Andreev bound states at the interface of antiferromagnets and *d*-wave superconductors

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We set up a simple transfer matrix formalism to study the existence of bound states at interfaces and in junctions between antiferromagnets and *d*-wave superconductors. The well-studied zero energy mode at the {110} interface between an insulator and a $d_{x^2\text{-}y^2}$ wave superconductor is spin split when the insulator is an antiferromagnet. This has, as a consequence, that any competing interface induced superconducting order parameter that breaks the time reversal symmetry needs to exceed a critical value before a charge current is induced along the interface.

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The discovery of the symmetry of the superconducting order parameter has been one of the most successful studies of high-T_c materials. Angular resolved photoemission spectroscopy has revealed the nodes in the gap function, and tunneling experiments have proven the sign change between adjacent lobes of the $d_{x^2\text{-}y^2}$ wave gap.[1–3] It was first shown by Hu[4] that this sign change can lead to zero energy Andreev bound states (ZEBS) at the surface of an insulator and a *d*-wave superconductor. These Andreev bound states were later identified with the zero bias conductance peaks observed in tunneling experiments. The experiments by Covington *et al.*[5] indicated, however, that the surface states were spontaneously split by a minigap. Several ideas were proposed for this effect;[6] one of which included the induction of a time reversal symmetry breaking *is* component of the order parameter near the interface.[7] The resulting gap $d+is$ lowers the condensation energy by lifting the directional degeneracy of the ZEBS.[8] Later Honerkamp *et al.*[9] used a tight-binding model with on-site repulsion and spin dependent nearest neighbor interaction to self-consistently study the competition between additional induced orders near the surface of an insulator and a $d_{x^2\text{-}y^2}$ wave superconductor.

The motivation for studying close domains of antiferromagnetism and superconductivity arises from the existence of striped domains in the cuprate materials. This was further emphasized by recent elastic neutron scattering experiments showing that static antiferromagnetic order is induced in a superstructure around the vortices in the mixed state of $La_{2-x}Sr_xCuO_4$ (Ref. 10) and $La_2CuO_{4+\delta}$.[11] These experiments are consistent with a static environment of alternating antiferromagnetic and *d*-wave superconducting stripes around the vortex cores. Thus the electronic states in such an environment is an important question.

Inspired by these experiments we set up a simple transfer matrix method to identify bound states on interfaces and junctions between antiferromagnets and *d*-wave superconductors. In particular we discuss a single interface separating antiferromagnetic and *d*-wave superconducting half-planes (AF/dSC), and point out a few differences from the conventional nonmagnetic insulator–*d*-wave superconductor interface (I/dSC). Note that the antiferromagnetism forces us to study a lattice model which is contrary to the usual discussion of Andreev interference in terms of semi-classical continuum models.

A simple lattice model that includes both *d*-wave superconductivity and antiferromagnetism is given by the Hamiltonian

$$H=-t\sum_{\langle n,m\rangle\sigma} c^\dagger_{n\sigma}c_{m\sigma}+\text{H.c.}-\mu\sum_{n\sigma} c^\dagger_{n\sigma}c_{n\sigma} \tag{1}$$

$$+\sum_{\langle n,m\rangle} \Delta_{n,m}c^\dagger_{n\uparrow}c^\dagger_{m\downarrow}+\text{H.c.} \tag{2}$$

$$+\sum_n M_n(c^\dagger_{n\uparrow}c_{n\uparrow}-c^\dagger_{n\downarrow}c_{n\downarrow}), \tag{3}$$

where $\langle n,m\rangle$ denotes nearest neighbors. M_n and $\Delta_{n,m}$ are the spatially dependent magnetic and superconducting order parameters. This Hamiltonian is quadratic and can be diagonalized by a Bogoliubov–de Gennes (BdG) transformation

$$\gamma^\dagger_\sigma=\sum_n u_\sigma(n)c^\dagger_{n\sigma}+\sigma v_\sigma(n)c_{n-\sigma}, \tag{4}$$

with σ equal to $+1$ (-1) for spin-up (-down). We use the notational convention that the spin indices on u_σ and v_σ follow that on the Bogoliubov operators $\gamma^\dagger_\sigma$.

