Theory of a Local Superconductor in a Magnetic Field

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The behavior of a superconductor in a static magnetic field $\mathbf{H}(\mathbf{r})$ is considered in the limit that the field and the gap function $\Delta(\mathbf{r})$ vary slowly in space compared with the correlation distance of a superconducting electron pair (local limit). The superconductor is described by a pair of coupled differential equations for $\Delta(\mathbf{r})$ and the induced vector potential $\mathbf{A}(\mathbf{r})$. The equations are analogous in form to those proposed phenomenologically by Ginzburg and Landau (GL), but contain additional nonlinear terms. When Δ is independent of position and $\mathbf{H}$ is weak, the equations reduce to those given by BCS for the dependence of Δ and the penetration depth on the temperature T. When $\Delta \ll T$, the equations reduce to those derived by Gor'kov, in confirmation of the GL theory. The region of validity of the derivation is examined, showing that while a local (London) electrodynamics can be correct for some materials over a wide range of T and H, $\Delta(\mathbf{r})$ is slowly varying for $T \ll T_c$ only if Δ is near to its equilibrium, zero-field value.

I. INTRODUCTION

IN 1950, Ginzburg and Landau[1] presented a phenomenological theory of the behavior of a superconductor in a magnetic field, based on Landau's general theory of second-order phase transitions. The central hypothesis is the existence of an order parameter, ψ, in the superconducting phase, which goes to zero at the transition point. This order parameter is taken to be a function of space, and GL wrote down a plausible free-energy functional which is to be stationary with respect to variations of $\psi(\mathbf{r})$ and the vector potential $\mathbf{A}(\mathbf{r})$. The corresponding Euler-Lagrange equations become a Schrödinger-like equation satisfied by ψ in the presence of $\mathbf{A}$, and Maxwell's equation for $\mathbf{A}$ with the current source expressed in terms of ψ. These coupled equations have been applied with great success to a number of experimental situations, such as the magnetization characteristics and field dependence of the energy gap in thin superconducting films.[2,3]

After the development of the[4] BCS microscopic theory of superconductivity, Gor'kov[5] recast the theory into the language of thermodynamic Green's functions, and showed[6] that in a well-defined limit the GL equations were an exact consequence. Corresponding to the order parameter of GL (except for normalization) was the "pair wave function" or "gap function" $\Delta(\mathbf{r})$, and the effective charge e^* of GL was determined to be $e^*=2e$, reflecting the existence of bound electron pairs characteristic of the microscopic theory.

Gor'kov's derivation, however, made critical use of the assumption that the temperature, T, was close to to the transition temperature, T_c. This single assumption justified several distinct approximations: (1) That the energy-gap function $\Delta(\mathbf{r},T)$ was small compared to T, and was thus a valid expansion parameter; (2) that $\Delta(\mathbf{r},T)$ varied only slowly over a coherence distance $\xi(T)$, characterizing the spatial extent of the electron pair correlations; (3) that the penetration depth $\delta(T)$ was much larger than $\xi(T)$, so that the magnetic field was also slowly varying over a coherence distance; (4) that the bulk critical field $H_c(T)$ was much smaller than $H_c(0)$, and hence, that all magnetic fields of interest were weak in strength; (5) and as a corollary of (4), that the cyclotron frequency was very small compared with T (both in energy units), thus allowing a semiclassical approximation for the one-electron Green's function in the normal state in the presence of the field.

Several authors[7,8] have speculated recently that the GL equations should be valid over a wider range of temperatures than that considered by Gor'kov. In particular, only assumptions (2) and (3) that the superconductor is described by parameters with slow spatial variation should really be necessary. That this is at least a minimum requirement may be understood by recalling that Landau's theory postulates the existence of a *local* order parameter; such a concept can be a sensible one only when, e.g., the superconductor obeys a local electrodynamics (London limit), and clearly not when the electrodynamics is nonlocal (Pippard limit). Assumption (3) holds for some pure superconductors over a fairly wide range of temperatures, and is well-obeyed for all T by superconducting alloys of negative surface energy.[9] On the other hand, the GL theory makes no explicit demands that the order parameter be small, and there is nothing in the underlying physics to suggest that it need be so; the theory is meant to be an adequate description throughout the superconducting phase. It would appear that Gor'kov's assumption (1) may be no more than a convenient mathematical simplification.

[1] V. L. Ginzburg and L. D. Landau, Zh. Eksperim. i Teor. Fiz. **20**, 1064 (1950); to be referred to as GL.
[2] V. L. Ginzburg, Zh. Eksperim. i Teor. Fiz. **34**, 113 (1958) [translation: Soviet Phys.—JETP **7**, 78 (1958)].
[3] D. H. Douglass, Phys. Rev. **124**, 735 (1961); IBM J. Res. Develop. **6**, 44 (1962).
[4] J. Bardeen, L. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[5] L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. **34**, 735 (1958) [translation: Soviet Phys.—JETP **7**, 505 (1958)].
[6] L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. **36**, 1918 (1959) [translation: Soviet Phys.—JETP **9**, 1364 (1959)].
[7] R. H. Parmenter, Phys. Rev. **118**, 1173 (1960).
[8] M. Tinkham, IBM J. Res. Develop. **6**, 49 (1962).
[9] A. A. Abrikosov, Zh. Eksperim. i Teor. Fiz. **32**, 1442 (1957) [translation: Soviet Phys.—JETP **5**, 1174 (1957)].

