Письма в ЖЭТФ

Boundary conditions for the contact between normal metal and multiband superconductors with unusual types of pairing

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To illustrate the procedure of derivation of such boundary conditions in tight-binding model, which are substantially different for each particular case, we consider one-dimensional model of the boundary between a normal metal and a superconductor, which has a quasimomentum-dependent order parameter. We start from the Hamiltonian H of the $1D$ chain of atoms (Fig. 1), whom electronic states are described in the tight-binding approximation, with the possibility of singlet superconducting pairing between neighboring atoms:

$$H = \sum_{j,\sigma} \left[-t_j \left(a^+_{\sigma,j} a_{\sigma,j+1} + h.c. \right) - \mu a^+_{\sigma,j} a_{\sigma,j} \right] + \\ + \sum_j \left[\Delta_j \left(a^+_{\uparrow,j} a^+_{\downarrow,j+1} - a^+_{\downarrow,j} a^+_{\uparrow,j+1} \right) + h.c. \right], \quad (1)$$

with creation (annihilation) operator $a^+_{\sigma,j}\,(a_{\sigma,j})$ of an electron with spin σ on j site, spatially inhomogeneous order parameter Δ_j, and chemical potential μ.

Diagonalization of the Hamiltonian Eq. (1) is produced by the following canonical transformation:

$$a_{\sigma,j} = \sum_\nu \left[u_{\nu,j} \alpha_{\nu,\sigma} + sign(\sigma) v^*_{\nu,j} \alpha^+_{\nu,-\sigma} \right], \quad (2)$$

which is a generalization of the Bogoliubov transformation to the case of a discrete lattice [17]. In the Eq. (2) operators $\alpha^+_{\nu,-\sigma}(\alpha_{\nu,\sigma})$ are operators of creation (annihilation) of quasiparticles satisfying Fermi anticommutation relations, $u_{\nu,j}$ и $v_{\nu,j}$ are the electron and hole amplitudes. The substitution of the discrete Bogoliubov transformations Eq. (2) to the Hamiltonian Eq. (1) leads to the following equations for the electron $u_{\nu,j}$ and hole $v_{\nu,j}$ amplitudes:

$$\begin{cases} t_j u_{\nu,j+1} + t_{j-1} u_{\nu,j-1} + \mu u_{\nu,j} + \\ + \Delta_j v_{\nu,j+1} + \Delta_{j-1} v_{\nu,j-1} = -\varepsilon_\nu u_{\nu,j}, \\ t_j v_{\nu,j+1} + t_{j-1} v_{\nu,j-1} + \mu u_{\nu,j} + \\ - \Delta^*_j u_{\nu,j+1} - \Delta^*_{j-1} u_{\nu,j-1} = \varepsilon_\nu v_{\nu,j}. \end{cases} \quad (3)$$

The system of equations Eq. (3) together with the corresponding self-consistent equations for the order parameter Δ_j allows, in principle, to consider any space-inhomogeneous problem for an arbitrary set of hopping parameters between sites t_j. However, this problem can be solved only numerically, even for the considered one dimensional model. At the same time, the greatest interest is the situation of the contact of a normal metal with constant hopping amplitude between sites t' and $\Delta_j = 0,\ j \le 0$, with the superconductor, described by constant in the space the order parameter $\Delta_j = \Delta,\ j \ge 1$, and hopping amplitude between sites t. The boundary between a metal and a superconductor described by the hopping amplitude γ (see Fig. 1).

For the coherent matching of the wave function at the boundary of a normal and superconducting metals with different amplitudes of hopping in them and piecewise-continuous order parameter (see Fig. 1) one can generalize known in the theory of semiconductor heterostructures method [18] to the case of superconducting heterostructures. The method proposed in [18] not limited by the assumption of quadratic single-particle excitation spectrum (using concepts of effective masses of electrons in the electrode contact) and reduces to the matching of extended solutions of discrete equations of the form Eq. (3) with $\Delta_j = 0$ from the left normal metal on one site to the region of the rigth normal metal and vice versa (see Fig. 1):

$$\begin{cases} t'\Phi_1 = \gamma\Psi_1, \\ \gamma\Phi_0 = t\Psi_0. \end{cases} \quad (4)$$

In Eq. (4) discrete electron wave functions $\Psi_i(\Phi_i)$ belong to the right (left) metal, respectively. In the continuum limit the boundary conditions Eq. (4) transform into the usual boundary conditions in effective mass approximation and provide the conservation of probability flow J across the interface:

$$J_{j<-1} = \frac{2t'}{\hbar} Im(\Phi^*_{j+1}\Phi_j) = J_{j>0} = \frac{2t}{\hbar} Im(\Psi^*_{j+1}\Psi_j). \quad (5)$$