In the case of a $d_{x^2\text{-}y^2}$-wave superconductor there are two qualitatively different orientations of the interface: the {100} and {110} directions corresponding to a vertical and diagonal stripe respectively. Both cases are studied below with the x-axis (y-axis) chosen perpendicular (parallel) to the interface which is placed at $x=0$. The lattice constant is set to unity. Assuming translational invariance along the y-direction the AF/dSC interface reduces to a one dimensional problem. For the {100} interface the resulting Bogoliubov–de Gennes equations have the forms

$$\begin{aligned}\epsilon_\sigma u_{q\sigma}(x)=&-t[u_{q\sigma}(x+1)+u_{q\sigma}(x-1)+2\cos(q)u_{q\sigma}(x)]\\&-\mu u_{q\sigma}(x)+\sigma M_x u_{q+Q\sigma}(x)\\&+(\Delta^d_{x+1,x})v_{q\sigma}(x+1)+(\Delta^d_{x-1,x})v_{q\sigma}(x-1)\\&+2\cos(q)(-\Delta^d_x)v_{q\sigma}(x),\end{aligned} \tag{5}$$

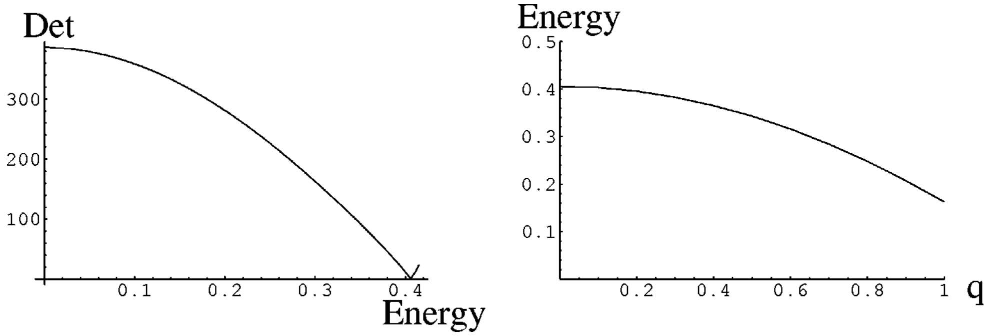

FIG. 1. {100} interface between an antiferromagnet and a d-wave superconductor: (a) Determinant of α_r as a function of energy ϵ for $q=0.1$. There is a de Gennes/Saint-James bound state close to the superconducting gap edge which is located at $\epsilon=0.42t$ for $q=0.1$. As seen in (b), their dispersion has the expected downward cosine form until it merges with the continuum.

$$\begin{aligned}\epsilon_\sigma v_{q\sigma}(x)=&t[v_{q\sigma}(x+1)+v_{q\sigma}(x-1)+2\cos(q)v_{q\sigma}(x)]\\&+\mu v_{q\sigma}(x)+\sigma M_x v_{q+Q\sigma}(x)\\&+(\Delta^{*d}_{x+1,x})u_{q\sigma}(x+1)+(\Delta^{*d}_{x-1,x})u_{q\sigma}(x-1)\\&+2\cos(q)(-\Delta^{*d}_x)u_{q\sigma}(x),\end{aligned}\tag{6}$$

after Fourier transforming along the y direction. The corresponding equations for the Fourier components $u_{q+Q\sigma}$ and $v_{q+Q\sigma}$ are obtained by simply performing the substitution $q\rightarrow q+Q$. These BdG equations are diagonal in the spin index with the only difference between spin-up and -down being the sign of the magnetic term.

A simple way to study bound states at the interface is in terms of the transfer matrix method.[12] Thus we introduce a (q,ϵ)-dependent matrix $T(x+1,x)$ defined by

$$\Psi(x+1)=T(x+1,x)\Psi(x),\tag{7}$$

which transfers the spinor Ψ from site x to site $x+1$. For a model with nearest neighbor coupling, Ψ takes the explicit form $\Psi(x)=[\psi(x),\psi(x-1)]$, where

$$\psi(x)=[u_{q\sigma}(x),v_{q\sigma}(x),u_{q+Q\sigma}(x),v_{q+Q\sigma}(x)].\tag{8}$$