In this paper, we re-examine Gor'kov's derivation, relaxing approximation (1) but retaining the others. We derive coupled equations determining $\Delta(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$ analogous to those of GL and Gor'kov, but which contain additional nonlinear terms. These terms are associated with the fact that $\Delta(\mathbf{r})$ is not normalized in the same way as the GL order parameter; this may also be seen by reconstructing the free-energy functional whose variation leads back to the dynamical equations. In the limit in which Δ does not vary in space, these equations reduce to those originally obtained by BCS for the energy gap and for the London penetration depth as functions of temperature. As $T\rightarrow T_c$ and $\Delta\rightarrow 0$, we recover Gor'kov's derivation. For low temperatures, on the other hand, an examination of the equations reveals limitations in their validity. First of all, the semiclassical approximation (5) in fields no greater than the critical field is accurate down to reduced temperatures $T/T_c \sim 10^{-2}$ or perhaps even less, but does fail at $T=0$. With this one mild restriction, the expression for the current can be correct for almost all T in some materials. The equation for $\Delta(\mathbf{r})$, however, derived by assuming this quantity to be slowly varying, shows the assumption (2) to be justified here only when $\Delta(\mathbf{r})$ is close to its zero-field value. Thus, while equations of the GL form can be suitably extended to much lower temperatures than indicated by Gor'kov's derivation, the equation for Δ (being highly nonlinear) is no longer an approximate description for all values of its solution. Nevertheless, if for low temperatures the transition at the critical field is of first order, so that, in fact, Δ is not substantially reduced by the field, than our Δ equation may be expected to hold for all $H\leq H_c$ and almost all T; a separate explicit calculation for each configuration would be needed, however, to determine the order of the transition.

II. DERIVATION

Our derivation begins by adopting Gor'kov's equations for the thermodynamic Green's functions G and $F^\dagger$ appropriate to a superconductor in a magnetic field, as stated in Eq. (2) of Ref. 6:

$$\left[i\omega+\frac{1}{2m}\left(\frac{\partial}{\partial\mathbf{r}}-\frac{ie}{c}\mathbf{A}(\mathbf{r})\right)^2+\mu\right]G_\omega(\mathbf{r},\mathbf{r}') = \delta^3(\mathbf{r}-\mathbf{r}')-\Delta(\mathbf{r})F_\omega{}^\dagger(\mathbf{r},\mathbf{r}'),$$
$$\left[-i\omega+\frac{1}{2m}\left(\frac{\partial}{\partial\mathbf{r}}+\frac{ie}{c}\mathbf{A}(\mathbf{r})\right)^2+\mu\right]F_\omega{}^\dagger(\mathbf{r},\mathbf{r}') = \Delta^*(\mathbf{r})G_\omega(\mathbf{r},\mathbf{r}'). \tag{1}$$

Reviewing the notation, ω is a discrete index, $=(2n+1)\pi T$ with n an integer; μ is the chemical potential; and $\Delta(\mathbf{r})$ is the gap function, defined by

$$\Delta^*(\mathbf{r})\equiv VT\sum_n F_\omega{}^\dagger(\mathbf{r},\mathbf{r}), \tag{2}$$

with V being the interaction constant. In addition, following Gor'kov, we introduce the single-particle Green's function $\tilde{G}_\omega(\mathbf{r},\mathbf{r}')$ for the electrons in the normal state, satisfying

$$\left[i\omega+\frac{1}{2m}\left(\frac{\partial}{\partial\mathbf{r}}-\frac{ie}{c}\mathbf{A}(\mathbf{r})\right)^2+\mu\right]\tilde{G}_\omega(\mathbf{r},\mathbf{r}')=\delta^3(\mathbf{r}-\mathbf{r}'), \tag{3a}$$

and the adjoint equation

$$\left[-i\omega+\frac{1}{2m}\left(\frac{\partial}{\partial\mathbf{r}'}+\frac{ie}{c}\mathbf{A}(\mathbf{r}')\right)^2+\mu\right]\tilde{G}_\omega(\mathbf{r},\mathbf{r}')=\delta^3(\mathbf{r}-\mathbf{r}'). \tag{3b}$$

It is worth noting that the Hartree-Fock contribution to the various Green's functions has been neglected.

