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Odd-frequency pairing in superconducting heterostructures

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Abstract
We review the theory of odd-frequency pairing in superconducting heterostructures, where an odd-frequency pairing component is induced near interfaces. A general description of the superconducting proximity effect in a normal metal or a ferromagnet attached to an unconventional superconductor (S) is given within quasiclassical kinetic theory for various types of symmetry state in S. Various possible symmetry classes in a superconductor are considered which are consistent with the Pauli principle: even-frequency spin-singlet even-parity (ESE) state, even-frequency spin-triplet odd-parity (ETO) state, odd-frequency spin-triplet even-parity (OTE) state and odd-frequency spin-singlet odd-parity (OSO) state. As an example, we consider a junction between a diffusive normal metal (DN) and a p-wave superconductor (even-frequency spin-triplet odd-parity symmetry), where the pairing amplitude in DN belongs to an odd-frequency spin-triplet even-parity symmetry class. We also discuss the manifestation of odd-frequency pairing in conventional superconductor/normal (S/N) proximity systems and its relation to the classical McMillan–Rowell oscillations.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

It is well established that superconductivity is realized due to the formation of Cooper pairs consisting of two electrons. In accordance with the Pauli principle, it is customary to distinguish spin-singlet even-parity and spin-triplet odd-parity pairing states in superconductors, where odd (even) refer to the orbital part of the pair wavefunction. For example, s-wave and d-wave pairing states belong to the former case while the p-wave state belongs to the latter one [1]. In both cases, the pair amplitude is an even function of energy. However, the so-called odd-frequency pairing states when the pair amplitude is an odd function of energy can also exist. Then, the spin-singlet odd-parity and the spin-triplet even-parity pairing states are possible.

The possibility of realizing the odd-frequency pairing state was first proposed by Berezinskii in the context of ^{3}He, where the odd-frequency spin-triplet pairing was discussed [2]. Odd-frequency superconductivity was then discussed in the context of various mechanisms of superconductivity involving strong correlations [3–5]. The odd-frequency pairing state was recently proposed in ferromagnet/superconductor heterostructures with inhomogeneous magnetization [6–11]. However, the very important issue of the manifestation of the odd-frequency pairing in proximity systems without magnetic ordering has not received any attention. This question is addressed in the present paper.

Coherent charge transport in structures involving diffusive normal metals (DN) and superconductors (S) has been extensively studied during the past decade both experimentally and theoretically. However, almost all previous work was restricted to junctions based on conventional s-wave superconductors [12]. Recently, a new theoretical approach for studying charge transport in junctions based on p-wave and d-wave superconductors was developed and applied to the even-frequency pairing state [13, 14]. It is known that in the anisotropic paring state, due to the sign change of the pair potential on the Fermi surface, a so-called midgap Andreev resonant state (MARS) is formed at the interface [15, 16]. As was found in [13, 14], MARS competes with the proximity effect in contacts with spin-singlet superconductors, while it coexists with the proximity effect in junctions with spin-triplet superconductors. In the latter case, it was predicted that the induced pair amplitude in the DN has a peculiar energy dependence and the resulting local density of states (LDOS) has a zero energy peak (ZEP) [14]. Here we review a general theory of the proximity effect in the N/S junctions, both in the clean and in the dirty limit [17], applicable to any type of symmetry state in a superconductor forming the junction in the absence of spin-dependent electronic scattering at the N/S interface.

2. Junctions in the dirty limit

Let us first discuss the case of a diffusive normal metal attached to a superconductor (DN/S junction). Before proceeding with a formal discussion, let us present qualitative arguments illustrating the main conclusions of the paper. Two constraints should be satisfied in the considered system: (1) only the s-wave even-parity state is possible in the DN due to isotropization by impurity scattering, (2) the spin structure of induced Cooper pairs in the DN is the same as in an attached superconductor. Then the Pauli principle provides the unique relations between the pairing symmetry in a superconductor and the resulting symmetry of the induced pairing state in the DN. Namely, for even-parity superconductors, even-frequency spin-singlet even-parity (ESE) and odd-frequency spin-triplet even-parity (OTE) states, the pairing symmetry in the DN should remain ESE and OTE. On the other hand, for odd-parity superconductors, even-frequency spin-triplet odd-parity (ETO) and odd-frequency spin-singlet odd-parity (OSO) states, the pairing symmetry in the DN should be OTE and ESE, respectively. The generation of the OTE state in the DN attached to the ETO p-wave superconductor is of particular interest. A similar OTE state can be generated in superconducting junctions with diffusive ferromagnets [6–11] but due to a different physical mechanism. Although the symmetry properties can be derived from the basic arguments given above, the quantitative model has to be considered to prove the existence of nontrivial solutions for the pairing amplitude in the DN in each of the above cases. These solutions and their main features will be discussed below.

Let us start with the general symmetry properties of the quasiclassical Green's functions in the considered system. The elements of retarded and advanced Nambu matrices $\widehat{g}^{R,A}$

$$\widehat{g}^{R,A} = \begin{pmatrix} g^{R,A} & f^{R,A} \\ \bar{f}^{R,A} & \bar{g}^{R,A} \end{pmatrix} \tag{1}$$

are composed of the normal $g^R_{\alpha,\beta}(\boldsymbol{r}, \varepsilon, \boldsymbol{p})$ and anomalous $f^R_{\alpha,\beta}(\boldsymbol{r}, \varepsilon, \boldsymbol{p})$ components with spin indices α and β. Here $\boldsymbol{p} = \boldsymbol{p}_F/|\boldsymbol{p}_F|$, $\boldsymbol{p}_F$ is the Fermi momentum, $\boldsymbol{r}$ and ε denote coordinate and energy of a quasiparticle measured from the Fermi level.

