Rigorous study of the gap equation for an inhomogeneous superconducting state near T_c†

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A rigorous analytic study of the self-consistent gap equation (symobolically $\Delta = \mathfrak{F}_T[\Delta]$), for an inhomogeneous superconducting state, is presented in the Bogoliubov formulation. The gap function $\Delta(\vec{r})$ is taken to simulate a planar normal-superconducting phase boundary: $\Delta(\vec{r}) = \Delta_\infty \tanh(\alpha\Delta_\infty z/v_F)\Theta(z)$, where $\Delta_\infty(T)$ is the equilibrium gap, v_F is the Fermi velocity, and $\Theta(z)$ is a unit step function. First a special space integral of the gap equation $\propto \int_{0+}^{\infty}(\mathfrak{F}_T - \Delta)(d\Delta/dz)dz$ is evaluated essentially exactly, except for a nonperturbative WKBJ approximation used in solving the Bogoliubov–de Gennes equations. It is then expanded near the transition temperature T_c in power of $\Delta_\infty \propto (1-T/T_c)^{1/2}$, demonstrating an exact cancellation of a subseries of "anomalous-order" terms. The leading surviving term is found to agree in order, but not in magnitude, with the Ginzburg-Landau-Gor'kov (GLG) approximation. The discrepancy is found to be linked to the slope discontinuity in our chosen Δ. A contour-integral technique in a complex-energy plane is then devised to evaluate the local value of $\mathfrak{F}_T - \Delta$ exactly. Our result reveals that near T_c this method can reproduce the GLG result essentially everywhere, except within a BCS coherence length [not $\xi(T)$!] from a singularity in Δ, where $\mathfrak{F}_T - \Delta$ can have a singular contribution with an "anomalous" local magnitude, not expected from the GLG approach. This anomalous term precisely accounts for the discrepancy found in the special integral of the gap equation as mentioned above, and likely explains the ultimate origin of the anomalous terms found in the free energy of an isolated vortex line by Cleary.

I. INTRODUCTION AND SUMMARY

Recently, there has been a growing effort to study various inhomogeneous superconducting states from a microscopic viewpoint. Prominent examples of space-dependent superconducting states include vortex lines in type-II materials, normal (N)–superconducting (S) phase boundaries in type-I materials, surface superconductivity near a sample boundary, proximity effects, etc.

All existing microscopic theories of inhomogeneous superconductors are the outgrowth of the celebrated Bardeen-Cooper-Schrieffer (BCS) theory,[1] and are basically generalized Hartree-Fock theories. The central physical quantity is a complex order-parameter function $\Delta(\vec{r})$, also loosely called the gap function, which is always determined via a self-consistency condition, often referred to as the gap equation. In Gor'kov's formulation,[2] two electronic Green's functions, $G(\vec{r},\vec{r}\,')$ and $F(\vec{r},\vec{r}\,')$, are determined via a pair of partial differential equations of linear inhomogeneous type (the Gor'kov equations), coupled by $\Delta(\vec{r})$ as a space-dependent coefficient. The gap equation in this formulation reads simply $\Delta(\vec{r}) = gF(\vec{r},\vec{r})$, where g is the BCS coupling constant. In the alternative formulation due originally to Bogoliubov,[3] which we adopt here, the central equations are the Bogoliubov-de Gennes (BdG) equations[4]:

$$E_n U_n(\vec{r}) = \hat{h}\,U_n(\vec{r}) + \Delta(\vec{r})\,V_n(\vec{r}) \,,$$
$$E_n V_n(\vec{r}) = -\hat{h}^* V_n(\vec{r}) + \Delta^*(\vec{r})\,U_n(\vec{r}) \,, \qquad (1.1)$$

where $\hat{h} \equiv (2m_e)^{-1}[-i\vec{\nabla} - e\vec{A}(\vec{r})]^2 - E_F$; m_e is the electronic mass, E_n is the energy of the nth elementary excitation with corresponding particle and hole amplitudes U_n and V_n, $E_F = (2m_e)^{-1}k_F^2$ is the Fermi energy, $\vec{A}$ is the vector potential corresponding to an external magnetic field $\vec{B}$, and units have been chosen such that $\hbar = c =$ Boltzmann's constant $= 1$. In this BdG theory, the gap equation takes the form

$$\Delta(\vec{r}) = g \sum_{E_n>0} U_n(\vec{r})\,V_n^*(\vec{r}) \tanh\frac{E_n}{2T} \equiv \mathfrak{F}_T(\vec{r}) \,, \qquad (1.2)$$

where T is the temperature. The two formulations are completely equivalent, as may be shown easily.[5]

Many successful applications[6] of these theories are based on solving the Gor'kov or the BdG equations by perturbation or iteration methods, which are presumed valid when $\Delta(\vec{r})$ is either small or nearly constant everywhere in space. In the case when neither condition is met, the self-consistency condition is rather difficult to satisfy, and, so far, theorists have generally been contented with qualitative studies based on intuitive guesses on the spatial dependence of $\Delta(\vec{r})$, or with various numerical techniques for achieving approximate self-consistency. It is clear that one can have much more confidence on such approximate or numerical methods, if one has a better understanding of the nature and the properties of the self-consistency condition on the gap function. To this goal we present below an analytical study of the gap equation in the Bogoliubov formulation, Eq. (1.2). It is based on the recent discovery by Bar-Sagi and Kuper[7] that in the absence of a field $\vec{B}$, the BdG equations (1.1) may be solved analytically in a *nonperturbative* WKBJ approximation,[8] if the order parameter is taken to have the following simple space dependence:

$$\Delta(\vec{r}) = \Delta_\infty \tanh(\alpha \Delta_\infty z/v_F) \equiv \Delta_\infty X , \quad (1.3)$$

where $\Delta_\infty(T)$ is the equilibrium value of Δ at temperature T, $v_F = k_F/m_e$ is the Fermi velocity, and α is a dimensionless free parameter. The WKBJ method requires only that $\xi_0 \equiv v_F/\pi\Delta_\infty(0) \gg k_F^{-1}$, or, equivalently, that the transition temperature $T_c \ll E_F$. It therefore presumably has a much wider region of validity than an iterative or perturbative method for solving the Gor'kov or the BdG equations. In this approximation, Bar-Sagi and Kuper solved Eq. (1.1) analytically in the region $z>0$, assuming Eq. (1.3), $A \equiv 0$, and the boundary conditions that $U=V=0$ at $z=0$. They then used these solutions to explicitly analyze the gap equation (1.2) near T_c. However, we find that their analysis of the gap equation has missed some very important points, and some of their main conclusions are built on rather questionable grounds (see Sec. II). This observation has prompted us to present here a more rigorous analysis of the gap equation. In order to avoid some unnecessary complications, as explained in Sec. II, we have chosen to study a slightly different inhomogeneous state, for which $\Delta(\vec{r})$ is given by Eq. (1.3) for $z>0$ only, and is identically zero for $z<0$. With $\alpha=\sqrt{3}$, this $\Delta(\vec{r})$ is the *only* "solution" of the Ginzburg-Landau (GL) equation,[9] in the absence of an external field, that has the property of a planar N-S phase boundary, although rigorously speaking the plane $z=0$ is singular for this $\Delta(\vec{r})$, and the GL equation is actually violated there. If a magnetic field of critical strength is also introduced in the region $z<0$, such a $\Delta(\vec{r})$ would, according to GL theory, well approximate an actual N-S phase boundary that can appear in the intermediate state of an otherwise homogeneous type-I superconductor, if the latter has a very small GL parameter κ. In an earlier work[10] we have shown that introducing a magnetic field in the normal region does not produce important changes in the excitation spectrum, the free energy, and most likely also the self-consistency requirement. We shall therefore loosely refer to our chosen $\Delta(\vec{r})$ as the gap function for an N-S phase boundary, although we shall not consider a magnetic field anywhere. Our chosen $\Delta(\vec{r})$ may likely also describe a bulk superconductor in proximity with a thick layer of a magnetic metal,[11] although we do not intend to include magnetic scatterings in our present analysis either. In any case, our choice for this $\Delta(\vec{r})$ does not stem mainly from a physical consideration, but rather from its mathematical simplicity, so that we could possibly complete our rigorous study of the gap equation *by purely analytical method, without neglecting any contribution.* Indeed, despite the fact that our choice of $\Delta(\vec{r})$ may not be exactly realistic, our study still revealed much useful information, and also removed some misconception about the self-consistency condition on the gap function. Furthermore, the mathematical techniques developed here for explicitly evaluating the gap equation of a nontrivial inhomogeneous state are most likely also useful for studying other more realistic space-dependent superconducting states.

Another principal motivation for this work concerns the exact relation between the Bogoliubov theory and the phenomenological GL theory. It is well known that Gor'kov[12] has derived the GL equations from his microscopic Green's-function theory of superconductivity by assuming that near T_c $\Delta(\vec{r})$ is small $[\propto (1-T/T_c)^{1/2}]$, as well as slowly varying [i.e., varying only in a scale $\xi(T) \propto \xi_0(1-T/T_c)^{-1/2} \gg \xi_0$, where $\xi_0 \propto v_F/T_c$ is the BCS coherence length]. Under these assumptions he solved the "Gor'kov's equations" by an iterative method, and expanded the gap equation with respect to Δ and the space-differentiation operation. The procedure was later extended by Neumann and Tewordt (NT)[13] to the next order, revealing an expansion in powers of $1-T/T_c$. De Gennes[4] has further shown that if the BdG equations are solved by the Rayleigh-Schrödinger perturbation theory, then the gap equation (1.2) can also be reduced to a GL equation. This second derivation of the GL equations is less rigorous, because the Rayleigh-Schrödinger method is valid for $E \gg \max|\Delta|$ only, but it has been used for all E in order to simplify Eq. (1.2). (We shall see that the low-energy contributions are not negligible, contrary to what one might attempt to assume near T_c.) Recently, Bardeen *et al.*[14] have developed a *nonperturbative* scheme to simplify the Bogoliubov theory which employs the WKBJ method for solving the BdG equations, and also replaces the self-consistent gap equation by a variational principle on a free-energy expression. They applied this method to study, among other quantities, the excess free-energy associated with an isolated vortex line. Later, Cleary[15] found that near T_c this excess free energy could be expanded in powers of the small parameter $\epsilon \equiv \Delta_\infty/2T \propto (1-T/T_c)^{1/2}$, and found somewhat surprising results: the second term in the expansion was found to agree exactly with the Ginzburg-Landau-Gor'kov (GLG)[9,12] prediction, but the leading term, which is a factor ϵ^{-1} larger than the GLG term, was completely unexpected. Since then, Jacobs[16] has extended this analysis to two more orders in ϵ, and found the NT result to appear in the fourth term, while the third term is again "anomalous" (i.e., not expected from the GLG-NT approach). (In applying the same scheme to study a N-S phase boundary, the author has also reconfirmed these findings in that new geometry.[10]) These results cast some doubt on the validity of perturbative or iterative methods near T_c, thus making the exact relation between the microscopic and the GL theories of superconductivity a puzzle. However, in the works described above, the chosen inhomogeneous states are all too complex to allow an explicit evaluation of the anomalous terms. It is therefore not possible to determine from those works what is the origin of such anomalous terms. The present study was initiated with the intention of throwing some definitive light on this problem. We have chosen to study the gap equation instead of the free energy, because the original relevant works of Gor'kov and NT were based on the gap equation. Indeed, we have succeeded in evaluating *all* contributions to the gap equation essentially exactly, except for the WKBJ approximation employed in solving the BdG equations. But Gor'kov and NT have also assumed an equivalent approximation (the semiclassical approximation) in their relevant works. The approximation, therefore, should not be regarded as a weak point in our rigorous analysis toward resolving the puzzle. Near T_c we have also succeeded in explicitly expanding the gap equation in powers of ϵ, so as to compare with the perturbative result of GLG and NT. Our result reveals, as we shall see in the subsequent sections, that the anomalous terms may be linked directly to the singularities in the space dependence of $\Delta(\vec{r})$, since, using our $\Delta(z)$, which has a slope singularity at $z=0$, we find that $\mathfrak{F}_T(z)-\Delta(z)$ contains not just the regular terms expected from the GLG-NT approach, but also a singular contribution which has an anomalous local magnitude and is localized to within ξ_0 of $z=0$. To confirm that singularities in $\Delta(\vec{r})$ are indeed the cause of the anomalous terms, it is necessary also to study the gap equation for a different choice of $\Delta(\vec{r})$, which has no discontinuity of any sort anywhere, and then to establish that indeed no terms other than those expected from the GLG-NT approach will appear in that case. This task has also been accomplished very recently by D. Chen and the author, and details of it will be reported in a future publication.