Since Gor'kov assumes Δ to be small, his derivation proceeds by iterating Eqs. (1) to a low order. However, by rearranging Eqs. (1) and (3), separate exact integral equations for G and $F^\dagger$ may be written, in terms of Δ, Δ^* and $\tilde{G}$ only:

$$\int d^3s\, K_\omega(\mathbf{r},\mathbf{s})G_\omega(\mathbf{s},\mathbf{r}')=\delta^3(\mathbf{r}-\mathbf{r}'),$$
$$\int d^3s\, K_{-\omega}(\mathbf{s},\mathbf{r})F_\omega{}^\dagger(\mathbf{s},\mathbf{r}')=\Delta^*(\mathbf{r})\tilde{G}_\omega(\mathbf{r},\mathbf{r}'), \tag{4}$$

where the kernel K is defined as

$$K_\omega(\mathbf{r},\mathbf{s})\equiv\delta^3(\mathbf{r}-\mathbf{s})\left[i\omega+\frac{1}{2m}\left(\frac{\partial}{\partial\mathbf{s}}-\frac{ie}{c}\mathbf{A}(\mathbf{s})\right)^2+\mu\right] +\Delta(\mathbf{r})\tilde{G}_{-\omega}(\mathbf{s},\mathbf{r})\Delta^*(\mathbf{s}). \tag{5}$$

We note the close mathematical similarity of the problem at hand to that studied by Baraff and Borowitz,[10] and by DuBois and Kivelson,[11] in the somewhat different physical context of the Thomas-Fermi atom. In both cases, a not necessarily weak perturbation, inhomogeneous but slowly varying, is being applied to an otherwise homogeneous system, and relevant observables are being examined for their spatial dependence, to some low order in the rapidity of their spatial variation. As in Refs. (10) and (11), then, we introduce sum and difference coordinates, and Fourier transform with respect to the difference coordinates. Thus, we define

$$K_\omega(\mathbf{p},\mathbf{R})\equiv\int d^3(r-s)e^{-i\mathbf{p}\cdot(\mathbf{r}-\mathbf{s})}K_\omega(\mathbf{r},\mathbf{s}), \tag{6}$$

with $\mathbf{R}\equiv\frac{1}{2}(\mathbf{r}+\mathbf{s})$, and similarly for G, $F^\dagger$, and $\tilde{G}$. Then

[10] G. A. Baraff and S. Borowitz, Phys. Rev. **121**, 1704 (1961); G. A. Baraff, *ibid.* **123**, 2087 (1961).

[11] D. F. DuBois and M. G. Kivelson, Phys. Rev. **127**, 1182 (1962).

Eqs. (4) transform to

$$\Theta[K_\omega(\mathbf{p},\mathbf{R})G_\omega(\mathbf{p}',\mathbf{R}')]=1\,, \tag{7}$$
$$\Theta[K_{-\omega}(-\mathbf{p},\,\mathbf{R})F_\omega^\dagger(\mathbf{p}',\mathbf{R}')]=\Theta[\Delta^*(\mathbf{R})\tilde{G}_\omega(\mathbf{p}',\mathbf{R}')]\,,$$

where Θ is the differential operator

$$\Theta\equiv\lim_{\mathbf{R}'\to\mathbf{R},\mathbf{p}'\to\mathbf{p}}\exp\left[\frac{i}{2}\left(\frac{\partial}{\partial\mathbf{R}}\cdot\frac{\partial}{\partial\mathbf{p}'}-\frac{\partial}{\partial\mathbf{p}}\cdot\frac{\partial}{\partial\mathbf{R}'}\right)\right]. \tag{8}$$

Combining Eqs. (5) and (6), we find

$$K_\omega(\mathbf{p},\mathbf{R})=i\omega-\epsilon(\mathbf{p},\mathbf{R})+\lim_{\mathbf{R}',\mathbf{R}''\to\mathbf{R}}\exp\left[\frac{i}{2}\frac{\partial}{\partial\mathbf{p}}\cdot\left(\frac{\partial}{\partial\mathbf{R}'}-\frac{\partial}{\partial\mathbf{R}''}\right)\right]$$
$$\times\Delta(\mathbf{R}')\tilde{G}_{-\omega}(-\mathbf{p},\,\mathbf{R})\Delta^*(\mathbf{R}'')\,, \tag{9}$$

with the notation

$$\epsilon(\mathbf{p},\mathbf{R})\equiv\epsilon\left(\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{R})\right)\equiv\frac{1}{2m}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{R})\right)^2-\mu\,. \tag{10}$$

We next expand (at least formally) each of the quantities in Eqs. (7) according to the degree of inhomogeneity, e.g.,

$$K=K^{(0)}+K^{(1)}+K^{(2)}+\cdots\,,$$

and equate terms of like degree in Eqs. (7) separately to zero. Thus, we obtain the set

$$\Theta^{(0)}[K^{(0)}G^{(0)}]=1\,,$$
$$\Theta^{(0)}[K^{(1)}G^{(0)}]+\Theta^{(0)}[K^{(0)}G^{(1)}]+\Theta^{(1)}[K^{(0)}G^{(0)}]=0\,, \tag{11}$$

etc., and a similar set for the $F^{\dagger(n)}$ with appropriate right-hand sides.

