Surface behavior of the gap parameter in short-coherence-length superconductors: Photoemission and critical currents

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We examine how the behavior of the gap parameter near the boundary between a short-coherence-length superconductor and an insulator can be studied by using several experimental probes. We show how photoemission can be used directly to infer the profile of the gap near such a boundary. We show that photoemission and critical-current experimental results for high-temperature superconductors are all indicative of a nondepleted gap near the surface. This is inconsistent with standard Ginzburg-Landau results, but in agreement with recent microscopic calculations.

I. INTRODUCTION

The behavior of the gap parameter near the surface of a superconductor is of considerable importance in interpreting experimental results. Many of the probes that are used to infer bulk properties of superconductors are in fact surface probes and measure properties only within a small distance of the boundary. In particular, phenomena such as tunneling, photoemission spectra, and critical currents all require, for their interpretation, a detailed understanding of the behavior of the order parameter near a surface.

The realization that high-T_c superconductors (HTSC's) have very short coherence lengths, ξ_0, compared to those of "classical" superconductors, has prompted a reexamination of this question. It was pointed out[1] some time ago that extrapolation of the standard theory,[2] for the profile of the gap parameter near an interface to the case of short coherence lengths, leads to a severe depletion of the gap near a superconductor-insulator boundary. Such a depletion was suggested[1] as an explanation for the low critical-current values in high-T_c superconductors, and, if present, would have a variety of additional experimental consequences.

The extrapolation of the Ginzburg-Landau (GL) based theory[2] to the case where ξ_0 is small is not obviously justified, and there are recent indications that it may lead to incorrect results. Experimentally, both photoelectron spectroscopy[3] and tunneling,[4] which are essentially surface probes, have yielded values of the energy gap Δ substantially in excess of the weak-coupling value. The large values of Δ thus obtained would be hard to reconcile with any substantial boundary depletion. Furthermore critical-current values have been steadily increasing. From the theoretical point of view, the gap profile has been microscopically calculated in Ref. 5 for a jellium model. Although this calculation is only valid right at the transition, it shows that, for short coherence lengths, the gap is not depleted near the surface, that it has Friedel oscillations (reflecting the standard charge-density oscillations[6]), and that it may, in fact, be enhanced, under certain cases. Different theoretical considerations[7] point to a possible pairing interaction enhancement near the surface of a HTSC, again possibly leading to gap enhancement.

In this paper we consider, in view of the above considerations, the implications of the behavior of the gap near an interface for the analysis of photoemission experiments, critical currents, and tunneling. We emphasize the difference between the conclusions obtained using the standard result[2] and those obtained using a nondepleted gap. We model the latter case from the specific results of Ref. 5 although one should stress that the results depend chiefly on whether the gap is depleted or not, rather than on the specific model. In particular (i) we explain how photoemission spectra can be used to study the depth dependence of the gap parameter $\Delta(z)$ (z is the direction perpendicular to the surface), by collecting electrons from different escape depths (a preliminary version of this point is found in Ref. 8) (ii) we show that the experimental data on critical currents is consistent with a nondepleted gap; and (iii) we mention the implications for tunneling current measurements in short ξ_0 superconductors.

This paper is organized as follows: The next section (Sec. II) briefly recalls the result of Refs. 2 and 5 for the gap profile. Section III shows how photoemission can be used as a probe of $\Delta(z)$, while Sec. IV deals with critical currents and tunneling. Section V recapitulates the results.

II. THE GAP PARAMETER $\Delta(z)$

The behavior of the gap parameter $\Delta(z)$ near a surface may be quite different in a short-coherence-length superconductor ($\xi_0 \gtrsim l$, l is the average lattice spacing), than in the ordinary case where $\xi_0 \gg l$. We begin by briefly reviewing the conventional model[2] for the gap parameter profile. In this model, $\Delta(z)$ is given, near an interface, by the expression derived from GL theory:

$$\Delta(T,z)=\Delta_0(T)\tanh[(z+z_0)/\sqrt{2}\xi(T)] , \qquad (1)$$

where $\xi(T)$ is the temperature-dependent coherence length and Δ_0 is the gap parameter in the bulk. The quantity z_0, which is the position of the interface, is determined from the condition

$$\left.\frac{d\Delta(z)}{dz}\right|_{z=0} = \frac{\Delta(z=0)}{b} , \qquad (2)$$

where b is the "extrapolation length," $b \approx \xi_0^2/l$. One finds z_0 by solving these two equations. As has been clearly shown elsewhere (see Fig. 1 in Refs. 1 and 8), the solutions for the case of a small ξ_0 superconductor and for a conventional superconductor differ very significantly at the surface. When ξ_0 is small, the gap is severely depleted near the surface, while in the ordinary case it is not, except unobservably close to T_c.