Using method proposed in [18] one can obtain from Eq. (3) the following boundary conditions for the description of the contact of a normal metal and a superconductor (see Fig. 1):

$$\begin{cases} t'\Phi_1 = \gamma\Psi_1, \\ t'\bar{\Phi}_1 = \gamma\bar{\Psi}_1, \\ \gamma\Phi_0 = t\Psi_0 + \Delta\bar{\Psi}_0, \\ \gamma\bar{\Phi}_0 = t\bar{\Psi}_0 - \Delta^*\Psi_0. \end{cases} \quad (6)$$

In equation Eq. (6) discrete electron wave functions $\Psi_i(\Phi_i)$ as well as in Eq. (4) belong to the right (left) metal, respectively. The functions $\Psi_i(\Phi_i)$ in the Eq. (6) describe the electron states and $\bar{\Psi}_i(\bar{\Phi}_i)$ describe hole states:

$$\begin{cases} \Phi_n = \exp(iq_1nl) + b\ \exp(-iq_1nl), \\ \bar{\Phi}_n = a\ \exp(iq_2nl), \\ \Psi_n = c\ u\exp(iknl) + d\ \widetilde{u}\ \exp(i\widetilde{k}nl), \\ \bar{\Psi}_n = c\ v\exp(iknl) + d\ \widetilde{v}\ \exp(i\widetilde{k}nl). \end{cases} \quad (7)$$

The wave functions of a normal metal and a superconductor contain four unknowns a, b, c, d, describing the Andreev and normal reflected in a normal metal waves (a and b, respectively) and two transmitted in the superconductor waves (c and d). These four unknowns (a, b, c, d) are uniquely defined from four boundary conditions Eq. (6). In Eq. (7) l is the distance between sites in a normal metal and a superconductor (for clarity, we consider them to be equal, but this restriction is not necessary [18]), $q_1, q_2, k, \widetilde{k}$ are wave vectors in a normal metal and a superconductor, corresponding to the energy E of propagating waves. These wave vectors are the space-homogeneous solutions of Eq. (3) for a normal metal and a superconductor, respectively. Electron and hole Bogolyubov coefficients $u, v; \widetilde{u}, \widetilde{v}$, corresponding to propagating waves in the bulk of a superconductor with wave vectors $k; \widetilde{k}$ are also the space-homogeneous solutions of Eq. (3) with $\Delta_j = \Delta$. One can show that obtained wave function after using boundary conditions Eq. (7) provide the conservation of the probability flow. The expression for the probability flow on a discrete lattice (Fig. 1) follows from the Bogolyubov-de Gennes equations on the sites of the crystal lattice Eq. (3):

$$J_s = \frac{2}{\hbar} Im(t\Psi^*_{j+1}\Psi_j - t\bar{\Psi}^*_{j+1}\bar{\Psi}_j + \Delta\Psi^*_{j+1}\bar{\Psi}_j + \Delta^*\bar{\Psi}^*_{j+1}\Psi_j). \quad (8)$$

It is necessary to note that the condition of the conservation of probability flow at the interface between a normal metal and a superconductor, having the form of discrete sums (differences) in the crystal lattice: $J = J_s$ (Eqs. (5), (8)), can be written as a product of squares of the amplitudes of the probability to be in states with wave vectors $q_1, -q_1, q_2, k, \widetilde{k}$ on the group velocities in these states:

$$\frac{\partial\varepsilon_n}{\partial q}|_{q=q_1} - |a|^2\frac{\partial\varepsilon_n}{\partial q}|_{q=q_2} + |b|^2\frac{\partial\varepsilon_n}{\partial q}|_{q=-q_1} = |c|^2\frac{\partial\varepsilon_s}{\partial q}|_{q=k} + |d|^2\frac{\partial\varepsilon_s}{\partial q}|_{q=\widetilde{k}}. \quad (9)$$

Eq. (9) is similar to the corresponding expression in [19].