Before proceeding with the superconducting problem, it is convenient at this point to obtain an approximate expression for the normal state Green's function. Replacing $K\to\tilde{K}$, $G\to\tilde{G}$ in Eqs. (11), and noting from definition (8) that $\Theta^{(0)}=1$, the first equation yields

$$\tilde{G}_\omega^{(0)}(\mathbf{p},\mathbf{R})=[\tilde{K}_\omega^{(0)}(\mathbf{p},\mathbf{R})]^{-1}=[i\omega-\epsilon(\mathbf{p},\mathbf{R})]^{-1}. \tag{12}$$

But since $\tilde{K}^{(1)}=0$, and since $\Theta^{(1)}[X,X^{-1}]=0$ for any function $X(\mathbf{p},\mathbf{R})$, the second of Eqs. (11) gives[10,11] $\tilde{G}^{(1)}=0$. Hence, to an approximation sufficient for our purposes, $\tilde{G}=\tilde{G}^{(0)}$, and we shall follow Gor'kov[6] in using this expression throughout.

Returning to the superconducting situation, Eqs. (11) can be solved for $G\cong G^{(0)}+G^{(1)}$;

$$G_\omega^{(0)}(\mathbf{p},\mathbf{R})=[K_\omega^{(0)}(\mathbf{p},\mathbf{R})]^{-1}$$
$$=\{i\omega-\epsilon(\mathbf{p},\mathbf{R})+|\Delta(\mathbf{R})|^2\times[-i\omega-\epsilon(-\mathbf{p},\,\mathbf{R})]^{-1}\}^{-1}\,, \tag{13}$$

$$G_\omega^{(1)}(\mathbf{p},\mathbf{R})=-K_\omega^{(1)}(\mathbf{p},\mathbf{R})G_\omega^{(0)}(\mathbf{p},\mathbf{R})/K_\omega^{(0)}(\mathbf{p},\mathbf{R})$$
$$=-\{[i\omega-\epsilon(\mathbf{p},\mathbf{R})]\times[-i\omega-\epsilon(-\mathbf{p},\,\mathbf{R})]+|\Delta(\mathbf{R})|^2\}^{-2}$$
$$\times\frac{i}{2}\left[\Delta^*(\mathbf{R})\frac{\partial\Delta(\mathbf{R})}{\partial\mathbf{R}}-\frac{\partial\Delta^*(\mathbf{R})}{\partial R}\Delta(\mathbf{R})\right]\cdot\frac{1}{m}\left[\mathbf{p}+\frac{e}{c}\mathbf{A}(\mathbf{R})\right]. \tag{14}$$

The observable of most immediate interest obtainable from G is the current. In general, the average value of this operator is given by

$$\mathbf{j}(\mathbf{R})=\frac{2e}{m}T\sum_n\lim_{\mathbf{r}'\to\mathbf{r}}\left[\frac{i}{2}\left(\frac{\partial}{\partial\mathbf{r}'}-\frac{\partial}{\partial\mathbf{r}}\right)-\frac{e}{c}\mathbf{A}(\mathbf{R})\right]G_\omega(\mathbf{r},\mathbf{r}')$$
$$=\frac{2e}{m}T\sum_n\int\frac{d^3p}{(2\pi)^3}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{R})\right)G_\omega(\mathbf{p},\mathbf{R})\,. \tag{15}$$

An approximate result for $\mathbf{j}$ is obtained by substituting expressions (13) and (14) into Eq. (15). Now although we have made a formal iteration in the degree of spatial variation, so that quantities with superscript (i) are homogeneous of order i in the gradient operator, so far these derivatives act on Δ and Δ^*. We are, indeed, expecting $|\Delta|$ to be slowly varying, but arg Δ need not be; any restrictions on arg Δ imply lack of full gauge invariance. Analogously, since $\mathbf{H}$ is no greater than a critical field, it may be considered as "weak"; but $\mathbf{A}$ need by no means be small, again due to the freedom of a gauge transformation. Nevertheless, quantities such as the current may be expanded in $\mathbf{A}$ as well as $\partial\Delta/\partial\mathbf{R}$ provided the resulting terms are regrouped into an expansion in the gauge-invariant combination

$$\left(\frac{\partial}{\partial\mathbf{R}}-\frac{2ie}{c}\mathbf{A}\right)\Delta\,,$$

which may very well be small. When such an expansion and regrouping is carried out for $\mathbf{j}$, keeping just the first nonvanishing contribution, and when, furthermore, the integration over angles of $\mathbf{p}$ indicated in Eq. (15) is performed, $\mathbf{j}$ becomes