In view of the obvious uncertainties involved in using this formulation in the regime $\xi_0 \approx l$, where the GL approach need not apply, one should consider other possible models. One alternative is to calculate $\Delta(z)$ microscopically. This has been done recently in Ref. 5 for a simple three-dimensional jellium model with a boson-mediated interaction. Results for the gap profile at the transition were obtained by solving the normal-state Bethe-Salpeter equation in the presence of a boundary to find the superconducting instability. It was found that the gap is not depleted but actually enhanced (by up to $\sim 25\%$) near the surface, and that there are Friedel-type oscillations in $\Delta(z)$. Although it is likely that inhomogeneities and impurities would wash out the oscillations, this would not result in depletion of the average gap.

The numerical results of Ref. 5 can be very roughly but conveniently represented in the limit where $\xi_0 \sim l$ as

$$\Delta(Z) = \Delta_0 \left[1 - \frac{\sin(Z+Z_0)}{(Z+Z_0)} \right] , \qquad (3)$$

where $Z \equiv 2k_F z$, k_F is the Fermi wave vector, and Z_0 is determined from the condition of charge neutrality.[9] The resulting value, $Z_0 = 3\pi/4$, is not very different, in this case, from that obtained from Eq. (2). In the remaining of this paper we will use Eq. (3), not only near T_c, but also, as a model of an undepleted gap, at temperatures well below T_c where some of the experiments we will discuss are performed. In Fig. 1, we have plotted Eq. (3). In order to show the contrast between Eqs. (1) and (3), we have included in this figure the plot (dashed line) of the result for $\Delta(z)$ obtained from the standard model [Eqs. (1) and (2)], for the same parameter values, and $\xi(T) \simeq \xi_0$. The depletion in the conventional model would be even larger for increased $\xi(T)$.

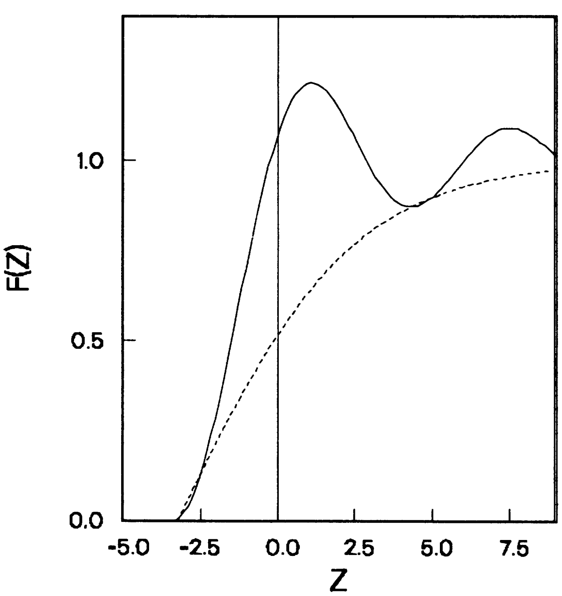

FIG. 1. Contrast of the gap profiles for $k_F\xi_0 = k_F l = 2$ as given by Eq. (3) (solid curve) and Eqs. (1) and (2) with $\xi(T) = \xi_0$ (dashed curve). The quantity plotted is defined by $\Delta(Z) = \Delta_0 F(Z)$ where Δ_0 is the bulk value. The vertical line is the superconductor boundary.

III. PHOTOEMISSION AS A PROBE OF $\Delta(z)$

Photoemission has long been used to study electronic states in solids. In a superconductor, an energy gap 2Δ forms around the Fermi surface in the electronic density of states and in principle ought to be reflected, along with a square-root singularity at $E_F - \Delta$, in the photoelectron spectrum.[10] Consequently, photoemission would be a natural probe of the gap characteristics. Photoemission as a tool to study superconductivity, however, is a relatively new technique because the energy gap for conventional superconductors is much too small (~ 1 meV) for typical instrument resolution (~ 25 meV), whereas the high-T_c superconductors have much larger gaps (up to 30 meV). Thus, measurements are currently possible in HTSC materials. In this section, we show how photoemission experiments in HTSC can be used to infer the profile function $\Delta(z)$ through measurements of the photoelectron spectra.