The function f^R and the conjugated function $\bar{f}^R$ satisfy the following relation [18, 19]

$$\bar{f}^R_{\alpha,\beta}(\boldsymbol{r}, \varepsilon, \boldsymbol{p}) = -[f^R_{\alpha,\beta}(\boldsymbol{r}, -\varepsilon, -\boldsymbol{p})]^*. \tag{2}$$

The Pauli principle is formulated in terms of the retarded and the advanced Green's functions in the following way [18]

$$f^A_{\alpha,\beta}(\boldsymbol{r}, \varepsilon, \boldsymbol{p}) = -f^R_{\beta,\alpha}(\boldsymbol{r}, -\varepsilon, -\boldsymbol{p}). \tag{3}$$

By combining the two above equations, we obtain $\bar{f}^R_{\beta,\alpha}(\boldsymbol{r}, \varepsilon, \boldsymbol{p}) = [f^A_{\alpha,\beta}(\boldsymbol{r}, \varepsilon, \boldsymbol{p})]^*$. Further, the definitions of the even-frequency and the odd-frequency pairing are $f^A_{\alpha,\beta}(\boldsymbol{r}, \varepsilon, \boldsymbol{p}) = f^R_{\alpha,\beta}(\boldsymbol{r}, -\varepsilon, \boldsymbol{p})$ and $f^A_{\alpha,\beta}(\boldsymbol{r}, \varepsilon, \boldsymbol{p}) = -f^R_{\alpha,\beta}(\boldsymbol{r}, -\varepsilon, \boldsymbol{p})$, respectively. Finally we get

$$\bar{f}^R_{\beta,\alpha}(\boldsymbol{r}, \varepsilon, \boldsymbol{p}) = [f^R_{\alpha,\beta}(\boldsymbol{r}, -\varepsilon, \boldsymbol{p})]^* \tag{4}$$

for the even-frequency pairing and

$$\bar{f}^R_{\beta,\alpha}(\boldsymbol{r}, \varepsilon, \boldsymbol{p}) = -[f^R_{\alpha,\beta}(\boldsymbol{r}, -\varepsilon, \boldsymbol{p})]^* \tag{5}$$

for the odd-frequency pairing. In the following, we focus on Cooper pairs with $S_z = 0$, remove the external phase of the pair potential in the superconductor and will concentrate on the retarded part of the Green's function.

We consider a junction consisting of a normal (N) and a superconducting reservoirs connected by a quasi-one-dimensional diffusive conductor (DN) with a length L much larger than the mean free path. The Green's function in the superconductor can be parameterized as $g_\pm(\varepsilon)\hat{\tau}_3 + f_\pm(\varepsilon)\hat{\tau}_2$ using Pauli matrices, where the suffix $+(-)$ denotes the right (left) going quasiparticles. $g_\pm(\varepsilon)$ and $f_\pm(\varepsilon)$ are given by $g_+(\varepsilon) = g^R_{\alpha,\beta}(\boldsymbol{r}, \varepsilon, \boldsymbol{p}) g_-(\varepsilon) = g^R_{\alpha,\beta}(\boldsymbol{r}, \varepsilon, \bar{\boldsymbol{p}}) f_+(\varepsilon) = f^R_{\alpha,\beta}(\boldsymbol{r}, \varepsilon, \boldsymbol{p})$, and $f_-(\varepsilon) = f^R_{\alpha,\beta}(\boldsymbol{r}, \varepsilon, \bar{\boldsymbol{p}})$, respectively, with $\bar{\boldsymbol{p}} = \bar{\boldsymbol{p}}_F/|\boldsymbol{p}_F|$ and $\bar{\boldsymbol{p}}_F = (-p_{Fx}, p_{Fy})$. Using the relations (4), (5), we obtain that $f_\pm(\varepsilon) = [f_\pm(\varepsilon)]^*$ for the even-frequency pairing and $f_\pm(\varepsilon) = -[f_\pm(-\varepsilon)]^*$ for the odd-frequency pairing, respectively, while $g_\pm(\varepsilon) = [g_\pm(-\varepsilon)]^*$ in both cases.

In the DN region only the s-wave even-parity pairing state is allowed due to isotropization by impurity scattering. The resulting pair amplitude in the DN can be parameterized by $\cos\theta\hat{\tau}_3 + \sin\theta\hat{\tau}_2$ in a junction with an even-parity superconductor and by $\cos\theta\hat{\tau}_3 + \sin\theta\hat{\tau}_1$ in a junction with an odd-parity superconductor. The function θ satisfies the Usadel equation [20] with the corresponding boundary condition at the DN/S interface and at the N/DN interface [13].

In the following, we will consider four possible symmetry classes of superconductor forming the junction and consistent with the Pauli principle: ESE, ETO, OTE and OSO pairing states. We will use the fact that only the even-parity s-wave pairing is possible in the DN due to the impurity scattering and that the spin structure of pair amplitude in the DN is the same as in an attached superconductor.

(1) *Junction with ESE superconductor.* In this case, $f_\pm(\varepsilon) = f^*_\pm(-\varepsilon)$ and $g_\pm(\varepsilon) = g^*_\pm(-\varepsilon)$ are satisfied. Then, the Usadel equations and the boundary conditions are consistent with each other only when $\sin\theta^*(-\varepsilon) = \sin\theta(\varepsilon)$ and $\cos\theta^*(-\varepsilon) = \cos\theta(\varepsilon)$. Thus the ESE state is formed in the DN, in accordance with the Pauli principle.

