Order parameter near a superconductor-insulator interface

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(Received 1 June 1992)

We examine the behavior of the superconducting order parameter near a superconductor-insulator interface by self-consistently solving the Gor'kov equations in a slab geometry. We obtain results as a function of temperature and the coherence length ξ_0. We find that even for small values of ξ_0 there is no significant depletion of the gap parameter near such an interface over any extended temperature range. This is in agreement with experimental information and in contrast with results obtained from an extrapolation of standard Ginzburg-Landau based results. We also find that quantum-size effects, which are present in the large ξ_0 case, disappear as ξ_0 decreases.

I. INTRODUCTION

The study of boundary effects in superconductors has a long history. A great deal of work on the subject was done over a quarter of a century ago. The results of that work were eventually embodied in review articles[1] and textbooks.[2] The view that emerged at that time makes heavy use of phenomenological descriptions of the order-parameter behavior based on the Ginzburg-Landau[3] (GL) free energy functional. A basic assumption[4] in GL theory is that the superconducting coherence length ξ_0 is much larger than the Fermi wavelength $\lambda_F \approx 2\pi/k_F$ (k_F is the Fermi wave vector). This assumption certainly holds in ordinary metallic superconductors, where the methodologies of the textbook theory are certainly justified. As a result the theory has proved very successful over the years in describing a large variety of experimental situations.

It is now well established, however, that there are low carrier concentration superconductors (e.g., high-transition-temperature oxide superconductors) for which the condition $k_F\xi_0 \gg 1$ is violated. This has disturbed the harmony between theory and experiment. It has been pointed out by several authors[5] that the standard theory, if straightforwardly extrapolated to the case where $k_F\xi_0$ is not large, predicts a very considerable depletion of the gap function (pair potential) near the interface between a superconductor and an insulator (or the vacuum). Such a depletion would occur over a very extended temperature range, while for conventional superconductors it occurs only at temperatures extremely close to the transition temperature T_c and is therefore often unimportant. This depletion would entail, for short coherence length materials, rather drastic experimental consequences.

The importance of understanding the behavior of the gap function $\Delta(z)$ (we denote by z the direction normal to the surface) near a superconductor-insulator (SI) interface is hard to underestimate. Information concerning the presumed behavior of a superconductor in the bulk is usually gathered through the use of experimental techniques which often probe only properties quite near the surface. Tunneling, for example, probes a sample within a region of order of the coherence length from the surface,[6] while photoemission experiments, from which detailed information about the gap structure can be extracted,[7] when the transition temperature is high enough, collect electrons from within an escape depth which, in practice, is also very small.[8] Indeed the fact that superconducting properties are measured at all by such probes[6,7] provides a rather obvious argument[9] against the existence of any dramatic depletion in $\Delta(z)$.

The question at issue, from a theoretical point of view, can be described as the need to determine whether the results of a microscopic calculation would agree, at small values of ξ_0, with those obtained from the usual phenomenology extrapolated to such values. Not much work has been done on this point. A solution of the Bethe-Salpeter equation above T_c for a BCS-type jellium model[10] gave support to the notion that a surface is not inimical to superconductivity when ξ_0 is small, since it was found that, in that case, the transition temperature at the surface is very slightly increased with respect to the bulk value, and the eigenvalue profile at the superconducting instability in enhanced, rather than depleted, at the interface as the temperature T approaches T_c from above. Other studies have focused[11,12] on the effect of a possible modification of the pairing interaction very near the surface, rather than on the purely geometric effects that we emphasize here.

In this work we approach the problem from a simple, but purely microscopic point of view. We write down the Gor'kov equations for the standard BCS model and we solve them, not for an infinite system, but for a thick slab, half of which is a representation of a semi-infinite system. We vary the relevant parameters in the problem to study systems with shorter and longer coherence lengths, and we obtain results as a function of temperature. The method we use is rather similar to that previously developed[13] within the context of ^{3}He films, except that certain important modifications (as will be seen in detail later) are required to properly treat the problem when $k_F\xi_0$ is not large, and that we assume in this work s-wave pairing. The use of a simple BCS model may be questioned on the grounds that since $k_F\xi \approx 0.36(T_F/T_c)$, a

decreasing value of $k_F\xi_0$ indicates the approach of the strong-coupling region. However, the results that we find cover a region of moderate and large values of this parameter, and we find that they are determined largely by the geometrical constraints inherent to the problem. Therefore they should be robust with respect to changes in the details of the treatment. We will return to this point when recapitulating our conclusions in the Sec. IV.

Our main results can be summarized as follows: our calculation, presented in this paper, shows that near a superconductor-insulator interface there is no significant depletion in the superconducting order parameter (gap function) over any broad temperature range even in short ξ_0 superconductors. We show that the standard theory[2] can be quantitatively applied only to the cases when ξ_0 is large. Thus, surface probes can indeed yield direct information on the bulk behavior of short coherence length superconductors, a result which agrees with experiment.

This paper is organized in the following way: In the next section we set up the Gor'kov equations for our model, and discuss the methods required for their solution. Then, in Sec. III, we present results for the gap parameter as a function of z for a variety of values of the relevant input quantities. We also present results for the variation of quantum oscillation effects in the average order parameter with ξ_0. We then discuss the significance of our results in Sec. IV.

II. THEORY AND METHODS

In this section we introduce the model we use and the methods we employ to solve it. Our method is based on the self-consistent solution of the Gor'kov equations. The solution of these equations leads us to results for physical quantities such as the shape of the order parameter near the insulator-superconductor interface.

