \phi_k^{(0)} \) to denote solutions of Eq. (2) for \( \mathbf{a} = 0 \).

In this paper, we will not consider the case of a general periodic scalar potential \( U(x) \) (i.e., we will not consider in this paper how the details of an electronic energy band structure may affect properties of the superconducting state). Instead, for simplicity in presenting the theory, we will use the solutions for free electrons in the following.

### C. Diagonalization of \( \hat{H} \)

Having obtained \( \epsilon_k \) and \( \phi_k(x) \), we can move on to diagonalize Hamiltonian \( \hat{H} \) of Eq. (1), which now becomes a local quantity, because \( \epsilon_k \) and \( \phi_k(x) \) are obtained locally at \( \mathbf{x}' \) for \( \mathbf{a} = \mathbf{a}(x') \).

An important step in the diagonalization of Hamiltonian \( \hat{H} \) is assuming that the pairings \( \langle c_{-k\uparrow} c_{k\uparrow} \rangle \) of electrons of opposite momenta and spins holds even for \( \mathbf{a} \neq 0 \). I.e., for a pair of \( (\mathbf{k}\uparrow) \) and \( (-\mathbf{k}\downarrow) \) electrons, we assume

\[
\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle \neq 0
\]
when the electrons are superconducting (here the angle brackets $\langle \cdots \rangle$ denote a thermal average).

The diagonalization of Hamiltonian $\hat{H}$ is the same as in the case of $a = 0$, except that we have $\epsilon_{-k} \neq \epsilon_k$ for $a \neq 0$. The results of the diagonalization are as follows.

The energy gap parameter is defined as

$$\Delta_k = -\sum_{k'} V_{k,k'} (c_{-k'}, c_k).$$

(9)

The diagonalized Hamiltonian is

$$\hat{H} = \sum_k \left( U_k + E_k \gamma_k^\dagger \gamma_k + E_{-k} \gamma_{-k}^\dagger \gamma_{-k} \right),$$

(10)

where

$$U_k = \frac{\xi_k + \xi_{-k}}{2} - E_k^{(s)} + \frac{|\Delta_k|^2}{2E_k^{(s)}} (1 - f_k - f_{-k});$$

(11)

$$\xi_k = \epsilon_k - \epsilon_F$$

(12)

is the single-electron energy in the normal state, measured relative to the Fermi energy $\epsilon_F$;

$$E_k = E_k^{(s)} + \frac{\xi_k - \xi_{-k}}{2}$$

(13)

the quasi-particle excitation energy in the superconducting state;

$$E_k^{(s)} = \sqrt{\left( \frac{\xi_k + \xi_{-k}}{2} \right)^2 + |\Delta_k|^2}$$

(14)

the symmetric part of $E_k$;

$$f_k = \left( e^{E_k/k_B T} + 1 \right)^{-1}$$

(15)

the Fermi function; and $\gamma_{k\sigma}^\dagger$ and $\gamma_{k\sigma}$ are the Fermi operators for quasi-particles in the superconducting state.

The operators $\gamma_{k\sigma}^\dagger$ and $\gamma_{k\sigma}$ are related to $c_{k\sigma}$ and $c_{k\sigma}$ via the Bogoliubov transformation

$$\begin{pmatrix} c_{k\sigma} \\ c_{-k\sigma}^\dagger \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v_k^\ast & u_k^\ast \end{pmatrix} \begin{pmatrix} \gamma_k^\dagger \\ \gamma_{-k} \end{pmatrix},$$

(16)

where the coefficients $u_k$ and $v_k$ satisfy the following relations:

$$|u_k|^2 = \frac{1}{2} \left( 1 + \frac{\xi_k + \xi_{-k}}{2E_k^{(s)}} \right),$$

(17)

$$|v_k|^2 = \frac{1}{2} \left( 1 - \frac{\xi_k + \xi_{-k}}{2E_k^{(s)}} \right),$$

(18)

and

$$\Delta_k u_k v_{-k}^\ast = \frac{|\Delta_k|^2}{2E_k^{(s)}}.$$

(19)

After the diagonalization of Hamiltonian $\hat{H}$, Eq. (9) can be expressed as

$$\Delta_k = -\sum_{k'} V_{k,k'} \frac{1 - f_{k'} - f_{-k'}}{2E_{k'}^{(s)}} \Delta_{k'}. $$

(20)

With regard to the above-described diagonalization of Hamiltonian $\hat{H}$, the following are worth emphasizing.

(i) Interaction matrix element $V_{k,k'}$ is $a$-independent, because $\phi_k(x) = \phi_k^{(0)}(x)$.

(ii) For $a \neq 0$, since $\epsilon_{-k} \neq \epsilon_k$, we have $\xi_{-k} \neq \xi_k$, $E_{-k} \neq E_k$, and $f_{-k} \neq f_k$. However, we still have $U_{-k} = U_k$, $E_{-k}^{(s)} = E_k^{(s)}$ and $\Delta_{-k} = \Delta_k$, as one can see from Eqs. (11), (12) and (20).

(iii) Fermi energy $\epsilon_F$, relative to which energies such as $\xi_k$ and $E_k$ are measured, is a local quantity, i.e., $\epsilon_F = \epsilon_F(a(x'))$. This can be understood as follows. In the superconducting ground state, all electrons are paired. For each pair of electrons, we have $(\epsilon_k + \epsilon_{-k}) \neq 2\epsilon_k^{(0)}$ for $a \neq 0$. Thus, we expect $\epsilon_F \neq \epsilon_F^{(0)}$ for $a \neq 0$. We further expect that $\epsilon_F > \epsilon_F^{(0)}$ for $a \neq 0$ in the superconducting state, where the increase in the Fermi energy is due to a flow of the paired electrons.

For an electronic energy spectrum of the form of Eq. (20), Fermi energy $\epsilon_F$ is determined by $\epsilon_F = (\epsilon_{kF} + \epsilon_{-kF})/2$, which gives

$$\epsilon_F = \epsilon_F^{(0)} + \frac{e^2}{2mc^2} a^2.$$ 

(21)

With the help of Eqs. (20) and (21), we also have

$$\frac{\xi_k + \xi_{-k}}{2} = \epsilon_k^{(0)},$$

(22)

and

$$\frac{\xi_k - \xi_{-k}}{2} = \frac{\hbar}{mc} k \cdot a,$$

(23)

where

$$\xi_k^{(0)} = \epsilon_k^{(0)} - \epsilon_F^{(0)}.$$

(24)

From the above-described diagonalization of Hamiltonian $H$, we see the following: Electronic states (or quasi-particles) in the superconducting state are each characterized by a wave-vector $k$ and a spin $\sigma$, and are in one-to-one correspondence with those in the normal state (this point is the same as in the case of $a = 0$). The superconducting state is different from the normal state because (i) there exists an energy gap parameter $\Delta_k$ for an electronic excitation in the superconducting state; and (ii) Fermi energy $\epsilon_F$ is vector potential $a$ dependent in the superconducting state. Both the existence of $\Delta_k$ and the $a$-dependence of $\epsilon_F$ originate from the pairing of $(k \uparrow)$ and $(\bar{k} \downarrow)$ electrons.
D. Free energy density \( F \)

From diagonalized Hamiltonian \( \hat{H} \) [Eq. (10)], the following expression for free energy density \( F \) at location \( \mathbf{x} \) (we can drop the prime in \( \mathbf{x}' \) hereafter) in the superconductor can be derived:

\[
F = \sum_{\mathbf{k}} \left[ U_k - k_BT \ln \left( 1 + e^{-E_k/k_BT} \right) \right] + \frac{ne^2}{2mc^2} a^2 + \frac{\left( \nabla \times a \right)^2}{8\pi}.
\tag{25}
\]

The first of the three terms in the above expression comes from \(-k_BT \ln \left[ \text{Tr} \left( e^{-\hat{H}/k_BT} \right) \right] \), which is the usual statistical electronic free energy density \( \hat{E} \). The second term comes from \( n(\epsilon_r - \epsilon_r^{(0)}) \), where \( n \) is the density of electrons, and we have used Eq. (21). This term is added to \( F \) because electronic energies in the expression for Hamiltonian \( \hat{H} \) are measured relative to \( \epsilon_r \). The third term is the magnetic field energy density.

