Surface effects in two-band superconductors: Application to MgB_2

E. Bascones* and F. Guinea
Instituto de Ciencia de Materiales, Consejo Superior de Investigaciones Científicas, Cantoblanco, 28049 Madrid, Spain
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Metals with many bands at the Fermi level can have different band dependent gaps in the superconducting state. The absence of translational symmetry at an interface can induce interband scattering and modify the superconducting properties. We dicuss the relevance of these effects to recent experiments in MgB_2.

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I. INTRODUCTION

Recent experiments[1] report the existence of superconductivity at nearly 40 K in MgB_2. Its origin is not completely elucidated. The material shows a pronounced isotope effect,[2] and the density of states is well approximated by the BCS theory.[3,4] Tunneling experiments suggest that the superconducting properties at the surface of the material differ from the expected bulk behavior.[3,4] In addition, photoemission results[5] suggest the existence of an *s*-like gap, Δ, such that $\Delta \leqslant 3k_BT_c$. A possible explanation of this result is that the measured Δ is the average of different gaps. The present work is motivated by the persistent discrepancy between the gap values measured in different experiments, and, particularly, the excellent fit to a BCS gap too low to explain the value of the critical temperature observed in tunneling experiments reported in Ref. 3.

Band structure calculations suggest that there are, at least, two types of bands at the Fermi surface: a hole band, built up of boron σ orbitals, with a weak dispersion in the direction perpendicular to the boron planes, and a broader band, built up mainly of π boron orbitals, which shows a significant dispersion in the direction perpendicular to the boron planes. Theoretical arguments favor, as the origin of the superconductivity, the holelike σ band,[6–9] or the π band.[10] The existence of two bands with different physical properties is assumed in other models for the superconducting properties of MgB_2.[11,12] It has been argued that the upper critical field can be best modeled if the superconducting properties depend on the specific band at the Fermi level.[13,14] On general grounds, it is reasonable to assume that the σ and π bands in MgB_2 will have different contributions to the superconducting properties, and that the superconducting gap needs not be the same in the two bands.

The existence of many bands at the Fermi level, with very different physical properties, is probably a generic feature of intermetallic superconductors.[15,16] In these materials, it can be expected that the pairing interaction which gives rise to the superconductivity will depend on the details of each band. If this is the case, there is not a uniform gap at the Fermi level. The superconducting state resembles, in this respect, that of an anisotropic superconductor. The effects of interband scattering on the bulk properties of a superconductor with two different bands at the Fermi level was studied in Ref. 17. Those results were extended in Ref. 18.

Interband scattering can be induced by any defect which breaks the translational symmetry of the lattice, including lattice imperfections, phonons, and surfaces or grain boundaries. Thus, in materials with many bands crossing the Fermi level, one can expect the superconducting properties near a surface to differ from those at the bulk. This effect should be more pronounced in systems with many irregular interfaces, such as ceramic and granular materials.

In the present work, we study pair breaking effects at the surfaces of many band superconductors. The main difference with the theory developed in Refs. 17, 18 is that, when interband scattering is restricted to the surface region, the superconducting gaps are inhomogeneous, because the value of the gaps within the bulk of the system is not affected by the presence of a surface. In order to take this effect into account, we develop a method which differs from the standard treatment of pair breaking effects in conventional[19] or unconventional[20] superconductors. We use the simplest possible model where non trivial effects are expected, presented in the next section. Section III presents the main results, and the main conclusions which can be drawn from them are discussed in Sec. IV.

II. THE MODEL

A. The Hamiltonian

Superconductors with different bands at the Fermi level, where each of these bands have different pairing interactions have already been discussed in the literature.[21,22] The simplest model contains two bands, with two different densities of states and pairing interactions. The generic Hamiltonian of the system is