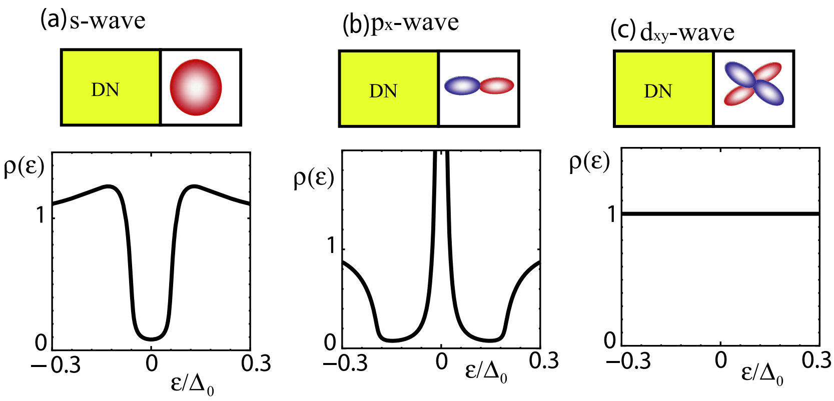

Figure 1. Local density of states in the diffusive normal metal DN in a contact with s-wave superconductor (a), p_x-wave superconductor (b) and d_{xy}-wave superconductor (c).

(2) *Junction with ETO superconductor.* Now we have $f_{\pm}(\varepsilon) = f_{\pm}^{*}(-\varepsilon)$ and $g_{\pm}(\varepsilon) = g_{\pm}^{*}(-\varepsilon)$. Then, $f_S(-\varepsilon) = -f_S^{*}(\varepsilon) = -f_S^{*}$ and $g_S(-\varepsilon) = g_S^{*}(\varepsilon) = g_S^{*}$. As a result, the boundary value problem is consistent if $\sin\theta^{*}(-\varepsilon) = -\sin\theta(\varepsilon)$ and $\cos\theta^{*}(-\varepsilon) = \cos\theta(\varepsilon)$. Thus the OTE state is formed in the DN. Remarkably, the appearance of the OTE state is the only possibility to satisfy the Pauli principle, as we argued above. Interestingly, the OTE pairing state can also be realized in superconductor/ferromagnet junctions [6–11], but the physical mechanism differs from the one considered here.

(3) *Junction with OTE superconductor.* In this case $f_{\pm}(\varepsilon) = -f_{\pm}^{*}(-\varepsilon)$ and $g_{\pm}(\varepsilon) = g_{\pm}^{*}(-\varepsilon)$. Then $f_S(-\varepsilon) = -f_S^{*}(\varepsilon)$ and $g_S(-\varepsilon) = g_S^{*}(\varepsilon)$ and we obtain $\sin\theta^{*}(-\varepsilon) = -\sin\theta(\varepsilon)$ and $\cos\theta^{*}(-\varepsilon) = \cos\theta(\varepsilon)$. Due to the absence of the spin flip scattering, these relations mean that the OTE pairing state is induced in the DN.

(4) *Junction with OSO superconductor.* We have $f_{\pm}(\varepsilon) = -f_{\pm}^{*}(-\varepsilon)$, $g_{\pm}(\varepsilon) = g_{\pm}^{*}(-\varepsilon)$ and $f_S(-\varepsilon) = f_S^{*}(\varepsilon)$, $g_S(-\varepsilon) = g_S^{*}(\varepsilon)$. One can show that $\sin\theta^{*}(-\varepsilon) = \sin\theta(\varepsilon)$ and $\cos\theta^{*}(-\varepsilon) = \cos\theta(\varepsilon)$. Following the same lines as in case (1), we conclude that the ESE pairing state is induced in the DN.

The central conclusions are summarized in the table below.

	Symmetry of the pairing in superconductors	Symmetry of the pairing in the DN
(1)	Even-frequency spin-singlet even-parity (ESE)	ESE
(2)	Even-frequency spin-triplet odd-parity (ETO)	OTE
(3)	Odd-frequency spin-triplet even-parity (OTE)	OTE
(4)	Odd-frequency spin-singlet odd-parity (OSO)	ESE

Note that for even-parity superconductors the resulting symmetry of the induced pairing state in the DN is the same as that of a superconductor (the cases (1), (3)). On the other hand, for odd-parity superconductors, the induced pairing state in the DN has a symmetry different from that of a superconductor (the cases (2), (4)).

In order to illustrate the main features of the proximity effect in all the above cases, we calculate the LDOS $\rho(\varepsilon) = \mathrm{Real}[\cos\theta]$ in the middle of the DN layer.

We start from junctions with ESE superconductors and choose the s-wave pair potential with $\Psi_{\pm} = 1$. The LDOS has a gap (figure 1(a)) and the real (imaginary) part of $f(\varepsilon)$ is an even (odd) function of ε consistent with the formation of the even-frequency pairing.

In junctions with ETO superconductors, we choose a p_x-wave pair potential with $\Psi_{+} = -\Psi_{-} = \cos\phi$ as a typical example. In this case, an unusual proximity effect is induced where the resulting LDOS has a zero energy peak (ZEP) [14] as illustrated in figure 1(b). The resulting LDOS has a ZEP [14] since $f(\varepsilon = 0)$ becomes a purely imaginary number. This is consistent with $f(\varepsilon) = -f^{*}(-\varepsilon)$ and the formation of the OTE pairing in the DN.

It is instructive to compare the ETO state with a p_x-wave pair potential and the ESE state with a d_{xy}-wave pairing. In the latter case, as seen from figure 1(c), there is no subgap structure at all in the LDOS in DN. This feature can be used to distinguish the p_x-wave state from the d_{xy}-wave one in tunneling experiments.