Note that the expression for \( F \) involves \(|\Delta_k|\) (through \( U_k, E_k \) and \( E_{-\mathbf{k}} \)). As we will see in the next subsection, \(|\Delta_k|\) is a function of \( \mathbf{k}, T \) and \( \mathbf{a} \), i.e., \(|\Delta_k| = |\Delta_k(T, \mathbf{a})|\), and the function \(|\Delta_k(T, \mathbf{a})|\) is determined by the self-consistency of the diagonalization of \( \hat{H} \). Thus, we see that \( F \) is a function of \( T \) and \( \mathbf{a} \), i.e., \( F = F(T, \mathbf{a}) \). [As can be shown, free energy density \( F \), excluding the magnetic field energy density, becomes \( \mathbf{a} \)-independent when \(|\Delta_k| = 0 \) for all electronic states.]

E. First equation: Implicit solution for \(|\Delta_k(T, \mathbf{a})|\)

The following equation is derived as a condition for the self-consistency of the diagonalization of Hamiltonian \( \hat{H} \):

\[
\frac{1 - f_{\mathbf{k}} - f_{-\mathbf{k}}}{E_{\mathbf{k}}^{(s)}} = \text{independent of } T \text{ and } \mathbf{a}.
\tag{26}
\]

For \( \mathbf{a} = 0 \), this equation was previously derived by the author in Ref. 8. We present the details of the derivation of this equation for \( \mathbf{a} \neq 0 \), which is similar to that for \( \mathbf{a} = 0 \), in Appendix A.

By using \( 1 - 2f_{\mathbf{k}} = \tanh(\mathcal{E}_{\mathbf{k}}/2k_BT) \) and the condition that \(|\Delta_k| = 0 \) at \((T, \mathbf{a}) = (T_c, 0)\), we can express the above equation as

\[
\frac{2}{\sqrt{\left( \xi_k^{(0)} \right)^2 + |\Delta_k|^2}} \left\{ \tanh \left[ \left( \sqrt{\left( \xi_k^{(0)} \right)^2 + |\Delta_k|^2} + \frac{\hbar c}{mc} \mathbf{k} \cdot \mathbf{a} \right)/2k_BT \right] \right\} + \tanh \left[ \left( \sqrt{\left( \xi_k^{(0)} \right)^2 + |\Delta_k|^2} - \frac{\hbar c}{mc} \mathbf{k} \cdot \mathbf{a} \right)/2k_BT \right] \right\} = \tanh \left[ \frac{\left| \xi_k^{(0)} \right| / 2k_BT_c}{\left| \xi_k^{(0)} \right|} \right].
\tag{27}
\]

F. Second equation: Relation between \( \mathbf{j} \) and \( \mathbf{a} \)

Having obtained an expression for \( F(T, \mathbf{a}) \) [i.e., the expression given by Eq. (26)], with \(|\Delta_k(T, \mathbf{a})|\) being implicitly given by Eq. (27)], we are now ready to consider determination of \( \mathbf{a}(\mathbf{x}) \). In thermodynamic equilibrium, the overall free energy, given by the volume integral of \( F(T, \mathbf{a}(\mathbf{x})) \), must be stationary with respect to arbitrary variation of \( \mathbf{a}(\mathbf{x}) \). This variational problem leads to

\[
\mathbf{j} = \frac{ne^2}{mc} \mathbf{a} + \frac{\hbar c}{m} \sum_k (f_{-\mathbf{k}} - f_{\mathbf{k}}) \mathbf{k},
\tag{29}
\]

where \( \mathbf{j} \) is the electrical current density, and we have used the relations \( \nabla \times \mathbf{j} = \nabla \times \mathbf{b} = \nabla \times \nabla \times \mathbf{a} \), with \( \mathbf{b} = \nabla \times \mathbf{a} \) being the magnetic flux density.

The first term on the right-hand side of Eq. (29) represents a uniform flow of all the electrons, which originates from the pairing of \((\mathbf{k}^\uparrow)\) and \((-\mathbf{k}^\downarrow)\) electrons. The second term is due to quasi-particle excitations and de-paired electrons, and tends to cancel the first term. When all
the electrons are in the superconducting ground state, the second term is zero. On the other hand, when $|\Delta_k| = 0$ for all the electrons (i.e., when the superconductor is in the normal state), the two terms cancel each other, and we have $j = 0$.

Equation (29) was also derived by BCS. However, the BCS derivation of Eq. (29) is based on a linear-response approach (i.e., vector potential $a$ is treated as a small perturbation), and thus, is valid only in the low-field limit.

Note that Eq. (29) is not gauge invariant (this feature is the same for the London equation). This is because the pairing of $(k \uparrow)$ and $(-k \uparrow)$ electrons fixes the total (canonical) momentum of the electrons, and thereby also the gauge of the vector potential. Namely, the theory became not-gauge-invariant at the point when the pairing assumption [Eq. (8)] was made. For the same reason, the expression for $F(T, a)$ [Eq. (25)] and the implicit solution for $|\Delta_k(T, a)|$ [Eq. (27)] are also not gauge invariant. Since, as can be shown, $\partial F / \partial a > 0$ (which means that a larger value of $a$ is energetically less favorable), we see that the gauge of vector potential $a$ in the present theory is such that $a \to 0$ deep inside a bulk superconductor, i.e., the London gauge.

### G. Dimensionless units

It is convenient to introduce a set of units so that physical quantities involved in the theory become dimensionless. The units that we choose to use are listed in Table 1, where $\lambda_0$ is the magnetic field penetration depth at $T = 0$ in the limit of zero magnetic field, and satisfies $\lambda_0^2 = mc^2 / 4\pi n e^2$; and $H_{c0}$ is the thermodynamic critical magnetic field at $T = 0$, and satisfies $H_{c0}^2 / 8\pi = (\pi^2 / 6)(k_B T_c)^2 N_0$, where $N_0$ is the density of states at the Fermi level ($N_0 = m k_F / 2\pi e^2$ for free electrons). The result for $H_{c0}$ was previously obtained by the author in Ref. 9.

