Surface effects in multiband superconductors. Application to MgB$_2$.

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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 discuss the relevance of these effects to recent experiments in MgB$_2$.

I. INTRODUCTION

Recent experiments report the existence of superconductivity at nearly 40K in MgB$_2$. Its origin is not completely elucidated. The material shows a pronounced isotope effect, and the density of states is well approximated by the BCS theory. Tunneling experiments suggest that the superconducting properties at the surface of the material differ from the expected bulk behavior. In addition, photoemission results suggest the existence of an s-like gap, $\Delta$, such that $\Delta \leq 3k_BT_c$. A possible explanation of this result is that the measured $\Delta$ 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 [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 $\sigma$ orbitals, with a weak dispersion in the direction perpendicular to the boron planes, and a broader band, built up mainly of $\pi$ 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 hole like $\sigma$ band, or the $\pi$ band. The existence of two bands with different physical properties is assumed in other models for the superconducting properties of MgB$_2$. 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. On general grounds, it is reasonable to assume that the $\sigma$ and $\pi$ bands in MgB$_2$ will have different contributions to the superconducting phases, 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. 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 [1].

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. The simplest model contains two bands, with two different densities of states and pairing interactions. We will consider the hamiltonian:

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

$$
\mathcal{H}_0 = \sum_{i=1,2;\vec{k},\sigma} \epsilon_{i,\vec{k}} c_{i,\vec{k},\sigma}^\dagger c_{i,\vec{k},\sigma}
$$

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

$$
\mathcal{H}_{\text{pb}} = \sum_{\vec{k},\sigma} \frac{1}{2} \sum_{i,j=1,2} \sum_{\vec{k},\vec{k}'} \alpha_{ij} \langle \sigma_{\vec{k},\vec{k}'} \rangle c_{i,\vec{k},\sigma}^\dagger c_{j,\vec{k}',\sigma}
$$
Electrons within each band experience a different pairing interaction, \( g_i \), leading to two superconducting gaps. The two 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 \( \omega_0 \) is a cutoff related to the pairing mechanism. Specific heat measurements \( [22] \) seem to exclude this possibility in MgB\(_2\). Figit intraband scattering, which does not give rise to pair breaking effects, at least to lowest order \( [22] \). Fi-}

\[
\mathcal{H}_{pb} = \sum_{s} \int d^3 \mathbf{r} f(z) \psi_{1,s}^\dagger(\mathbf{r}) \psi_{2,s}(\mathbf{r})
\]

(1)

B. Pair breaking effects.

The lack of translational symmetry induced by the surface makes it convenient to solve directly the the Bogoliubov-de Gennes equations derived from (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 with 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:

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{int} + \mathcal{H}_{pb}
\]

\[
\mathcal{H}_0 = \sum_{l,i,j,s} t_{ij} c_{l,i,s}^\dagger c_{l,j,s} + \text{h.c.}
\]

\[
\mathcal{H}_{int} = -\sum_{l,i} U_{l} c_{l,i,\uparrow}^\dagger c_{l,i,\downarrow} c_{l,i,\downarrow}^\dagger c_{l,i,\uparrow} - \sum_{i} U' c_{i,\uparrow}^\dagger c_{i,\downarrow} c_{2,i,\downarrow}^\dagger c_{2,i,\uparrow}
\]

\[
\mathcal{H}_{pb} = \sum_{s,i \in \ell} V c_{1,i,s}^\dagger c_{2,i,s}
\]

(2)

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

III. RESULTS

The BCS equations are solved using the standard equivalence of the attractive Hubbard model in a bipar- tite lattice to the repulsive Hubbard model \( [23] \). The semiinfinite model is solved using transfer matrix tech- niques \( [24] \), which are described in the Appendix. The gaps are calculated selfconsistently in a layer of \( m \) sites, which are coupled to an homogeneous chain where the gaps take the bulk values, where the gaps are defined as:

\[
\Delta_i = \frac{U_{l}}{2} (c_{l,i,\uparrow}^\dagger c_{l,i,\uparrow}) + \frac{U'}{2} (c_{i,\uparrow}^\dagger c_{i,\downarrow})
\]

(3)

We present results obtained with \( m = 32 \). This ideal- ized one dimensional model can be viewed as an approxi- mation 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 unphys- ical one dimensional features.
The gaps are almost uniform, suggesting that the influence of the interband scattering on the value of the gaps is very small.

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, where the results at T=36K 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 $V = t_1 \approx 0.3\text{eV}$. 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 [25].

IV. CONCLUSIONS

We have analyzed the effects of interband scattering at the surface, in a superconductor with a many 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, a minimum gap, below which the density of states near the surface vanishes. This gap, $\Delta_{\text{min}}$, has a weak temperature dependence until close to the bulk critical temperature.

We have used a set of parameters appropriate 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 $\pi$ 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.

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 1.7 T$_c$ [27].

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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VI. APPENDIX

The problem defined by the Hamiltonian in eq. (3) with the geometry shown in Fig. 1 reduces to the calculation of the density of states in 2$m$ sites, with gap values $\Delta_i$ and connected by hoppings 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:

$$
c_i \rightarrow d_i
$$

$$
c_i \uparrow \rightarrow d_i \uparrow
$$

$$
c_i \downarrow \rightarrow (-1)^i d_i \downarrow
$$

$$
c_i \rightarrow (-1)^i d_i
$$

(4)

The superconducting order parameter, $\Psi_i = \langle c_i \dagger c_i \rangle$, is mapped onto a staggered magnetization in the transverse direction. At half filling, there is an additional symmetry which allows us to rotate this magnetization to the z-axis. Then, $\Psi_i = ((-1)^i(c_i \dagger c_i' - c_i c_i'))$. 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, $t_{1,2}$, and energy levels, $\epsilon_i$, which are related to the local value of the gaps. The gaps must be determined selfconsistency from the values of the $\Psi_i$'s.

The fractions:

$$
g_{n,n+1}(\omega) = t_{n,n+1} \frac{G_{n,n+1}(\omega)}{G_{n,n+1,n'}(\omega)}
$$

are independent of $n'$, and satisfy:

$$
g_{n,n+1}(\omega) = \frac{1}{\omega - \epsilon_{n,n+1} - t_{n,n+1,n+2,2}(\omega)}
$$

and:

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

Thus, the problem can be solved by iteration from the boundaries, provided that one knows the values of $g_{\pm m,\pm m+1}$. These values can be easily be calculated, if one assumes that the values of the $\epsilon_i$'s are constant beyond position $m$ [26]. Finally, the selfconsistency requirement for the values of $\epsilon_i$, $i = 1, 2m$ must be satisfied.

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