In summary, in this section we considered four symmetry classes in a superconductor allowed by Pauli principle: (1) even-frequency spin-singlet even-parity (ESE), (2) even-frequency spin-triplet odd-parity (ETO), (3) odd-frequency spin-triplet even-parity (OTE) and (4) odd-frequency spin-singlet odd-parity (OSO). We have found that the resulting symmetry of the induced pairing state in the DN is (1) ESE (2) OTE (3) OTE and (4) ESE corresponding to the above four classes. When the even (odd) frequency pairing is induced in the DN, the resulting LDOS has a gap (peak) at zero energy.

3. Junctions in the clean limit

In this section we present the results of the theoretical study of the induced odd-frequency pairing state in ballistic normal metal/superconductor (N/S) junctions where a superconductor has even-frequency symmetry in the bulk and a normal metal layer has an arbitrary length.

We show that if a superconductor has even-parity pair potential (spin-singlet s-wave state), the odd-frequency pairing component with odd-parity is induced near the N/S interface, while in the case of odd-parity pair potential (spin-triplet p_x-wave or spin-singlet d_{xy}-wave) the odd-frequency component with even-parity is generated. In conventional s-wave junctions, the amplitude of the odd-frequency pairing state is strongest in the case of a fully transparent N/S interface and is enhanced at energies corresponding to the peaks in the local density of states (LDOS). In p_x- and d_{xy}-wave junctions, the amplitude of the odd-frequency component on the S side of the N/S interface is enhanced at zero energy where the midgap Andreev resonant state (MARS) appears due to the sign change of the pair potential. The odd-frequency component extends into the N region and exceeds the even-frequency component at energies corresponding to the LDOS peak positions, including the MARS. At the edge of the N region the odd-frequency component is nonzero while the even-frequency one vanishes.

In the following, we consider an N/S junction as the simplest example of non-uniform superconducting system without impurity scattering. Both cases of spin-triplet odd-parity and spin-singlet even-parity symmetries are considered in the superconductor. We assume a thin insulating barrier located at the N/S interface ($x = 0$) with N ($-L < x < 0$) and S ($x > 0$). The length of the normal region is L.

The quasiclassical Green's functions in a normal metal (N) and a superconductor (S) in the Matsubara frequency representation are parameterized as

$$\hat{g}^{(i)}_{\pm} = f^{(i)}_{1\pm}\hat{\tau}_1 + f^{(i)}_{2\pm}\hat{\tau}_2 + g^{(i)}_{\pm}\hat{\tau}_3, \qquad (\hat{g}^{(i)}_{\pm})^2 = \hat{1} \tag{6}$$

where the subscript i(=N, S) refer to N and S, respectively. Here, $\hat{\tau}_j$ ($j = 1, 2, 3$) are Pauli matrices and $\hat{1}$ is a unit matrix. The subscript $+(-)$ denotes the left (right) going quasiparticles [18]. Functions $\hat{g}^{(i)}_{\pm}$ satisfy the Eilenberger equation [21]

$$\mathrm{i}v_{\mathrm{F}x}\hat{g}^{(i)}_{\pm} = \mp[\hat{H}_{\pm}, \hat{g}^{(i)}_{\pm}] \tag{7}$$

with

$$\hat{H}_{\pm} = \mathrm{i}\omega_n\tau_3 + \mathrm{i}\bar{\Delta}_{\pm}(x)\tau_2.$$

Here $v_{\mathrm{F}x}$ is the x component of the Fermi velocity, $\omega_n = 2\pi T(n + 1/2)$ is the Matsubara frequency, n is an integer number and T is the temperature. $\bar{\Delta}_{+}(x)$ ($\bar{\Delta}_{-}(x)$) is the effective pair potential for left (right) going quasiparticles. In the N region, $\bar{\Delta}_{\pm}(x)$ is set to zero due to the absence of a pairing interaction in the N metal. The above Green's functions can be expressed as

$$\begin{aligned} f^{(i)}_{1\pm} &= \pm\mathrm{i}(F^{(i)}_{\pm} + D^{(i)}_{\pm})/(1 - D^{(i)}_{\pm}F^{(i)}_{\pm}), \\ f^{(i)}_{2\pm} &= -(F^{(i)}_{\pm} - D^{(i)}_{\pm})/(1 - D^{(i)}_{\pm}F^{(i)}_{\pm}), \\ g^{(i)}_{\pm} &= (1 + D^{(i)}_{\pm}F^{(i)}_{\pm})/(1 - D^{(i)}_{\pm}F^{(i)}_{\pm}). \end{aligned} \tag{8}$$

Functions $D^{(i)}_{\pm}(x)$ and $F^{(i)}_{\pm}(x)$ satisfy the Riccati equations [22] in the N and S regions, supplemented by the proper boundary conditions [17].

Here, we consider the situation without mixing of different symmetry channels for the pair potential. Then the pair potential $\bar{\Delta}_{\pm}(x)$ is expressed by

$$\bar{\Delta}_{\pm}(x) = \Delta(x)\Phi_{\pm}(\theta)\Theta(x) \tag{9}$$

with the form factor $\Phi_{\pm}(\theta)$ given by $\Phi_{\pm}(\theta) = 1, \pm\sin 2\theta$, and $\pm\cos\theta$ for s-wave, d_{xy}-wave, and p_x-wave superconductors, respectively. The pair potential $\Delta(x)$ is determined by the self-consistent equation

$$\Delta(x) = \frac{2T}{\log\frac{T}{T_{\mathrm{C}}} + \sum_{n\geqslant 1}\frac{1}{n-\frac{1}{2}}}\sum_{n\geqslant 0}\int_{-\pi/2}^{\pi/2}\mathrm{d}\theta\, G(\theta) f_{2+} \tag{10}$$

with $G(\theta) = 1$ for the s-wave case and $G(\theta) = 2\Phi(\theta)$ for other cases, respectively [23]. T_{C} is the transition temperature of the superconductor. The condition in the bulk is $\Delta(\infty) = \Delta_0$. Since the pair potential $\bar{\Delta}(x)$ is a real quantity, the resulting $f_{1\pm}$ is an imaginary quantity and $f_{2\pm}$ is a real one.