We also make the substitution $\sum_k \to (1/8\pi^3) \int d^3 k$, and, as usual, assume that $\epsilon^{(0)}_p \gg k_B T_c$, so that the substitution $\int_0^\infty d\xi (0) \to \int_0^\infty d\xi (0)$ and the approximation $k \cdot a = k a_z \simeq k_F a_z$ hold, where $k_F = \cos \alpha_k$, with $\alpha_k$ being the angle between $k$ and $a$.

By using the units shown in Table 1 and the above-mentioned assumption and approximation, Eq. (25) becomes

$$F = \frac{6}{\pi^2} \int_{-\infty}^\infty d\zeta^{(0)}_k \int_0^1 d\zeta_k \left[ U_k - T \ln \left( 1 + e^{-E_k/T} \right) \left( 1 + e^{-E_{-k}/T} \right) \right] + a^2 + (\nabla \times a)^2$$

(30)

with

$$U_k = \zeta^{(0)}_k - \sqrt{\left( \zeta^{(0)}_k \right)^2 + |\Delta_k|^2 + \frac{\tanh \left( \zeta^{(0)}_k / 2 \right)}{2 |\zeta^{(0)}_k|}}$$

and

$$E_{\pm k} = \sqrt{\left( \zeta^{(0)}_k \right)^2 + |\Delta_k|^2 \pm \frac{\pi}{\sqrt{2} a_z}};$$

and Eqs. (27) and (29) become

$$\left[ 2 \sqrt{\left( \zeta^{(0)}_k \right)^2 + |\Delta_k|^2} \right]^{-1} \left\{ \tanh \left( \sqrt{\left( \zeta^{(0)}_k \right)^2 + |\Delta_k|^2 + \sqrt{2} a_z} \right) / 2T \right\}$$

$$+ \tanh \left( \sqrt{\left( \zeta^{(0)}_k \right)^2 + |\Delta_k|^2 - \frac{\pi}{\sqrt{2} a_z}} \right) / 2T \right) \right\} \frac{\tanh \left( \zeta^{(0)}_k / 2 \right)}{\left| \zeta^{(0)}_k \right|}$$

(31)

and

$$j = -n a,$$

(32)

respectively, where the “effective superconducting elec-
tron density$^{\dagger}$
\[ n_s = 1 - \frac{3\sqrt{2}}{\pi a} \int_0^\infty df_{k}^{(0)} \int_0^1 d\zeta_k \zeta_k (f_{-k} - f_k) \quad (33) \]

with
\[ f_{\pm k} = \left[ e \left( \sqrt{\xi_k^0 + |\Delta_k|^2 \pm \frac{\xi_k}{2} a z_k} / T \right) / 1 \right]^{-1} \quad (34) \]

Note that Eq. (32) is the same as the London equation, except that our $n_s$, given by Eq. (33), is both $T$- and $a$-dependent, whereas $n_s$ is only $T$-dependent in the London theory.

The condensation energy density is defined as
\[ F_c = F'_n - F'_s, \quad (35) \]
where $F'_n = F - (\nabla \times a)^2$ is the superconducting state free energy density excluding the magnetic field energy density; and $F'_s$ is the normal state counterpart of $F'_n$. The quantity $F_c$ can be used as a measure of the difference between the normal and superconducting states.

As can be shown, the following relation exists:
\[ n_s = \frac{1}{2a} \frac{\partial F'_s}{\partial a} \quad (36) \]
\[ = -\frac{1}{2a} \frac{\partial F_c}{\partial a}, \quad (37) \]
where the second expression holds because $F'_s$ is $a$-independent.

For an isotropic superconductor (as in the present case), $n_s$ and $F_c$ are functions of temperature $T$ and the magnitude of vector potential $a$, i.e., $n_s = n_s(T, a)$ and $F_c = F_c(T, a)$.

We analyze the functions $|\Delta_k(T, a)|$, $n_s(T, a)$ and $F_c(T, a)$ in the next subsection.

H. $|\Delta_k(T, a)|$, $n_s(T, a)$, and $F_c(T, a)$

We solve Eq. (31) to obtain $|\Delta_k(T, a)|$ by using an iterative method $^{24}$ [Note that the variables $(k \not\equiv 0$, $T$, $a)$ for the function $|\Delta_k(T, a)|$ appear in Eq. (31) in the forms of $(|\xi_k^0|$, $T$, $a z_k)$; and remember that $a z_k = a \cos \alpha_k$ is the component of $a$ along $k$]. When solving Eq. (31), it is important to note the following:

(i) We define temperature $T_{ck}$ such that Eq. (31) has no $|\Delta_k| > 0$ solution for given $|\xi_k^0|$, $T$ and $a z_k$ if $T > T_{ck}$. Note that $T_{ck}$ is a function of $|\xi_k^0|$, $T$ and $a z_k$. Only for $a = 0$ is $T_{ck} = T_{c}$ the same for all the electronic states.

(ii) Similarly, we define vector potential magnitude $a_{ck}$ as such that Eq. (31) has no $|\Delta_k| > 0$ solution for given $|\xi_k^0|$, $T$ and $a z_k$ if $a > a_{ck}$. Note that $a_{ck}$ is a function of $|\xi_k^0|$, $T$ and $a z_k$.

(iii) Depending on $|\xi_k^0|$, $T$ and $a z_k$, a $|\Delta_k| > 0$ solution of Eq. (31) may be an unstable solution, because the normal state solution $|\Delta_k| = 0$ may be energetically more favorable.

Point (iii) can be understood as follows. Note that for given $|\xi_k^0|$, $T$ and $a z_k$, there are always two possible solutions for $|\Delta_k|$ if $T < T_{ck}$ or $a < a_{ck}$; the $|\Delta_k| > 0$ solution of Eq. (31) and the $|\Delta_k| = 0$ solution. The free energy associated with a pair of $(k \not\equiv 0$, $T$, $a)$ excitations with $|\Delta_k| > 0$ is

\[ F_{sk} = |\xi_k^0| - F''_k + \frac{\tan \left( |\xi_k^0| / 2 \right)}{2|\xi_k^0|} - T \ln \left[ 1 + e^{-\left( F''_k + \frac{|\xi_k^0|}{2} a z_k \right) / T} \right] \left[ 1 + e^{-\left( F''_k - \frac{|\xi_k^0|}{2} a z_k \right) / T} \right], \quad (38) \]

where $F''_k = \sqrt{\left( |\xi_k^0| \right)^2 + |\Delta_k|^2}$. For $|\Delta_k| = 0$, it becomes

\[ F_{nk} = |\xi_k^0| - |\xi_k^0| - T \ln \left[ 1 + e^{-\left( |\xi_k^0| + \frac{|\xi_k^0|}{2} a z_k \right) / T} \right] \left[ 1 + e^{-\left( |\xi_k^0| - \frac{|\xi_k^0|}{2} a z_k \right) / T} \right], \quad (39) \]

Both $F_{sk}$ and $F_{nk}$ are functions of $|\xi_k^0|$, $T$ and $a z_k$. For given $|\xi_k^0|$, $T$ and $a z_k$, the $|\Delta_k| > 0$ solution is the stable solution if $F_{sk} < F_{nk}$. Otherwise, the $|\Delta_k| = 0$ solution is the stable solution.