We begin with the Gor'kov equations in their standard form for a system without translational invariance, in the absence of a magnetic field ($\mathbf{A}=\mathbf{0}$):[14]

$$(i\omega_n+\nabla^2/2m+\mu)G(\mathbf{r},\mathbf{r}',\omega_n)+\Delta(\mathbf{r})F^*(\mathbf{r},\mathbf{r}',\omega_n)=\delta(\mathbf{r}-\mathbf{r}')\ , \quad (2.1a)$$

$$(-i\omega_n+\nabla^2/2m+\mu)F^*(\mathbf{r},\mathbf{r}',\omega_n)-\Delta^*(\mathbf{r})G(\mathbf{r},\mathbf{r}',\omega_n)=0\ , \quad (2.1b)$$

where G and F are the standard single-particle Green's functions, ω_n are the Matsubara frequencies given by $\omega_n=(2n+1)\pi T$, and the order parameter (gap function or pair potential) satisfies the self-consistency equation:

$$\Delta(\mathbf{r})=gT\sum_n F(\mathbf{r},\mathbf{r},\omega_n)\ . \quad (2.2)$$

In our model we shall assume that electrons with energy within a range ω_0 of the Fermi surface interact through an attractive point contact interaction of strength g. The physical origin of this interaction is left unspecified. In a given gauge Δ can be taken to be real without loss of generality.

We consider these equations in a slab geometry, with the slab being infinite in the x and y directions and having a thickness d in the z direction. The superconductor is in the region $0<z<d$. In this geometry the above equations are clearly translationally invariant in the x,y plane and it is convenient to perform a spatial Fourier transform in this plane. One then obtains

$$(i\omega_n-\epsilon_\perp+\nabla_z^2/2m+\mu)G(z,z',k_\perp,\omega_n)+\Delta(z)F^*(z,z',k_\perp,\omega_n)=\delta(z-z')\ , \quad (2.3a)$$

$$(-i\omega_n-\epsilon_\perp+\nabla_z^2/2m+\mu)F^*(z,z',k_\perp,\omega_n)-\Delta^*(z)G(z,z',k_\perp,\omega_n)=0 \quad (2.3b)$$

with

$$\epsilon_\perp=\frac{1}{2m}\mathbf{k}_\perp^2 \quad (2.4)$$

and $\mathbf{k}_\perp$ is the wave vector in the transverse (x,y plane) direction. In order to consider the z dependence of the order parameter we find it useful to expand the relevant functions in terms of the complete set of eigenfunctions $u_\nu(z)$ of a one-dimensional box:

$$G(z,z',k_\perp,\omega_n)=\sum_{\nu\nu'}u_\nu(z)u_{\nu'}(z')g_{\nu\nu'}(k_\perp,\omega_n)\ , \quad (2.5a)$$

$$F(z,z',k_\perp,\omega_n)=\sum_{\nu\nu'}u_\nu(z)u_{\nu'}(z')f_{\nu\nu'}(k_\perp,\omega_n)\ , \quad (2.5b)$$

where

$$u_\nu(z)=\sqrt{2/d}\sin(k_\nu z),\quad k_\nu\equiv\frac{\nu\pi}{d}\ . \quad (2.6)$$

These functions obviously satisfy the boundary conditions $u_\nu(z=0)=u_\nu(z=d)=0$, corresponding to an infinite potential barrier at the surfaces. In fact, these boundary conditions are not exactly correct, due to the "leak" of electronic wave functions outside the metal boundaries as shown by Sugiyama.[15] More precisely, one should assume that the electronic density vanishes at $z=-\delta$ and $z=d+\delta$. Nevertheless, since the value of δ is known to be[16] $k_F\delta\sim 1$, our boundary conditions are still appropriate for the thicknesses we will consider here ($k_Fd\gg 1$). Note that we have assumed here s-wave pairing. If we assumed pairing in a higher-order partial wave, it would be necessary to take into account the depairing effects of scattering by random surface inhomogeneities as was done in Ref. 17. In the s-wave case the surface roughness enters the theory in the same way as nonmagnetic bulk impurities[18] (see also remarks in Ref. 17) and therefore its effects can be neglected to a good approximation.

The order parameter is, of course, not a constant in space, as it would be in the bulk geometry. However, it varies only in the z direction. Then one can also expand the order parameter as

$$\Delta(z)=\sum_\nu^N u_\nu(z)\Delta_\nu\ . \quad (2.7)$$

Since $\Delta(z)$ should be symmetric with respect to a plane bisecting the slab at $z=d/2$, it is sufficient to take only odd ν values in (2.7). In Eq. (2.7) the upper limit in the

sum, N, is determined by

$$N=[(k_F d/\pi)\sqrt{1+\omega_0/E_F}] \tag{2.8}$$

where the square brackets denote the integer part of the expression they enclose and E_F is the Fermi energy. Physically, this corresponds to the degeneracy of the usual Fermi sphere into a set of rings (Fig. 1), distinguished by a quantized $k_z=k_\nu$ as in previous work.[19] N corresponds to the maximum number of rings within a sphere of radius $E_F+\omega_0$.

By defining

$$\lambda_\beta=\frac{1}{2m}k_\beta^2=\frac{1}{2m}\left[\frac{\beta\pi}{d}\right]^2, \tag{2.9}$$

$$\gamma^\beta_{nk_\perp}=i\omega_n-\epsilon_\perp-\lambda_\beta+\mu \tag{2.10}$$

and making use of the orthogonality of the u_ν's, the Gor'kov equations transform into a set of equations for the matrix elements:

$$\gamma^\beta_{nk_\perp}g_{\beta\rho}(k_\perp,\omega_n)+\sum_{\nu\nu'}\Delta_\nu f^*_{\nu'\rho}(k_\perp,\omega_n)J_{\nu\nu'\beta}=\delta_{\beta\rho}\ , \tag{2.11a}$$

$$(\gamma^\beta_{nk_\perp})^* f^*_{\beta\rho}(k_\perp,\omega_n)-\sum_{\nu\nu'}\Delta_\nu g_{\nu'\rho}(k_\perp,\omega_n)J_{\nu\nu'\beta}=0 \tag{2.11b}$$

