Properties of the zero-energy Andreev bound state in a two-sublattice SNS junction

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Abstract – We study properties of the zero energy Andreev bound state in a superconductor-normal metal-superconductor (SNS) junction consisting of two intrinsic degrees of freedom. The superconductors on either sides of the normal metal are assumed to have two sublattices with an intra-sublattice pairing with a phase equal to zero or π between the two sublattices. In addition, we add a uniform inter-sublattice pairing and study its effect on the local density of states (LDOS). In particular, we find that as the inter-sublattice pairing is turned on, the zero-bias peak (ZBP) is unstable (robust) when the phase difference across the sublattices is π (zero). We discuss the relevance of our results to the recently proposed odd-parity η pairing ground states in iron-based superconductors (FeSCs).

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Introduction. – The study of electronic transport through the normal metal-superconductor interface has provided a wealth of information regarding the ground states of the constituent materials forming such an interface. A case of particular interest is the transport of an electron having an energy less than that of the superconducting gap, which, when incident onto the interface from the normal metal region, gets retro-reflected as a hole with opposite spin. Such a reflection conserves momentum (up to order Δ/Ef, where Δ is the gap and Ef is the Fermi energy) and is accompanied by the transmission of a charge 2e Cooper pair into the superconductor. This process, termed as Andreev reflection [1,2], has had a widespread applicability in probing a variety of condensed-matter systems for several decades, including superconducting ground states [3], polarization in ferromagnets [4,5], and, more recently, topological matter [6–8].

Probing the superconducting gap and its pairing symmetry is, perhaps, one of the most important uses of the Andreev reflection spectroscopy [3]. The sensitivity of the Andreev in-gap bound-state energies to the phase of the superconducting gap gives it a special advantage over probes like the ARPES, STM or Raman ones which do not contain any phase information. As an example, the surface of a d-wave superconductor, when oriented perpendicular to the nodal direction of the order parameter, was predicted to host a zero-energy surface bound state [9]. Kashiwaya and coworkers [10–12] generalized the works of refs. [2,9] to a d-wave symmetry of the gap for arbitrary orientations of the surface. Such ZBPs have since been widely observed in experiments (see refs. [13–15] and refs. [3,10] for a review) providing a crucial confirmation of the d-wave pairing gap in the cuprates. Additionally, the effects of a magnetic field and surface roughness [16–18] on the ZBP, and a broken time-reversal component [16,18] of the d-wave order parameter have all been taken into account. Similarly, characteristic features of the Andreev tunneling spectrum have been calculated [19] and observed [20] in the spin triplet p-wave superconductor Sr2RuO4. More recently, a topological index theorem for the stability of dispersionless surface Andreev bound states on the interface of a normal metal-superconductor was proven [21]. Here, the authors derived general conditions for the existence of dispersionless Andreev bound states for different angular momenta as well as mixed pairing symmetries using the bulk-boundary correspondence.
In multiorbital systems, the resolution of the pairing symmetry using Andreev and tunneling spectroscopy [22,23] is complicated by the fact that several bands contribute to the density of states at the Fermi level. For example, in the iron-based superconductors [24–31], all the iron $d$-orbitals are known to have a non-vanishing density of states at $E_F$ resulting in multiple pockets around the $\Gamma$ and $M$ points in the Brillouin zone [32]. To add to it, unlike the cuprates, the phase distribution of the order parameter across the Fermi surface is not symmetry protected; as a result, phase-sensitive probes like those used in the cuprates are hard to design. So far, several new pairing phases in the iron-based superconductors have been proposed, including, $s$-wave [33–38] and $d$-wave pairing symmetries [39,40]. Within the $s$-wave pairing symmetry, there are a variety of possibilities including the sign changes between different pockets (so-called $s^{\pm}$ [33–36]), or between bands featured by different orbitals [41–44], or between two sublattices [43] (the $\eta$ pairing). Therefore, a systematic study of these ground-state characteristics using the Andreev spectroscopy is called for.