The associated 8×8 transfer matrix has the general form

$$T(x+1,x)=\begin{pmatrix}A & B\\ 1 & 0\end{pmatrix},\tag{9}$$

where A (B) denotes the 4×4 coefficient-matrix connecting $\psi(x+1)$ and $\psi(x)$ $[\psi(x-1)]$ determined from the BdG equations (5) and (6). In the simplest case of a sharp interface we have the following spatial dependences of M_x and Δ_x:

$$M_x=M(-1)^x \quad \text{for} \quad x\leqslant 0,\tag{10}$$

$$\Delta_x=\Delta_d \quad \text{for} \quad x>0.\tag{11}$$

Thus there are effectively three different transfer matrices: one in the bulk magnetic region T_M, one in the bulk superconducting region T_{SC}, and one associated with transfer through the interface T_I. By diagonalizing T_M and T_{SC} there exist decaying, growing, or propagating eigenstates depending on whether the eigenvalues are less than, larger than or equal to 1, respectively. Here decaying and growing are refer to propagation along the axis for increasing x. If PET_M denotes the matrix obtained after propagating the eigenvectors of the bulk magnetic transfer matrix through the interface, we introduce a matrix α given by

$$PET_M=ET_{SC}\alpha,\tag{12}$$

where ET_{SC} is the matrix containing the eigenvectors of the bulk superconducting region as column vectors. The dot indicates matrix multiplication. Now let S^m_g and S^{sc}_g denote the subspace of growing eigenstates of PET_M and ET_{SC}, respectively, and consider the following linear combination of the *growing* states of PET_M:

$$\begin{aligned}\sum_{i\in S^m_g}\beta_i|PET_M i\rangle&=\sum_{i\in S^m_g}\sum_{j\in S^{sc}_g}\beta_i\alpha_{ji}|ET_{SC}j\rangle\\&=\sum_{j\in S^{sc}_g}\left(\sum_{i\in S^m_g}\alpha_{ji}\beta_i\right)|ET_{SC}j\rangle.\end{aligned}\tag{13}$$

From Eq. (13) it is evident that to have a bound state at the interface the vector β must belong to the null space of the reduced matrix α_r, which is the $S^{sc}_g\times S^m_g$ upper left part of the original matrix α since the matrices PET_M and ET_{SC} are

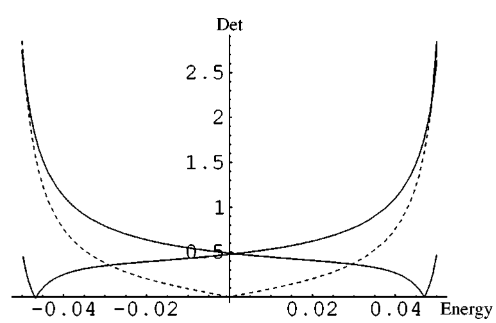

FIG. 2. Determinant of α_r vs the energy ϵ for the {110} AF/dSC interface. Again this is plotted inside the superconducting gap and with $q=0.1$. The dashed curve is the usual case of an I/dSC interface which clearly contains a ZEBS (the insulator state is obtained by performing the substitution $M_n\rightarrow -M_n$ for the hole part of the BdG equations only). The solid curves show the spin splitting of the ZEBS for this particular value of q.

organized to have the eigenstates with the largest eigenvalues as column vectors to the left. In the case that the two subspaces S_g^{sc} and S_g^m have the same dimension a bound state at the interface is characterized by the vanishing of the determinant of α_r:

$$\text{Bound states:} \quad \det(\alpha_r)=0. \tag{14}$$

Plots of the wave functions with values of (q,ϵ) that satisfy Eq. (14) verifies that these states indeed are bound to the interface (not shown). The following explicit values of the input parameters are chosen: $t=1$, $\Delta_d=0.14$, $M=2.0$, and $\mu=-0.99$ (for simplicity we ignore next-nearest neighbor coupling). Figure 1(a) shows the determinant plotted as a function of energy for the $\{100\}$ interface. There are bound states close to the superconducting gap edge that disperses downward in a cosine form [Fig. 1(b)].

These are the well-known de Gennes/Saint-James states existing on the surface of an insulator and a superconductor.[13,14] These subgap states are bound to the interface and disappear when $M\to 0$.

The induction of additional gap symmetries, extended *s* or p wave, near the $\{100\}$ interface of a *d*-wave superconductor and an antiferromagnet, was studied self-consistently by Kuboki.[15] These local gap perturbations will slightly modify the graphs in Fig. 1. There is no spin splitting of the dGSJ mode in this geometry.