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\rm int} + \mathcal{H}_{pb}$$

$$\mathcal{H}_0 = \sum_{i=1,2;\vec{\mathbf{k}},s} \epsilon_{i,\vec{\mathbf{k}}} c^\dagger_{i,\vec{\mathbf{k}},s} c_{i,\vec{\mathbf{k}},s} + \text{H. c.}$$

$$\mathcal{H}_{\rm int} = \sum_{i=1,2;\vec{\mathbf{k}}\vec{\mathbf{k}}'} -g_i c^\dagger_{i,\vec{\mathbf{k}}\uparrow} c^\dagger_{i,-\vec{\mathbf{k}}\downarrow} c_{i,\vec{\mathbf{k}}'\uparrow} c_{i,-\vec{\mathbf{k}}'\downarrow}$$

$$- \sum_{\vec{\mathbf{k}}\vec{\mathbf{k}}'} g' c^\dagger_{1,\vec{\mathbf{k}}\uparrow} c^\dagger_{1,-\vec{\mathbf{k}}\downarrow} c_{2,\vec{\mathbf{k}}'\uparrow} c_{2,-\vec{\mathbf{k}}'\downarrow},$$

$$\mathcal{H}_{pb} = \sum_s \int d^3\vec{\mathbf{r}} V f(z) \psi^\dagger_{1,s}(\vec{\mathbf{r}}) \psi_{2,s}(\vec{\mathbf{r}}). \quad (1)$$

Electrons within each band experience a different pairing interaction g_i, leading to two superconducting gaps. The two

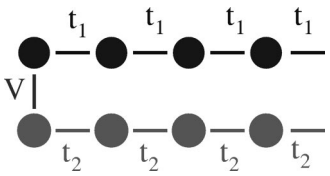

FIG. 1. Sketch of the lattice solved in the text.

bands are coupled by the interaction g'. Otherwise, in the absence of interband scattering the two gaps open at different temperatures $T_{c,i} \propto \omega_0 \exp(-W_i/g_i)$, where W_i is the bandwidth and ω_0 is a cutoff related to the pairing mechanism. Specific heat measurements[23] seem to exclude this possibility in MgB_2. We neglect intraband scattering, which does not give rise to pair breaking effects, at least to lowest order.[24] Finally, we assume a constant interband scattering term, localized near the surface. The function $f(z)$ is peaked near the surface, located at $z=0$. The width of $f(z)$ is of the order of a lattice spacing. With these restrictions, the model described in Eq. (1) includes six parameters, with dimensions of energy: the density of states at the Fermi level of each band $N_i(\epsilon_F)$, the pairing interactions g_i and g', and the scattering potential V.

B. Pair breaking effects

The lack of translational symmetry induced by the surface makes it convenient to solve directly the Bogoliubov–de Gennes equations derived from Eq. (1). We use a discrete tight binding model for this purpose. We assume that each band can be described by a single orbital per site, and that there are local attractive interactions which induce the pairing. The model reduces, in the absence of interband scattering, to two coupled negative U Hubbard models. In this basis, interband scattering can be included by allowing for hopping from one orbital to the other at any given lattice site. Our discretized model in real space becomes

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\rm int} + \mathcal{H}_{pb},$$

$$\mathcal{H}_0 = \sum_{l;ijs} t_l c^\dagger_{l,i,s} c_{l,j,s} + \text{H. c.},$$

$$\mathcal{H}_{\rm int} = -\sum_{l,i} U_l c^\dagger_{l,i,\uparrow} c_{l,i,\uparrow} c^\dagger_{l,i,\downarrow} c_{l,i,\downarrow} - \sum_i U' c^\dagger_{1,i,\uparrow} c_{1,i,\uparrow} c^\dagger_{2,i,\downarrow} c_{2,i,\downarrow},$$

$$\mathcal{H}_{pb} = \sum_{s, i \in i_s} V c^\dagger_{1,i,s} c_{2,i,s}. \qquad (2)$$

We assume that the lattice is a semi-infinite chain, and that interband scattering is restricted to the outermost site, as schematically depicted in Fig. 1.