The main focus of this work will be to analyze the properties of SNS junctions formed by such exotic, odd-parity $\eta$ paired superconducting states proposed for multiorbital systems [42,43]. Before we outline the details of our calculations, we briefly summarize previous works by one of the present authors [42,43] so that the distinction between the mixed $\eta$ and the commonly studied $s$-pairing states is clarified. In order to accommodate the two crucial experimental features of $i$ a $(\pi/2, \pi)$ resonance in the 245 chalcogenide and $ii$ an isotropic, nodeless gap on both the electron pockets in most iron superconductors, one needs to include both nearest-neighbor (NN) even-parity pairing, $\langle c_{k\sigma}^\dagger \sigma c_{k\sigma} \rangle$, and the next-nearest-neighbor (NNN) odd-parity $\eta$ pairing, $\langle c_{k\sigma}^\dagger \sigma c_{k+\hat{Q}\sigma} \rangle$. Here $c_{k\sigma}$ is the electron creation operator at quasi-momentum $\vec{k}$ and spin $\sigma$, and $\hat{Q} = (\pi, \pi)$ is the reciprocal lattice wave vector in the 2-Fe unit cell. While the former brings about the sign change between the inner and outer electron and hole pockets in the two-Fe BZ (thus providing a possible explanation of the resonance peak), the latter removes the nodes at the intersection point of the two electron pockets giving a completely nodeless gap on the electron pockets. A natural consequence of the odd-parity pairing is that if we convert the $\langle c_{k\sigma}^\dagger \sigma c_{k+\hat{Q}\sigma} \rangle$ order parameter in terms of the pairing in the $A$ and $B$ sublattices (by re-writing $c_{k\sigma}$ and $c_{k+\hat{Q}\sigma}$ in terms of $c_{A\sigma}$ and $c_{B\sigma}$), we find that the order parameter between the two sublattices $A$ and $B$ should change sign. This real-space sign distribution of the gap function as well as its momentum space counterpart are, therefore, clearly distinct from the $s_\pm$ scenario.

To begin our detailed analysis of the bound-state properties of an SNS junction formed by the pairing state described above, we model the lattice with two intrinsic degrees of freedom, say two sublattices. We assume that the superconductors on either side of the normal metal have two kinds of local pairings—type-(a) NNN intra-sublattice pairing with a relative phase equal to 0 or $\pi$ between the two sublattices and type-(b) NN uniform inter-sublattice pairing in each of the two superconductors (see fig. 1). We also maintain an overall $\pi$ phase difference between the two superconductors on either side of the normal metal—a condition which gives a ZBP at the NS interface in the absence of the $(b)$ pairing type. Our central result is that, as the inter-sublattice pairing type $(b)$ is turned on, the ZBP is unstable (robust) when the phase difference between the sublattices is $\pi$ (zero). This result, as will be discussed later, rules out a pure finite-momentum $\eta$ pairing. In the following section, we will present an analytic result for a simplified toy model of an SNS junction. In the third section we will discuss our numerical results supporting the conclusions in the second section. Finally, in the last section we will end with our discussions and provide an experimental context to our results through FeSCs.

**Analytical treatment.** $i$) Sign change case: We begin with the case in which we have two sublattices in each superconductor, labelled by $A$ and $B$. For the superconductor on the right, we assume a positive sign of the gap on $A$ and negative on $B$. On the left, we swap the signs of the gaps leaving the magnitudes the same (see fig. 1). The B-dG equations in the bulk of the right superconductor take the form

\[
\begin{align*}
\epsilon u_R^L &= -H_e u_R^L + \Delta v_R^L + \Delta_\epsilon v_R^L, \\
\epsilon v_R^L &= H_e v_R^L + \Delta u_R^L + \Delta_\chi u_R^L, \\
\epsilon u_R^R &= -H_e u_R^R - \Delta v_R^R + \Delta_\epsilon v_R^R, \\
\epsilon v_R^R &= H_e v_R^R - \Delta u_R^R + \Delta_\chi u_R^R.
\end{align*}
\]

![Fig. 1: SNS geometry for the two-sublattice case. A normal metal of thickness $2d$ is sandwiched between the two SCs. The origin is taken to be at the right NS interface.](image)

Here $u_R^{L,R}$, $v_R^{L,R}$ are the B-dG wave functions for the left (L) and right (R) superconductors, $\Delta, \Delta_\epsilon$ are the intra- and inter-sublattice pairing, respectively, $H_e$ is the kinetic part of the Hamiltonian and $\epsilon$ is the eigenvalue. We can solve the ensuing differential equations to get the B-dG solutions $u_R^L, v_R^L$ in the right superconductor as

\[
u_R^L(x) = \alpha_R^L e^{ik_1x} + \alpha_R^L e^{-ik_2x},
\]