Before performing actual numerical calculations, we now discuss general properties of the pair amplitude. In the following, we explicitly write $f^{(i)}_{1\pm} = f^{(i)}_{1\pm}(\omega_n, \theta)$, $f^{(i)}_{2\pm} = f^{(i)}_{2\pm}(\omega_n, \theta)$, $F^{(i)}_{\pm} = F^{(i)}_{\pm}(\omega_n, \theta)$ and $D^{(i)}_{\pm} = D^{(i)}_{\pm}(\omega_n, \theta)$. For the limit $x = \infty$, we obtain

$$\begin{aligned} f^{(S)}_{1\pm}(\omega_n, \theta) &= 0, \\ f^{(S)}_{2\pm}(\omega_n, \theta) &= \frac{\Delta_0\Phi_{\pm}(\theta)}{\sqrt{\omega_n^2 + \Delta_0^2\Phi_{\pm}^2(\theta_{\pm})}}. \end{aligned} \tag{11}$$

Note that $f^{(i)}_{1\pm}(\omega_n, \theta)$ becomes finite due to the spatial variation of the pair potential and it does not exist in the bulk. One can show that $D^{(i)}_{\pm}(-\omega_n, \theta) = 1/D^{(i)}_{\pm}(\omega_n, \theta)$ and $F^{(i)}_{\pm}(-\omega_n, \theta) = 1/F^{(i)}_{\pm}(\omega_n, \theta)$. After simple manipulation, we obtain

$$\begin{aligned} f^{(i)}_{1\pm}(\omega_n, \theta) &= -f^{(i)}_{1\pm}(-\omega_n, \theta), \\ f^{(i)}_{2\pm}(\omega_n, \theta) &= f^{(i)}_{2\pm}(-\omega_n, \theta), \end{aligned} \tag{12}$$

for any x. It is remarkable that functions $f^{(i)}_{1\pm}(\omega_n, \theta)$ and $f^{(i)}_{2\pm}(\omega_n, \theta)$ correspond to odd-frequency and even-frequency components of the pair amplitude, respectively. Function $f^{(1)}_{1\pm}(\omega_n, \theta)$ describes the odd-frequency component of the pair amplitude penetrating from the superconductor.

Next, we discuss the parity of these pair amplitudes. The even-parity (odd-parity) pair amplitude should satisfy the following relation $f^{(i)}_{j\pm}(\omega_n, \theta) = f^{(i)}_{j\mp}(\omega_n, -\theta)$ [$f^{(i)}_{j\pm}(\omega_n, \theta) = -f^{(i)}_{j\mp}(\omega_n, -\theta)$], with $j = 1, 2$. For an even-parity (odd-parity) superconductor, $\Phi_{\pm}(-\theta) = \Phi_{\mp}(\theta)$ [$\Phi_{\pm}(-\theta) = -\Phi_{\mp}(\theta)$]. Then, we can show that for the even-parity case

$$D^{(i)}_{\pm}(-\theta) = D^{(i)}_{\mp}(\theta), \qquad F^{(i)}_{\pm}(-\theta) = F^{(i)}_{\mp}(\theta) \tag{13}$$

and for the odd-parity case

$$D^{(i)}_{\pm}(-\theta) = -D^{(i)}_{\mp}(\theta), \qquad F^{(i)}_{\pm}(-\theta) = -F^{(i)}_{\mp}(\theta)$$

respectively.

The resulting $f_{1\pm}^{(i)}(\omega_n,\theta)$ and $f_{2\pm}^{(i)}(\omega_n,\theta)$ satisfy

$$\begin{aligned} f_{1\pm}^{(i)}(\omega_n,\theta) &= -f_{1\mp}^{(i)}(\omega_n,-\theta),\\ f_{2\pm}^{(i)}(\omega_n,\theta) &= f_{2\mp}^{(i)}(\omega_n,-\theta), \end{aligned} \tag{14}$$

for an even-parity superconductor and

$$\begin{aligned} f_{1\pm}^{(i)}(\omega_n,\theta) &= f_{1\mp}^{(i)}(\omega_n,-\theta),\\ f_{2\pm}^{(i)}(\omega_n,\theta) &= -f_{2\mp}^{(i)}(\omega_n,-\theta), \end{aligned} \tag{15}$$

for an odd-parity superconductor, respectively. Note that the parity of the odd-frequency component $f_{1\pm}^{(i)}(\omega_n,\theta)$ is always different from that in the bulk superconductor.

As shown above, the odd-frequency component $f_{1\pm}^{(i)}(\omega_n,\theta)$ is a purely imaginary quantity. The underlying physics behind this formal property is the follows. Due to the breakdown of translational invariance near the N/S interface, the pair potential $\bar{\Delta}(x)$ acquires a spatial dependence which leads to the coupling between even-parity and odd-parity states. Since the bulk pair potential has an even-frequency symmetry, the Fermi–Dirac statistics requires that the order parameter component induced near the interface should be odd in frequency. The phase of the induced pair amplitude undergoes a $\pi/2$ shift from that in the bulk S, thus removing internal phase shift between the even- and odd-frequency components and making the interface-induced state compatible with the time reversal invariance. As a result, function $f_{1\pm}^{(i)}(\omega_n,\theta)$ becomes a purely imaginary quantity.