with

$$\begin{aligned} J_{\nu\nu'\beta}&=\int_0^d dz\, u_\nu(z)u_{\nu'}(z)u_\beta(z)\ ,\\ J_{\nu\nu'\beta}&=\frac{1}{\pi\sqrt{2d}}\tilde{J}_{\nu\nu'\beta}\ ,\\ \tilde{J}_{\nu\nu'\beta}&=[1-(-1)^{\nu\pm\nu'+\beta}]\left[\frac{1}{\nu+\nu'-\beta}+\frac{1}{-\nu+\nu'+\beta}\right.\\ &\quad\left.+\frac{1}{\nu-\nu'+\beta}-\frac{1}{\nu+\nu'+\beta}\right], \end{aligned} \tag{2.12}$$

and the self-consistency equation becomes

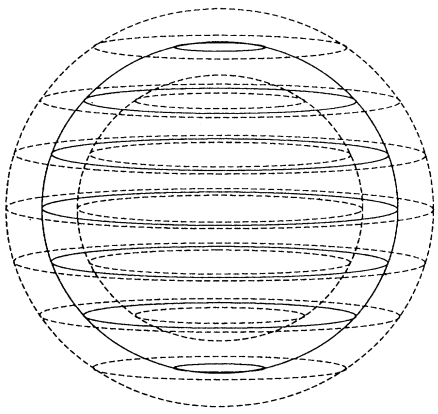

FIG. 1. Momentum space in a slab geometry: the Fermi surface degenerates into a set of circles represented by solid lines. The dashed lines indicate the range $E_F\pm\omega_0$ in momentum space where the electron coupling occurs. The number of rings is given by Eq. (2.8).

$$\Delta_\beta=gT\sum_{\nu\nu'}^{N}J_{\nu\nu'\beta}\int\frac{d^2k_\perp}{(2\pi)^2}\sum_n f_{\nu\nu'}(k_\perp,\omega_n)\ . \tag{2.13}$$

We have assumed that electron pairing occurs only for electrons with wave vectors lying in a shell of thickness $2\omega_0$ around the Fermi surface. Therefore, as ω_0/E_F increases, as in short ξ_0 superconductors, the limits of integration in Eq. (2.13) depend increasingly on the indices ν and ν', as well as on the parameter $k_F d$. From Eq. (2.12) we see that the indices in the sum in Eq. (2.13), ν and ν', must be of the same parity, since, as mentioned before, β is an odd integer.

At any finite thickness d, one has to solve the system (2.11) together with the self-consistency condition (2.13). This is done numerically, using an iterative procedure to ensure that (2.13) is satisfied as explained in the next section. These equations can be conveniently recast in matrix form. One can define the following matrices (all of order $N\times N$):

$$\begin{aligned} &C_{\beta\rho}=\sum_\nu\Delta_\nu J_{\nu\beta\rho},\quad \Gamma_{\beta\rho}=\gamma^\beta_{nk\perp}\delta_{\beta\rho}\ ,\\ &G_{\beta\rho}=g_{\beta\rho}(k_\perp,\omega_n),\quad F_{\beta\rho}=f_{\beta\rho}(k_\perp,\omega_n)\ , \end{aligned} \tag{2.14}$$

and (2.11) can be rewritten as matrix equations,

$$\underline{\Gamma}\,\underline{G}+\underline{C}\,\underline{F}^*=\underline{1}_N\ , \tag{2.15a}$$

$$\underline{C}\,\underline{G}-\underline{\Gamma}^*\underline{F}^*=\underline{0}\ . \tag{2.15b}$$

One easily finds the formal solution for $\underline{F}$:

$$\underline{F}=[\underline{1}_N+(\underline{\Gamma}^{-1}\underline{C})^*\underline{\Gamma}^{-1}\underline{C}]^{-1}(\underline{\Gamma}^{-1}\underline{C})^*\underline{\Gamma}^{-1}\ . \tag{2.16}$$

In the $3-d$ limit $\Delta(z)$ is a constant, and therefore

$$\Delta_\beta=\frac{2\sqrt{2d}}{\pi}\frac{1}{\beta}\ . \tag{2.17}$$

From Eq. (2.16) we see that the matrix $\underline{F}$ is, in that case, diagonal, since $C_{\beta\rho}=\sum_\nu\Delta_\nu J_{\nu\beta\rho}\to\Delta_{\rm bulk}\delta_{\beta\rho}$, where $\Delta_{\rm bulk}$ is the temperature-dependent three-dimensional gap. Then one can substitute $f_{\beta\rho}(k_\perp,\omega_n)$ into (2.13) and obtain the familiar equation[14] for $\Delta_{\rm bulk}$ in cylindrical coordinates. In a slab, however, one finds $\underline{F}$ and $\underline{G}$ to have off-diagonal matrix elements different from zero, which makes the self-consistent calculation, in particular the matrix inversion in (2.16), much harder. For finite thickness, and for the parameter values that we will consider here, one cannot neglect the off-diagonal elements. Nevertheless, the off-diagonal elements of the matrices $\underline{G}$ and $\underline{F}$ are small compared to the diagonal ones, which simplifies the calculations somewhat.

One can then write $\underline{F}$ as

$$\underline{F}=(\underline{D}+\underline{\theta})^{-1}(\underline{\Gamma}^{-1}\underline{C})^*\underline{\Gamma}^{-1}\ , \tag{2.18}$$

where $\underline{D}$ is the larger diagonal part, which is given by

$$\underline{D}_{\beta\rho}=\delta_{\beta\rho}\left[1+\left|\frac{C_{\beta\beta}}{\gamma^\beta_{nk_\perp}}\right|^2\right]$$

and $\underline{\theta}$ is the remaining, off-diagonal part. Then one can use the expansion

$$(\underline{D}+\underline{\theta})^{-1}=(\underline{1}+\underline{D}^{-1}\theta)^{-1}\underline{D}^{-1}$$
$$=\underline{D}^{-1}-\underline{D}^{-1}\underline{\theta}\,\underline{D}^{-1}+\underline{D}^{-1}\underline{\theta}\,\underline{D}^{-1}\underline{\theta}\,\underline{D}^{-1}-\ldots . \tag{2.19}$$

to calculate $\underline{F}$ as accurately as desired. In our calculations we have required only the first two terms and estimated that the relative error incurred in neglecting the remaining terms was at most of order 10^{-3}.