This paper will proceed as follows. In Sec. II we review the explicit solutions of the BdG equations in the WKBJ approximation found by Bar-Sagi and Kuper, and point out why their crude argument confirming that the gap equation will reduce to the GLG theory near T_c is invalid. We then proceed to our more rigorous study of the gap equation for a slightly different choice of $\Delta(\vec{r})$, namely, that of a N-S phase boundary as defined early in this section. In Sec. III we find all bound-state solutions ($E_n<\Delta_\infty$) of the BdG equations (1.1) for such a system, and evaluate explicitly their total contribution to $\mathfrak{F}_T$, which we denote as $\mathfrak{F}_B$. In Sec. IV we find all scattering-state solutions to Eq. (1.1). Their total contribution to $\mathfrak{F}_T$, denoted as $\mathfrak{F}_S$, is found to consist of two parts of very different spacial behavior, a direct contribution $\mathfrak{F}_{SD}$ and an interference contribution $\mathfrak{F}_{SI}$. In examining all these terms, it then becomes clear that the integral

$$\int_0^1 (\mathfrak{F}_T-\Delta)\,dX \equiv N(0)g\Delta_\infty \mathcal{J} \tag{1.4}$$

is particularly simple to study for our chosen geometry. [$N(0)=mk_F/2\pi^2$ is the usual normal-state density of states per spin at the Fermi surface.] In Sec. V, therefore, we obtain a natural expansion of the quantity $\mathcal{J}$ defined in Eq. (1.4) in powers of ϵ which can actually be carried out explicitly to *all* orders. It is shown that its bound-state contribution $\mathcal{J}_B$ has only odd powers of ϵ, while its scattering-state contribution $\mathcal{J}_S$ has all integer powers greater than 0. Adding them up to give an expansion for $\mathcal{J}$, we find that *all* odd-power terms cancel out *exactly*, leaving an expansion in $\epsilon^2 \propto 1-T/T_c$. We thus have established that there are no terms of anomalous orders in $\mathcal{J}$ *to all orders*, despite the fact that they do appear in the separate contributions $\mathcal{J}_B$ and $\mathcal{J}_S$. *This points to the caution needed in approximate or numerical studies of an inhomogeneous superconducting state via the Bogoliubov approach, since one might lose such an exact cancellation as a consequence, which can then have particularly severe effects near T_c.* Next we explicitly evaluate the GLG and NT contributions to $\mathcal{J}$ (of order ϵ^2 and ϵ^4, respectively), and find them to agree only in order, but not in magnitude, with the leading two terms in our expansion of $\mathcal{J}$. The result at first seems to suggest some sort of a breakdown of the GLG-NT theories, but we then notice that our Δ is not exactly "slowly varying" everywhere in the sense defined by Gor'kov. Noticing that our Δ has a slope discontinuity at $z=0$, and that the GLG approximation to $\mathfrak{F}_T$ has a term $\propto d^2\Delta/dz^2$, which for our Δ would have a δ-function singularity at $z=0$, we find that the discrepancy in the leading term of $\mathcal{J}$ could be removed if one interprets the integral in Eq. (1.4) to be right from the middle of the δ function when evaluating $\mathcal{J}_{\rm GLG}$. Realizing that such an argument cannot be made rigorous, we then proceed to study the local behavior of $\mathfrak{F}_T$ in Sec. VI. We first develop a mathematical technique to evaluate the sum over states in Eq. (1.2) analytically. Essentially we find that $\sum_n U_n(\vec{r})V_n(\vec{r})^*\delta(E-E_n)$ may be expressed in terms of a function which is analytic in the whole upper half-plane of a complex-energy variable $\tilde{E}$. The bound- and scattering-state contributions to Eq. (1.2) are then combined into a single complex-energy integral just above the real line, which can then be evaluated by closing the contour with a large semicircle in the upper half-plane. Contributions to this integral arise mainly from the poles of the hyperbolic tangent function in Eq. (1.2). Near T_c all of these poles are far above the real line in the scale of $\Delta_\infty(T)$. *This result suggests the true reason why de Gennes can use the Rayleigh-Schrödinger perturbation theory to solve the* BdG *equations near* T_c. Indeed, in a subsequent paper we will show for a smooth $\Delta(\vec{r})$ how the GLG-NT expansion for $\mathfrak{F}_T$ can be obtained near T_c by this method, *without assuming the validity of any iteration or perturbation method.* For our present choice of $\Delta(\vec{r})$, which has a slope discontinuity at $z=0$, we find $\mathfrak{F}_T(z)$ to agree *almost everywhere* with the GLG-NT approach, except near the plane $z=0$, where $\mathfrak{F}_T$ is found to have an additional subseries of "singular" contributions. Near T_c the dominant term in this subseries has the shape of a symmetric cusp, with its peak amplitude being a factor ϵ^{-1} larger than the GLG contribution, but it dies off on both sides essentially exponentially within a distance $\xi_0 \propto \epsilon\xi(T)$. *This contribution is therefore rapidly varying in Gor'kov's criterion, anomalous as judged from its local magnitude, and, when substituted into Eq.* (1.4), *it precisely accounts for the singular contribution needed to explain the discrepancy between the leading term in the quantity* $\mathcal{I}$ *mentioned above and the corresponding* GLG *result.*

These results have led us to a consistent picture about the asymptotic behavior of the superconductive gap equation as T approaches T_c. This conclusion is presented in the Sec. VII, together with a discussion of the possible significance and implications of our findings.

II. WKBJ METHOD AND THE BAR-SAGI–KUPER SOLUTION

In this section we wish to briefly review a recent work by Bar-Sagi and Kuper[7] in which a method was presented to solve the BdG equations analytically in the WKBJ approximation for a semi-infinite superconducting slab. In that work they have also studied the gap equation (1.2) and have shown that their method retrieves the GLG theory near T_c, but we shall point out here why their argument is actually invalid and misleading. We shall then introduce a slightly different inhomogeneous state in order to perform a more rigorous analysis of the gap equation, which we present in the following sections.

The principal assumption for solving Eq. (1.1) in the WKBJ approximation is that the equation admits *special* solutions of the form

$$\begin{pmatrix} U \\ V \end{pmatrix} = \hat{g}\, e^{i\vec{k}_F\cdot\vec{r}} , \qquad (2.1)$$

where $\vec{k}_F$ is a vector on the Fermi surface, and the pseudospinor $\hat{g} \equiv (u, v)^{tr}$ is assumed to vary in a scale $\xi_0 \gg k_F^{-1}$ only, so that we can ignore the second derivative of $\hat{g}$ in Eq. (1.1). Then the equation for $\hat{g}$ is, in the case when $\Delta = \Delta(z)$, $\vec{A} \equiv 0$,

$$E\hat{g}_a(z) = \left(-i\sigma_z a p v_F \frac{d}{dz} + \Delta\sigma_x \right) \hat{g}_a(z) , \qquad (2.2)$$

where $a = \mathrm{sgn}(\vec{k}_F\circ\hat{z})$, $p = |\vec{k}_F\circ\hat{z}|/k_F$, $(\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices, and by putting "a" as the subscript to $\hat{g}$, we have anticipated our later need and have explicitly emphasized the dependence of $\hat{g}$ on a.

Bar-Sagi and Kuper (BK) observed that Eq. (2.2) may be decoupled by the transformation $f_{1,2} = u \pm iv$, in the sense that if one denotes $\hat{f}_a \equiv (f_{1a}, f_{2a})^{tr}$, then Eq. (2.2) may be rewritten

$$E\hat{f}_a = \left(-iapv_F\sigma_x \frac{d}{dz} - \Delta\sigma_y \right) \hat{f}_a . \qquad (2.3)$$

From Eq. (2.3) one can easily deduce

$$E^2\hat{f}_a = \left(-(pv_F)^2 \frac{d^2}{dz^2} + \Delta^2 - apv_F \frac{d\Delta}{dz}\sigma_z \right) \hat{f}_a , \quad (2.4)$$

in which the equations for the two components of $\hat{f}_a$ are decoupled.

When $\Delta(z)$ is given by Eq. (1.3), BK introduced the new variable $X = \tanh(\alpha\Delta_\infty z/v_F)$. Equation (2.4) is then converted to

$$(1-X^2)\frac{d^2\hat{f}_a}{dX^2} - 2X\frac{d\hat{f}_a}{dX} + \left(a\nu(a\nu + \sigma_z) + \frac{\mu^2}{1-x^2} \right) \hat{f}_a = 0 , \qquad (2.5)$$

where $\nu = (\alpha p)^{-1} > 0$, and $\mu = \nu(\Lambda^2-1)^{1/2}$ with $\Lambda = E/\Delta_\infty$. Equation (2.5) is seen to be the equation for the associated Legendre functions[17] $P^{\pm i\mu}_{\pm a\nu}(X)$, where the upper ± sign refers to the two independent solutions of Eq. (2.5), and the lower ± sign refers to the two components of the pseudospinor $\hat{f}_a$.