$$\mathbf{j}(\mathbf{R})=\frac{2e}{m}\left[-\frac{i}{2}\left(\Delta^*(\mathbf{R})\frac{\partial\Delta(\mathbf{R})}{\partial\mathbf{R}}-\frac{\partial\Delta^*(\mathbf{R})}{\partial\mathbf{R}}\Delta(\mathbf{R})\right)-\frac{2e}{c}|\Delta(\mathbf{R})|^2\mathbf{A}(\mathbf{R})\right]T\sum_n\int\frac{d^3p}{(2\pi)^3}\frac{p^2/3m}{(\omega^2+E^2(\mathbf{p},\mathbf{R}))^2}, \tag{16}$$

where

$$E(\mathbf{p},\mathbf{R})\equiv[\epsilon^2(\mathbf{p})+|\Delta(\mathbf{R})|^2]^{1/2}. \tag{17}$$

Equation (16) is similar to the corresponding expression for $\mathbf{j}$ found by Gor'kov, except for the factor explicitly containing the temperature. In fact, when

$\Delta \ll \pi T$,

$$T\sum_n \int \frac{d^3p}{(2\pi)^3}\frac{p^2/3m}{(\omega^2+E^2)^2} \equiv \frac{N}{2}g_2(|\Delta|^2) \to \frac{N}{2}\frac{7\zeta(3)}{8(\pi T)^2}, \quad (18)$$

(where N is the number of particles per unit volume and ζ is the Riemann function), which is precisely the result[6] of Gor'kov. In general, however, $2|\Delta|^2 g_2$ is closely related to the temperature-dependent London penetration depth as computed by BCS (Λ/Λ_T in their notation.) Carrying out the ω summation, we have

$$2|\Delta|^2 g_2 = \int_{-\infty}^{\infty} d\epsilon \frac{|\Delta|^2}{E^2}\left(\frac{df(E)}{dE}+\frac{1-2f(E)}{2E}\right) = 1+\int_{-\infty}^{\infty} d\epsilon \frac{df(E)}{dE}, \quad (19)$$

where f is the usual Fermi function. Expression (19) is identical to Λ/Λ_T, although in the present case, where Δ is a local function of position, Λ/Λ_T becomes position dependent as well.

The procedure just used to solve approximately for G can also be used to obtain $F^\dagger$. Here, however, it will be important to work through order $F^{\dagger(2)}$, one order higher than for G. Referring to Eqs. (6) and (10), it is seen that

$$K_{-\omega}^{(0)}(-\mathbf{p},\mathbf{R})F_\omega^{\dagger(0)}(\mathbf{p},\mathbf{R}) = \Delta^*(\mathbf{R})\tilde{G}_\omega(\mathbf{p},\mathbf{R}),$$

or

$$F_\omega^{\dagger(0)}(\mathbf{p},\mathbf{R}) = \Delta^*(\mathbf{R})[(i\omega-\epsilon(\mathbf{p},\mathbf{R})) \times(-i\omega-\epsilon(-\mathbf{p},\mathbf{R}))+|\Delta(\mathbf{R})|^2]^{-1}. \quad (20)$$

The next two approximations to $F^\dagger$ may be generated straightforwardly but the resulting expressions are quite lengthy and will not be quoted here. What is of more interest is to use $F^\dagger$ to construct an equation determining $\Delta^*(\mathbf{R})$. In the mixed representation, Eq. (2) reads

$$\Delta^*(\mathbf{R}) = VT\sum_n \int \frac{d^3p}{(2\pi)^3}F_\omega^\dagger(\mathbf{p},\mathbf{R}). \quad (21)$$

As was done for G, we also expand $F^\dagger \cong F^{\dagger(0)}+F^{\dagger(1)}+F^{\dagger(2)}$ in powers of $\mathbf{A}$: to order A^2 in $F^{\dagger(0)}$, A in $F^{\dagger(1)}$ and A^0 in $F^{\dagger(2)}$. The angular integration indicated in Eq. (21) removes all terms linear in the vector $\mathbf{p}$, and the integration over energies removes all terms linear in $\epsilon(\mathbf{p})$, (i.e., terms odd under particle-hole interchange about the Fermi surface[12]). The remaining terms can be combined so that Eq. (19) finally becomes

$$\Delta^* = VT\sum_n \int \frac{d^3p}{(2\pi)^3}\left\{\frac{\Delta^*}{\omega^2+E^2}+\left[\left(\frac{\partial}{\partial\mathbf{R}}+\frac{2ie}{c}\mathbf{A}\right)^2\Delta^* +\Delta\left(\left(\frac{\partial}{\partial\mathbf{R}}+\frac{2ie}{c}\mathbf{A}\right)\Delta^*\right)^2\frac{\partial}{\partial|\Delta|^2}+\frac{\Delta^*}{3}\frac{\partial^2|\Delta|^2}{\partial\mathbf{R}^2}\frac{\partial}{\partial|\Delta|^2} +\frac{\Delta^*}{6}\left(\frac{\partial|\Delta|^2}{\partial\mathbf{R}}\right)^2\frac{\partial^2}{\partial(|\Delta|^2)^2}\right]\frac{p^2/6m^2}{(\omega^2+E^2)^2}\right\}. \quad (22)$$

[12] V. Ambegaokar and L. P. Kadanoff, Nuovo Cimento **22**, 914 (1961).