Let us now focus on the values of the pair amplitudes at the edge of N region (at $x=-L$). We concentrate on two extreme cases with (I) $\Phi_+(\theta)=\Phi_-(\theta)$ and (II) $\Phi_+(\theta)=-\Phi_-(\theta)$. In case (I), the MARS is absent since there is no sign change of the pair potential felt by the quasiparticle at the interface. Then the relation $D_+^{(\mathrm{N})}=D_-^{(\mathrm{N})}$ holds. On the other hand, in case (II), the MARS is generated near the interface due to the sign change of the pair potential and the relation $D_+^{(\mathrm{N})}=-D_-^{(\mathrm{N})}$ is satisfied [15]. At the edge $x=-L$, it is easy to show that $F_\pm^{(\mathrm{N})}=-D_\pm^{(\mathrm{N})}$ for the former case and $F_\pm^{(\mathrm{N})}=D_\pm^{(\mathrm{N})}$ for the latter one. As a result, $f_{1\pm}^{(\mathrm{N})}=0$ for case (I) and $f_{2\pm}^{(\mathrm{N})}=0$ for case (II), respectively. Thus we can conclude that in the absence of the MARS only the even-frequency pairing component exists at $x=-L$, while in the presence of the MARS only the odd-frequency one exists.

In order to understand the angular dependence of the pair amplitude in a more detail, we define $\hat{f}_1^{(i)}$ and $\hat{f}_2^{(i)}$ for $-\pi/2<\theta<3\pi/2$ with $\hat{f}_{1(2)}^{(i)}=f_{1(2)+}^{(i)}(\theta)$ for $-\pi/2<\theta<\pi/2$ and $\hat{f}_{1(2)}^{(i)}=f_{1(2)-}^{(i)}(\pi-\theta)$ for $\pi/2<\theta<3\pi/2$. We decompose $\hat{f}_{1(2)}^{(i)}$ into various angular momentum components as follows,

$$\hat{f}_{1(2)}^{(i)}=\sum_m S_m^{(1(2))}\sin(m\theta)+\sum_m C_m^{(1(2))}\cos(m\theta) \tag{16}$$

with $m=2l+1$ for the odd-parity case and $m=2l$ for the even-parity case with integer $l\geqslant 0$, where l is the quantum number of the angular momentum. Here, $C_m^{(1(2))}$ and $S_m^{(1(2))}$ are defined for all x. It is straightforward to show that the only nonzero components are (1) $C_{2l}^{(2)}$ and $C_{2l+1}^{(1)}$ for the even-parity superconductor without sign change at the interface (*i.e.*, s-wave or $\mathrm{d}_{x^2-y^2}$-wave), (2) $S_{2l+2}^{(2)}$ and $S_{2l+1}^{(1)}$ for d_{xy}-wave, (3) $C_{2l+1}^{(2)}$ and $C_{2l}^{(1)}$ for p_x-wave, and (4) $S_{2l+1}^{(2)}$ and $S_{2l}^{(1)}$ for p_y-wave junctions, respectively. The allowed angular momenta for odd-frequency components are $2l+1$, $2l+1$, $2l$, and $2l+2$ corresponding to each of the above four cases.

In order to get better insight into the spectral property of the odd-frequency pair amplitude, we perform an analytical continuation from the Matsubara frequency ω_n to the quasiparticle energy ε measured from the chemical potential. The retarded Green's function corresponding to equation (1) is defined as $\hat{g}_\pm^{(i)R}=f_{1\pm}^{(i)R}\hat{\tau}_1+f_{2\pm}^{(i)R}\hat{\tau}_2+g_\pm^{(i)R}\hat{\tau}_3$. One can show that $f_{1\pm}^{(i)R}(-\varepsilon)=-[f_{1\pm}^{(i)R}(\varepsilon)]^*$, $f_{2\pm}^{(i)R}(-\varepsilon)=[f_{2\pm}^{(i)R}(\varepsilon)]^*$, and $g_\pm^{(i)R}(-\varepsilon)=[g_\pm^{(i)R}(\varepsilon)]^*$. The LDOS $\rho(\varepsilon)$ at the N/S interface at $x=0$ normalized to its value in the normal state is given by

$$\rho(\varepsilon)=\int_{-\pi/2}^{\pi/2}\mathrm{d}\theta\ \mathrm{Real}\left(\frac{g_+^{(i)R}(\varepsilon)+g_-^{(i)R}(\varepsilon)}{2\pi}\right). \tag{17}$$

Let us discuss the case of s-wave superconductor junctions as shown in figure 2. By changing the length L of the N region and the transparency at the interface, we calculate the spatial dependence of the pair potential and the pair amplitudes in the Matsubara frequency representation. We only concentrate on the lowest angular momentum of the even-frequency pair amplitude $C_0^{(2)}$. As regards the odd-frequency pair amplitudes, we focus on the $C_1^{(1)}$, $C_3^{(1)}$ and $C_5^{(1)}$ components which all have odd-parity and depend on θ as $\cos\theta$, $\cos 3\theta$ and $\cos 5\theta$, respectively, and correspond to the p_x-wave, f_1-wave and h_1-wave components shown in figure 1. In all cases, the even-frequency component is constant in the S region far away from the interface and the corresponding odd-frequency components are absent. The s-wave pair potential is suppressed for the fully transparent case ($Z=0$), while it is almost constant for the low transparent case ($Z=5$). It does not penetrate into the N region due to the absence of the attractive interaction in the N metal. On the other hand, in all considered cases, the spatial variation of the even-frequency s-wave pair amplitude is rather weak in the S region, while in the N region it is strong for $Z=0$ and is reduced for $Z=5$ since the proximity effect is weaker in the latter case. The odd-frequency component always vanishes at $x=-L$ and does not have a jump at the N/S interface even for nonzero Z. Its amplitude is strongly enhanced near the N/S interface especially for fully transparent junctions. Note that not only the p_x-wave but also the f_1-wave and the h_1-wave have sufficiently large magnitudes as shown in figures 2(a) and (c). With the decrease of the transparency of the N/S interface, the odd-frequency components are suppressed as shown in figures 2(b) and (d).