We define temperature $T_{ck}$ and vector potential magnitude $a_{ck}$ as such that the $|\Delta_k| = 0$ solution becomes the stable solution for $T \geq T_{ck}$ or $a \geq a_{ck}$. By definition, we have $T_{ck} \leq T_{ck}$ and $a_{ck} \leq a_{ck}$. Note that a pair of $(k \not\equiv 0$, $T$, $a)$ electrons becomes de-paired (having $|\Delta_k| = 0$) for $T \geq T_{ck}$ or $a \geq a_{ck}$.

Numerical results for $T_{ck}$ and $a_{ck}$ are shown in Fig. 1 [Figs. 1(a)-(c)]. Figure 1(a) shows $T_{ck}$ versus $|\xi_k^0|$ for different values of $a z_k$; Fig. 1(b) shows $a_{ck} z_k$ versus $|\xi_k^0|$ for different values of $T$; and Fig. 1(c) shows $T_{ck}$ versus...
Fig. 1: (a) $T_{ck}$ versus $|\xi_k^{(0)}|$ for different values of $a \Delta k$; (b) $a \Delta k \xi_k$ versus $|\xi_k^{(0)}|$ for different values of $T$; (c) $T_{ck}$ versus $a \Delta k$ for different values of $|\xi_k^{(0)}|$. The dotted curves show the corresponding results for $T_{ck}$ or $a \Delta k \xi_k$.

For constant $|\xi_k^{(0)}|$, the values of $T_{ck}$ and $a \Delta k$ are lowest when $\mathbf{k}$ is parallel to $\mathbf{a}$, because $\mathbf{a}$ appears in Eq. (31) only in the form of $a \Delta k$, which is largest (therefore, most effective as a de-pairing force) when $z_k = 1$.

For two electronic states with wave-vectors $\mathbf{k}'$ and $\mathbf{k}$, respectively, if $|\xi_{k'}^{(0)}| = |\xi_k^{(0)}|$ and $\mathbf{k}$ is parallel to $\mathbf{a}$, then, the following relations hold: $T_{ck}(a) = T_{ck||a}(a \Delta k')$; and $a \Delta k(T) = a \Delta k||a(T)/\xi_{k'}$. Note that $T_{ck||a}(a)$ is the lowest value of $T_{ck}(a)$, i.e., $T_{ck||a}(a) = T_{ck,\min}(a)$. Similarly, $a \Delta k||a(T)$ is the lowest value of $a \Delta k(T)$, i.e., $a \Delta k||a(T) = a \Delta k,\min(T)$. The function $T_{ck||a}(a)$ [or its inverse function $a \Delta k||a(T)$], which is shown by the $|\xi_k^{(0)}| = 0$ curve in Fig. 2 (c) (for $z_k = 1$), is of particular importance. When $T < T_{ck||a}(a)$ [or $a < a \Delta k||a(T)$] in a region in a superconductor [remember that $\mathbf{a} = \mathbf{a}(\mathbf{x})$ is a location-dependent
quantity), this region is in a “all-paired state,” in which $|\Delta_k| > 0$ for all the electrons. On the other hand, when $T > T_{ck}|a|(a)$ [or $a > a_{ck}|a|(T)$] in a region in a superconductor, this region is in a “partly-paired state,” in which electrons with $T_{ck}(a_{zk})$ in the range $T_{ck}|a|(a) < T_{ck}(a_{zk}) < T$ [or with $a_{ck}(T)$ in the range $a_{ck}|a|(T) < a_{ck}(T) < a$] become de-paired (having $|\Delta_k| = 0$), while electrons with $T_{ck}(a_{zk}) > T$ [or $a_{ck}(T) > a$] remain paired (having $|\Delta_k| > 0$).

Numerical results for $|\Delta_k|$ versus $|\xi_k^{(0)}|$ for different values of $T$ and $a_{zk}$ are shown in Fig. 2 [Figs. 2(a)-2(c)]. Figure 2(a) shows the case of $a = 0$. In this case, $|\Delta_k|$ is a monotonic decreasing function of $|\xi_k^{(0)}|$ for all temperatures below $T_c$; and $|\Delta_k|$ vanishes at the same temperature $T_c$ for all values of $|\xi_k^{(0)}|$.

Figure 2(b) shows an example of the case of $0 < a < a_{ck}|a|(0)$ [note that $\pi a_{ck}|a|(0)/\sqrt{2} = 1$ (in dimensionless units)]. In this case, the $|\Delta_k|$-versus-$|\xi_k^{(0)}|$ curve for $T = 0$ is the same as in the case of $a = 0$. However, as $T$ increases, $|\Delta_k|$ for a smaller $|\xi_k^{(0)}|$ is more strongly suppressed, and decreases faster, so that the $|\Delta_k|$-versus-$|\xi_k^{(0)}|$ curve eventually becomes non-monotonic, with a maximum located away from $|\xi_k^{(0)}| = 0$. As $T$ increases further, $|\Delta_k|$ for a smaller $|\xi_k^{(0)}|$ vanishes at a lower temperature [namely, $T_{ck}$ is smaller for smaller $|\xi_k^{(0)}|$, a feature that is also shown by Fig. 1(a)]. The $|\Delta_k|$-versus-$|\xi_k^{(0)}|$ curve then has two parts: a $|\Delta_k| = 0$ part for low energies, for which $T_{ck}(a_{zk}) < T$ [or $a_{ck}(T) < a$], and a $|\Delta_k| > 0$ part for higher energies, for which $T_{ck}(a_{zk}) > T$ [or $a_{ck}(T) > a$].

Figure 2(c) shows an example of the case of $a > a_{ck}|a|(0)$. In this case, the $|\Delta_k|$-versus-$|\xi_k^{(0)}|$ curve has a $|\Delta_k| = 0$ part even for $T = 0$. Namely, at $T = 0$, $|\Delta_k| = 0$ for those electronic states with $a_{ck}(0) < a$. The vertical rises in the $|\Delta_k|$-versus-$|\xi_k^{(0)}|$ curves for low temperatures (i.e., the curves for $T = 0; 0.3$ and $0.5$) in Fig. 2(c) indicate discontinuities. The dotted curves in Fig. 2(c) show corresponding unstable solutions of Eq. (31) for $T$ in the range $T_{ck} < T < T_{ck}^*$ (or for $a$ in the range $a_{ck} < a < a_{ck}^*$).

Figures 3 and 4 show, respectively, the $T$-dependence and $a_{zk}$-dependence of $|\Delta_k|$. The dotted curves in Figs 3 and 4 show corresponding unstable solutions of Eq. (31) in the range $T_{ck} < T < T_{ck}^*$ or $a_{ck} < a < a_{ck}^*$. As shown in the figures, $|\Delta_k|$ is a monotonic decreasing function of $T$ and $a_{zk}$, except that at $T = 0$, $|\Delta_k| > 0$ is a constant for $a < a_{ck}(0)$. Note that, at $T = T_{ck}$ or $a = a_{ck}$, $|\Delta_k|$ may become zero continuously or discontinuously, depending on $|\xi_k^{(0)}|$, $T$ and $a_{zk}$. The vertical drops in
that are monotonic decreasing functions of $\pi a^2$. For $T = 0$ and $a < a_{cKF}|\pi a(0)|$, we have $F_c = 1 - a^2$ which can be derived either from the expression for $F_c$, or by solving Eq. (37) for $n_s = 1$ and $F_c(0, 0) = 1$. This is shown in Fig. 6(b), where we can see that the $F_c$-versus-$a$ curve for $T = 0$ is parabolic for $0 \leq \pi a/\sqrt{2} \leq 1$. Namely, in this case, all the electrons are paired and no thermal excitations exist, so that the decrease in $F_c$ (i.e., the $-a^2$ term) is entirely due to the kinetic energy associated with the uniform flow of all the electrons. At $T = 0$, as $a$ increases further so that $a > a_{cKF}|\pi a(0)|$ (i.e., $\pi a/\sqrt{2} > 1$), de-paired electrons (having $|\Delta_k| = 0$) begin to appear, and we have $n_s < 1$.