For $E < \Delta_\infty$ (the "bound" states), it is convenient to put $\mu = i\bar{\mu}$, so that $\bar{\mu} = \nu(1-\Lambda^2)^{1/2} > 0$. Then the solution of Eq. (2.5) (unnormalized) that also satisfies Eq. (2.3) and the boundary condition that $\hat{f}_a \to 0$ as $z \to \infty$ (i.e., $X \to 1$) is[7]

$$\hat{f}_a = N_a \begin{pmatrix} e^{i\pi/4}(1 + a\bar{\mu}/\nu)^{1/2} P^{-\bar{\mu}}_{a\nu}(X) \\ e^{-i\pi/4}(1 - a\bar{\mu}/\nu)^{1/2} P^{-\bar{\mu}}_{-a\nu}(X) \end{pmatrix} . \qquad (2.6)$$

For $E > \Delta_\infty$ (the "scattering" states), μ is real and positive. There are two independent solutions of Eq. (2.3), characterized by $b = \pm$, which were normalized by BK to approach the normalized BCS solutions of a bulk superconductor[7] as $z \to \infty$:

$$\hat{f}^b_a = \Gamma(1 - iab\mu) \begin{pmatrix} e^{ib\phi} P^{iab\mu}_{a\nu}(X) \\ b\, e^{-ib\phi} P^{iab\mu}_{-a\nu}(X) \end{pmatrix} , \qquad (2.7)$$

where $\phi = \frac{1}{2}\tan^{-1}(\nu/\mu) = \frac{1}{2}\tan^{-1}(\Lambda^2-1)^{-1/2}$. In deducing the above, one needs the identity[17]

$$P_\nu^{\pm i\mu}(X) = \frac{1}{\Gamma(1\mp i\mu)}\left(\frac{1+X}{1-X}\right)^{\pm i\mu/2} \times F(-\nu,\ \nu+1,\ 1\mp i\mu,\ \tfrac{1}{2}-\tfrac{1}{2}X) = \Gamma^{-1}(1\mp i\mu)\, e^{\pm iqz} F\ , \tag{2.8}$$

where $q=(E^2-\Delta_\infty^2)^{1/2}/v_F p$. Physically, $b=+(-)$ corresponds to particle (hole)-like excitations, and $ab=+(-)$ implies that the *group* velocity of the elementary excitation has a z component which is positive (negative).

Using the above special solutions of Eq. (2.3), BK constructed all solutions of the BdG equations (1.1) that satisfy the boundary conditions $U=V=0$ at $z=0$. These solutions were then used to evaluate the quantity $\mathfrak{F}_T$ defined in the gap equation (1.2). The solutions were said to correspond to a superconductor filling the half-space $z>0$ with a vacuum or an insulator filling the other half. This identification is questionable because for such a system the equilibrium order parameter would not be given by Eq. (1.3). Rather, it would take the constant value Δ_∞ everywhere except within atomic distances from the surface, where the order parameter should then plunge to zero in some way as $z\to 0$, in order to conform with the boundary condition that[18] $UV^*=0$ at $z=0$. Nevertheless, it is still *mathematically sound* to study the properties of $\mathfrak{F}_T$ under BK's choice of $\Delta(\vec{r})$ in conjunction with their boundary conditions for U and V. This goal has been partly accomplished by BK, as they have calculated $U_n V_n^*$ explicitly for both the bound and the scattering states. They correctly concluded that the bound-state contribution to $\mathfrak{F}_T$ is of the order $\Delta_\infty^2 \propto 1-T/T_c$ for T near T_c, but they incorrectly deduced from this observation that the bound-state contributions are negligible near T_c, since they failed to observe that the GLG contribution to $\mathfrak{F}_T$ is only of the order Δ_∞^3 (*vide infra*). For the scattering states they found

$$UV^* = \Xi_1 + \Xi_2 + \text{O.T.}\ , \tag{2.9}$$

where Ξ_1 is a direct contribution, Ξ_2 is an interference contribution which oscillates in the length scale $\xi(T)$, and O.T. designates a contribution oscillating in the atomic scale which is known to exist near a superconductor-vacuum (or insulator) boundary.[18] They argued that Ξ_2 may be ignored near T_c, but we shall see that this argument is also fallacious. For the term Ξ_1 they obtained an explicit expansion with respect to $\Delta_\infty/(E^2-\Delta_\infty^2)^{1/2}$, which is small only if $E\gg\Delta_\infty$. The leading term of the expansion was found to make the gap equation an identity, while the second term, after summing over all directions of propagation, was found to be proportional to $1-\frac{1}{3}\alpha^2$. This was taken by them as evidence that their solution agrees with the GLG theory near T_c, since Eq. (1.3) with $\alpha=\sqrt{3}$ gives precisely a solution of the GLG equations. However, if their expansion of Ξ_1 ($\cong U_n V_n^*$ according to their argument) is substituted into Eq. (1.2) and is then summed over all scattering states with $E>\Delta_\infty$, then all terms except the leading one will give rise to divergent coefficients. To avoid this difficulty, BK had to consider only those states with $E>\epsilon_{\max}=10\,\Delta_\infty$, and cited their numerical investigation as evidence that the states below $\epsilon_{\max}$ are negligible. This argument, besides being obviously not rigorous, is probably also misleading, in view of the findings that we shall present below, which reveal that the states with energy $\lesssim\Delta_\infty$ will always be important, no matter how close T is to T_c.

Since previous works[10,15,16] have revealed a puzzling relation between the Bogoliubov theory and the GL theory of superconductivity, as we have reviewed in the introduction, and because the recent work of BK has not really clarified the situation, but has in fact created some misconception, it is apparent that a more rigorous study of the self-consistent gap equation is in order. In such a study, only purely analytical methods should be used, and not a single contribution should be ignored without a clear justification. We have precisely accomplished such a task, but only for a slightly modified geometry, namely, the geometry of an "N-S phase boundary" as described in Sec. I. To facilitate normalization of the elementary-excitation wavefunctions and calculation of the density-of-state function, we have also introduced vanishing boundary conditions for U and V at $z=+D$ and $-L$. However, by letting $D\gg L\gg\xi(T)$, we have saved $\mathfrak{F}_T$ from being plagued by terms oscillating in the atomic scale, the presence of which would constitute an *inessential* complication to the gap equation, and which, if present but neglected, would become a weak point of our rigorous analysis. Also, by having a normal region of thickness $L\gg\xi(T)$, we have made the excitation spectrum below the gap Δ_∞ quasicontinuous, which at first appealed to us as being easier to cope with than a discrete spectrum.[19] We thus will study the gap equation in the subsequent sections for this choice of geometry.

III. BOUND-STATE CONTRIBUTION

In this section we determine the bound-state excitation energies and their corresponding wave functions for the "N-S phase boundary" problem as defined in the previous sections, and then evaluate the total bound-state contribution $\mathfrak{F}_B$ to the quantity $\mathfrak{F}_T$ of Eq. (1.2).

Since we have introduced the boundary conditions $U=V=0$ at $z=+D$ and $-L$, and because the system has translational invariance in the x-y directions, we expect the stationary eigensolutions of Eq. (1.1) to be made of the following linear combination of the special solutions discussed in and below Eq. (2.1):

$$\begin{pmatrix} U \\ V \end{pmatrix} = e^{i\vec{k}_{F\perp}\cdot\vec{r}_\perp} \sum_{a=\pm 1} a\hat{g}_a e^{iak_F p(z+L)} . \qquad (3.1)$$

For $z<0$, the most general solution of Eq. (2.2) which makes $U=V=0$ at $z=-L$ is

$$\hat{g}_a = \begin{pmatrix} A\exp[iaE(z+L)/v_F p] \\ B\exp[-iaE(z+L)/v_F p] \end{pmatrix} , \qquad (3.2)$$

where the constants A and B may be taken as real. Since we wish to consider the bound states here, with $\Lambda = E/\Delta_\infty < 1$, we may use Eq. (2.6) to determine $\hat{g}_a \equiv ((f_1+f_2)/2,\ (f_1-f_2)/2i)_a^{tr}$ in the region $z>0$. The two expressions of $\hat{g}_a$, for the respective regions $z \gtrless 0$, can then be matched at $z=0$, giving

$$N_\pm = (\pm i)^n N, \quad A = \tfrac{1}{2}NS_0 = (-1)^n B , \qquad (3.3)$$

$$2E_n L/v_F p + \phi_0 = (n+\tfrac{1}{2})\pi , \qquad (3.4)$$

where n is an integer, $S_0 \equiv S(X=0)$, with

$$S(X) = [(1+\bar{\mu}/\nu)P_\nu^{-\bar{\mu}}(X)^2 + (1-\bar{\mu}/\nu)P_{-\nu}^{-\bar{\mu}}(X)^2]^{1/2} , \qquad (3.5)$$

and

$$\phi_0 = 2\tan^{-1}\frac{(1-\bar{\mu}/\nu)^{1/2}P_{-\nu}^{-\bar{\mu}}(0)}{(1+\bar{\mu}/\nu)^{1/2}P_\nu^{-\bar{\mu}}(0)} . \qquad (3.6)$$

The constant N is determined by normalization, which gives

$$NS_0 = L^{-1/2}[1+O(\xi/L)] . \qquad (3.7)$$

The density of bound states at fixed $\vec{k}_{F\perp}$, hence fixed p, may be obtained by differentiating Eq. (3.4):

$$\rho_p(E) = \frac{2L}{\pi v_F p} + \pi^{-1}\frac{d\phi_0}{dE} , \qquad (3.8)$$

where the first term is the bulk contribution from the N region, and the second term is important only if one wishes to calculate the surface energy of the phase boundary.

We may now evaluate the total bound-state contribution to $\mathfrak{F}_T$, which we shall denote as $\mathfrak{F}_B$. First, we use the stationary eigensolutions to find that for $z \leqslant 0$,

$$\begin{aligned} U_n V_n^* &= (-1)^n (2L)^{-1}\{\cos[2E_n(z+L)/v_F p] \\ &\quad - \cos[2k_F p(z+L)]\} \qquad (3.9a) \\ &= (2L)^{-1}\{\sin[\phi_0(p,E) - 2E_n z/v_F p] \\ &\quad - (-1)^n\cos[2k_F p(z+L)]\} , \qquad (3.9b) \end{aligned}$$

where we have used Eq. (3.4). On the other hand, for $z \geqslant 0$, we obtain

$$\begin{aligned} U_n V_n^* &= (2LS_0^2)^{-1}\{2(1-\bar{\mu}^2/\nu^2)^{1/2} P_\nu^{-\bar{\mu}}(X)P_{-\nu}^{-\bar{\mu}}(X) \\ &\quad - (-1)^n S^2(X)\cos[2k_F p(z+L)]\} , \qquad (3.10) \end{aligned}$$

where $S(X)$ is defined in Eq. (3.5).