It is instructive to discuss the spectral properties of the induced pairing state in the N region. Here, we concentrate on the situation when the N/S interface is fully transparent ($Z=0$) and $L=5L_0$. In this case the LDOS in the N region and at the N/S interface coincide with each other. The LDOS has multiple peaks due to the existence of the multi-subgap structures due to electron–hole interference effects in the N region [24, 25].

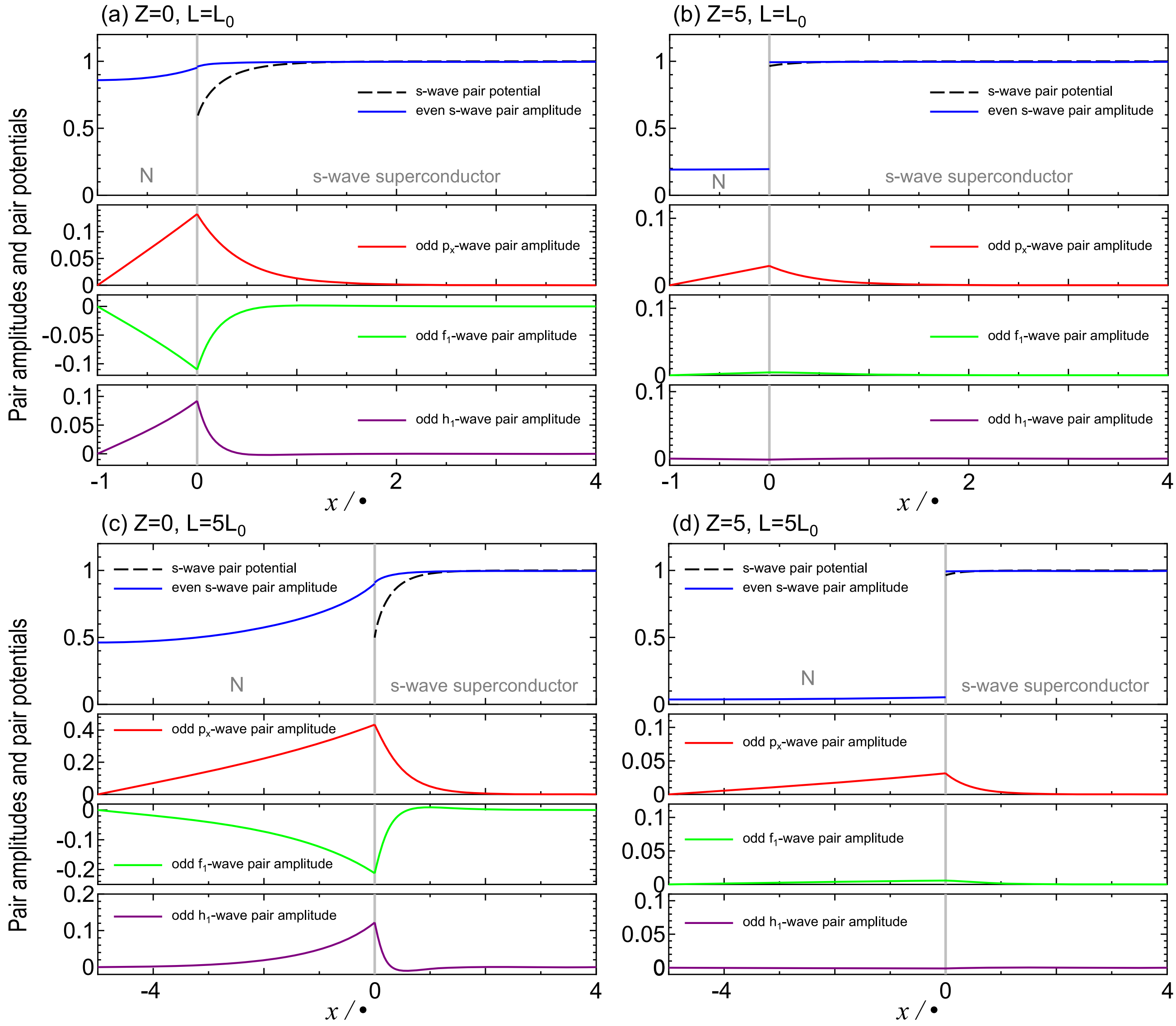

Figure 2. Spatial dependence of the normalized pair potential, even-frequency pair amplitude and odd-frequency components of the pair amplitude for s-wave superconductor junctions. Here, we choose $\xi = v_F/\Delta_0$ in the S region ($x > 0$) and $\xi = L_0 = v_F/2\pi T_C$ in the N region. The pair amplitudes $C_0^{(2)}$, $C_1^{(1)}$, $C_3^{(1)}$, and $C_5^{(1)}$ are denoted as even s-wave, odd p$_x$-wave, odd f_1-wave, and odd h_1-wave pair amplitudes. (a) $Z = 0$, $L = L_0$, (b) $Z = 5$, $L = L_0$, (c) $Z = 0$, $L = 5L_0$, and (d) $Z = 5$, $L = 5L_0$, respectively.