It is of interest here to discuss the range of applicability of the approximation where one assumes that the matrices $\underline{G}$ and $\underline{F}$ are diagonal. An equivalent assumption was tacitly made in Refs. 13, 19, 20, and 21 to calculate quantities such as the average gap parameter in films. There are two cases where this approximation is justified. The first is for the calculation of the average value of the order parameter over a very thick slab, $k_F d \gg 1$. We have already mentioned that, as this quantity tends to infinity, $\underline{G}$ and $\underline{F}$ are diagonal and $\Delta_\beta \sim 1/\beta$. One can then show that off-diagonal corrections will affect the quantities involving sums over ν indices by an amount of order $1/k_F d$.[22]

The other case where the off-diagonal terms are negligible is when $k_F d$ is very small. (Note, however, that other problems may arise in general with the method in that limit.[12]) Fermions with different values of the ν and ν' indices are uncoupled when the transverse projections of the corresponding rings in Fig. 1 do not overlap. This is the case if $2\omega_0/(\lambda_\nu-\lambda_{\nu'})<1$ which will hold for all values of ν and ν', if

$$\frac{\omega_0}{4\lambda_1}=\frac{\omega_0/E_F}{4(\pi/k_F d)^2}<1$$

or equivalently

$$(k_F d)^2<4\pi^2 E_F/\omega_0 . \tag{2.20}$$

The right-hand side of the last equation can be rewritten in terms of the bulk coupling constant λ, related to the zero-temperature bulk order parameter $\Delta^0_{\rm bulk}$ by $\Delta^0_{\rm bulk}=\omega_0/\sinh(1/\lambda)$, and ξ_0 through the use of the BCS relation

$$k_F\xi_0=(2/\pi)(E_F/\Delta^0_{\rm bulk}) . \tag{2.21}$$

We see that for long coherence length materials, and for the purpose of the work in the references mentioned above, the diagonal approximation is sufficiently accurate. But in order to study the gap profile when $k_F\xi_0$ is not large the off-diagonal terms must be taken into account.

To conclude this section, we point out that it is convenient to rewrite Eq. (2.13) as

$$\tilde{\Delta}_\beta=\frac{\Delta_\beta}{\Delta^0_{\rm bulk}\sqrt{d}}$$
$$=\frac{\lambda\sqrt{2}}{k_F d}\sum_{\nu\nu'}\tilde{J}_{\nu\nu'\beta}I_{\nu\nu'}(k_F d,\tilde{\Delta}_\nu) \tag{2.22}$$

where $\tilde{\Delta}_\beta$ and $\tilde{J}_{\nu\nu'\beta}$ are dimensionless [from Eqs. (2.7) and (2.12)], and $I_{\nu\nu'}(k_F d,\tilde{\Delta}_\nu)$ is the result of performing the sum and integral on the right-hand side of Eq. (2.13).

III. RESULTS

In this section we present the results of our model and their analysis. We show and discuss our results for the order parameter $\Delta(z)$ as a function of distance z from the boundary at various temperatures. At temperatures close to the transition temperature T_c we compare our results for the function $\Delta(z)$ near the interface with the standard Ginzburg-Landau based theory. At $T=0$ we also discuss the average value of the gap function Δ, as a function of thickness d for moderate values of this quantity, emphasizing the dependence of the quantum-size effects for this average quantity on ξ_0.

We briefly review the phenomenological[12] result for the order-parameter profile, developed for conventional, long ξ_0 superconductors. One finds that, in the presence of an interface, $\Delta(z)$ is given by

$$\Delta(z)=\Delta_{\rm bulk}(T)\tanh\frac{z+z_0}{\xi(T)\sqrt{2}} , \tag{3.1}$$

where $\xi(t)$ is the GL temperature-dependent coherence length, $\Delta_{\rm bulk}(T)$ is the gap parameter in the bulk, z_0 is determined by

$$\left.\frac{d\Delta(z)}{dz}\right|_{z=0}=\frac{1}{b}\Delta(z=0) , \tag{3.2}$$

and b is the extrapolation length, microscopically estimated, for a SI interface, as $b\approx\xi_0^2/a$, with $a\approx\pi/k_F$. Straightforward application[5] of this model to shorter ξ_0 superconductors gives a large depletion of the gap near the surface over a broad temperature range.

Before presenting our results, it is necessary to introduce a convenient choice of dimensionless parameters for this problem. The physical parameters of our model are the characteristic frequency ω_0, the zero-temperature bulk order parameter $\Delta^0_{\rm bulk}$, the Fermi energy E_F, the thickness of the slab d, and the temperature T. The first three parameters characterize the general, bulk properties of the superconductor. In a finite system, two of these parameters are independent, as pointed out already in Ref. 10. Therefore, recalling Eq. (2.21), we choose as two of our dimensionless parameters $\Delta^0_{\rm bulk}/\omega_0$ and $k_F\xi_0$. The frequency ω_0 is approximately the same in both short and long ξ_0 materials.[23] In addition we take $k_F d$ as our dimensionless measure of the slab thickness, and $t\equiv 1-T/T_c$ as the dimensionless temperature. Note that this is different from the parameter T/T_c often denoted by t in superconductivity theory. The chemical potential μ is calculated as a function of d as indicated in Ref. 13. We take μ equal to E_F in our calculations, which is adequate at the temperatures we are considering. Alternative choices for the bulk parameters are possible. We could have for example, as in Ref. 10, used the bulk transition temperature $T_c^{\rm bulk}$ instead of $\Delta^0_{\rm bulk}$. However, these quantities are simply related to each other in the BCS theory[24] and therefore are equivalent.