Using Eq. (3.9a), and noticing the $(-1)^n$ factor, we conclude that $\mathfrak{F}_B$ vanishes if $z+L \ll L$, i.e., for the region far to the left of the phase boundary. On the other hand, to the immediate left of the phase boundary, where $|z| \ll L$, Eq. (3.9b) is more convenient, giving

$$\begin{aligned} \mathfrak{F}_B &= N(0)g\int_0^1 dp\int_0^{\Delta_\infty} dE \\ &\quad \times \sin\left(\phi_0(p,E) - \frac{2Ez}{v_F p}\right)\tanh\frac{E}{2T} , \qquad (3.11) \end{aligned}$$

where we have used the fact that summing a smooth function of E over all bound states, in the limit $L \gg \xi(T)$, is equivalent to the operation

$$\begin{aligned} &(2\pi)^{-2}\int d^2k_{F\perp}\int_0^{\Delta_\infty} dE\,\rho_p(E)(\cdots) \\ &\cong 2LN(0)\int_0^1 dp\int_0^{\Delta_\infty} dE(\cdots) . \qquad (3.12) \end{aligned}$$

For $z>0$, we substitute Eq. (3.10) into Eq. (1.2), obtaining

$$\begin{aligned} \mathfrak{F}_B &= N(0)g\int_0^1 dp\int_0^{\Delta_\infty} dE\frac{E}{\Delta_\infty}\tanh\frac{E}{2T} \\ &\quad \times[2S_0^{-2}P_\nu^{-\bar{\mu}}(X)P_{-\nu}^{-\bar{\mu}}(X)] . \qquad (3.13) \end{aligned}$$

Equations (3.11) and (3.13), for $z \lesseqgtr 0$, respectively, are the main results of this section.

IV. SCATTERING-STATE CONTRIBUTION

In this section we find all scattering-state solutions of Eq. (1.1) corresponding to $\Lambda = E/\Delta_\infty > 1$, and use them to evaluate the total scattering-state contribution $\mathfrak{F}_S$ to the quantity $\mathfrak{F}_T$ of Eq. (1.2).

Equation (3.1) is still the general form for the wave functions, and Eq. (3.2) is still valid in the region $z<0$. However, for $z>0$, we must in general let

$$\hat{g}_a = N_a(\hat{g}_a^+ e^{-ia\mu\alpha\bar{D}} + iC_a\hat{g}_a^- e^{+ia\mu\alpha\bar{D}}) , \qquad (4.1)$$

where, as before, $\hat{g}_a \equiv (u_a, v_a)^{tr}$, and $\hat{g}_a^\pm$ are related to the $\hat{f}_a^\pm$ of Eq. (2.7) by the transformation $f_{1,2} = u \pm iv$. We have also put $\bar{D} \equiv D\Delta_\infty/v_F$. Substituting this expression into Eq. (3.1), requiring $U=V=0$ at $z=+D$, and using the asymptotic behavior at $z=+D \gg \xi(T)$ that[7]

$$\begin{aligned} g_a^+ &\cong \begin{pmatrix} \cos\phi \\ \sin\phi \end{pmatrix} e^{ia\mu\alpha\bar{D}} , \\ g_a^- &\cong i^{-1}\begin{pmatrix} \sin\phi \\ \cos\phi \end{pmatrix} e^{-ia\mu\alpha\bar{D}} , \end{aligned} \qquad (4.2)$$

one can deduce that $N_\pm = Ne^{ia\gamma}$, $C_\pm = C$, with N, C, and γ being real constants. Furthermore, γ is found to satisfy the relation

$$\exp\{i[\gamma + k_F p(D+L)]\} = 1 . \qquad (4.3)$$

As we have pointed out in our earlier work,[10] it is convenient to allow k_F to have a very slight p dependence [of order $(D+L)^{-1}$]. Then we can let $\gamma = 0$. Next, we may match at $z=0$ our solutions for the regions $z \gtrless 0$, respectively, to obtain

$$\begin{aligned} A e^{i(\mu^2+\nu^2)^{1/2}\alpha\overline{L}} &= \tfrac{1}{2} N e^{\xi_{20}+i\eta_{10}/2} (e^{\eta_{20}/2+i\xi_{10}-i\mu\alpha\overline{D}} \\ &\quad + C e^{-\eta_{20}/2-i\xi_{10}+i\mu\alpha\overline{D}}, \\ B e^{-i(\mu^2+\nu^2)^{1/2}\alpha\overline{L}} &= \tfrac{1}{2} N e^{\xi_{20}-i\eta_{10}/2} (e^{-\eta_{20}/2+i\xi_{10}-i\mu\alpha\overline{D}} \\ &\quad + C e^{\eta_{20}/2-i\xi_{10}+i\mu\alpha\overline{D}}), \end{aligned} \tag{4.4}$$

where $\overline{L} = L\Delta_\infty/v_F$, and ξ_{10}, ξ_{20}, η_{10}, η_{20} are real quantities defined by

$$\begin{pmatrix} \Gamma(1-i\mu)[e^{i\phi}P_\nu^{i\mu}(0) + e^{-i\phi}P_{-\nu}^{i\mu}(0)] \\ i\Gamma(1+i\mu)[e^{-i\phi}P_\nu^{-i\mu}(0) - e^{i\phi}P_{-\nu}^{-i\mu}(0)] \end{pmatrix} \equiv e^{\xi_{20}+i\eta_{10}/2} \begin{pmatrix} e^{\eta_{20}/2+i\xi_{10}} \\ e^{-\eta_{20}/2-i\xi_{10}} \end{pmatrix}. \tag{4.5}$$

Equation (4.4) is nominally identical to Eqs. (2.29a) and (2.29b) of Ref. 10, and can be analyzed accordingly. Multiplying the two equations by $2N^{-1}\exp \times[\mp i(\mu^2+\nu^2)^{1/2}\alpha\overline{L} - \xi_{20}]$ and taking the imaginary part of both sides, one can deduce immediately that $C=\pm 1$, $B=\pm A$ are real constants, and that the respective sets of eigenenergies are determined by

$$\tan(\mu\alpha\overline{D} - \xi_{10}) + \frac{1 \pm e^{-\eta_{20}}}{1 \mp e^{-\eta_{20}}} \tan[(\mu^2+\nu^2)^{1/2}\alpha\overline{L} - \tfrac{1}{2}\eta_{10}] = 0 . \tag{4.6}$$

To proceed further with our rigorous analysis, we shall assume that $D \gg L \gg \xi(T)$. It is then convenient to rewrite Eq. (4.6) in the form:

$$n\pi = \mu\alpha\overline{D} - \xi_{10} + \delta_0 , \tag{4.7}$$

where δ_0 is the arctangent of the second term in Eq. (4.6). Regarding n as a continuous function of E, and differentiating both sides of Eq. (4.7) with respect to E, one obtains the density-of-state function at given $\vec{k}_{F\perp}$ (thus p) and C, for $E > \Delta_\infty$:

$$\rho_p^{(\pm)}(E) = \frac{1}{\pi}\left[\left(\frac{(\mu^2+\nu^2)^{1/2}}{\mu}\frac{D}{v_F p} - \frac{d\xi_{10}}{dE}\right) + Y_\pm(E)\left(\frac{L}{v_F p} - \frac{1}{2}\frac{d\eta_{10}}{dE}\right)\right], \tag{4.8}$$

where

$$Y_\pm(E) = \frac{[(1\pm e^{-\eta_{20}})/(1\mp e^{-\eta_{20}})]\sec^2[(\mu^2+\nu^2)^{1/2}\alpha\overline{L} - \frac{1}{2}\eta_{10}]}{1 + \{[(1\pm e^{-\eta_{20}})/(1\mp e^{-\eta_{20}})]\tan[(\mu^2+\nu^2)^{1/2}\alpha\overline{L} - \frac{1}{2}\eta_{10}]\}^2} \tag{4.9}$$

is a function oscillating in the energy scale $\pi v_F p/L$, which is small in comparison with Δ_∞ owing to our assumption $L \gg \xi(T)$, yet large in comparison with the level spacing $\sim[(E^2-\Delta_\infty^2)/E](\pi v_F p/D)$, since we assumed $D \gg L$. Such oscillations in the density-of-state function for $E > \Delta_\infty$ clearly result from resonances due to repeated scatterings between the matter boundary at $z=-L$ and the phase boundary at $z=0$. They are interference effects first discussed by Rowell and McMillan,[20] and are akin to the Tomasch oscillations observed in tunneling experiments.[21] If one is not interested in the size-quantization effects, one could average $\rho_p^{(\pm)}(E)$ with respect to many periods of such oscillations, and obtain the "smoothed" density-of-state function which is just[22] Eq. (4.8) with $Y_\pm$ replaced by $\langle Y_\pm\rangle_{\rm osc} = 1$. We must, however, proceed further in our rigorous analysis using the exact Eq. (4.8), because the average of a product is not always equal to the product of averages.

Our next step is to determine the normalization constants $N^{(\pm)}$ for the two scattering modes $C=\pm 1$. For $D, L \gg \xi(T)$, we have $\int(|U|^2+|V|^2)d^3r \cong 4N^2D + 4A^2L$; so we must require

$$N^2 = \tfrac{1}{4}[D + (A^2/N^2)L]^{-1} . \tag{4.10}$$

In Appendix A, we show that, for the two modes with $C=\pm 1$,

$$(A^2/N^2)^{(\pm)} = [\mu/(\mu^2+\nu^2)^{1/2}]Y_\pm(E) . \tag{4.11}$$

We thus find, using Eqs. (4.8), (4.10), and (4.11), that

$$[N^2\rho_p(E)]^{(\pm)} = [(\mu^2+\nu^2)^{1/2}/\mu](4\pi v_F p)^{-1} \tag{4.12}$$

is the same for the two scattering modes, while

$$[A^2\rho_p(E)]^{(\pm)} = (4\pi v_F p)^{-1} Y_\pm(E) \tag{4.13}$$

still has a size-quantization oscillation which depends on C.

We are now ready to calculate $\mathfrak{F}_S$. For $z<0$, we first obtain

$$\begin{aligned} (U_n V_n^*)^{(\pm)} = \pm 2[A^{(\pm)}]^2\{&\cos[2(\mu^2+\nu^2)^{1/2}\alpha(\overline{z}+\overline{L})] \\ &- \cos[2k_F p(z+L)]\} , \end{aligned} \tag{4.14}$$

where $\overline{z} \equiv z\Delta_\infty/v_F$. The summation over all scattering states is carried out using the prescription (compare with Eq. (3.12) for the bound-state case)

$$\sum_{E_n > \Delta_\infty}(\cdots) = (2\pi)^{-1}k_F^2\int_0^1 p\,dp \sum_{C=\pm}\int_{\Delta_\infty}^\infty dE\,\rho_p^{(C)}(E)(\cdots). \tag{4.15}$$

The energy integral may be carried out in two steps, the first step being to average out the size-quantization oscillations. For $z+L \ll L$, i.e., in the N region far away from the phase boundary, the quantities in the curly bracket of Eq. (4.14) are slowly varying functions of E. The relevant averaging is simply $\langle (A^{(\pm)})^2 \rho_p^{(\pm)} \rangle_{\rm osc} = (4\pi v_F p)^{-1}$. The $\pm$ sign in front of Eq. (4.14) then shows that the two scattering modes give exactly opposite contributions to $\mathfrak{F}_S$, implying that

$$\mathfrak{F}_S \equiv 0 \quad \text{for } z+L \ll L . \tag{4.16}$$

For $-\xi(T) \lesssim z < 0$, the second term in Eq. (4.14) still makes no contribution. For the first term, the relevant averaging is[22]

$$\langle (A^{(\pm)})^2 \rho_p^{(\pm)} \cos[2(\mu^2+\nu^2)^{1/2}\alpha(\bar{z}+\bar{L})]\rangle_{\rm osc} = \pm (4\pi v_F p)^{-1} e^{-\eta_{20}} \cos(2Ez/v_F p + \eta_{10}) . \tag{4.17}$$