We begin with a description of the depths probed by photoemission. Photoelectrons collected in a photoemission experiment originate on a layer determined by the "escape depth" λ (basically the mean free path of the photoelectrons in the solid). The value of λ depends on the electron energy. Typical calculations are in Ref. 11 and are shown in Fig. 2. One can see that the value of λ as a function of electronic energy has a minimum at roughly 5–10 Å. Experiments[3] have been performed up to now only near this minimum. The electron energy, and therefore the escape depth λ, can readily be changed by varying the incoming photon energy. This allows one,

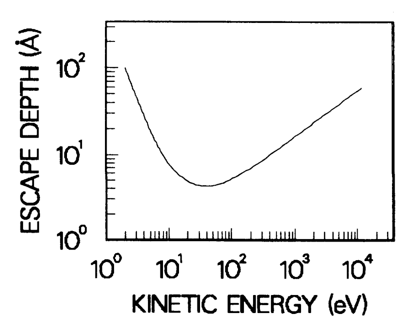

FIG. 2. Photoelectron escape depth vs electron energy from Ref. 11. Note the sharp minimum at about 5 Å.

in principle, to dial up the desired escape depth by changing the frequency of the ultraviolet photons. Thus one can perform a "depth spectroscopy."

To illustrate how this depth spectroscopy works, we consider a jellium model. In practice one is interested in photoelectrons originating near the Fermi surface, within an energy of roughly the order of the gap. This is a very narrow energy range in terms of the overall energy scale determined by the incoming ultraviolet photons. Since observed photoelectrons near the Fermi edge are little affected by multiple scattering their spectrum reflects the electronic density of states. In the presence of a z-dependent gap, the density of states would have to be the properly weighted average over the escape depth λ of the local density of states. This average can be written as:

$$n_{\mathrm{eff}}(E,\lambda) \propto \int_0^\infty \frac{dz}{\lambda} e^{-z/\lambda} \frac{|E|}{\sqrt{E^2-\Delta(z)^2}} , \tag{4}$$

where the energy E is measured from the Fermi surface, the argument of the square root is always positive, the factor of $|E|/\sqrt{E^2-\Delta(z)^2}$ is the familiar enhancement factor in the superconductivity density of states,[12] and the exponential is the probability of escaping from a depth z.

One can use Eq. (4) to calculate $n_{\mathrm{eff}}(E,\lambda)$ for any model of $\Delta(z)$. If $\Delta(z)$ is a Θ function (i.e., a constant in the superconductor), $n_{\mathrm{eff}}(E,\lambda)$ becomes the quasiparticle density, with a square-root singularity at the gap value. In general, n_{eff} will have broad peaks, the position of which will depend on λ and will reflect the behavior of $\Delta(z)$.

As illustrations, we have computed the right-hand side of Eq. (4) both for the model given by Eq. (3) and for the standard case of Eqs. (1) and (2). In both cases the sensitivity to λ is quite remarkable. In the first case [Eq. (3)] the results are shown in Fig. 3 for three different values of λ in the region around the experimentally accessible range. The results are convolved with a Gaussian to take into account instrument resolution. One can clearly see that the spectrum with short λ, with its peak farther away from the Fermi edge, reflects the enhanced value of the gap near the surface. As one increases λ, it is evident that the peak moves to the right, towards the bulk value of the gap. ($\Delta_0=0.1$ in the units used.) Note also how the shoulders in the solid curve correspond to the minima and maxima of the curve in Fig. 1. It is clear that, in general, spectra taken at different values of λ will reflect the function $\Delta(z)$ in considerable detail.

In Fig. 4 we show the results of the standard model for parameter values similar to those used in Fig. 3. We see that, as we increase the escape depth, the peak moves to the left, the opposite of the direction of movement for Fig. 3. The movement of the peak to the left reflects the larger value of the gap being probed. Tracking the movement of peaks as a function of the escape depth is one of the ways that photoemission can be used to reveal the properties of the gap function $\Delta(z)$.

The above examples are intended only as an illustration of the method. Obviously, a realistic calculation of the photoelectron spectrum should include band structure, matrix elements, final-state effects, and, in the case of most high-temperature materials, the effects of quasi-two-dimensionality. Yet, the effects that we are discussing are qualitative, and should therefore be very robust: If the spectrum shows a peak attributable to the energy gap and the energy gap varies with z, then the position of the peak will vary as one changes the photon energy (and hence λ), and the direction and size of the variation will be determined by the specific behavior of the function $\Delta(z)$.