In determining the parameter ranges to be explored,

we have kept in mind the experimental results,[23,25] which show that both quantities, T_c and $\Delta^0_{\rm bulk}$ often take much higher values in short ξ_0 superconductors than in conventional ones, while the Fermi energy is somewhat lower.[25] Therefore we have explored a wide range of parameter values keeping $\Delta^0_{\rm bulk}/\omega_0$ smaller whenever $k_F\xi_0$ is taken to be larger. We vary $k_F\xi_0$ in a range from several thousands with $\Delta^0_{\rm bulk}/\omega_0$ of order 0.01, values which are of the order of those found in traditional superconductors such as aluminum or tin, to values less than 10 (somewhat higher than those found in high-temperature superconductors) with $\Delta^0_{\rm bulk}/\omega_0$ as high as 0.5. Our results for the shape of $\Delta(z)$ (normalized to its bulk value) depend on $k_F\xi_0$ and on the temperature, but hardly at all on $\Delta^0_{\rm bulk}/\omega_0$. We vary k_Fd from ~ 50 up to many thousands as necessary to attain the condition that our results for $\Delta(z)$ near the surface become independent of k_Fd. This turns out to be the same as requiring that d be large enough so that $\Delta(z)$ attains essentially its bulk value away from the edges of the slab. We explore the temperature range between 0 and T_c, with special emphasis on zero temperature and on the region where t is small. As explained at the end of the previous section, the ratio $\Delta^0_{\rm bulk}/\omega_0$ is a measure of the strength of the interaction, while $k_F\xi_0$ gives the length scale for the variation of the relevant functions (F and Δ) in the problem. Both parameters combined give us the domain in momentum space where pairing occurs. Again, here we do not make any assumptions as to the actual mechanism of the electron coupling, but only as to its energy range and length scale.

We now turn to the results. We begin by considering zero temperature. At $T=0$ one can solve Eqs. (2.13) and (2.16) analytically to the specified accuracy and then one must perform only the self-consistent gap calculation numerically. At finite temperatures the integration in the former equation must be done numerically. The self-consistent calculation is performed by starting with some reasonable guess for the gap [we usually set the initial values for the coefficients Δ_β to their bulk values given in Eq. (2.17)] and then iterating the set of equations until self-consistency is achieved, as determined by the relative change in the average $\Delta(z)$ becoming less than 10^{-4}. The accuracy of the results, of course, does not depend on the initial guess for the shape of the order parameter.

The results for $\Delta(z)$ at zero temperature are shown in Figs. 2 and 3. In these and subsequent figures for $\Delta(z)$ we show results for the region $0<z<d/2$ as necessary to show detail. Figure 2 shows the shape of the order parameter in a superconducting slab with large ξ_0 ($\pi k_F\xi_0=20\,000$, $\Delta^0_{\rm bulk}/\omega_0=0.01$). The set of relevant parameter values employed in each figure is specified in the captions. As expected, at zero temperature there is no depletion of the pair potential near the surface. The wiggles in the $\Delta(z)$ function seen in this and many of the subsequent figures reflect the Friedel oscillation behavior in the density of states, due to the discontinuity in the occupation of states at the Fermi energy, caused by geometric reasons. Oscillations are more significant very near the surface than farther in the interior of the slab, where they eventually disappear as $k_Fd\to\infty$. The same enhancement effect was found in the eigenvalue profile in Ref. 10.

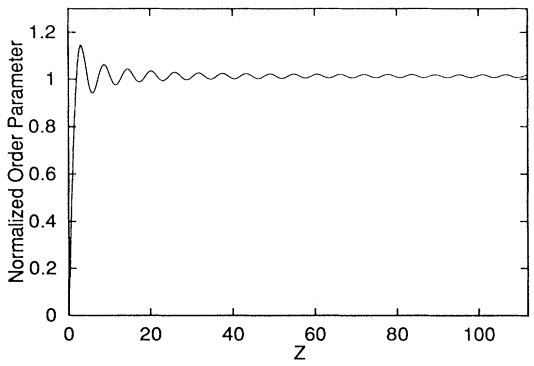

FIG. 2. The normalized order parameter, defined as $\Delta(z)/\Delta^0_{\rm bulk}$, vs $Z\equiv k_Fz$, the distance from the SI interface measured in units of k_F^{-1}. The results shown in this figure are at $T=0$ for $\pi k_F\xi_0=2\times10^4$ as in an ordinary superconductor.

The number of oscillations is equal to $[(N+1)/2]$, where N is defined in Eq. (2.8). One can also observe the saturation of the order parameter away from the boundary of a slab to the bulk value, showing that our results have the correct behavior in the $3-d$ limit.

Zero-temperature results for a smaller value of $k_F\xi_0$ ($\pi k_F\xi_0=20$, $\Delta^0_{\rm bulk}/\omega_0=0.5$) are in Fig. 3. One can see that for short ξ_0 superconductors the shape of $\Delta(z)$ is essentially the same, at zero temperature, as for standard superconductors. The behavior of $\Delta(z)$ at $T=0$ is practically independent of the coherence length ξ_0.[26] This is as expected. For this reason, we have not included intermediate values of ξ_0 at zero temperature.

We now take a brief detour from our main topic to consider the question of quantum-size effects in the gap, in thick films, as a function of k_Fd. These effects have been considered in the past in long coherence length materials.[12,13,19–21] In the case of long ξ_0 superconductors quantum-size effects have been experimentally observed (at very low temperatures).[27] We show our results in Fig. 4 for three values of $k_F\xi_0$. The quantity plotted is the value of the order parameter, averaged over the thickness of the film, as a function of film thickness. It can be seen

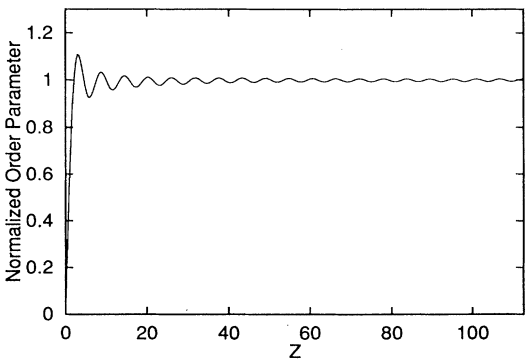

FIG. 3. As in Fig. 2 ($T=0$) for a short ξ_0 superconductor: $\pi k_F\xi_0=20$.