Equation (22) reduces to familiar expressions in two different limits. In the absence of a magnetic field and in an otherwise homogeneous system, Δ^* is independent of position; performing the sum over frequencies reduces Eq. (22) to the standard BCS result for Δ^* as a function of temperature:

$$\Delta^* = V\int \frac{d^3p}{(2\pi)^3}\frac{\tanh(\frac{1}{2}\beta E)}{2E}\Delta^*. \quad (23)$$

Furthermore, for T near the transition temperature T_c, Eq. (22) may be expanded in powers of $|\Delta|^2$. Recalling that in the homogeneous situation T_c is determined by the condition

$$1 = V\int \frac{d^3p}{(2\pi)^3}\frac{\tanh(\frac{1}{2}\beta_c\epsilon)}{2\epsilon}, \quad (24)$$

to first order Δ^* can be shown to satisfy

$$0 = \left\{\ln\frac{T_c}{T}-\frac{7\zeta(3)}{8(\pi T)^2}|\Delta(\mathbf{R})|^2 +\frac{7\zeta(3)}{8(\pi T)^2}\frac{p_F^2}{6m^2}\left(\frac{\partial}{\partial\mathbf{R}}+\frac{2ie}{c}\mathbf{A}(\mathbf{R})\right)^2\right\}\Delta^*(\mathbf{R}). \quad (25)$$

This is again precisely the result found by Gor'kov, agreeing with the GL theory.

It is also of interest to verify that the coupled dynamical equations (16) and (22) can be obtained by requiring that a certain functional $\mathfrak{F}$ be stationary with respect to variations of $\Delta(\mathbf{R})$ and $\mathbf{A}(\mathbf{R})$. The functional for which Eqs. (16) and (22) are the corresponding Euler-Lagrange

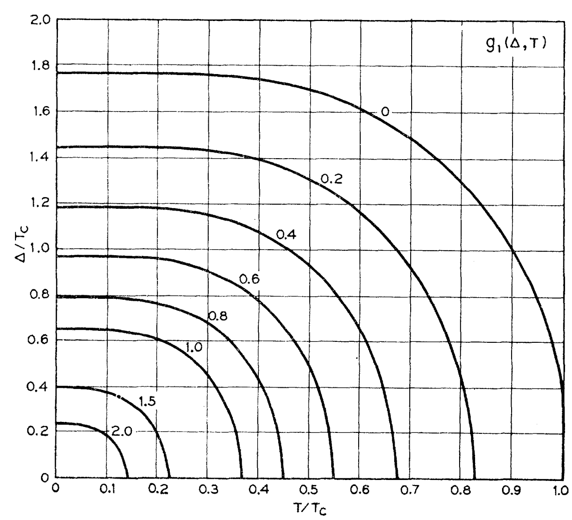

FIG. 1. Contour lines of the function $g_1(|\Delta|,T)$ defined by Eq. (29) in the dimensionless $(\Delta/T_c, T/T_c)$ plane. The curve $g_1=0$ reproduces the temperature dependence of the zero-field energy gap in the BCS theory. The region $g_1 \ll 1$ is that for which the gap function $|\Delta(\mathbf{r})|$ is a slowly varying function of position.

equations [the latter with Eq. (24) subtracted, to remove the divergence] is

$$\mathfrak{F}=\int d^3R\left\{\int\frac{d^3p}{(2\pi)^3}\left[\frac{1}{\beta}\ln\frac{1+\cosh\beta E(\mathbf{p},\mathbf{R})}{1+\cosh\beta\epsilon(\mathbf{p})}-|\Delta(\mathbf{R})|^2\frac{\tanh\frac{1}{2}\beta_c\epsilon(\mathbf{p})}{2\epsilon(\mathbf{p})}\right]\right.$$
$$\left.+\frac{1}{2m}\left|\left(\frac{\partial}{\partial\mathbf{R}}-\frac{2ie}{c}\mathbf{A}(\mathbf{R})\right)\Delta(\mathbf{R})\right|^2\frac{N}{2}g_2(|\Delta|^2)+\frac{1}{2m}\frac{\partial|\Delta(\mathbf{R})|^2}{\partial\mathbf{R}}\cdot\frac{N}{12}\frac{\partial g_2(|\Delta|^2)}{\partial\mathbf{R}}+\frac{|\mathbf{H}(\mathbf{R})-\mathbf{H}_a|^2}{8\pi}\right\},\qquad(26)$$

where $\mathbf{H}_a$ is the field applied externally. In fact, the stationary value of $\mathfrak{F}$ can be shown to be just the (Gibbs) free-energy difference between the superconducting and normal states. A convenient proof uses, along with Eqs. (22) and (24), the well-known formula for the free-energy difference in terms of an integration of the potential energy over coupling constants, given for instance by Gor'kov's[6] Eq. (19). Consistent with this interpretation, $\mathfrak{F}$ vanishes when $\Delta=0$, and it reduces to the BCS expression for the free-energy difference when $H_a=0$.