The present analysis provides a possible explanation for the experimentally observed non-vanishing Knight shifts in the superconducting state near $T = 0$ (for example, Refs. 14 and 15). Namely, at $T = 0$, electrons in a superconducting sample are all paired only when the applied magnetic field is weak so that we have $a < a_{cKF}|\pi a(0)|$ everywhere in the sample; this gives zero spin-polarization, and therefore, zero Knight shift (which is proportional to the density of spin polarization12). However, we note that the applied magnetic fields that were used for the Knight shift measurements14,15 are comparable to the thermodynamic critical magnetic fields of the samples. Therefore, it is likely that we actually had $a > a_{cKF}|\pi a(0)|$ over a significant portion of the sample, where a finite fraction of the electrons were de-paired and
spin-polarized, giving rise to a non-zero Knight shift. The previous theoretical prediction of a zero Knight shift in the superconducting state for \( T \to 0 \) by Yoshida\cite{Yoshida1962} is valid only for weak magnetic fields. Although the present theory is developed for highly-local superconductors, we expect qualitative conclusions of the theory, including the prediction for a non-vanishing Knight shift near \( T = 0 \) for a not-so-weak magnetic field, to be valid also for non-local superconductors.

### III. APPLICATIONS

We present in this section a few examples of application of the theory. We consider the case of a semi-infinite superconductor in an applied magnetic field \( H_a \) parallel to the surface of the superconductor and the case of an isolated vortex in an infinite superconductor. We determine, in each case, spatial variations of vector potential \( \mathbf{a} \), magnetic flux density \( \mathbf{b} \), electrical current density \( \mathbf{j} \), energy gap parameter amplitude \( |\Delta_k| \), “effective superconducting electron density” \( n_s \) and condensation energy density \( F_c \). We also calculate magnetic field penetration depth \( \lambda(T, H_a) \) and lower critical magnetic field \( H_{c1}(T) \).

#### A. Semi-infinite superconductor

We consider a semi-infinite superconductor in an applied magnetic field \( H_a \) parallel to the surface of the superconductor. Let the superconductor occupy the half space \( x > 0 \) and \( H_a \) be applied along the \( z \)-axis. In terms of the Cartesian coordinates \( (x, y, z) \) and the unit vectors \( (\hat{x}, \hat{y}, \hat{z}) \), we can write \( \mathbf{b} = b(x)\hat{z} \), \( \mathbf{j} = j(x)\hat{y} \), and \( \mathbf{a} = -a(x)\hat{y} \). Then, Eq. (32) and the relation \( \mathbf{b} = \nabla \times \mathbf{a} \) become

\[
b'(x) = -n_s(x)a(x) \quad (40)
\]

and

\[
a'(x) = -b(x), \quad (41)
\]

respectively, where a “prime” indicates a derivative with respect to \( x \); \( n_s(x) = n_s(a(x)) \) is given by Eq. (33), where \( |\Delta_k(x)| = |\Delta_k(a(x))| \) is determined by Eq. (31); and the relation \( j(x) = -b'(x) \) has been used.

This is a non-linear second-order boundary-value problem with boundary conditions

\[
b(0) = -a'(0) = H_a \quad (42)
\]

and

\[
a(\infty) = b(\infty) = 0. \quad (43)
\]

Note that, for the convenience of numerical calculation, we have expressed this second-order boundary-value problem as a system of two first-order differential equations. The numerical method for solving this boundary-value problem is explained in Appendix B.

#### B. Magnetic field penetration depth \( \lambda(T, H_a) \)

The solution for \( a(x) \) obtained in Sec. IIIA for the case of a semi-infinite superconductor can be used to calculate magnetic field penetration depth \( \lambda(T, H_a) \), which, for a semi-infinite superconductor, is defined as

\[
\lambda = \frac{1}{H_a} \int_0^\infty b(x)dx = \frac{a(0)}{H_a}, \quad (44)
\]

where \( a(0) \) is the value of \( a(x) \) at the surface of the superconductor.

Numerical results for \( \lambda(T, H_a) \) are shown as \( \lambda^2(0)/\lambda^2 \) versus \( T \) for different values of \( H_a \) in Fig. 9(a), and \( \lambda^2(0)/\lambda^2 \)
versus $H_a$ for different values of $T$ in Fig. 9(b).

The dotted curve in Fig. 9(a) shows M"uhlschlegel’s numerical result for $\lambda_0^2/\lambda_1^2(T)$. As we mentioned earlier, the M"uhlschlegel’s result is based on a linear-response approach, and corresponds to our $n_s(T, a)/n$ for $a = 0$, which is the same as $\lambda_0^2/\lambda_1^2(T, H_a)$ for $H_a = 0$, i.e., $\lambda_0^2/\lambda_1^2(T) = \lim_{a \to 0} n_s(T, a)/n = \lim_{H_a \to 0} \lambda_0^2/\lambda_1^2(T, H_a)$. The quantitative difference between M"uhlschlegel’s $\lambda_0^2/\lambda_1^2(T)$ and our $n_s(T, a)/n$ for $a = 0$, or $\lambda_0^2/\lambda_1^2(T, H_a)$ for $H_a = 0$, is due to the use of the cut-off approximation in M"uhlschlegel’s work.

As shown in Fig. 9(b), for $H_a$ up to about $H_a(T)/2$, $\lambda_0^2/\lambda_1^2(T)$ is $H_a$-independent or nearly $H_a$-independent for low temperatures, and only weakly $H_a$-dependent for higher temperatures. However, for $H_a$ above about $H_a(T)/2$, $\lambda_0^2/\lambda_1^2(T)$ drops rapidly as $H_a$ increases. Note that the case of $H_a$ below about $H_a(T)/2$ corresponds to the case shown in Figs. 7(a) and 8(a), where $a < a_{ckF\|a}(T)$ at the surface of the superconductor so that no de-paired electrons exist in the superconductor, whereas the case of $H_a$ above about $H_a(T)/2$ corresponds to the case shown in Figs. 7(b), 7(c), 8(b) and 8(c), where $a > a_{ckF\|a}(T)$ at the surface of the superconductor so that de-paired

FIG. 7: Variations of $a(x)$, $b(x)$, $j(x)$, $n_c(x)$, $|\Delta_{KF\|a}(x)|$, and $F_c(x)$ near the surface at $T = 0$ and different values of $H_a$: $H_a/H_{co} = 0.4$ (a), 0.6 (b), and 0.8 (c). The quantities $a(x)$, $b(x)$, $j(x)$, $n_c(x)$, $|\Delta_{KF\|a}(x)|$, and $F_c(x)$ are measured in units of $\lambda_0 H_a$, $H_a$, $H_a/\lambda_0$, $n_s(\infty)$, $|\Delta_{KF}(\infty)|$, and $F_c(\infty)$, respectively.