Thus, for $-\xi(T) \lesssim z < 0$, we obtain

$$\mathfrak{F}_S = N(0) g \int_0^1 dp \int_{\Delta_\infty}^{\infty} dE\, e^{-\eta_{20}} \times \cos\left(\frac{2Ez}{v_F p} + \eta_{10}\right) \tanh \frac{E}{2T} . \tag{4.18}$$

For $z>0$, we show in Appendix B that

$$\sum_{C=\pm} \langle (UV^* \rho_p)^{(C)} \rangle_{\rm osc} = (\pi v_F p)^{-1} (1+\nu^2/\mu^2)^{1/2} |\Gamma(1+i\mu)|^2 \times \mathrm{Im}[e^{2i\phi} P_\nu^{i\mu}(X) P_{-\nu}^{-i\mu}(X) + R P_\nu^{i\mu}(X) P_{-\nu}^{i\mu}(X)] , \tag{4.19}$$

where

$$R \equiv \frac{e^{-i\phi} P_\nu^{-i\mu}(0) - e^{i\phi} P_{-\nu}^{-i\mu}(0)}{e^{i\phi} P_\nu^{i\mu}(0) + e^{-i\phi} P_{-\nu}^{i\mu}(0)} . \tag{4.20}$$

We thus find, after using Eq. (4.15), that for $z>0$

$$\mathfrak{F}_S = N(0) g \int_0^1 dp \int_{\Delta_\infty}^{\omega_D} dE \left(1+\frac{\nu^2}{\mu^2}\right)^{1/2} |\Gamma(1+i\mu)|^2 \tanh\frac{E}{2T} \times \mathrm{Im}[e^{2i\phi} P_\nu^{i\mu}(X) P_{-\nu}^{-i\mu}(X) + R P_\nu^{i\mu}(X) P_{-\nu}^{i\mu}(X)] \equiv \mathfrak{F}_{SD} + \mathfrak{F}_{SI} , \tag{4.21}$$

where ω_D is the usual Debye-frequency cutoff. We may identify $\mathfrak{F}_{SD}$ and $\mathfrak{F}_{SI}$ as the "scattering-direct" and the "scattering-interference" contributions. We note that $\mathfrak{F}_{SD}$ is identical to the contribution from the term $(UV^*)_1$ in the work of BK (denoted as Ξ_1 in their second paper),[7] while $\mathfrak{F}_{SI}$ is similar but not identical to their Ξ_2 contribution. We also find no terms oscillating in the atomic scale, contrary to the case studied by BK, owing to our not introducing a matter boundary at or near the phase boundary at $z=0$.

Since our derivation of Eq. (4.21) is mathematically tedious (though conceptually simple), and because the precise form of this equation is crucial to our following analysis, we have presented in Appendix C an alternate derivation, based on a theorem in quantum scattering theory that a complete set of "outgoing" scattering solutions[23] of a Schrödinger equation, if normalized according to their incident parts, form a complete orthonormal set of basic states, if to them are also added all normalized bound-state solutions. This method was also used by BK for discussing the scattering contributions to $\mathfrak{F}_T$ in their superconductor-vacuum geometry. It is actually a simpler method for obtaining, e.g., our Eq. (4.21), but because our first method has more potential usefulness for studying, e.g., finite-L or -D effects, we have therefore chosen to elaborate our first method here with details, and only outline the alternative method in an appendix to ensure the readers that Eq. (4.21) is correct.

Equations (4.18) and (4.21) are the main results of the present section.

V. ANALYSIS OF A SPECIAL SPACE INTEGRAL OF THE GAP EQUATION NEAR T_c

We return to Eq. (3.13). In Appendix D it is shown that

$$S_0^2 = 2 \int_0^1 P_\nu^{-\bar{\mu}}(X) P_{-\nu}^{-\bar{\mu}}(X)\, dX , \tag{5.1}$$

where S_0 is defined directly above Eq. (3.5). Now Eq. (3.13), taken together with this identity, implies immediately that

$$\mathcal{I}_B \equiv [N(0) g \Delta_\infty]^{-1} \int_0^1 \mathfrak{F}_B\, dX = \int_0^1 \Lambda \tanh \epsilon\Lambda\, d\Lambda = \tfrac{1}{3}\epsilon - \tfrac{1}{15}\epsilon^3 + \tfrac{2}{105}\epsilon^5 + \cdots , \tag{5.2}$$

where $\epsilon \equiv \Delta_\infty / 2T$. This observation suggests that the quantity $\mathcal{I}$, defined in Eq. (1.4), may be particularly simple to study for our chosen geometry. To do so, we proceed to study the scattering-state contribution to $\mathcal{I}$, namely,

$$\mathcal{I}_S \equiv [N(0) g \Delta_\infty]^{-1} \int_0^1 (\mathfrak{F}_S - \Delta)\, dX , \tag{5.3}$$

where $\mathfrak{F}_S$ in the region $0<X<1$ is given by Eq. (4.21). In Appendix D, we have indicated how we have derived the following identities:

$$\int_0^1 P_\nu^{i\mu}(X) P_{-\nu}^{-i\mu}(X)\, dX = \frac{-i\mu}{\nu |\Gamma(1+i\mu)|^2} + \frac{1}{2}\left(1+\frac{i\mu}{\nu}\right)[|P_\nu^{i\mu}(0)|^2 + |P_{-\nu}^{i\mu}(0)|^2] , \tag{5.4}$$

$$\int_0^1 P_\nu^{i\mu}(X)P_{-\nu}^{i\mu}(X)\,dX$$

$$= -\tfrac{1}{2}i\left(1+\frac{\mu^2}{\nu^2}\right)^{1/2}\left[e^{2i\phi}P_\nu^{i\mu}(0)^2 - e^{-2i\phi}P_{-\nu}^{i\mu}(0)^2\right], \quad (5.5)$$

where for $e^{2i\phi}$ one is reminded of Eq. (A5) of Appendix A.

Combining these identities with the definition of R in Eq. (4.20), we obtain the following simple result:

$$\int_0^1 dX\,\mathrm{Im}[e^{2i\phi}P_\nu^{i\mu}(X)P_{-\nu}^{-i\mu}(X) + RP_\nu^{i\mu}(X)P_{-\nu}^{i\mu}(X)]$$

$$= \frac{\mu}{\nu}\left(1 - \frac{\mu}{(\mu^2+\nu^2)^{1/2}}\right)\frac{1}{|\Gamma(1+i\mu)|^2}, \quad (5.6)$$

where Eq. (A4) of Appendix A has been used.

Substituting Eq. (4.21) into Eq. (5.3), and using Eq. (5.6), we obtain

$$\mathfrak{F}_S = \int_1^\infty d\Lambda[\Lambda - (\Lambda^2-1)^{1/2} - \tfrac{1}{2}(\Lambda^2-1)^{-1/2}]\tanh\epsilon\Lambda, \quad (5.7)$$

where the last term arises from the Δ term in Eq. (5.3), after using the equilibrium gap equation[1]:

$$[N(0)g]^{-1} = \int_1^{\omega_D/\Delta_\infty} d\Lambda\,(\Lambda^2-1)^{-1/2}\tanh\epsilon\Lambda. \quad (5.8)$$

[The upper limit of the Λ integral in Eq. (5.7) has been put as infinity instead of the cutoff ω_D/Δ_∞, because the integral is now convergent.] The expansion of Eq. (5.7) with respect to ϵ for $T \gtrsim T_c$ can perhaps be done in a number of ways, but one systematic method is to use a formula previously derived by the author [see Appendix B of Ref. 10]. We give below the result only:

$$\mathcal{J}_S = -\tfrac{1}{3}\epsilon + [7\zeta(3)/8\pi^2]\epsilon^2 + \tfrac{1}{15}\epsilon^3 - [31\zeta(5)/8\pi^4]\epsilon^4 - \tfrac{2}{105}\epsilon^5 + [1905\zeta(7)/128\pi^6]\epsilon^6 + \cdots. \quad (5.9)$$

Adding up Eqs. (5.2) and (5.9), we obtain the expansion of $\mathcal{J}$ as defined in Eq. (1.4):

$$\mathcal{J} = \frac{7\zeta(3)}{8\pi^2}\epsilon^2 - \frac{31\zeta(5)}{8\pi^4}\epsilon^4 + \frac{1905\zeta(7)}{128\pi^6}\epsilon^6 + \cdots, \quad (5.10)$$

which contains no odd-power terms to all orders. We now show that the odd orders are precisely the anomalous orders unexpected from the GLG-NT approach. In Gor'kov's derivation of the GL equation,[12] he gives the following approximate expression for $\mathfrak{F}_T - \Delta$:

$$(\mathfrak{F}_T - \Delta)_{\mathrm{GLG}}$$

$$= N(0)g\left(\ln\frac{T_c}{T}\Delta + \frac{7}{48}\frac{\zeta(3)v_F^2}{(\pi T)^2}(\vec{\nabla} - 2ie\vec{A})^2\Delta - \frac{7\zeta(3)}{8(\pi T)^2}|\Delta|^2\Delta\right). \quad (5.11)$$

If Eq. (1.3) and $A \equiv 0$ are substituted into this expression, and if the lower limit of the X integral in Eq. (1.4) is interpreted as being 0_+, then one finds

$$\mathcal{J}_{\mathrm{GLG}} = (7\zeta(3)/8\pi^2)(1 - \tfrac{1}{3}\alpha^2)\epsilon^2, \quad (5.12)$$

which agrees with the leading term in Eq. (5.10) only in the power of ϵ, but not quite in the front coefficient. To understand the discrepancy, we note that Eq. (5.11) contains a term $d^2\Delta/dz^2$. It therefore contains a δ-function singularity at $z=0$ for our choice of Δ, which is Eq. (1.3) times a unit step function. If we interpret the lower limit of integration in Eq. (1.4) as being right from the *middle* of this singularity, one would obtain an extra contribution to Eq. (5.12):

$$\mathcal{J}_{\mathrm{singular}} = \frac{1}{2}\frac{7\zeta(3)v_F^2}{48(\pi T)^2\Delta_\infty}\int_{0_-}^{0_+}\frac{d^2\Delta}{dz^2}\left(\frac{\alpha\Delta_\infty}{v_F}\right)dz$$

$$= \frac{7\zeta(3)}{8\pi^2}\frac{\alpha^2}{3}\epsilon^2, \quad (5.13)$$

which precisely accounts for the difference between Eq. (5.12) and the first term in Eq. (5.10).