We now turn to the more interesting configuration of a $\{110\}$ interface. Allowing for a possible interface induced subgap order with extended s wave symmetry the Bogoliubov–de Gennes equations have the forms

$$\begin{aligned}\epsilon_\sigma u_{q\sigma}(x)=&-2t\cos(p)[u_{q\sigma}(x+1)+u_{q\sigma}(x-1)]-\mu u_{q\sigma}(x)\\&+\sigma M_x u_{q\sigma}(x)-2i\sin(q)[\Delta^d_{x+1,x}v_{q\sigma}(x+1)\\&-\Delta^d_x v_{q\sigma}(x-1)]+2i\cos(q)[\Delta^s_{x+1,x}v_{q\sigma}(x+1)\\&+\Delta^s_x v_{q\sigma}(x-1)],\end{aligned} \tag{15}$$

$$\begin{aligned}\epsilon_\sigma v_{q\sigma}(x)=&2t\cos(p)[v_{q\sigma}(x+1)+v_{q\sigma}(x-1)]+\mu v_{q\sigma}(x)\\&+\sigma M_x v_{q\sigma}(x)-2i\sin(q)[\Delta^{*d}_{x+1,x}u_{q\sigma}(x+1)\\&-\Delta^{*d}_x u_{q\sigma}(x-1)]-2i\cos(q)[\Delta^{*s}_{x+1,x}u_{q\sigma}(x+1)\\&+\Delta^{*s}_x u_{q\sigma}(x-1)],\end{aligned} \tag{16}$$

These equations are diagonal in the Fourier component q obtained after fourier transforming parallel to the $\{110\}$ interface since there is no staggering of the moments along a diagonal line in a square antiferromagnetic lattice. In Fig. 2 we again plot the determinant of the reduced matrix α_r as a function of energy ϵ when $\Delta^s=0$. As seen the spin degeneracy of the ZEBS (dashed curve) is lifted at a $\{110\}$ AF/dSC