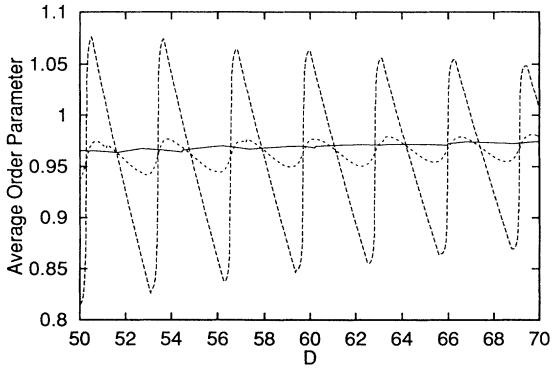

FIG. 4. Disappearance of the quantum-size effects as $k_F\xi_0$ decreases. The quantity displayed is the zero-temperature order parameter, averaged over the film thickness d and normalized with respect to Δ^0_{bulk}. It is plotted vs $D \equiv k_F d$. The solid line corresponds to $\pi k_F \xi_0 = 20$, the dotted line corresponds to $\pi k_F \xi_0 = 250$, while the dashed line corresponds to $\pi k_F \xi_0 = 2 \times 10^4$.

that the oscillations occur at large values of $k_F\xi_0$, in agreement with the previous work mentioned above, but that they become much less prominent as this quantity decreases. This can be understood as follows: quantum oscillations can occur any time N, defined in Eq. (2.8), increases by one. This appears to be simply the usual condition for having standing electron waves of wave vector k_F in an infinite potential well of width d. The correct calculations, however, include higher-order corrections in ω_0/E_F to the shape of the resonances which were neglected in previous work and must be included in the general case. Physically, this corresponds to the fact that although k_F is a function of thickness d at fixed density,[20] in a correct treatment one must recall that the electronic wave vectors are smeared in the region given by the condition $(E_F - \omega_0 < k^2/2m < E_F + \omega_0)$. This region is relatively larger when $k_F\xi_0$ is smaller, which broadens, and eventually flattens out the resonances. This purely geometrical effect is quite different, as pointed out in the Introduction, from that explored in Ref. 12, where the finite-size effects in the phonon interaction in very thin films were considered. We have chosen to display in this figure a range of values of $k_F d$ corresponding to relatively small slab thicknesses ($k_F d \sim 50$), since at larger thicknesses the oscillations become washed out even for large values of the coherence length, as $k_F d$ reaches values comparable to $k_F\xi_0$. Mathematically, this is due to the dependence on ω_0/E_F of the limits of integration in Eq. (2.13). The approximations used in previous works hold only in the limit of long ξ_0 superconductors where ω_0/E_F is a very small quantity. It is interesting to speculate on whether other resonance effects, which occur, e.g., in layered structures, are similarly affected. This seems likely, and it is a question we plan to address in future work.

We now return to $\Delta(z)$ and proceed with the finite-temperature case. We first calculate the transition temperature $T_c(d)$. This function exhibits quantum oscillations, as a function of thickness, which for an s-wave superconductor are similar to those found for the order parameter and shown in Fig. 4. To calculate T_c, we use the fact that when $T \to T_c$ one can expand $\underline{F}$ in terms of Δ_β's, and the self-consistent Eq. (2.13) transforms into

$$\Delta_\beta \approx \sum_\alpha \Phi^\alpha_\beta \Delta_\alpha \ , \tag{3.3}$$

where

$$\Phi^\alpha_\beta = g/2 \sum_{\nu\nu'} J_{\nu\nu'\alpha} J_{\nu\nu'\beta} \int \frac{d^2k_\perp}{(2\pi)^2} \frac{\tanh(E_{\nu\nu'}/2T) + \tanh(E_{\nu'\nu}/2T)}{E_{\nu\nu'} + E_{\nu'\nu}} \tag{3.4}$$

and

$$E_{\nu\nu'} = \epsilon_\perp + \frac{\lambda_\nu - \lambda_{\nu'}}{2} - \mu \ . \tag{3.5}$$

This equation is only approximately correct at any temperature other than T_c where it becomes exact. One can recognize an eigenvalue problem in Eq. (3.3) which must have an eigenvalue equal to one at $T = T_c$. It enables us to obtain the critical temperature T_c. This eigenvalue procedure is similar to that used above T_c.[10] As in that case, Eq. (3.3) can be used for the determination of $\Delta(z)$ at T_c up to an arbitrary multiplicative factor. We used this method to double check the results of our self-consistent calculation of the order parameter very close to the transition temperature.

Once T_c is calculated, we can specify the value of the parameter $t \equiv 1 - T/T_c$ and compute $\Delta(z)$ at different temperatures. We expect that the gap function will show some depletion near the boundary for sufficiently small t. Physically, we might say that the coupling becomes weaker, at higher temperatures, for electrons with higher values of k_z. One can see from Fig. 1 that, at constant t, the effect will be smaller when $k_F\xi_0$ is larger and $\omega_0 \ll E_F$. The important question however, is to find quantitatively how important this effect is for reasonable values of the temperature, for short or long coherence length superconductors, and to elucidate whether or not the depletion of the gap is strong enough and extends over a wide enough temperature range to become an important factor in the planning or the analysis of experiments. This is one of the main motivations of this work.

We begin by presenting our results at high temperature (small t). Consider first the standard, large $k_F\xi_0$ case ($\pi k_F \xi_0 = 20\,000$ with $t = 0.01$ in Fig. 5). We see that the pair potential retains its square wave zero-temperature shape, the only difference being a decline in the bulk value of Δ. For these parameters values, this is in agreement with the standard theory, which predicts a change only extremely close to T_c ($t \lesssim 10^{-6}$).