where $\alpha_R^L$ are numbers, $j = 1, 2$ and similar equations follow for $v_R^L(x)$ with coefficients $\beta_R^L$. We have defined $k_1$ and $k_2$ as $k_1 = \sqrt{E_f + \sqrt{E_f^2 - (\Delta^2 + \Delta_\chi^2)}}$ and $k_2 = \sqrt{E_f - \sqrt{E_f^2 - (\Delta^2 + \Delta_\epsilon^2)}}$. The above solutions are
where $\eta$ and similar equations follow for $\epsilon$ ratio of the in gap bound-state energy ($\alpha$ of the interface at $e$ try are modified to take into account the no sign change that the sign of the order parameters is swapped. The same procedure for the case of the left superconductor not- wave vectors in the normal metal ($\beta$ there is a sign change of this substitution, the condition in eq. (4) states that when infinitesimally diagonalizes the pairing sector, that turning on the inter- a unitary transformation to the Hamiltonian which di- will destroy the ZBP. It is easy to show, by performing the determinant of the linear equation matrix to zero, the condition for the existence of a solution by equat- ing the previous result in i) to the case in which there is no in- fferioral interface of the right SN junction, see fig. 1)

We have defined $k'_1 = \sqrt{E_f + \epsilon}$ and $k'_2 = \sqrt{E_f - \epsilon}$. As a next step, we match boundary conditions on the two sides of the interface at $x = 0$ using (the origin is chosen as the interface of the right SN junction, see fig. 1)

$$u^N_i(x = 0) = u^R_i(x = 0),$$

$$u^{N}_{i\pm}(x = 0) = u^{R}_{i\pm}(x = 0),$$

and similar equations follow for $x = 2d$ and for the $u^s_i$. Here $i = 1, 2$, and the subscript $x$ refers to derivatives. With these boundary conditions we obtain sixteen equations with sixteen variables to solve for. We can determine the condition for the existence of a solution by equating the determinant of the linear equation matrix to zero, which then yields the condition

$$\cos(2\Xi) - \cos[2(k'_1 - k'_2 - \phi)] = 0,$$

which implies that

$$k'_1 - k'_2 - \phi = \Xi + n\pi,$$

where $\Xi = \frac{1}{2}\cos^{-1}\left[\frac{\Delta^2 - \Delta^2_l}{\Delta^2 + \Delta^2_l}\right]$ and $\cos\phi_2 = -\frac{\epsilon}{\sqrt{\Delta^2 + \Delta^2_l}}$. The ratio of the in gap bound-state energy ($\epsilon$) and the Fermi energy ($E_f$) is small, and as a result, the difference of the wave vectors in the normal metal ($k'_1 - k'_2$) is proportional to $\epsilon$, which is, in turn, proportional to cos $\phi_2$. Making this substitution, the condition in eq. (4) states that when there is a sign change of $\pi$ between the sublattices, even an infinitesimally small inter-sublattice uniform pairing will destroy the ZBP. It is easy to show, by performing a unitary transformation to the Hamiltonian which diagonalizes the pairing sector, that turning on the inter- sublattice pairing is equivalent to the effects of a non-zero inter-sublattice hopping matrix element. The condition is simplified in the limit of $\Delta_e \ll \Delta$, where we keep only the linear terms to get

$$k'_1 - k'_2 - \phi = \frac{\pi}{2} - \eta + n\pi$$

with $\eta \equiv \frac{\Delta}{2\Delta_l}$. Thus, the presence of even a small but non-zero $\eta$ leaves the ZBP unstable.

ii) No sign change case: We now wish to compare our previous result in i) to the case in which there is no internal sign change between sublattices A and B. Just like before, we wish to study the effect of the nearest-neighbor uniform pairing ($\Delta_e$). To this end, the Bd-G equations for the right and left superconductor of the new geometry are modified to take into account the no sign change condition. We again solve the simultaneous equations for the coefficients $\beta^R_{ij}$ and $\alpha^R_{ij}$ [3]. We can follow the same procedure for the case of the left superconductor noting that the sign of the order parameters is swapped. The general solutions of the Bd-G equation in the normal metal are given by $u^R_i(x) = p_{j1} \sin[k'_1(x + d)] + p_{j2} \cos[k'_2(x + d)]$, where $p_{j1}$ are numbers, $j = 1, 2$, and similar equations follow for $u^N_i(x)$ with coefficients $q_{ij}$ and $k'_1$ replaced by $k'_2$.