Photoemission experiments[3] in HTSC materials have been performed at $\lambda \simeq 5-10$ Å. Hence, only a very narrow surface layer has been probed as yet. The reason for

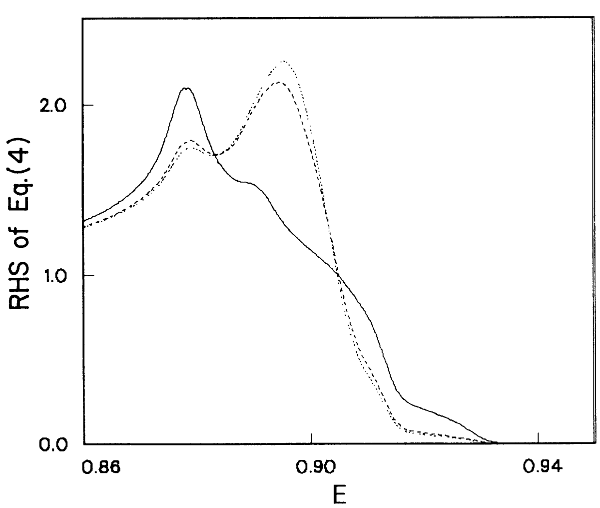

FIG. 3. Illustration of the photoemission "depth spectroscopy" method of the model gap profile of Eq. (3). The plotted quantity is the right-hand side of Eq. (4). The energy is in units of E_F and, at $k_F=0.40$ Å^{-1}, the three escape depth values are $\lambda=5$, 15, and 20 Å (solid, dashed, and dotted lines respectively).

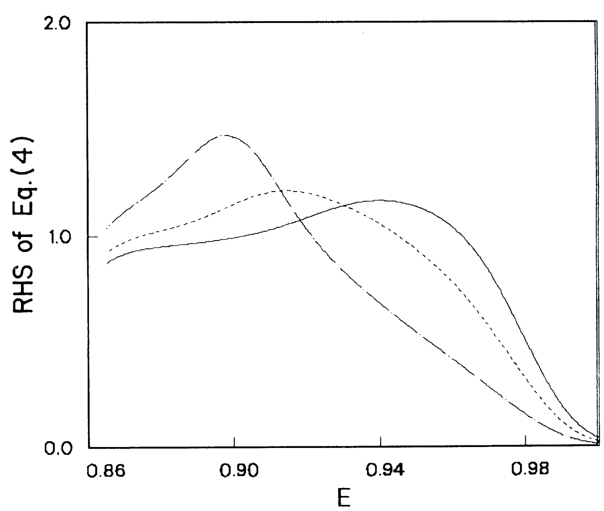

FIG. 4. The same calculation as in Fig. 3 for the standard gap profile [Eqs. (1) and (2)]. The parameter values are as in Fig. 3 with an addition, $\xi(T)=15$ Å, and the escape depths are $\lambda=5$ Å (solid curve), $\lambda=10$ Å (dashed curve), and $\lambda=20$ Å (dotted chain).

this choice is that, in the materials used, the corresponding photon energy is very close to the maximum in the photoemission cross section.[13] Thus, use of this particular energy maximizes photoelectron yield and produces better statistics. However, it is still possible[14] to vary the photon energy to obtain a sufficiently large change in λ and still have reasonable statistics in the experiment. Increasing the escape depths in these experiments will, we propose, manifest the surface behavior of the gap parameter.

Considering the very shallow range probed and the large values of the gap found (considerably in excess of weak-coupling values), the experimental results indicate that the order parameter is not depleted near the surface and are compatible with an enhancement. Any increase in the value of Δ with increasing λ is extremely unlikely because of its already large magnitude. Therefore the relevance of the standard model is put in question. The validity is further questioned in the next section.

IV. $\Delta(T)$ AND CRITICAL CURRENTS IN GRANULAR SUPERCONDUCTORS

In this section, we discuss critical-current measurements and how they also indicate a nondepleted surface gap. We will begin with the Ambegaokar-Baratoff[15] formula, which determines the critical current in a Josephson weak line:

$$I_c(T)=[\pi\Delta(T)/2eR_n]\tanh[\Delta(T)/2k_BT] , \tag{5}$$

where R_n is the normal metallic resistance of the weak link. This equation is valid for a wide range of temperatures and coherence lengths since it is not based on GL theory but rather on a microscopic calculation in which thermodynamic Green's function were used. Thus, $I_c(T)$ measures the gap Δ within a distance of the interface of the order of the coherence length. Sufficiently near to T_c Eq. (5) can be rewritten as

$$I_c(T)\simeq(\pi/4eR_nk_BT_c)\Delta^2(T) . \tag{6}$$

If one then simply replaces the temperature dependence of the gap function with the standard bulk Bardeen-Cooper-Schrieffer result $\Delta(T)\propto t^{1/2}$ (t is the reduced temperature), then one obtains near the transition, $I_c(T)\propto t$. This is correct if one neglects any temperature dependence induced by the depletion of the gap near the surface as one would do, for example, within the theory of Ref. 5 where no temperature-dependent length scale is involved.