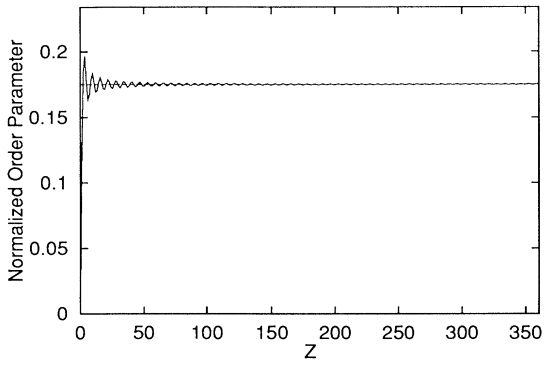

FIG. 5. The order parameter in a conventional superconductor at $t \equiv (T_c - T)/T_c = 0.01$ [$\pi k_F \xi_0 = 2 \times 10^4$ and $k_F \xi(t) = 4.7 \times 10^4$]. The extrapolation length b is extremely long ($k_F b \approx 2 \times 10^7$). The solid line represents our result. The dashed line, which is nearly indistinguishable, shows the corresponding phenomenological theory result from Eqs. (3.1) and (3.2). Again, the order parameter is normalized with respect to Δ^0_{bulk}.

We next turn to the opposite case of short ξ_0 ($\pi k_F \xi_0 = 20$) and very small t ($t \approx 10^{-4}$), which is shown in Fig. 6. The solid line in this figure represents the microscopically calculated order parameter, while the dashed line represents the curve obtained from Eqs. (3.1) and (3.2). Here we can see a glaring discrepancy between the microscopic results and those obtained from extrapolation of the large ξ_0 phenomenology. It is obvious that, although a depletion of the gap does occur near the boundary, even at these high temperatures it is only of order 10%, much smaller then what the standard theory predicts. Farther away from T_c, the depletion, although it still exists, becomes completely inconsequential. Our results show that the value of the order parameter reaches a level very close to its bulk value at distances from the surface of order k_F^{-1}. Moreover, since the superconducting energy gap in a slab is, to a good approximation, equal to the minimum value of the order parameter along its cross section,[1] one should be able to observe a significant energy gap even at temperatures close to the transition temperature, and certainly there should be no problems at the temperatures typical tunneling and photoemission experiments are performed.[6,7] We have carried out the calculations for this figure in an extremely thick slab, to ensure that the condition $\xi(t) \ll d$ [where $\xi(t)$ is the phenomological temperature-dependent coherence length] is satisfied and note that the dashed curve reaches the correct bulk value in the center of the slab.[28]

An additional example, for the same parameter values as in Fig. 6, but at a somewhat lower temperature (approximately the same as in Fig. 5, with which it should be contrasted) is shown in Fig. 7. The disagreement between the two results is again evident. The depletion is now minimal in the microscopic calculation.

The discrepancy that we find at short coherence lengths is rather gratifying, since it confirms what is indicated by many experiments: that the order parameter is present near a boundary such as we are considering. While with the benefit of hindsight it is not really surprising that GL based theory does not work for shorter coherence lengths, the magnitude of the discrepancy is quite startling, particularly in the case shown in Fig. 6. From the experimental point of view, it is worthwhile to emphasize that one could not have *a priori* assumed that the breakdown of GL theory would lead to a larger, rather than to an even smaller, value of the gap function near the surface.

In order to investigate at what ξ_0 the discrepancy occurs we obtained the shape of the order parameter at intermediate values of the coherence length. As an example, we show our computations for a value of $\pi k_F \xi_0 = 250$ in Fig. 8, for a value of t of the same order as that used in Figs. 5 and 7. We obtain a much better agreement between the results of the two theories. The discrepancy

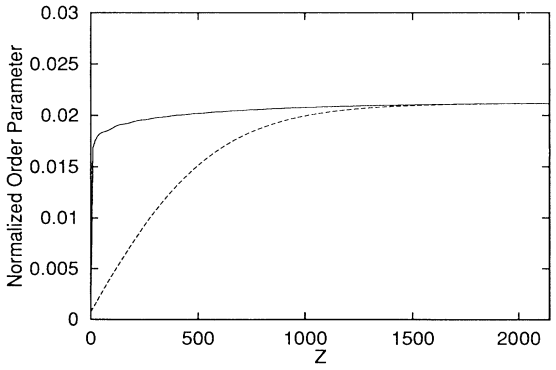

FIG. 6. The same calculation as in Fig. 5 for a shorter ξ_0 superconductor ($\pi k_F \xi_0 = 20$ as in Fig. 3). The GL coherence length is $k_F \xi(T) = 410$ and $k_F b = 20.3$. Here the temperature is extremely close to T_c ($t = 1 \times 10^{-4}$). The microscopic and phenomenological results are clearly different. Note the very extended Z range shown.

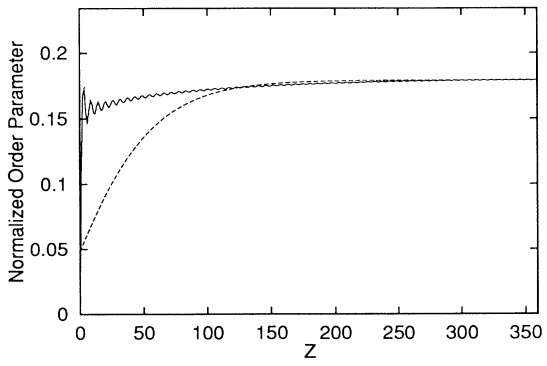

FIG. 7. Results for the normalized order parameter at $\pi k_F \xi_0 = 20$ (as in Figs. 3 and 6) and $t = 0.01$, as in Fig. 5. Again, the solid line represents the microscopic result and the dashed line the phenomenological result. This figure should be compared with Fig. 5.