The amplitudes of the corresponding even-frequency and odd-frequency components are enhanced at energies ε corresponding to the LDOS peak positions, while the ratio of these components depends on the energy and location in the N region. To clarify this point further, we concentrate on the ratio of the odd- and even-frequency components in the N region. The ratio of the magnitude of the odd-frequency component $f_{1+}^{(\mathrm{N})}(\varepsilon,\theta)$ to the even-frequency one $f_{2+}^{(\mathrm{N})}(\varepsilon,\theta)$ is

$$\frac{\left|f_{1+}^{(\mathrm{N})}(\varepsilon,\theta)\right|}{\left|f_{2+}^{(\mathrm{N})}(\varepsilon,\theta)\right|} = \left|\tan\left(\frac{2\varepsilon}{v_{\mathrm{F}x}}(L+x)\right)\right|. \qquad (18)$$

At the edge of the N region, $x = -L$, the odd-frequency component vanishes at all energies. On the other hand, a very interesting situation occurs at the N/S interface, $x = 0$, as will be shown below. In figure 3, we plot this ratio for $\theta = 0$ and $x = 0$.

It is remarkable that at some energies the amplitude of the odd-frequency pair amplitude exceeds that of the even-frequency one.

Let us clarify the relation between the positions of the bound states and the above ratio of the odd-to-even pair amplitude. In the limit $L \gg L_0$ the bound states are determined by the simple relation [24, 25]

$$\varepsilon_n = \frac{\pi v_{\mathrm{F}x}}{2L}(n+1/2), \qquad n = 0, 1, 2, \ldots. \qquad (19)$$

That means that at the subgap peak energies the odd-frequency component dominates over the even-frequency one at the N/S interface. This is a remarkable property of the odd-frequency pairing, which makes it relevant to the classical

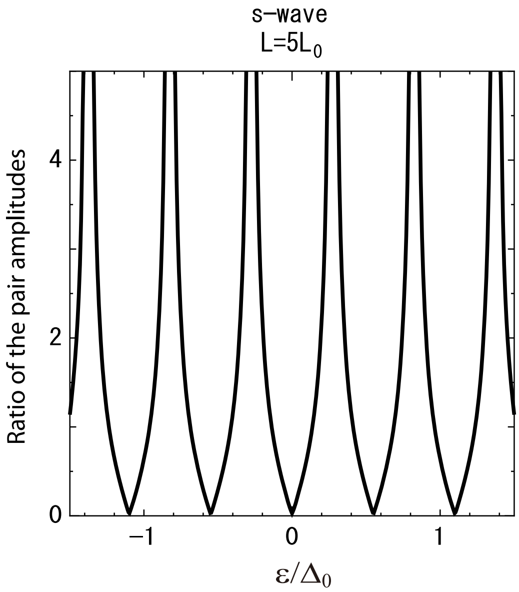

Figure 3. Ratio of the pair amplitudes $f_{1+}^{(\mathrm{N})}(\varepsilon,\theta)/f_{2+}^{(\mathrm{N})}(\varepsilon,\theta)$ on the N side of the N/S interface in s-wave junction as a function of energy ε for $\theta = 0$ and $L = 5L_0$.

McMillan–Rowell oscillations in the N/S geometry [25]. To summarize, we have shown that the odd-frequency component is present even in the standard case of a ballistic N/S system, and it dominates at energies when the LDOS has subgap peaks.

In summary, using the quasiclassical Green's function formalism, we have shown that the odd-frequency pairing state is ubiquitously generated in the normal metal/superconductor (N/S) ballistic junction system, where the length of the normal region is finite. It is shown that the even-parity (odd-parity) pair potential in the superconductor induces the odd-frequency pairing component with spin-singlet odd-parity (spin-triplet even-parity). Even for conventional s-wave junctions, the amplitude of the odd-frequency pairing state is enhanced at the N/S interface with a fully transparent barrier. By analyzing the spectral properties of the pair amplitudes, we found that the magnitude of the resulting odd-frequency component at the interface can exceed that of the even-frequency one. For the case of p_x-wave and d_{xy}-wave junctions, the magnitude of the odd-frequency component at the S side of the N/S interface is significantly enhanced. The magnitude of the induced odd-frequency component is enhanced in the presence of the midgap Andreev resonant state due to the sign change of the anisotropic pair potential at the interface. The LDOS has a zero energy peak (ZEP) both at the interface and in the N region. At the edge of the N region, only the odd-frequency component is nonzero.

The underlying physics behind these phenomena is related to the breakdown of translational invariance near the N/S interface where the pair potential $\bar{\Delta}(x)$ acquires a spatial dependence. As a result, an odd-frequency component is quite generally induced near the interface. The breakdown of translational invariance is strongest when the pair potential changes sign upon reflection as in the case of p_x-wave and d_{xy}-wave junctions, then the magnitude of odd-frequency component is the largest. Moreover, the phase of the interface-induced odd-frequency component has a $\pi/2$ shift from that in the bulk of S. Therefore, as shown above, the odd-frequency component $f_{1\pm}^{(i)}(\omega_n,\theta)$ becomes a purely imaginary quantity and the peak structure in the LDOS naturally follows from the normalization condition.

We have also shown that in N/S junctions with s-wave superconductors the classical McMillan–Rowell oscillations [25] can also be reinterpreted in terms of odd-frequency pairing. At the energies corresponding to the subgap peaks in the N/S junction, the odd-frequency component dominates over the even-frequency one. This is a remarkable application of the odd-frequency pairing concept.

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