With these boundary conditions we obtain sixteen equations which then yields the condition

$$0 = (\beta^2 - \alpha^2) \cos[2(k'_1 - k'_2)] + (\alpha^2 + \beta^2) \cosh 2\Gamma$$

$$- 2\alpha \beta \sin[2(k'_1 - k'_2)],$$

(6)

with the definitions

$$\sqrt{\epsilon^2 - (\Delta + \Delta_e)^2} - \epsilon \equiv i\alpha + \beta,$$

(7)

and $\frac{\Delta}{\sqrt{\Delta^2 - \Delta^2_l}} \equiv \cosh\Gamma$. Here, we look for solutions $\epsilon < (\Delta + \Delta_e)$ with $\alpha$ and $\beta$ being real in the case $\Delta_e < \Delta$. In the limit $\eta = \frac{\Delta}{\Delta_l} \ll 1$ we have $\alpha \approx \phi + \frac{\sin \phi}{\sin \phi_2}$, $\beta \approx -\cos \phi$ and $1 \approx \cosh 2\Gamma$, with $\phi$ defined as $\cos \phi = \epsilon/\Delta$. In the limit $\eta \ll 1$ we can rewrite the condition in eq. (6) as

$$0 = 2\cos^2[k'_1 - k'_2 - \phi] - 2\eta \cos[2(k'_1 - k'_2)] + 2\eta \left(\frac{\pi}{2} - \eta + n\pi\right),$$

(8)

where, again, $k'_1 - k'_2$ is proportional to $\Delta \cos \phi$. The above condition allows for a zero-energy bound-state solution (i.e. in the limit of $\phi \to \pi/2$, implying that the ZBP is robust under a small perturbation $\Delta_e$). However, as one must expect, the ZBP is destroyed in the other limit where $\Delta_e \gg \Delta$.

Numerics.

a) Model and method. We now verify the conclusions in the previous section using a more concrete, two-dimensional, lattice model. For the purposes of numerical illustration, we start with a two-sublattice model consisting of a single orbital per sublattice. A model ideally suited for such a calculation is a single subspace of the doublet model presented in [45] for FeSCs. The parameters are chosen in such a way that there are only hole pockets centered around the $\Gamma$-point. We do this to be able to obtain a fully gapped spectrum in the bulk of the superconductor; for the chosen model, this is not possible with a pure type-(a) pairing (with a $\pi$ phase between $A$ and $B$) when the electron pockets close to the edges of the Brillouin zone are present. If we insist that such a band structure and Fermi surface must indeed describe a specific system, we can keep in mind the case of the extremely hole-doped pnictide KFe$_2$As$_2$, where ARPES sees only hole pockets at the $\Gamma$-point [46]. However, as we saw in the earlier section, the results are more generic and can be applied to a wide category of systems. The following sets of parameters are chosen in the two-sublattice model [45]:

$$(t_{1s}, t_{1d}, t_{2s}, t_{2d}, t_{3s}, t_{3d}, \mu, \epsilon) = (0.2, -0.03, 0.3, 0.2, 0.05, ...$$
where $H_e(r, r')$ contains the kinematics in real space in the form of single orbital NN, NNN and 3rd NN hopping. The gap structure in the superconducting state, $\Delta(r, r')$, corresponds to NNN intra-sublattice pairing which changes sign between the sublattices (pure type-(a) pairing) with no NN pairing initially. The matrix in real space is diagonalized on a $40 \times 40$ lattice and the B-dG factors, $v_n(r)$ and $u_n(r)$, are obtained along with the eigenvalues $\epsilon_n$. One can then go on to obtain the LDOS [18]. For the two-sublattice, single-orbital band structure parameters with a purely type-(a) pairing (with $\pi$ phase difference), a relatively large value of the intra-sublattice pairing parameter ($\Delta_a = 0.4–0.5$) is needed to open a considerable full gap ($\sim 0.08$ eV) on the Fermi surface. In the following subsection, we will study the effects of type-(b) pairing on the ZBP.