FIG. 8: Variations of $a(x)$, $b(x)$, $j(x)$, $n_c(x)$, $|\Delta_{KF\|a}(x)|$, and $F_c(x)$ near the surface at $T/T_c = 0.6$ and different values of $H_a$: $H_a/H_{co} = 0.3$ (a), 0.4 (b), and 0.5 (c) $|H_a/H_{c1}(T) = 0.49$ (a), 0.65 (b), and 0.81 (c)]. The quantities $a(x)$, $b(x)$, $j(x)$, $n_s(x)$, $|\Delta_{KF\|a}(x)|$, and $F_c(x)$ are measured in units of $\lambda_L(T) H_a$, $H_a$, $H_a/\lambda_L(T)$, $n_s(\infty)$, $|\Delta_{KF}(\infty)|$, and $F_c(\infty)$, respectively, where $\lambda_L(T) = \lim_{H_a \to 0} \lambda(T, H_a)$.
electrons exist in the region near the surface of the superconductor.

As shown in Figs. 9(a) and 9(b), $\lambda^2 / \lambda^2 \to 0$ when $H_a \to H_c(T)$, or $T \to T_c(H_a)$ [here $T_c(H_a)$ is the inverse function of $H_c(T)$]. However, we should note that this is not true for a type-II superconductor, for which superconductivity is completely suppressed only at the upper critical magnetic field $H_c2$, which is usually much higher than $H_c$ for a highly-local superconductor. This is because the definition for $\lambda$, i.e., Eq. (41), is valid only when the superconductor is in the Meissner state. In the mixed state of a type-II superconductor, in which vortices exist, this definition for $\lambda$ is no longer valid. Further, we note that the definition of Eq. (41) is valid only for bulk samples with dimensions much larger than the magnetic field penetration depth.

C. Isolated vortex

We consider an isolated vortex in an infinite superconductor. Let the vortex be centered on the $z$-axis. In terms of the cylindrical coordinates $(r, \phi, z)$ and the unit vectors $(\hat{r}, \hat{\phi}, \hat{z})$, we can write $\mathbf{b} = b(r) \hat{z}$, $\mathbf{j} = j(r) \hat{\phi}$, and $\mathbf{a} = -a(r) \hat{\phi}$. Then, Eq. (42) and the relation $\mathbf{b} = \nabla \times \mathbf{a}$ become

$$b'(r) = -n_s(r)a(r)$$

and

$$a'(r) = -b(r) - \frac{a(r)}{r},$$

respectively, where a “prime” indicates a derivative with respect to $r$; $n_s(r) = n_s(a(r))$ is given by Eq. (43) where $|\Delta_k(r)| = |\Delta_k(a(r))|$ is determined by Eq. (31); and the relation $j(r) = -b'(r)$ has been used.

This is a non-linear second-order boundary-value problem with boundary conditions

$$b(\infty) = a(\infty) = 0$$

and

$$\frac{1}{a} = \int_0^\infty dr b(r).$$

The last boundary condition comes from flux quantization, i.e., $\Phi_0 = 2\pi \int_0^\infty dr rb(r)$ in conventional units, where $\Phi_0$ is the flux quantum. The parameter $\kappa$ is defined as

$$\kappa = 2\pi \lambda_0^2 H_c0/\Phi_0.$$ 

Note the difference between the present definition for $\kappa$ and the one in the Ginzburg-Landau (GL) theory. $\kappa^{(GL)} = 2\sqrt{2}\pi \lambda^2 H_c/\Phi_0$. Besides the difference between $\lambda_0^2 H_c0$ for $\kappa$ of Eq. (49) and $\lambda^2 H_c$ for $\kappa^{(GL)}$, there is an extra factor $\sqrt{2}$ in the expression for $\kappa^{(GL)}$. In the GL theory, $\kappa^{(GL)}$ can also be expressed as a ratio between the magnetic field penetration depth and the coherence length. A similar expression for $\kappa$ does not exist in the present theory, because the coherence effect (or the non-local effect) is not accounted for in the present theory.

For the convenience of numerical calculation, the above-described second-order boundary-value problem has been expressed as a system of two first-order differential equations. The numerical method for solving this boundary-value problem is explained in Appendix C.

Numerical results for $a(r)$, $b(r)$, $j(r)$, $n_s(r)$, $|\Delta_k||\mathbf{a}(r)|$ and $F_r(r)$ near the vortex core are shown in Fig. 10 for $\kappa = 5$ at several different temperatures as indicated in the figure. Here, as an example of $|\Delta_k(r)|$, $|\Delta_k||\mathbf{a}(r)|$ is shown in the figure.

Let $r_0$ denote the location at which $a = a_{c-k}(a)(T)$. We have $|\Delta_k||\mathbf{a}(r)| = 0$ for $0 \leq r < r_0$, and $|\Delta_k||\mathbf{a}(r)| > 0$ for $r > r_0$. Paired electrons (with $|\Delta_k| > 0$) and de-paired electrons (with $|\Delta_k| = 0$) co-exist in the region $0 \leq r < r_0$, whereas no de-paired electrons exist (i.e., $|\Delta_k| > 0$ for all the electrons) in the region $r > r_0$.

As shown in Fig. 10, as $r \to 0$, we have $a \to \infty$, $n_s \to 0$, $j \to 0$ and $F_r \to 0$. It also appears that $b(r)$, $j(r)$ and $n_s(r)$ have zero slopes at $r = 0$, while $F_r(r)$ has a finite slope at $r = 0$ and is nearly linear for small $r$. The electrical current density $j(r)$ has a maximum located near $r_0$.  

![Graph of $\lambda^2 / \lambda^2$ versus $T$ for different values of $H_a$ as indicated on the curves; (b) $\lambda^2 / \lambda^2$ versus $H_a$ for different values of $T$ as indicated on the curves. The dotted curve in (a) shows the Mühlhöchle's result for $\lambda_0^2 / \lambda_2^2(T)$](image-url)
FIG. 10: Variations of $a(r)$, $b(r)$, $j(r)$, $n_s(r)$, $|\Delta_{k_F}[a(r)]|$, and $F_c(r)$ near the vortex core at $T/T_c = 0.0$ (a), 0.6 (b), and 0.9 (c), for $\kappa = 5$. The quantities $a(r)$, $b(r)$, $j(r)$, $n_s(r)$, $|\Delta_{k_F}[a(r)]|$, and $F_c(r)$ are measured in units of $\lambda_0 H_{c0}$, $b(0)$, $cH_{c0}/4\pi\lambda_0 n_s(\infty)$, $n_s(\infty)$, $|\Delta_{k_F}(\infty)|$, and $F_c(\infty)$, respectively.