Equation (5.11) has been extended to the next order in $1 - T/T_c \sim \epsilon^2$ by NT.[13] The corresponding contribution to $\mathcal{J}$ has also been evaluated by us, assuming again that the integration in Eq. (1.4) is from 0_+ up:

$$\mathcal{J}_{\mathrm{NT}} = -(31\zeta(5)/8\pi^4)(1 - \tfrac{1}{5}\alpha^4)\epsilon^4. \quad (5.14)$$

It is seen to have the same power in ϵ as the second term in Eq. (5.10), but differs again in the front coefficient. The discrepancy must again be due to some singular contributions, resulting from the slope-discontinuity of our Δ at $z=0$. But a similar quantitative account of the discrepancy, as we have done above for the lowest-order term, is now difficult, because the NT expression for $\mathfrak{F}_T - \Delta$ contains the fourth derivative of Δ, which is highly ill-defined for our choice of $\Delta(\vec{r})$ at $z=0$.

We conclude this section with the following statements: (i) With respect to the quantity $\mathcal{J}$ studied in this section, any contribution proportional to an odd power of ϵ must be termed anomalous, since they are not obtained in the GLG-NT approach. (ii) Our essentially exact calculation of $\mathcal{J}$ reveals that no such anomalous-order terms exist to *all* orders, although they *do* appear in the separate bound-state and scattering-state contributions. (iii) The leading two terms in the expansion of $\mathcal{J}$ with respect to ϵ are of orders ϵ^2 and ϵ^4, respectively. They have the same powers in ϵ as, but disagree in magnitude with, the GLG and NT contributions. (iv) The discrepancy with GLG-NT results is found to be due to singular contributions resulting from the slope discontinuity at $z=0$ in our chosen form for the gap function. (v) In order to trace out the exact nature of such singular contributions, we proceed to study the *local* behavior of $\mathfrak{F}_T$ in the next section.

VI. LOCAL ANALYSIS OF THE GAP EQUATION NEAR T_c

We turn to examine the local behavior of $\mathfrak{F}_T = \mathfrak{F}_B + \mathfrak{F}_S$ near T_c. To explain our method for evaluating $\mathfrak{F}_T$ locally, it is convenient to define a function $\sigma(\vec{r}, E)$ such that

$$\mathfrak{F}_T(\vec{r}) = N(0)g\int_0^{\omega_D} \sigma(\vec{r}, E)\tanh\frac{E}{2T}\,dE\,. \qquad (6.1)$$

Comparing this expression with Eq. (1.2), we obtain

$$\sigma(\vec{r}, E) = [N(0)]^{-1}\sum_{E_n>0} U_n(\vec{r})V_n(\vec{r})\delta(E-E_n)\,. \qquad (6.2)$$

It thus may be identified as the spectral weight function for the Gor'kov's function[2] $F(\vec{r}, \vec{r})$. We then note that if we could decompose $\sigma(\vec{r}, E)$ into the form

$$\sigma(\vec{r}, E \geq 0) = \Sigma(\vec{r}, E+i\epsilon) - \Sigma(\vec{r}, -E+i\epsilon)\,, \qquad (6.3)$$

such that $\Sigma(\vec{r}, \tilde{E})$ is an *analytic function in the whole upper half-plane of the complex-energy variable* $\tilde{E}$, then we could evaluate

$$\mathfrak{F}_T = N(0)g\int_{-\omega_D+i\epsilon}^{\omega_D+i\epsilon} \Sigma(\vec{r}, \tilde{E})\tanh\frac{\tilde{E}}{2T}\,d\tilde{E} \qquad (6.4)$$

by closing up the contour with a large semicircle in the upper half-plane of radius ω_D. One would then obtain $\mathfrak{F}_T$ as the sum of the residue contributions from the poles of the hyperbolic tangent function in the upper half-plane, minus possibly the line integral along the large semicircle, should it not be negligible.

To see that this way of evaluating $\mathfrak{F}_T$ is indeed possible, we first look into the region $z<0$, for which $\mathfrak{F}_B$ and $\mathfrak{F}_S$ are given by Eqs. (3.11) and (4.18), respectively. [The relatively simple forms of these two equations make them especially suitable for illustrating the present method.] By comparing Eq. (6.1) with these two equations, we first obtain

$$\sigma(z\leq 0, E) = \begin{cases} \operatorname{Im}\int_0^1 dp\exp[-i(2Ez/v_Fp)+i\phi_0] & (\text{if } E<\Delta_\infty) \\ \operatorname{Im}\int_0^1 dp\exp[-i(2Ez/v_Fp)+i(\pi/2-\eta_{10})-\eta_{20}] & (\text{if } E>\Delta_\infty)\,, \end{cases} \qquad (6.5)$$

where ϕ_0 is given by Eq. (3.6), while η_{10} and η_{20} are defined in Eq. (4.5). It is then not difficult to verify that Eq. (6.3) and the analyticity requirement for Σ are both satisfied, if one takes

$$\Sigma(z\leq 0, \tilde{E}) = (2i)^{-1}\int_0^1 dp\exp\left(-i\frac{2\tilde{E}z}{v_Fp}\right)\Phi(\tilde{\lambda})\,, \qquad (6.6)$$

where

$$\Phi(\tilde{\lambda}) \equiv \frac{(1+\tilde{\mu}/\nu)P_\nu^{-\tilde{\mu}}(0) + i\tilde{\lambda}P_{-\nu}^{-\tilde{\mu}}(0)}{(1+\tilde{\mu}/\nu)P_\nu^{-\tilde{\mu}}(0) - i\tilde{\lambda}P_{-\nu}^{-\tilde{\mu}}(0)}\quad . \qquad (6.7)$$

In Eq. (6.7), $\tilde{\lambda}\equiv\tilde{E}/\Delta_\infty$, and $\tilde{\mu}\equiv\nu(1-\tilde{\lambda}^2)^{1/2}$ is the analytic function in the upper half-plane which reduces to $i\mu$, $\overline{\mu}$, and $-i\mu$, respectively, when $\tilde{E}$ approaches the segments $(-\infty, -\Delta_\infty)$, $(-\Delta_\infty, \Delta_\infty)$, and (Δ_∞, ∞) of the real line from above. Substituting Eq. (6.6) into Eq. (6.4), and realizing that the value of Σ is negligibly small as $|\tilde{E}|\to\omega_D$ in the upper half-plane for any $z\leq 0$, we obtain from the contour integration

$$\mathfrak{F}_T(z\leq 0) = 2\pi TN(0)g\sum_{n=0}^{\infty}\int_0^1 dp \times\exp\left(\frac{(2n+1)2\pi T}{v_Fp}z\right)\Phi\left(i\frac{(2n+1)\pi T}{\Delta_\infty}\right)\,. \qquad (6.8)$$

For $T\sim T_c$, $\epsilon\equiv\Delta_\infty/2T$ is small. Using Eqs. (6.7) and (A6), we can show that

$$\Phi(i\tau) = (4\nu\tau^2)^{-1}[1+O(\tau^{-2})] \quad \text{for real } \tau\gg 1. \qquad (6.9)$$

We thus find near T_c

$$\mathfrak{F}_T(z\leq 0) = N(0)g\Delta_\infty\left[\frac{\alpha\epsilon}{\pi}\int_0^1 p\,dp\sum_{n=0}^{\infty}(2n+1)^{-2} \times\exp\left((2n+1)\frac{2\pi Tz}{v_Fp}\right) + O(\epsilon^{-3})\right]\,. \qquad (6.10)$$

In particular, we find to leading order in ϵ:

(i)

$$\mathfrak{F}_T(0) = N(0)g\Delta_\infty(\pi\alpha\epsilon/16)\,, \qquad (6.11a)$$

(ii)

$$[d^n\mathfrak{F}_T(z)/dz^n]_{z\to 0^-} = \infty \quad \text{for all positive integers } n\,, \qquad (6.11b)$$

(iii)

$$\int_{-\infty}^{0}\frac{\mathfrak{F}_T(z)\,dz}{\mathfrak{F}_T(0)} = 7\zeta(3)v_F/3\pi^3T \cong 0.501\,\xi_0\,. \qquad (6.11c)$$

Because $\Delta(z)$ has been chosen to vanish identically in the region $z\leq 0$, what we have found for $\mathfrak{F}_T(z)$ is also true for $(\mathfrak{F}_T-\Delta)(z)$ in this region.

Next we consider the region $z>0$, for which $\mathfrak{F}_B$ and $\mathfrak{F}_S$ are given by Eqs. (3.13) and (4.21), respectively. Comparing these equations with Eq. (6.1), we obtain

$$\sigma(z \geqslant 0, E) = \begin{cases} \int_0^1 dp \frac{2E''}{\Delta_\infty} S_0^{-2} P_\nu^{-\tilde{\mu}}(X) P_{-\nu}^{-\tilde{\mu}}(X) & (\text{if } E < \Delta_\infty) \\ \int_0^1 dp \left(1 + \frac{\nu^2}{\mu^2}\right)^{1/2} |\Gamma(1+i\mu)|^2 \,\mathrm{Im}\{e^{2i\phi} P_\nu^{i\mu}(X) P_{-\nu}^{-i\mu}(X) + R P_\nu^{i\mu}(X) P_{-\nu}^{i\mu}(X)\} & (\text{if } E > \Delta_\infty)\,, \end{cases} \tag{6.12}$$

where S_0^{-2} is given by Eq. (5.1), $e^{2i\phi} = (\mu + i\nu)/(\mu^2 + \nu^2)^{1/2}$ as before, and R is given by Eq. (4.20). With a little effort, it can then be verified that Eq. (6.3) and the analyticity requirement for Σ are both satisfied if one takes

$$\Sigma(z \geqslant 0, \tilde{E}) = \int_0^1 dp \frac{\nu}{2i\tilde{\mu}} \Gamma(1+\tilde{\mu})\Gamma(1-\tilde{\mu}) \Bigg[\left(1 + \frac{\tilde{\mu}}{\nu}\right) P_\nu^{-\tilde{\mu}}(X) P_{-\nu}^{\tilde{\mu}}(X) + i\tilde{\lambda} \frac{(1+\tilde{\mu}/\nu) P_{-\nu}^{\tilde{\mu}}(0) + i\tilde{\lambda} P_\nu^{\tilde{\mu}}(0)}{(1+\tilde{\mu}/\nu) P_\nu^{-\tilde{\mu}}(0) - i\tilde{\lambda} P_{-\nu}^{-\tilde{\mu}}(0)} P_\nu^{-\tilde{\mu}}(X) P_{-\nu}^{-\tilde{\mu}}(X) \Bigg] . \tag{6.13}$$

It is interesting to note that the first term in this equation, when substituted into Eq. (6.4), gives only the scattering-direct contribution, while the second term in Eq. (6.13) gives the sum of the bound-state and scattering-interference contributions. We also note that $\Gamma(1-\tilde{\mu})$ has poles in the upper half-plane at $\tilde{\lambda} = i(n^2/\nu^2 - 1)$, where n is any integer $> \nu$, but these poles are removable ones in Σ, because the combination in the square brackets of Eq. (6.13) vanishes at these points, although the separate terms do not vanish there.