b) Results. In the presence of a pure intra-sublattice (NNN) pairing which changes sign between the two sublattices (i.e. type-(a) pairing with phase of $\pi$) we expect a ZBP in our model. We will now turn on the NN inter-sublattice uniform pairing (type (b)) and consider its effect on the ZBP. The B-dG equations are similar to what was presented before, except for additional terms which connect the particle-hole sections of the Hamiltonian generated from the nearest-neighbor pairing (denoted by $\Delta_c$). Figure 2 shows a comparison of the LDOS at the NS boundary of the +NN-geometry formed by sandwiching two normal metal layers between superconductors with global sign change of $\pi$ in the phase. The plot on the left shows the effect of $\eta = \frac{\Delta_c}{\Delta_a}$ on the ZBP for the case in which there is a sign change of $\pi$ between the $A$ and $B$ sublattices. Evidently, up to the accuracy of the given lattice size, even a small value of $\eta = 0.08$ is enough to destroy the ZBP. By choosing larger system sizes, this effect can be seen more clearly with even smaller values of $\eta$. On the other hand, when there is no sign change between the sublattices (fig. 2, right), even a relatively large value of $\eta = 0.4$ does not destroy the ZBP. These numerical results are consistent with our analytical result derived in the previous section. In the following, we will discuss the relevance of our results in the context of FeSCs.

Discussion. Recently, several new pairing phases in the FeSCs have been proposed including $s$-wave [33–38] and $d$-wave pairing symmetries [39,40]. Additionally, within the $s$-wave pairing symmetry, there is a variety of possibilities including the sign changes between different pockets (so-called $s^\pm$ [33–36]), or between bands featured by different orbitals [41–44], or between two sublattices [43]. For example, it was argued in [45] that the Fe lattice in the superconducting state can be divided into two sublattices, with the pairing amplitude changing sign between the two sublattices. The motivation of such state [43,45] is to gap out the regions where the electron pockets are degenerate so as to be consistent with ARPES. However, a pure NNN sublattice sign changing gap alone could not account for the experimentally observed neutron resonance peak close to $(\pi, \pi/2)$. An additional NN uniform pairing between the two sublattices was needed for such a sign changing ground state to be fully consistent with experiments. From the above theoretical analysis and the following experimental evidence, we argue that the Andreev bound-state spectroscopy also requires the presence of NN pairing as was done by neutron scattering, thus ruling out a pure NNN sign changing ground-state description of FeSCs. Several experimental groups have reported Andreev spectra in the 1111 [47–62], 111 [63], 11 [60,64] and 122 [52,53,65–69] families. Initially, there were several reports of the presence of a ZBP in the 1111 and 122 compounds. However, there were inconsistencies present in the data like the dependence of the ZBP on the sample position, temperature dependence, and dependence on the size of the metallic tip. Later it was shown that the ZBP was an artifact of excessive pressure applied on the tip. More consistent data followed once “soft contact” Ag tips were used (for a detailed review and discussion, the reader can refer to [53]). In the 1111 compounds (LaFeAsO$_{1-x}$F$_x$ and SmFeAsO$_{1-x}$F$_x$) the data was collected for polycrystalline samples with random orientations. No ZBP was observed in either of the cases and, as a result, it was concluded that no nodes were present and the gaps were completely isotropic [53] which—if it is to be understood in the odd-parity picture—corresponds...
to the presence of the NN uniform even-parity pairing. With respect to the 122 compounds, \((\text{Ba,K})\text{Fe}_2\text{As}_2\) and \((\text{Ba,Co})\text{Fe}_2\text{As}_2\) directional measurements along different crystal directions could be performed due to the availability of single crystals. Several measurements in different directions along the a-b plane again indicated the absence of ZBPs (see [53] and references therein). Point contact measurements along the \(c\)-axis of single crystals in the 111 compound \(\text{LiFeAs}\) [63] showed a zero-bias Josephson current, unrelated to the ZBP due to in gap states. A similar behavior was seen in polycrystalline samples of the 11 compound \(\text{FeSe}\) [60,64]. With such strong experimental support and our theoretical analysis, a pure NNN sublattice sign changing pairing, namely a pure \(\eta\) pairing state [43], is ruled out. But a mixed pairing state with both the \(\eta\) pairing and a NN uniform pairing is still possible.

To conclude, we have studied the properties of the zero-bias in-gap Andreev bound state for an SNS junction made of a lattice with two degrees of freedom. The superconducting state consists of a NNN pairing with opposite (same) sign on each sublattice and a uniform NN pairing between the two. We find that the zero-bias Andreev bound state is unstable (robust) to inter-sublattice NN uniform pairing when the phase difference between the two sublattices is \(\pi\) (zero). From existing experimental evidence for FeSCs, this necessarily means that a pure \(\eta\) pairing is ruled out. Our study suggests that it is difficult to detect a real-space pairing sign change without symmetry protection in SNS junctions. These results can also be extended to cases for pairing states with sign change among intrinsic degree of freedoms such as orbitals.

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