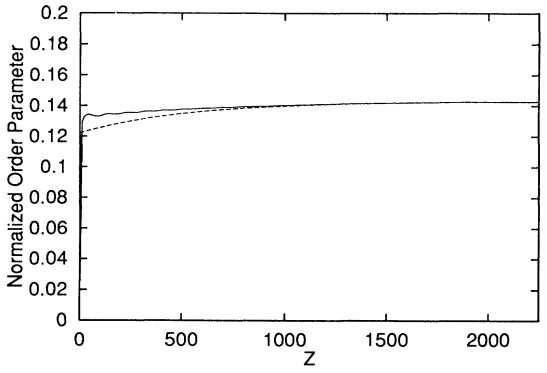

FIG. 8. The same calculation as in Fig. 6 for $\pi k_F \xi = 250$ and at $t = 2.12 \times 10^{-3}$ [$k_F \xi(T) = 1279$ and $k_F b = 3166$]. This is an intermediate case, where ξ_0 is neither extremely long nor very short.

still exists, but it is considerably smaller as can clearly be seen in the figure. At this temperature, both theories agree eventually at $k_F \xi_0 \sim 150$. The value of $k_F \xi_0$ we used in Fig. 8 is still smaller than that typical of standard BCS superconductors, but is nevertheless close to the textbook values for some of the metallic superconductors like niobium. Thus, we see that problems with the GL approach to this problem develop unless the condition $k_F \xi_0 \gg 1$ is very strictly satisfied.

It is nevertheless worthwhile to emphasize that some depletion of the gap function does occur near the surface, and we have investigated the temperature dependence of this depletion. We find that the depletion increases with temperature, but it is only at temperatures very close to T_c where a significant depletion occurs. A rough estimate, up to first order in ω_0/E_F and $1/k_F d$, which assumes that Δ_β's do not change too much from their bulk values except for β close to N, shows that the relative depletion $\delta\Delta/\Delta$ (averaged within one Fermi wavelength from the surface), at T very close to T_c, should satisfy

$$\frac{\delta\Delta(T)}{\Delta(T)} < \zeta \left[\frac{\omega_0}{E_F} - \frac{\pi}{k_F d} \right]$$

with a coefficient of proportionality ζ smaller than unity. The typical value of ω_0/E_F for a long coherence length superconductor is of order 0.01 or smaller, while in short ξ_0 superconductors ω_0/E_F takes values as large as 0.2. In the former case $1/k_F d$ is comparable to ω_0/E_F, which suggests a zero depletion, while in the latter case the relative depletion must be obvious but should not exceed 10%, which is in agreement with our results plotted in Fig. 6.

IV. CONCLUSIONS

We have studied boundary effects at a superconductor-insulator interface by examining the shape of the order parameter near such an interface. The results obtained are a function of ξ_0. When ξ_0 is very long at any temperature except extremely close to T_c, the order parameter, averaged over distances of order k_F^{-1}, has always a trivial constant shape, independent of the distance to the boundary. For smaller values of ξ_0, there is some depletion of the order parameter near the interface, physically due to the weaker coupling of high k_z electrons in this geometry. The depletion is, however, quite small, and the value of the order parameter at the surface remains very close to its bulk value. This is inconsistent with predictions based on extrapolation of GL theory which propose a dramatic depletion of the gap function near the interface, even at temperatures far from T_c. Our results make sense physically since the relevant lengths for short ξ_0 superconductors are of order k_F^{-1} and one cannot neglect all microscopic details as in standard GL theory. We also find that quantum-size effects, quite prominent in the large ξ_0 case, disappear as ξ_0 decreases.

Our results are consistent with recent experiments, measuring the energy gap in high-T_c oxides even at temperatures close to the transition temperatures.[6,7,9] This means that the boundary imposed geometrical factors, which we repeatedly emphasized, do not suppress superconductivity.

Although our method is not free of limitations, we believe that our conclusions apply to real materials with small ξ_0 such as oxide superconductors. There are two qualms that one could raise concerning the application of our procedures to real materials. The first is that, as ξ_0 decreases, the coupling becomes stronger and the simple BCS-like formalism that we use should be replaced by strong-coupling methods (e.g., for phonon coupling the Eliashberg[29] theory). However, there are good reasons to believe that this should not affect our qualitative conclusions because our results arise, in effect, from very general physical and geometrical principles. Consider first the weakening of the quantum oscillations: this is largely a reflection of the uncertainty principle. As the coupling increases, so does the range of wave vectors involved in the pairing, and the resonances must broaden as a result. Similarly, the behavior of $\Delta(z)$ can be understood (as remarked upon in Sec. III) from rather general considerations concerning the range of longitudinal and transverse wave vectors involved. Most important, our results show that the gap depletion is considerably smaller than predicted from GL even at moderate and relatively long values of $k_F \xi_0$ (see e.g., Fig. 8). We have, in fact, refrained from presenting here results for the very small values of $k_F \xi_0$ ($k_F \xi_0 \sim 1$) that would better correspond to high-temperature superconducting oxides. Thus, our qualitative conclusions regarding $\Delta(z)$ should hold.

The second consideration is that we have dealt only with isotropic materials here. Many short ξ_0 superconductors are highly anisotropic, layered structures consisting of superconducting and insulating layers. The general quantitative conclusions reached here as to the experimental observability of the gap should still apply. There may be additional interference effects occurring in such structures.[30] One also cannot disregard the difference in the energy dispersion relations for the motion in the x-y plane, as opposed to the transverse one. We plan to consider such effects elsewhere.

ACKNOWLEDGMENTS

We are indebted to S. W. Pierson, Z. Tešanović, and M. T. Béal-Monod for many useful discussions on this problem, and to A. M. Goldman for conversations on its experimental implications. We thank the Minnesota Supercomputer Institute for a grant of computer time. This work was supported in part by NSF under Grant No. DMR-8908094.

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