For large $|\tilde{\lambda}|$, it may be shown with Eq. (2.8) that the second term in Eq. (6.13) is negligibly small but the first term leads to the following asymptotic behavior:

$$\Sigma(z \geqslant 0, \tilde{E}) \to \int_0^1 dp \frac{\nu}{2i\tilde{\mu}} \left[\frac{\tilde{\mu}}{\nu} + X + O\left(\frac{\nu}{\tilde{\mu}}\right) \right] . \tag{6.14}$$

The contribution to $\mathfrak{F}_T$ from the large semicircle of radius ω_D therefore does not vanish in this case. However, instead of trying to evaluate this contribution, we shall subtract the following from both sides of Eq. (6.4):

$$\Delta(z) = N(0) g \Delta_\infty \int_{-\omega_D + i\epsilon}^{\omega_D + i\epsilon} d\tilde{E} \int_0^1 dp \frac{\nu}{2i\tilde{\mu}} \left(\frac{\tilde{\mu}}{\nu} + X\right) \times \tanh \frac{\tilde{E}}{2T} , \tag{6.15}$$

which is nothing but a slight variation of Eq. (5.8). We then obtain, after using Eq. (2.8), that for $z \geqslant 0$

$$\mathfrak{F}_T - \Delta = 2\pi T N(0) g \sum_{n=0}^{\infty} \int_0^1 dp \frac{\nu}{\tilde{\mu}_n} [\Omega_1(\tilde{\lambda}_n) + \Omega_2(\tilde{\lambda}_n)] , \tag{6.16}$$

where

$$\tilde{\lambda}_n = i(2n+1)\pi T/\Delta_\infty , \quad \tilde{\mu}_n = \nu(1 - \tilde{\lambda}_n^2)^{1/2} ,$$
$$\Omega_1(\tilde{\lambda}) = (1+\tilde{\mu}/\nu) F(-\nu, 1+\nu, 1+\tilde{\mu}, \tfrac{1}{2} - \tfrac{1}{2}X) F(\nu, 1-\nu, 1-\tilde{\mu}, \tfrac{1}{2} - \tfrac{1}{2}X) - (\tilde{\mu}/\nu + X) , \tag{6.17}$$

and

$$\Omega_2(\tilde{\lambda}) = i\tilde{\lambda} \frac{(1+\tilde{\mu}/\nu) F(\nu, 1-\nu, 1-\tilde{\mu}, \tfrac{1}{2}) + i\tilde{\lambda} F(-\nu, 1+\nu, 1-\tilde{\mu}, \tfrac{1}{2})}{(1+\tilde{\mu}/\nu) F(-\nu, 1+\nu, 1+\tilde{\mu}, \tfrac{1}{2}) - i\tilde{\lambda} F(\nu, 1-\nu, 1+\tilde{\mu}, \tfrac{1}{2})} \times \left(\frac{1+X}{1-X}\right)^{-\tilde{\mu}} F(-\nu, 1+\nu, 1+\tilde{\mu}, \tfrac{1}{2} - \tfrac{1}{2}X) F(\nu, 1-\nu, 1+\tilde{\mu}, \tfrac{1}{2} - \tfrac{1}{2}X) . \tag{6.18}$$

For a reason that will soon become clear, we shall call the Ω_1 part the "regular" contribution, and the Ω_2 part the "singular" contribution. Near T_c, we can expand Ω_1 and Ω_2 with respect to $\lambda_n^{-1} = -i|\lambda_n|^{-1}$ by employing the series expansion form for the hypergeometric function:

$$F(a, b, c, z) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{z^n}{n!} , \tag{6.19}$$

where $(a)_n = a(a+1) \cdots (a+n-1)$. To leading order, the result is

$$\Omega_1(\tilde{\lambda}_n) = \tfrac{1}{2}(1 - \nu^{-2}) |\tilde{\lambda}_n|^{-2} X (1 - X^2) + O(|\tilde{\lambda}_n|^{-4}) , \tag{6.20}$$

$$\Omega_2(\tilde{\lambda}_n) = (4\nu |\tilde{\lambda}_n|)^{-1} + O(|\tilde{\lambda}_n|^{-3}) . \tag{6.21}$$

Substituting these expressions into Eq. (6.16), we obtain an expansion of $\mathfrak{F}_T - \Delta$ in powers of ϵ for the region $z \geqslant 0$, made of a regular series due to Ω_1, and a singular series due to Ω_2:

$$(\mathfrak{F}_T - \Delta)_{\text{regular}} = N(0) g \Delta_\infty \{[7\zeta(3)/2\pi^2] \epsilon^2 (1 - \tfrac{1}{3}\alpha^2) X (1 - X^2) + O(\epsilon^4)\} , \tag{6.22}$$

$$(\mathfrak{F}_T - \Delta)_{\text{singular}} = N(0)g\Delta_\infty\left(\frac{\alpha\epsilon}{\pi}\int_0^1 p\,dp\sum_{n=0}^{\infty}(2n+1)^{-2} \times \exp\left(-(2n+1)\frac{2\pi Tz}{v_F p}\right) + O(\epsilon^3)\right). \qquad (6.23)$$

In Eq. (6.22), the leading term is just the GLG contribution, as may be shown by substituting our $\Delta(\vec{r})$ into Eq. (5.12). If the next-order term is also evaluated, one can expect an agreement with the NT theory, as the order of the error already suggests. On the other hand, the leading term in Eq. (6.23) may be combined with Eq. (6.10) to give a symmetric function of z which is localized within a distance ξ_0 about $z=0$. Its peak magnitude, as may be seen from Eq. (6.11a), is bigger than the GLG term by a factor ϵ^{-1}. All terms in Eq. (6.23) are clearly "anomalous" in the sense discussed in the introduction. If one substitutes Eqs. (6.22) and (6.23) into Eq. (1.4) to evaluate the quantity $\mathfrak{J}$ defined there, one finds that Eq. (6.22) leads exactly to Eq. (5.12), while Eq. (6.23) exactly accounts for the difference between the leading terms in Eq. (5.10) and Eq. (5.12). The leading regular and singular contributions to $\mathfrak{J}$ are now of the same order in ϵ owing to the "rapidly varying"[12] nature of the singular terms. We thus have obtained a completely consistent picture about the asymptotic behavior of the gap equation as $T\to T_c$ which is discussed in the following section together with other conclusions.

VII. CONCLUSIONS

From our present rigorous study of the gap equation $\Delta = \mathfrak{F}_T[\Delta]$ for an inhomogeneous superconducting state near T_c, we can draw the following conclusions:

(a) The present work has demonstrated explicitly that the low-lying eigensolutions of the BdG equations (with $E \lesssim \Delta_\infty$) can play a decisive role in shaping the spatial dependence of $\mathfrak{F}_T$, and thereby determining whether a given Δ is a self-consistent one, even at temperatures T very close to T_c when Δ_∞ is small. In particular, we find that it is not permissible in general to neglect the bound-state contributions and the quasiparticle-quasihole interference part of the scattering-state contributions when evaluating $\mathfrak{F}_T$ near T_c, contrary to what one might attempt to assume, as has been done recently by BK.[7]

(b) In general, $\mathfrak{F}_T - \Delta$ is made of a bound-state contribution, a scattering-direct contribution, and a scattering-interference contribution. However, we find it useful to regroup $\mathfrak{F}_T - \Delta$ into a regular contribution and a singular contribution. This decomposition comes about naturally after we introduce a contour-integration technique for evaluating $\mathfrak{F}_T - \Delta$. Then the regular contribution arises solely from the scattering-direct part, and the singular contribution arises from the bound-state-plus-scattering-interference part, *after* realizing a cancellation between the former and the latter of the effects due to a series of unphysical poles in the two parts [i.e., the poles due to the factor $\Gamma(1-\tilde{\mu})$, as discussed following Eq. (6.13)]. At finite T, the regular contribution will vary only in the scale of $\xi(T)$, thus it is "slowly varying" near T_c, in terms of Gor'kov's nomenclature.[12] On the other hand, the singular contribution will vary in the scale ξ_0 (and possibly k_F^{-1} also) at all T; so it is "rapidly varying" according to Gor'kov. For a $\Delta(z)$ which is slowly varying everywhere except at $z=0$, where it has a slope discontinuity, we find that the leading regular terms reproduce exactly the GLG-NT results near T_c, while the singular contribution is anomalous in the sense that it contains terms of local magnitudes, which is proportional to powers of Δ_∞ unexpected from the GLG-NT approach.

(c) In this work, the singular (or anomalous) contribution is found to be closely tied to singularities in the spatial dependence of $\Delta(\vec{r})$, and indeed in a subsequent paper we shall show that for a Δ which is everywhere slowly varying, only the regular contribution is obtained. However, $\Delta(\vec{r})$ is only one coefficient in the BdG equations, and it should be very plausible that a singular contribution to $\mathfrak{F}_T - \Delta$ can also arise from other sources of singularities in the BdG equations. In particular, we suggest that a singular contribution will possibly appear in the following situations; so the truly self-consistent $\Delta(\vec{r})$ must contain a rapidly varying part near T_c in order to compensate for that singular contribution, so that $\mathfrak{F}_T - \Delta$ can vanish identically everywhere. (i) Near a superconductor-vacuum (or insulator) boundary, either when a finite magnetic field is applied parallel to the surface, or for any Δ with a nonvanishing odd-order normal derivative at the boundary (after one has smoothed out any oscillation of Δ in the scale of k_F^{-1}). We have envisioned these conditions on the basis of our earlier study[24] of the linearized gap equation which indicates that a specular boundary may be equivalently taken into account by extending Δ into an even function, and the parallel magnetic field an odd function, across the boundary. (See, in particular, Eq. (28) of Ref. 24.) Indeed, in our previous study of the surface-nucleation critical field H_{c3} near T_c,[25] we already found that Δ contains rapidly varying terms near the boundary surface for T just outside the GL region. Now, the configuration considered by BK[7] has $d\Delta/dz \neq 0$ at a sample boundary located at $z=0$. In view of the complex bound-state and scattering-interference contributions obtained by them which they did not analyze carefully near

T_c, we feel that their conclusion of a retrieval of GL theory near T_c is at least premature if not fallacious. (ii) Near a discontinuity of any normal metal property such as a proximity boundary or even an impurity site. (iii) Near a vortex core where the Bogoliubov excitations see a centrifugal potential barrier which diverges at the vortex axis. [See, e.g., Ref. 14, Eq. (4.4).]

We are much less sure whether a centrifugal singularity is sufficient to bring about a singular contribution to $\mathfrak{F}_T - \Delta$, especially in view of the fact even Bogoliubov excitations in the Meissner state would see such a singularity if studied in cylindrical coordinates. However, if a singular contribution does exist near a vortex core, it would mean that the anomalous terms found by Cleary[15] in the free energy of an isolated vortex line near T_c are genuine, and their effect would be to modify the order parameter $\Delta(\vec{r})$ within a radius ξ_0 from the vortex axis, in a way not obtainable from the GLG-NT approach.

It is clearly desirable to study this last case further with the new insight about the "anomalous terms" obtained in this work.