III. DISCUSSION

The dynamical equations (16) and (22) coupling $\Delta(\mathbf{R})$ and $\mathbf{A}(\mathbf{R})$, or, equivalently, the free-energy functional (26) from which the requirement of stationarity recovers them, constitute our principal results. We have seen that these equations resemble in form the phenomenological Ginzburg-Landau theory, but contain $\Delta(\mathbf{R})$-dependent coefficients, which further complicate the dynamics. Because of this, no precise identification with the GL order parameter ψ can be made; the gap function Δ might still be interpreted to a certain extent as an order parameter, but it cannot be normalized in the same way as ψ, and is not related to the superfluid density in as simple a manner.

The equations also are similar to the standard BCS theory, to which, as we have seen, they reduce when the gap function becomes independent of $\mathbf{R}$. In this sense, they constitute a natural generalization of the BCS energy gap and London electrodynamic equations, to situations that are spatially inhomogeneous on a macroscopic scale. Our results are manifestly gauge invariant, and it here becomes clear that the generalization $\Delta\to\Delta(\mathbf{R})$ is all that is needed in the BCS context to obtain this invariance.[12]

It may now be asked, to what extent are the assumptions used in deriving Eqs. (16) and (22) valid? That is, under what circumstances are the solutions Δ and $\mathbf{A}$ indeed slowly varying compared with a coherence distance? To develop some feeling for this problem, we may temporarily skeletonize it by taking Δ to be real, and ignoring the $\mathbf{R}$ dependence of g_2. Then subtracting Eq. (24) from (22), and substituting Eq. (16) into the appropriate Maxwell equation, the equations we wish to examine can be written as

$$\nabla^2\mathbf{A}=(2|\Delta|^2g_2/\delta_L{}^2)\mathbf{A},\qquad(27)$$

$$0=\left\{g_1+\frac{p_F{}^2}{6m^2}g_2\left(\frac{\partial}{\partial\mathbf{R}}+\frac{2ie}{c}\mathbf{A}\right)^2\right\}\Delta.\qquad(28)$$

Here $\delta_L\equiv(4\pi Ne^2/mc^2)^{-1/2}$ is the London penetration depth, and

$$g_1(|\Delta|^2)\equiv\int_{-\infty}^{\infty}d\epsilon\left[\frac{\tanh\frac{1}{2}\beta E}{2E}-\frac{\tanh\frac{1}{2}\beta_c\epsilon}{2\epsilon}\right].\qquad(29)$$

From the definitions (18) and (29), it is seen that $g_2=-\partial g_1/\partial|\Delta|^2$.

Equation (28) now reveals that the coherence distance ξ, the characteristic distance of nonlocality for $\Delta(\mathbf{R})$, is just given by

$$\xi^2\sim\xi_0{}^2(\gamma\pi T_c)^2g_2,\qquad(30)$$

with $\xi_0\equiv v_F/\gamma\pi^2T_c$ being the BCS coherence distance (γ is Euler's constant). On the other hand, $\Delta(\mathbf{R})$ varies in space over characteristic lengths

$$\lambda\sim\xi g_1{}^{-1/2}.\qquad(31)$$

Thus, it is legitimate to regard $\Delta(\mathbf{R})$ as a local, slowly varying function only when $g_1\ll1$, so that $\lambda\gg\xi$. From another point of view, Eq. (28) represents the first two terms in an expansion which may be indicated schematically as

$$0=\left\{g_1+\xi^2\frac{\partial^2}{\partial R^2}+\xi^4\frac{\partial^4}{\partial R^4}+\cdots\right\}\Delta;$$

the third and higher terms may be neglected and Δ varies as $\cos R/\lambda$, only if $\lambda\gg\xi$.

Furthermore, the penetration depth δ of the magnetic field is given from Eq. (27) as

$$\delta=\delta_L(2|\Delta|^2g_2)^{-1/2}.\qquad(32)$$

Thus, the field is slowly varying compared to a coherence distance if $\xi\ll\delta$, or

$$\gamma\pi T_c|\Delta|g_2\ll\delta_L/\xi_0.\qquad(33)$$

The inequality not only depends on the values of T and $|\Delta|$, but also on the ratio of the London penetration depth to the BCS coherence distance. This ratio typically is small for pure soft superconductors (so that the electrodynamics can be local only for $T\approx T_c$), but may be of order unity or more for some pure transition metals such as niobium,[13] and for alloys (a situation not explicitly treated here) is expected to be much larger than one. In the latter cases, a local electrodynamics of the London type, Eq. (27), is appropriate even at comparatively low reduced temperatures.