The BCS equations are solved using the standard equivalence of the attractive Hubbard model in a bipartite lattice to the repulsive Hubbard model.[25] The semiinfinite model is solved using transfer matrix techniques,[26] which are described in the Appendix. The order parameters are calculated selfconsistently in a layer of m sites, which are coupled to an homogeneous chain where they take the bulk values. The position dependent values of the gaps can be expressed in terms of the local order parameters as

$$\Delta_i = \frac{U_i}{2} \langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle + \frac{U'}{2} \langle c^\dagger_{j\uparrow} c^\dagger_{j\downarrow} \rangle. \qquad (3)$$

We present results obtained with $m=32$. This idealized one-dimensional model can be viewed as an approximation to the inhomogeneous layered structure expected near the surface. Note that the BCS equations exclude the possibility of one-dimensional fluctuations, so that the solutions to be discussed below do not show unphysical one dimensional features.

III. RESULTS

We use as unit of energy one of the hopping parameters in Eq. (2), $t_1=1$. We assume that band 1 represents the total effect of the two σ bands in MgB_2. The density of states in the π band is roughly one third that of the two σ bands,[8] and we set $t_2=3t_1$. We assume that the superconductivity is mostly due to the σ band, and we choose the parameters U_1, U_2, and U' so that the smallest gap is less than one half the largest one, at zero temperature.[3] A reasonable combination is $U_1=0.5t_1, U_2=0$, and $U'=0.2t_1$ so that $\Delta_1=0.0212t_1$ and $\Delta_2=0.0079t_1$. The choice $U_2=0$ reflects the likely possibility that the π band, on its own, is not a superconductor, as in compounds with a similar structure, such as graphite. The critical temperature in these units is $T_c=0.011t_1$. Using the experimental value $T_c \approx 40$ K, the value of the unit of energy, t_1 is equal to 0.3 eV, and the bulk density of states of the σ band is 0.5 states/eV cell, which has the right order of magnitude.[8] Note that, with these parameters, the model is well into the BCS weak coupling regime. The coherence length, in lattice units, is given by $\xi_i \approx t_i/\Delta_i$, so that $\xi_\sigma \sim 50$ lattice units.

We finally must determine the strength of the interband scattering at the surface V. The mixing of the boron π and σ bands is strongly suppressed in the bulk. This effect is weakened if the relative angles between nearest neighbor B ions is modified at the surface, so that the σ bands are not built up of sp^2 orbitals only. The interband hopping associated with these deformations will be a fraction of the bulk hopping terms. We take in the following $V=0.4t_1 \approx 0.12$ eV, and restrict this interband hopping to the outermost layer. The order parameters near the surface, at zero temperature, are plotted in the inset in Fig. 2. They are almost uniform, suggesting the interband scattering at the surface does not change appreciably the order parameter.

Interband scattering has a stronger influence on the density of states near the surface. The results for the outermost site are plotted in Fig. 2. The coupling between the two bands shows in the existence of peaks in the density of states at the two gap positions, while, in the bulk, each band displays a single peak at the value of the corresponding gap.

The overall features in the density of states remain the same at relatively high temperatures, as shown in Fig. 3,

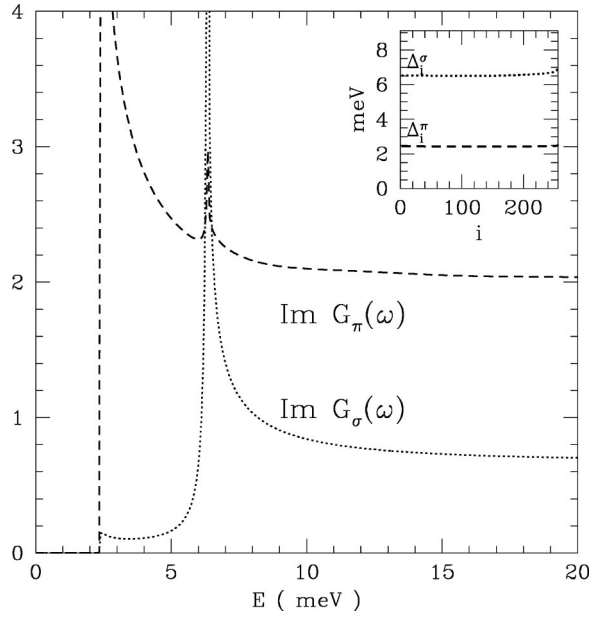

FIG. 2. Density of states at the surface at zero temperature. The inset shows the superconducting order parameters in each band as a function of position from the surface.