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APPENDIX A

To prove Eq. (4.11), we first obtain from Eq. (4.4), together with $C=\pm 1$, $B=\pm A$, that

$$(A^2/N^2)^{(\pm)} = \tfrac{1}{4} e^{2\xi_{20}}[(e^{\eta_{20}/2} \pm e^{-\eta_{20}/2})^2 \cos^2(\xi_{10} - \mu\alpha\bar{D}) + (e^{\eta_{20}/2} \mp e^{-\eta_{20}/2})^2 \sin^2(\xi_{10} - \mu\alpha\bar{D})] \ . \tag{A1}$$

Using Eq. (4.6) to eliminate the trigonometric functions of $\xi_{10} - \mu\alpha\bar{D}$, we obtain a smooth function of E in the scale of level spacings:

$$(A^2/N^2)^{(\pm)} = \tfrac{1}{2} e^{2\xi_{20}} \sinh\eta_{20} Y_\pm(E) \ , \tag{A2}$$

where $Y_\pm(E)$ is given by Eq. (4.9). Comparing it with the desired result Eq. (4.11), we see that we now need only prove

$$\tfrac{1}{2} e^{2\xi_{20}} \sinh\eta_{20} = \mu/(\mu^2 + \nu^2)^{1/2} \ . \tag{A3}$$

In view of the definition of ξ_{20} and η_{20} in Eq. (4.5), it is equivalent to prove that

$$e^{2i\phi} P_\nu^{i\mu}(0) P_{-\nu}^{-i\mu}(0) + \text{c.c.} = [2\mu/(\mu^2+\nu^2)^{1/2}] \,|\Gamma(1+i\mu)|^{-2} \ , \tag{A4}$$

which may be varified directly by using

$$e^{2i\phi} = (\mu + i\nu)/(\mu^2+\nu^2)^{1/2} \tag{A5}$$

[which follows from the definition of ϕ just below Eq. (2.7)], and

$$P_\nu^\mu(0) = 2^\mu \pi^{1/2}/\Gamma(1 - \tfrac{1}{2}\mu + \tfrac{1}{2}\nu)\Gamma(\tfrac{1}{2} - \tfrac{1}{2}\mu - \tfrac{1}{2}\nu) \tag{A6}$$

[see Ref. 17, Eq. (8.6.1)], together with the properties of the Γ function, such as Ref. 17, Eqs. (6.1.17) and (6.1.31).

APPENDIX B

To derive Eq. (4.19), the first step is to obtain straightforwardly from the scattering solutions in the region $z \geq 0$ that

$$(U_n V_n^*)^{(\pm)} = 2N^{(\pm)2}((|\Gamma_+|^2 \mathrm{Im}\, e^{2i\phi} P_+^+ P_-^- \pm \mathrm{Re}\, e^{-2i\mu\alpha\bar{D}} \Gamma_-^2 P_+^+ P_-^+) + \tfrac{1}{2}\cos[2k_F p(z+L)]\{\mathrm{Im}\, e^{-2i\mu\alpha\bar{D}} \Gamma_-^2 [e^{2i\phi}(P_+^+)^2 - e^{-2i\phi}(P_-^+)^2] \pm |\Gamma_+|^2 (|P_+^+|^2 + |P_-^+|^2)\}) \ , \tag{B1}$$

where we have introduced the shorthand $\Gamma_\pm \equiv \Gamma(1 \pm i\mu)$, and $P_\pm^\pm \equiv P_{\pm\nu}^{\pm i\mu}(X)$. The parenthesized superscript ($\pm$) still stands for the two scattering modes with $C = \pm$.

The next step is to eliminate the explicit $\bar{D}$ dependence, via Eq. (4.6), in order to obtain a smooth function of E in the scale of level spacings (for $z \ll D$). For this purpose we rewrite Eq. (4.6) as

$$e^{-2i(\mu\alpha\bar{D} - \xi_{10})} = 2\{1 - i[(1 \pm e^{-\eta_{20}})/(1 \mp e^{-\eta_{20}})] \times \tan[(\mu^2+\nu^2)^{1/2}\alpha\bar{L} - \tfrac{1}{2}\eta_{10}]\}^{-1} - 1 \ , \tag{B2}$$

which still exhibits a size-quantization oscillation. We then note from Eq. (4.12) that $[N^2\rho_p(E)]^{(\pm)}$ does not oscillate in this scale; we can therefore average Eq. (B2) over such oscillations before it is substituted into Eq. (B1). Following the averaging prescription,[22] we obtain

$$\langle e^{-2i\mu\alpha\bar{D}} \rangle_{\text{osc}}^{(\pm)} = \mp e^{-2i\xi_{10} - \eta_{20}} = \mp i[\Gamma(1+i\mu)/\Gamma(1-i\mu)]R \ , \tag{B3}$$

where R is given by Eq. (4.20). In deriving the first equality we have used the fact that $\eta_{20} > 0$, which follows from Eqs. (4.5) and (A4). The second equality in Eq. (B3) is then a straightforward consequence of Eq. (4.5). Substituting Eqs. (B3) and (4.12) into Eq. (B1) and summing over the two cases with $C = \pm 1$, we obtain Eq. (4.19), which no longer contains terms oscillating in the atomic scale [such as the second part in Eq. (B1)].

APPENDIX C

In this appendix, we consider directly the N-S system with $L = D = \infty$, find a complete set of its outgoing scattering solutions, and then use them to obtain an alternative derivation of Eq. (4.21). In the WKBJ approximation, we can now seek solutions that have the simple form of Eq. (2.1) everywhere, instead of the more complex form of Eq. (3.1) when there are ordinary surfaces present. But for $z \leq 0$, it is now more convenient to put:

$$\hat{g}_a = \begin{pmatrix} \mathcal{A}\exp(iaEz/v_F p) \\ \mathcal{B}\exp(-iaEz/v_F p) \end{pmatrix} \tag{C1}$$

in place of Eq. (3.2), and for $z \geq 0$, we rather rewrite Eq. (4.1) as

$$\hat{g}_a = \mathcal{C} g_a^+ + \mathcal{D} g_a^- . \tag{C2}$$

[Remember that $a \equiv \mathrm{sgn}(\vec{k}_F \cdot \vec{z})$, $p \equiv |\vec{k}_F \cdot \hat{z}|/k_F$.] The coefficients $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$, and $\mathcal{D}$ are related by requiring the two forms of $\hat{g}_a$ to match at $z = 0$, but to make the coefficients unique we need to further specify some of them. The usual choice for this specification is such that the states become the pure "outgoing" scattering eigenstates, which can then form an orthonormal set of basis states if they are further normalized according to their incident parts.[23] There are four types of such outgoing states here, corresponding to a particle or a hole incident from left or right. For a particle incident from left we take $a = +1$, $\mathcal{A}_{pl} = 1$ and $\mathcal{D}_{pl} = 0$. Then, matching Eqs. (C1) and (C2) at $z = 0$ gives

$$\begin{aligned} \mathcal{B}_{pl} &= 2/\Gamma(1 - i\mu)\mathcal{S} , \\ \mathcal{C}_{pl} &= -i\left[1 - 2e^{-i\phi}P_{-\nu}^{i\mu}(0)/\mathcal{S}\right] , \end{aligned} \tag{C3}$$

where

$$\mathcal{S} = e^{i\phi}P_\nu^{i\mu}(0) + e^{-i\phi}P_{-\nu}^{i\mu}(0) .$$

For a hole incident from left we take $a = -1$, $\mathcal{B}_{hl} = 1$, $\mathcal{C}_{hl} = 0$, and find $\mathcal{A}_{hl} = \mathcal{B}_{pl}$, $\mathcal{D}_{hl} = i\mathcal{C}_{pl}$. For a (quasi) particle incident from right, we take $a = -1$, $\mathcal{B}_{pr} = 0$, $\mathcal{C}_{pr} = 1$, and find

$$\begin{aligned} \mathcal{A}_{pr} &= \Gamma(1 + i\mu)\left[e^{2i\phi}P_\nu^{i\mu}(0)P_{-\nu}^{-i\mu}(0) + \text{c.c.}\right]/\mathcal{S} , \\ \mathcal{D}_{pr} &= -\frac{\Gamma(1 + i\mu)}{\Gamma(1 - i\mu)} \frac{e^{i\phi}P_{-\nu}^{-i\mu}(0) - e^{-i\phi}P_\nu^{-i\mu}(0)}{\mathcal{S}} . \end{aligned} \tag{C4}$$

Finally, for a (quasi) hole incident from right, we take $a = +1$, $\mathcal{A}_{hr} = 0$, $\mathcal{D}_{hr} = 1$, and find $\mathcal{B}_{hr} = -i\mathcal{A}_{pr}$, $\mathcal{C}_{hr} = -\mathcal{D}_{pr}$. These solutions may now be used to evaluate $\mathcal{F}_S$. The only remaining ingredient is that for incident-from-left states

$$\sum_n = (2\pi)^{-2}\int d^2k_{F\perp}\int \frac{dE}{(2\pi v_F p)} = \tfrac{1}{2}N(0)\int_0^1 dp \int_{\Delta_\infty}^\infty dE ,$$

while for incident-from-right states,

$$\sum_n = \tfrac{1}{2}N(0)\int_0^1 dp \int_{\Delta_\infty}^\infty dE \frac{E}{(E^2 - \Delta_\infty^2)} ,$$

because the left side is normal, while the right side is superconducting. Putting all of these together and with the help of Eq. (A4), we obtain precisely Eq. (4.21) in the region $z \geq 0$. We may also obtain Eqs. (4.18), (3.13), and (3.11) by this method, but we shall omit the details here.

APPENDIX D

In this appendix we briefly outline the derivation of three useful identities about the associated Legendre functions, i.e., Eqs. (5.1), (5.4), and (5.5). The common starting point is the differential equation[17]

$$(1 - X^2)\frac{d^2}{dX^2}P_a^b(X) - 2X\frac{d}{dX}P_a^b(X) + \left(a(a+1) - \frac{b^2}{1 - X^2}\right)P_a^b(X) = 0 . \tag{D1}$$

Applying a standard trick to this equation, we first obtain

$$\int_0^1 P_\nu^\mu(X)P_{-\nu}^{\pm\mu}(X)\,dX = (2\nu)^{-1}(X^2 - 1)\left(P_{-\nu}^{\pm\mu}\frac{d}{dX}P_\nu^\mu - P_\nu^\mu\frac{d}{dX}P_{-\nu}^{\pm\mu}\right)\Bigg|_{X=0}^{X=1} . \tag{D2}$$

The derivatives of P_ν^μ and $P_{-\nu}^{\pm\mu}$ may be eliminated by using the recurrence relation[17]

$$(X^2 - 1)\frac{d}{dX}P_a^b(X) = aXP_a^b(X) - (a+b)P_{-a}^b(X) . \tag{D3}$$

The upper limit at $X = 1$ may then be evaluated by using Eq. (2.8). This procedure leads easily to Eqs. (5.1), (5.4), and (5.5), when μ is replaced by $-\bar{\mu}$ and $i\mu$ in Eq. (D2).

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[23]See, for example, E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1970), Ch. 19, Sec. 5, and, in particular, Eq. (19.46).

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