D. Lower critical magnetic field $H_{c1}(T)$

The numerical solutions obtained in the last subsection for an isolated vortex can be used to calculate lower critical magnetic field $H_{c1}$ of the superconductor. By definition, at $H_a = H_{c1}$, the Gibbs free energy must be the same whether the first vortex exists or not, i.e., $G^{(\text{no vortex})} = G^{(\text{one vortex})}$ at $H_a = H_{c1}$. This condition leads to

$$H_{c1} = \frac{\kappa}{2} \int_0^\infty dr r \left( H_c^2 - F_c + b^2 \right).$$

(50)

FIG. 11: $H_{c1}/H_c$ versus $\kappa$ at different values of $T/T_c$ as indicated on the curves. The two curves for $T/T_c = 0.6$ and 0.9 are practically indistinguishable from each other. The dotted curve shows the Ginzburg-Landau results for $H_{c1}/H_c$ in the high-$\kappa$ limit.

Numerical results for $H_{c1}$ are shown in Fig. 11 as $H_{c1}/H_c$ versus $\kappa$ for several different temperatures.

The dotted curve in Fig. 11 shows the Ginzburg-Landau result for $H_{c1}/H_c$ for high-$\kappa$ superconductors.

$$\frac{H_{c1}^{(GL)}}{H_c} = \frac{1}{\sqrt{2}\kappa^{(GL)}} \left( \ln \kappa^{(GL)} + 0.50 \right)$$

$$= \frac{1}{2\kappa} \left( \ln \kappa + 0.85 \right),$$

(51)

where we have used $\kappa^{(GL)} = \sqrt{2}\kappa$ by replacing $\lambda^2 H_{c0}$ with $\lambda_0^2 H_{c0}$ in the expression for $\kappa^{(GL)}$.

As shown in Fig. 11, our result for $H_{c1}/H_c$ is only weakly $T$-dependent for low temperatures, and nearly $T$-independent for intermediate and high temperatures, as indicated by the fact that the two $H_{c1}/H_c$ versus $\kappa$ curves for $T = 0.6$ and 0.9 are practically indistinguishable from each other. This feature is to be compared with that $H_{c1}^{(GL)}/H_c$ is $T$-independent in the Ginzburg-Landau theory. Figure 11 also shows that our result for $H_{c1}/H_c$ and the Ginzburg-Landau result are quantitatively not very different for $\kappa \gg 1$.

For lower values of $\kappa$, the present theory underestimates the value of $H_{c1}$, because the coherence (or non-local) effect, which increases the energy associated with a vortex and thus leads to a larger $H_{c1}$, is not accounted for in the present theory.

IV. SUMMARY

We have presented a microscopic theory for superconductivity in a magnetic field based on a local approximation approach. The theory allows microscopic description of the suppression of superconductivity by an externally applied magnetic field.

In Sec. [I], we presented the details of the theory. The main results derived in Sec. [II] include an expression for
free energy density \( F \) as a function of temperature \( T \) and vector potential \( \mathbf{a} \), and two basic equations of the theory: the first is an implicit solution for energy gap parameter amplitude \(|\Delta_k|\) as a function of wave vector \( \mathbf{k} \), temperature \( T \) and vector potential \( \mathbf{a} \); and the second is a London-like relation between electrical current density \( \mathbf{j} \) and vector potential \( \mathbf{a} \), with an “effective superconducting electron density” \( n_s \) that is both \( T \)- and \( \mathbf{a} \)-dependent. The two equations allow determination of the spatial variations of \( \mathbf{a} \) and \(|\Delta_k|\) in a superconductor for given temperature \( T \), applied magnetic field \( \mathbf{H}_a \) and sample geometry. In the low-field limit, the theory reduces to the local-limit result of BCS. We also numerically analyzed the functions \(|\Delta_k(T,a)|, n_s(T,a)\) and \( F_c(T,a) \) (where \( F_c \) is the condensation energy density).

In Sec. III as examples, we applied the theory to the case of a semi-infinite superconductor in an applied magnetic field \( \mathbf{H}_a \) parallel to the surface of the superconductor and the case of an isolated magnetic vortex in an infinite superconductor, and determined, for each case, spatial variations of quantities such as \( \mathbf{a}, |\Delta_k|, n_s \) and \( F_c \). We also calculated magnetic field penetration depth \( \lambda(T,H_a) \) and lower critical magnetic field \( H_{c1}(T) \).

An important conclusion of the theory is that, depending on temperature \( T \), applied magnetic field \( \mathbf{H}_a \) and sample geometry, a “partly-paired state” can exist in which paired electrons (having \(|\Delta_k| > 0 \) and de-paired electrons (having \(|\Delta_k| = 0 \)) co-exist. Such a “partly-paired state” exists even at \( T = 0 \) when \( H_a \) is above a threshold for a given sample, giving rise to a non-vanishing Knight shift in the superconducting state at \( T = 0 \) for \( H_a \) above the threshold.

Since the non-local effect (or coherence effect) in the superconducting state is not accounted for in the present theory, we expect the theory to be valid only for highly-local superconductors (for which magnetic field penetration depth \( \lambda \) is much larger than coherence length \( \xi \)). However, when a more complete theory is developed that is able to account for the non-local effect (or coherence effect), we expect it to reduce to the present theory in the local limit.

**APPENDIX A: DERIVATION OF EQ. (20)**

For \( \mathbf{a} = 0 \), Eq. (20) was previously derived by the author in Ref. 8 (related discussions are also given in Refs. 3 and 10). The derivation of Eq. (20) for \( \mathbf{a} \neq 0 \) is similar to that for \( \mathbf{a} = 0 \). We now present the details of the derivation of Eq. (20).

For convenience, we define

\[
C_k = \frac{1 - f_k - f_{-k}}{2E_k^{(s)}},
\]

which is a real number. Then, the self-consistency equation, Eq. (20), can be rewritten as

\[
\Delta_k = -\sum_{k'} V_{kk'} C_{k'} \Delta_{k'}. \tag{A2}
\]

In the presence of an applied magnetic field, we expect \( \Delta_k \) to be a function of temperature \( T \) and vector potential \( \mathbf{a} = (a_1,a_2,a_3) \), where \( a_i \) \((i = 1,2,3)\) are the components of \( \mathbf{a} \). Let \( X \) denote any one of \( T, a_1, a_2 \) and \( a_3 \). We operate \( \partial/\partial X \) on both sides of Eq. (A2) to obtain

\[
\frac{\partial \Delta_k}{\partial X} = -\sum_{k'} V_{kk'} \left( \frac{\partial C_{k'}}{\partial X} \Delta_{k'} + C_{k'} \frac{\partial \Delta_{k'}}{\partial X} \right). \tag{A3}
\]

We next multiply both sides of the above equation by \( C_k \Delta_k^* \), and then take summation over \( k \), i.e.,

\[
\sum_k C_k \Delta_k^* \frac{\partial \Delta_k}{\partial X} = \sum_k \left( -\sum_{k'} V_{kk'} C_k \Delta_{k'}^* \right) \times \left( \frac{\partial C_{k'}}{\partial X} \Delta_{k'} + C_{k'} \frac{\partial \Delta_{k'}}{\partial X} \right). \tag{A4}
\]

The quantity inside the first pair of parentheses on the right-hand side of the above equation equals \( \Delta_k^* \) [according to Eq. (A2)] so that the second of the two terms on the right-hand side is the same as the term on the left-hand side. Thus, we have

\[
\sum_k |\Delta_k|^2 \frac{\partial C_k}{\partial X} = 0. \tag{A5}
\]

We want a \(|\Delta_k| > 0 \) solution. Clearly,

\[
C_k = \text{independent of } T \text{ and } \mathbf{a}, \tag{A6}
\]

which is Eq. (26) and satisfies

\[
\frac{\partial C_k}{\partial X} = 0, \tag{A7}
\]

is a solution of Eq. (A5).