On the other hand, as pointed out by Deutscher and Müller,[1] there is an additional temperature dependence in the gap profile as derived from Eqs. (1) and (2) that enters into Eq. (6). This arises from the t dependence of the GL coherence length. For $\xi(T)\gg z_0$, Eq. (1) can be written

$$\Delta(z=0,T)\propto\Delta_0(T)/\xi(T)\propto t , \tag{7}$$

where we have used $\xi(T)\propto t^{-1/2}$. Substitution of Eq. (7) into Eq. (6) produces the quadratic behavior $I_c\propto t^2$, in contradistinction to the $I_c\propto t$ behavior found in the absence of surface depletion.

The approximation used to obtain Eq. (7) is valid when $x\lesssim 0.4$ where x is the argument of the hyperbolic tangent in Eq. (5). Since[16] $\xi(T)=0.74\xi_0/t^{1/2}$, and $z_0\simeq b$ in the region of interest, this condition becomes

$$t^{1/2}\lesssim 0.4l/\xi_0 . \tag{8}$$

As an example, for $YBa_2Cu_3O_8$, $a\simeq4$ Å, $c\simeq12$ Å, $\xi_{ab}\simeq15$ Å, and $\xi_c\simeq4$ Å where a is the lattice spacing within the layer and c is the lattice spacing in the direction perpendicular to the layers; ξ_{ab} and ξ_c are the coherence lengths in the a and c directions, respectively. Since many experiments are done in bulk samples where the grains are randomly oriented, we believe it is best to average the directional dependences of the quantities to produce an effective coherence length and lattice spacing. One finds $\xi_{0\,\mathrm{eff}}\simeq l_{\mathrm{eff}}$. In this case the quadratic dependence would be valid for $T\gtrsim0.85T_c$. One could also argue that, since I_c will depend on the weak links with the smallest critical current, one should use the c-directional quantities, thereby producing a much wider temperature over which the quadratic behavior would be valid. This is consistent with the statement that the quadratic law holds "over a wide range of temperatures."[1] Our estimate is also consistent[17] with that of Ref. 18 for films which are strictly c-axis oriented, and one, therefore, would use the in-plane quantities a and ξ_{0ab}.

Experimentally, one can measure the temperature dependence of the critical current in weak links by exploiting the granular structure of the HTSC and treating the coupling between grains as Josephson coupling. This has been done extensively with the consensus of the results being the following: In the region, $0.1\lesssim t\lesssim0.3$, it is seen[19,20] that $I_c\propto t$. This crosses over to $I_c\propto t^{3/2}$ for $t\lesssim0.1$.[19–21] This crossover has been nicely explained by Ref. 19; the $\frac{3}{2}$ behavior is due to intragranular critical currents as modeled by Clem *et al.*,[22] which changes to the linear behavior of the intergranular critical currents when the condensation energy within the grains equals the Josephson coupling energy between them. Although Ref. 19 leaves it open that t^2 behavior may be seen extremely close to T_c, the data make it clear the t^2 behavior is not seen over the wide temperature range in which it was first predicted.[1] Note that the t^2 behavior, if it were present, should dominate the critical-current temperature dependence since it produces lower critical currents. Thus, the data are consistent with a nondepleted gap, as predicted by the microscopic model of Ref. 5.

Finally, we make a brief comment about the effect of the gap at the surface on tunneling experiments. Scanning tunneling microscopy (STM) has only recently proved successful in measuring the gap in HTSC's. Although these experiments were performed at very low temperatures, by attempting these experiments at progressively higher temperatures, STM can be used to study the nature of the gap by mapping its temperature dependence. By doing so, one ought to be able to draw more conclusions of the validity of the surface profile of Δ. A depleted gap at the surface would make the measurement of the gap by STM virtually impossible for temperatures closer to T_c. On the other hand, STM ought to be able to measure the gap for temperatures up to $0.9T_c$ if the gap is not depleted.

V. SUMMARY

We have studied the experimental implications of the surface behavior of the gap parameter. We have described how photoemission can be used as a "depth spectroscopy" tool to infer the gap profile function. We have shown that present experimental evidence is inconsistent with standard GL calculations of the gap profile, and agrees with models in which there is no gap depletion at the surface. Finally, we hope that this work encourages further study of the gap parameter near a surface, particularly through photoemission, critical-current measurements, and tunneling.

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