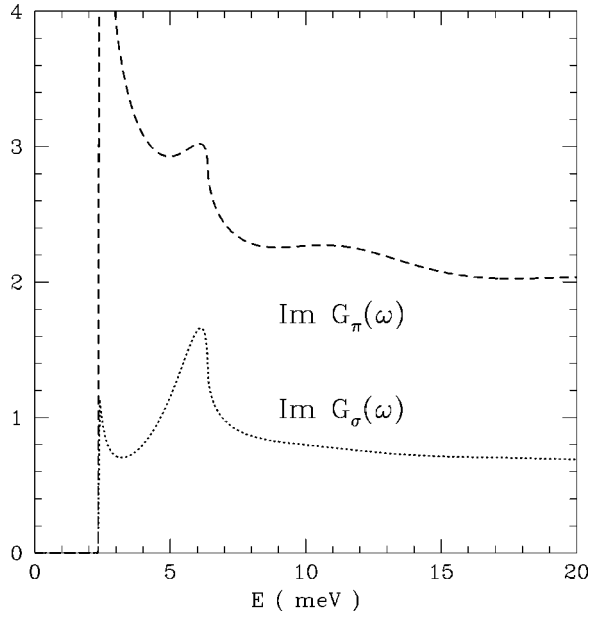

FIG. 4. Density of states at the surface at $T=0$ K, in the presence of strong interband scattering at the surface.

where the results at $T=36$ K are shown. The scale at which the smallest gap closes is determined by the largest gap.

In some experiments, like point contact spectroscopy, the probe can be an additional source of interband scattering, at the position where the measurement is being made. In the presence of strong interband scattering at the surface, the perturbation in the densities of states is more pronounced, as shown in Fig. 4, calculated using $V=t_1\approx 0.3$ eV. A single smeared gap will be observed in an experiment of this type.

It is interesting to note that, if the value of the gaps in the bulk were of opposite sign, a midgap state, induced by Andreev reflections, should arise. The problem considered here maps onto that of a dimerized chain. If the value of the dimerization changes sign, a gap state always arises, as extensively discussed in connexion to solitons in polyacetilene.[27] This situation, two gaps of opposite sign, is likely to occur when the pairing mechanism arises from repulsive interactions. Thus, the observation of surface Andreev states can give information about the nature of the pairing.

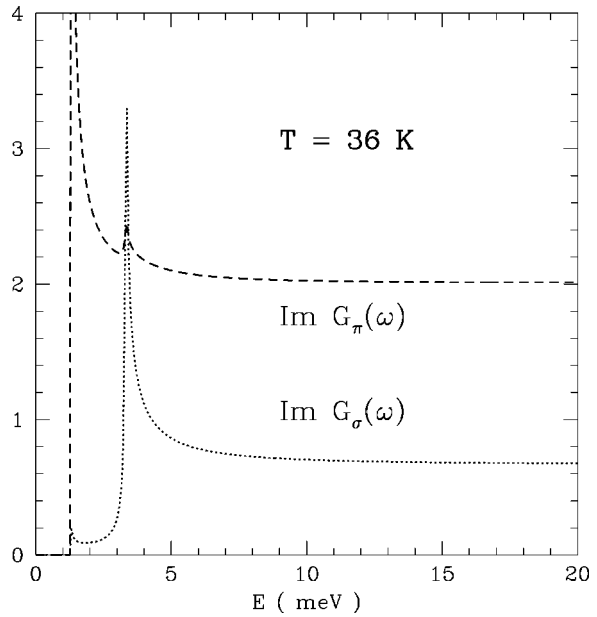

FIG. 3. Density of states at the surface at $T=36$ K.

IV. CONCLUSIONS

We have analyzed the effects of interband scattering at the surface, in a superconductor with a two bands at the Fermi level, and different pairing strengths for each band. Surface scattering, for reasonable values of the parameters, is ineffective in changing the gaps near the surface. This is consistent with the fact that, in a conventional weak coupling BCS superconductor, the coherence length is much greater than the surface layer where strong scattering is expected.