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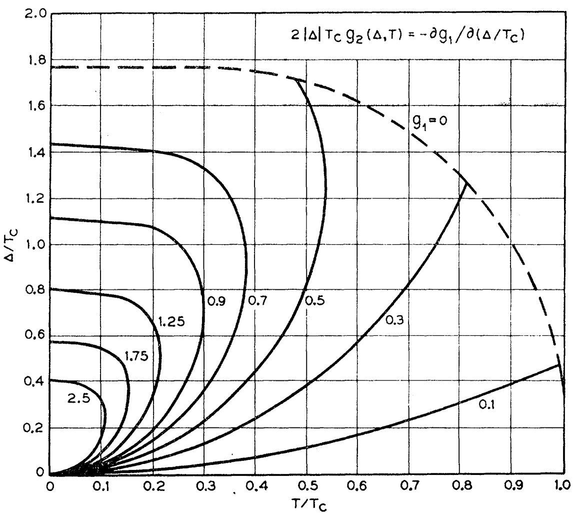

FIG. 2. Contour lines of the function $2T_c|\Delta|g_2(|\Delta|,T)$, with g_2 defined by Eq. (19), in the $(\Delta/T_c,T/T_c)$ plane. The dashed curve is the $g_1=0$ curve from Fig. 1. The region $2T_c|\Delta|g_2 \ll \delta_L/\xi_0$, depending on the ratio of London penetration depth to BCS coherence distance, is that for which the magnetic field is a slowly varying function of position and satisfies a local differential equation of the London form.

The results of the preceding paragraphs may be summarized graphically, illustrating the regions of validity of a local superconductivity. In Figs. 1 and 2 we plot contours of constant g_1 and $2T_c|\Delta|g_2$, respectively, as functions of the reduced variables $|\Delta|/T_c$ and T/T_c. The curve $g_1=0$ of Fig. 1 simply reproduces the temperature dependence of the energy gap, $\Delta_{\rm BCS}(T)$, in the BCS theory [note definition (29)], while the region of $g_1 \ll 1$ gives the values of (Δ,T) for which Δ is slowly varying and obeys the local Eq. (22). For $T \lesssim T_c$, Eq. (22) is seen to hold for all $0 \leq |\Delta| \leq \Delta_{\rm BCS}$; whereas for $T \ll T_c$, the equation is adequate only for $|\Delta| \lesssim \Delta_{\rm BCS}$, and so can describe the magnetic transition only if it is of first order, with $|\Delta|$ not greatly affected by the field. Similarly, Fig. 2 displays the region of validity of the local current expression (16), depending through Eq. (33) on the ratio of intrinsic parameters, δ_L/ξ_0. Illustrated are the standard results that for the usual soft superconductors with $\delta_L \ll \xi_0$, a London electrodynamics is valid at all Δ only when $T_c - T \ll T_c$; but in the much less common situation $\delta_L \gg \xi_0$, Eq. (16) is valid for almost all T and Δ.

At this point, however, it is worth noting that the above analysis, being devoted primarily to the relative size of the space derivatives [assumptions (2) and (3)], is only relevant for bulk specimens. In films thinner than the characteristic lengths ξ and δ, spatial variations are negligible and the real issue is assumption (4) on the relative strength of the field. The equations derived here reduce for the thin film case very nearly to those proposed by Bardeen.[14] The question of validity in this situation becomes lengthy and is postponed to a later paper.

One further result of some interest follows directly from the form of Eq. (16) for the current, without further computation. It has been shown by Bardeen,[15] Keller and Zumino,[16] and Ginzburg,[17] from the high temperature, small gap limit of Eq. (16) found previously by Gor'kov, that fluxoid quantization is an exact consequence of the microscopic theory; because of the presence of the "effective charge" $e^*=2e$, the natural quantum unit of flux is $\Phi_0 = hc/2e$, the value found experimentally,[18] and half the value originally predicted by London. Our establishment of Eq. (16) valid at all temperatures for which $\xi \ll \delta$ makes fluxoid quantization in units of Φ_0 an exact theoretical prediction for all superconductors in the London limit.

Finally, a number of generalizations of the calculation presented here are possible, and will also be the subject of a separate paper. It is entirely feasible to include: (1) Time-varying magnetic, and also electric fields. This would be of interest, e.g., for a computation (completely gauge invariant) of the magnetic field dependence of the microwave surface impedance of superconductors.[19] (2) The interaction of the magnetic field with the electron *spins* as well as their orbital motion. This would allow a systematic analysis of the role of the Zeeman energy in determining the critical field, especially in the high H_c superconducting alloys, as first discussed by Clogston.[20] Another generalization of practical interest is the inclusion of impurity scattering centers, so as to obtain the effect (e.g., on the penetration depth) of a finite electronic mean free path. Results in the "high-temperature" regime have already been obtained by Abrikosov and Gor'kov.[21]

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