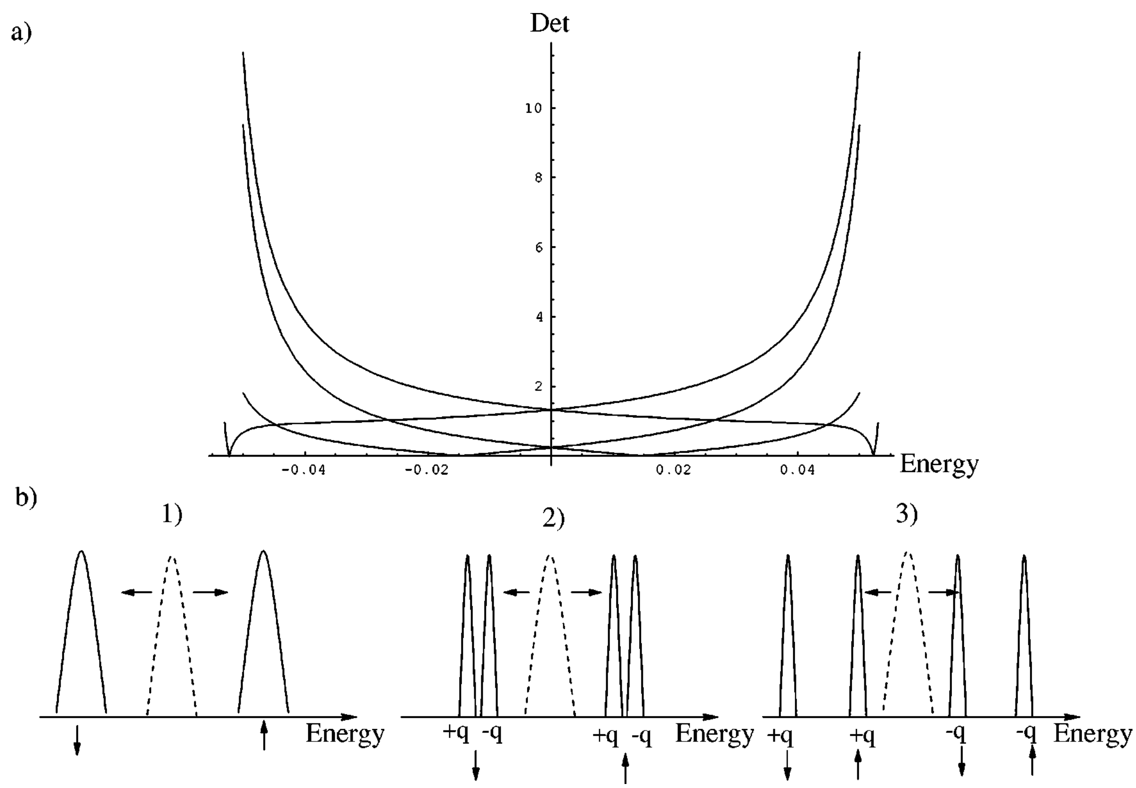

FIG. 3. (a) Same as in Fig. 2, but with an induced extended s-wave gap function near the interface, i.e., $d\to d+is$. For clarity we do not show the original ZEBS (dashed curve from Fig. 2). (b) Schematic representation of the splitting of the original zero energy Andreev bound state (dashed curve): (1) The antiferromagnetic interface breaks the spin degeneracy, as shown in Fig. 2. (2) Induction of a possible sub-dominant s-wave gap parameter Δ^s further splits the spin up/down states by breaking the directional degeneracy. (3) Only when Δ^s exceeds a critical value is an interface current induced. In this last figure, which corresponds to the situation from a), Δ^s is equal to Δ^d on the interface and decreases linearly to zero within 20 sites of the interface.

interface. As opposed to the usual dGSJ states in Fig. 1, this splitting is also caused by the fact that a {110} interface belongs to only one sublattice whereas the {100} interface studied above contains the same amount of spin-up and -down sites.

The splitting of the ZEBS by Δ^s mixing in the usual situation of a I/dSC interface has been extensively studied in the literature.[7–9] It is also well-known that a magnetic field further splits the ZEBS.[5] The above spin splitting at AF/dSC interfaces is similar to this magnetic field effect in the sense that the magnetic interface effectively acts as a local magnetic field. A similar effect caused by a correlation induced magnetization near the interface in the case of a I/dSC surface was discussed by Honerkamp *et al.*[9] This ''Zeeman'' effect is also directly related to the split zero energy Andreev mode observed in the center of vortex cores of underdoped cuprates where local antiferromagnetism has been shown to exist.[17–22]

To the best of our knowledge there has been no self-consistent calculation investigating any {110} AF/dSC interface induced subdominant order parameters. However, we know from the study of I/dSC surfaces[7,16] that the strong pair breaking effects of a {110} geometry, as opposed to a {100} surface, tends to stabilize the subdominant *s*-wave component. Thus, even though there is no Fermi surface instability begging for removal of the ZEBS from the Fermi level in the case of a AF/dSC {110} interface, one should still consider the effect of an additional local superconducting order parameter *is* competing with the splitting caused by the magnetism. The consequences of this competition for the ZEBS are discussed in Fig. 3.

The induction of a surface current is a well-known consequence of the time reversal symmetry broken state of I/dSC interfaces.[7,8] However, for the AF/dSC interface with a locally induced $d \pm is$ order parameter there is a critical value of Δ_c^s before a current runs along the interface.[23] In Fig. 3(a) we show the situation when the induced Δ^s has exceeded this critical value. Figure 3(b) is a schematic representation of the splitting of the original ZEBS with the first sketch corresponding to the parameters from Fig. 2 and the last sketch to those from Fig. 3(a). We stress that only a self-consistent model calculation can determine the magnitude of the directional splitting caused by *is* compared to the spin splitting caused by the antiferromagnetism, and hence the relevancy of the interface current.

In conclusion, we have set up a simple method so determine the existence of bound states at the interfaces of *d*-wave superconductors and antiferromagnets. In particular we studied the energetics of the notorious zero energy mode bound to {110} I/dSC interfaces first discovered by Hu.[4] This state is always spin split when the insulator is an antiferromagnet and is analogous to the split states found around the magnetic vortex cores of YBCO and BSCCO crystals. In the case of an array of junctions corresponding to a periodic domain of vertical or diagonal stripes these states will hybridize and eventually form a band. A current along the interface exists only when the effect of a competing, interface induced *is* component exceeds the spin splitting.

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