The influence of the surface scattering induces significant changes in the density of states near the surface. The density of states of each band shows peaks at the positions of the gaps associated with the other bands. There is, however, always a minimum gap, below which the density of states vanishes. This gap, $\Delta_{\min}$, has a weak temperature dependence until close to the bulk critical temperature.

We have used a set of parameters appropiate for MgB_2. We assume that there is a wide, delocalized band, and a narrower and more localized band, which determines mostly the superconducting properties. The wide band (derived from the π orbitals) has the smallest gap, and is weakly influenced by the narrow band. The narrow band shows stronger features at both the small and large gaps. Tunneling experiments are highly sensitive to the delocalization of the wave func-

tion. Hence, it is possible that they measure the density of states associated to the wider band (π orbitals). If this is the case, the observations will show a single gap, well approximated by the BCS expression. This gap should have a weak temperature dependence, until temperatures comparable to the bulk critical temperature.[3]

The strength of the interband scattering at the surface studied here can depend on the experimental setup, and it may be enhanced in some experiments. If that is the case, a single smeared gap will be observed, of magnitude comparable to $1.76\ T_c$.[28] Finally, it is interesting to note that, if the gaps in the two bands were of opposite signs, as expected from electron-electron pairing mechanisms, a surface state near the center of the gap should appear.

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APPENDIX

The problem defined by the hamiltonian in Eq. (2) with the geometry shown in Fig. 1 reduces to the calculation of the density of states in $2m$ sites, with gap values Δ_i and connected by hopping terms which can be either t_1, t_2, or V. The attractive Hubbard model $U_i<0$, can be mapped onto the repulsive Hubbard model, in a bipartite lattice, by the transformation

$$c^\dagger_{i\uparrow}\rightarrow d^\dagger_{i\uparrow},$$

$$c_{i\uparrow}\rightarrow d_{i\uparrow},$$

$$c^\dagger_{i\downarrow}\rightarrow(-1)^i d_{i\downarrow},$$

$$c_{i\downarrow}\rightarrow(-1)^i d^\dagger_{i\downarrow}. \tag{A1}$$

The anomalous expectation value in the superconducting state $\Psi_i=\langle c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}\rangle$ is mapped onto a staggered magnetization in the transverse direction $\Psi_i=(-1)^i\langle c^\dagger_{i\uparrow}c_{i\downarrow}+c^\dagger_{i\downarrow}c_{i\uparrow}\rangle$. At half filling, there is an additional symmetry which allows us to rotate this magnetization to the z axis. Then, $\Psi_i=\langle(-1)^i(c^\dagger_{i\uparrow}c_{i\uparrow}-c^\dagger_{i\downarrow}c_{i\downarrow})\rangle$. In this representation, the hamiltonian does not mix the spins, and it can be decomposed into two boxes, one for each spin direction. The problem is reduced to the calculation of the density of states in a tight binding chain with variable hoppings, $t_{i,i\pm1}$, and energy levels, ϵ_i, which are related to the local value of the gaps. The gaps must be determined selfconsistently from the values of the Ψ_i's.

The fractions

$$g_{n,n\pm1}(\omega)=t_{n,n\pm1}\frac{G_{n,n'}(\omega)}{G_{n\pm1,n'}(\omega)} \tag{A2}$$

are independent of n', and satisfy

$$g_{n,n\pm1}(\omega)=\frac{t^2_{n,n\pm1}}{\omega-\epsilon_{n,n\pm1}-t_{n\pm1,n\pm2}g_{n\pm1,n\pm2}(\omega)} \tag{A3}$$

and

$$G_{n,n}(\omega)=\frac{1}{\omega-\epsilon_n-t_{n,n-1}g_{n,n-1}(\omega)-t_{n,n+1}g_{n,n+1}(\omega)}. \tag{A4}$$

Thus, the problem can be solved by iteration from the boundaries, provided that one knows the values of $g_{\pm m,\pm m\pm1}$. These values can be easily be calculated, if one assumes that the values of the ϵ_i's are constant beyond position m.[29] Finally, the selfconsistency requirement for the values of $\epsilon_i, i=1,2m$ must be satisfied.

*Present address: Department of Physics, University of Texas at Austin, Austin, Texas 78712.

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