However, since Eq. (A6) is not the only possible solution of Eq. (A5) [as one can see, Eq. (A5) actually can have an infinite number of solutions], we need to justify that Eq. (A6) is the only physical solution.

Since the diagonalized Hamiltonian, Eq. (10), describes a set of independent quasi-particle excitations, there should be no coupling (except pair correlation) between the quasi-particle excitations. Therefore, we expect the thermal energy and entropy associated with each pair of \((\mathbf{k},-\mathbf{k})\) excitations to be

\[
\varepsilon_k = u_k + f_k E_k + f_{-k} E_{-k} \tag{A8}
\]

and

\[
S_k = -k_B \left[ f_k \ln f_k + (1 - f_k) \ln(1 - f_k) \right. \nonumber \\
+ f_{-k} \ln f_{-k} + (1 - f_{-k}) \ln(1 - f_{-k}) \right]. \tag{A9}
\]
between. Similarly, we expect the contribution to the electrical current density from each pair of \((k \uparrow, -k \downarrow)\) excitations to be

\[
j'_k = e f_k - f'_k v_k
\]  
(A10)

[here \(v_k = \hbar k/m\) for free electrons, and \(\sum_k j'_k\) corresponds to the second term on the right-hand side of Eq. (29).]

However, as compared to the above expressions for \(\varepsilon_k, S_k\), and \(j'_k\), those derived from the diagonalized Hamiltonian contain additional terms involving \(\partial^2 U_k/\partial X\), \(\partial^2 E_k/\partial X\) and \(\partial f_k/\partial X\) (where \(X = T\) in the case of \(\varepsilon_k\) or \(S_k\); and \(X = a_i\) in the case of \(j'_k\)).

Setting the sum of the additional terms to be zero, one gets Eq. (A7), and therefore Eq. (A6).

APPENDIX B: NUMERICAL METHOD FOR SOLVING THE BOUNDARY-VALUE PROBLEM OF SEC. III A

The boundary-value problem of Sec. III A as specified by the system of Eqs. (40) and (41), with boundary conditions given by Eqs. (43) and (48), can be solved by using the Runge-Kutta method.

In order to use the Runge-Kutta method, we first need to know values of \(a\) and \(b\) at one point on the \(r\)-axis. We know that far away from the vortex core, both \(a\) and \(b\) become small and \(n_s\) becomes a constant. For a constant \(n_s\), Eqs. (44) and (45) can be solved analytically (see, for example, Ref. [21]):

\[
a = \frac{C}{\sqrt{n_s}} K_1(r\sqrt{n_s})
\]  
(C1)

and

\[
b = CK_0(r\sqrt{n_s}),
\]  
(C2)

where \(C\) is a constant to be determined, and \(K_0(x)\) are the modified Bessel functions of the second kind.

Let \(r_0\) denote the \(r\)-coordinate of such a point located far away from \(r = 0\), the center of the vortex. We choose a value for \(r_0\) that is sufficiently large, and guess an initial value for constant \(C\), say \(C_0\), and obtain \(a(r_0)\) and \(b(r_0)\) from Eqs. (C1) and (C2), respectively, where \(n_s\) is obtained from Eq. (33) for \(a = 0\) (since the \(a\)-dependence of \(n_s\) is negligible when \(a\) is small) and given \(T\).

Once we know \(a(r_0)\) and \(b(r_0)\) at \(x = x_0\), we use the Runge-Kutta method to compute \(a(x_n)\) and \(b(x_n)\) for \(x_n = x_0 - nh\), where \(h\) is a small positive interval and \(n = 1, 2, \ldots, N\), until \(b(x_N) \geq H_a\) at \(x_N = x_0 - Nh\).

Usually, \(b(x_N)\) is greater than \(H_a\). If the difference between \(b(x_N)\) and \(H_a\) is small, we can simply use \(x_N\) as coordinate \(x_s\) of the surface of the superconductor. Or, we can obtain \(x_s\) by making a linear interpolation:

\[
x_s = x_{N-1} - \frac{H_a - b(x_{N-1})}{b(x_N) - b(x_{N-1})}.
\]  
(B2)

APPENDIX C: NUMERICAL METHOD FOR SOLVING THE BOUNDARY-VALUE PROBLEM OF SEC. III C

The boundary-value problem of Sec. III C as specified by the system of Eqs. (43) and (46), with boundary conditions given by Eqs. (45) and (48), can be solved by using the Runge-Kutta method.

In order to use the Runge-Kutta method, we need to know values of \(a\) and \(b\) at one point on the \(r\)-axis. We know that far away from the vortex core, both \(a\) and \(b\) become small and \(n_s\) becomes a constant. For a constant \(n_s\), Eqs. (44) and (45) can be solved analytically (see, for example, Ref. [21]):

\[
a = \frac{C}{\sqrt{n_s}} K_1(r\sqrt{n_s})
\]  
(C1)

and

\[
b = CK_0(r\sqrt{n_s}),
\]  
(C2)

where \(C\) is a constant to be determined, and \(K_0(x)\) are the modified Bessel functions of the second kind.

Let \(r_0\) denote the \(r\)-coordinate of such a point located far away from \(r = 0\), the center of the vortex. We choose a value for \(r_0\) that is sufficiently large, and guess an initial value for constant \(C\), say \(C_0\), and obtain \(a(r_0)\) and \(b(r_0)\) from Eqs. (C1) and (C2), respectively, where \(n_s\) is obtained from Eq. (33) for \(a = 0\) (since the \(a\)-dependence of \(n_s\) is negligible when \(a\) is small) and given \(T\). Once we know \(a(r_0)\) and \(b(r_0)\) at \(r = r_0\), the Runge-Kutta method allows us to compute \(a(r)\) and \(b(r)\) for any \(r\).

We then compute total magnetic flux \(\Psi\) associated with the vortex by numerically carrying out the integral on the right-hand side of Eq. (49). If total magnetic flux \(\Psi = \Psi_0\) for \(C = C_0\) is, for example, greater than flux quantum \(\Phi_0\), we reassign a smaller value for \(C\), say \(C_1\), and repeat the computation of \(a(r), b(r)\) and \(\Psi\).

For the \(i\)-th repetition \((i \geq 2)\), we can assign a value for \(C\) by making a linear interpolation or extrapolation, i.e.,

\[
C_i = C_{i-2} + \frac{\Phi_0 - \Psi_{i-2}}{\Psi_{i-1} - \Psi_{i-2}} (C_{i-1} - C_{i-2})
\]

The computation of \(a(r), b(r)\) and \(\Psi\) is repeated until the difference between total magnetic flux \(\Psi\) and flux quantum \(\Phi_0\) is within a predetermined range. In practice, it usually involves only a few repetitions.

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