The proposed method allows us to consider the coherent electron transport in $N - S_p$ (normal metal - superconducting pnictides) structures with non-zero misorientation angle also. In considering of the electron transport across $N - S_p$ contact with a nonzero misorientation angle it is necessary to take into account hopping at the two adjacent atom layers of pnictides (see Fig. 2). Hopping across the $N - S_p$ boundary for non-zero misorientation angle is described by larger number of parameters than at zero misorientation angle between crystallographic axes of the pnictides and the interface (see Fig. 2). In addition to hopping parameters γ_1, γ_2, we should use additional parameters of hopping across the boundary γ'_1, γ'_2. These parameters of hopping across the boundary take into account connection of orbitals from the last atom layer of pnictides with the penultimate from the boundary atom layer of the normal metal. Taking into account these processes is necessary due to the breaking at the boundary of the diagonal bonds in the crystal lattice of pnictides for non-zero angle of misorientation (see Fig. 2). Also in the normal metal together with the nearest neighbor hopping t'_1 we need to consider the diagonal hopping t'_2 in square lattice. The boundary conditions for the contact between a normal metal and pnictides, considered in the framework of the two-orbital model, for misorientation angle $\pi/4$ between crystallographic axes of the pnictides and the interface have the following form:

$$
\begin{cases}
t_1'\Phi_1(e^{ik_yl}+e^{-ik_yl})+t_2'\Phi_2=\Psi_1^{\alpha}(\gamma_1e^{ik_yl}+\gamma_2e^{-ik_yl})\\
+\Psi_1^{\beta}(\gamma_1e^{-ik_yl}+\gamma_2e^{ik_yl})+\gamma_1'\Psi_2^{\alpha}+\gamma_2'\Psi_2^{\beta},\\
t_1'\bar{\Phi}_1(e^{ik_yl}+e^{-ik_yl})+t_2'\bar{\Phi}_2=\bar{\Psi}_1^{\alpha}(\gamma_1e^{ik_yl}+\gamma_2e^{-ik_yl})\\
+\bar{\Psi}_1^{\beta}(\gamma_1e^{-ik_yl}+\gamma_2e^{ik_yl})+\gamma_1'\bar{\Psi}_2^{\alpha}+\gamma_2'\bar{\Psi}_2^{\beta},\\
\Phi_0(\gamma_1e^{ik_yl}+\gamma_2e^{-ik_yl})+\gamma_1'\Phi_{-1}=t_1\Psi_0^{\alpha}e^{ik_yl}\\
+t_2\Psi_0^{\alpha}e^{-ik_yl}+t_3\Psi_{-1}^{\alpha}-t_4\Psi_{-1}^{\beta}+\Delta_0\bar{\Psi}_{-1}^{\alpha},\\
\bar{\Phi}_0(\gamma_1e^{ik_yl}+\gamma_2e^{-ik_yl})+\gamma_1'\bar{\Phi}_{-1}=t_1\bar{\Psi}_0^{\alpha}e^{ik_yl}\\
+t_2\bar{\Psi}_0^{\alpha}e^{-ik_yl}+t_3\bar{\Psi}_{-1}^{\alpha}-t_4\bar{\Psi}_{-1}^{\beta}-\Delta_0\Psi_{-1}^{\alpha},\\
\Phi_0(\gamma_1e^{-ik_yl}+\gamma_2e^{ik_yl})+\gamma_2'\Phi_{-1}=t_1\Psi_0^{\beta}e^{ik_yl}\\
+t_2\Psi_0^{\beta}e^{-ik_yl}+t_3\Psi_{-1}^{\beta}-t_4\Psi_{-1}^{\alpha}+\Delta_0\bar{\Psi}_{-1}^{\beta},\\
\bar{\Phi}_0(\gamma_1e^{-ik_yl}+\gamma_2e^{ik_yl})+\gamma_2'\bar{\Phi}_{-1}=t_1\bar{\Psi}_0^{\beta}e^{ik_yl}\\
+t_2\bar{\Psi}_0^{\beta}e^{-ik_yl}+t_3\bar{\Psi}_{-1}^{\beta}-t_4\bar{\Psi}_{-1}^{\alpha}-\Delta_0\Psi_{-1}^{\beta},\\
\gamma_1'\Phi_0=t_3\Psi_0^{\alpha}-t_4\Psi_0^{\beta}+\Delta_0\bar{\Psi}_0^{\alpha},\\
\gamma_1'\bar{\Phi}_0=t_3\bar{\Psi}_0^{\alpha}-t_4\bar{\Psi}_0^{\beta}-\Delta_0\Psi_0^{\alpha},\\
\gamma_2'\Phi_0=t_3\Psi_0^{\beta}-t_4\Psi_0^{\alpha}+\Delta_0\bar{\Psi}_0^{\beta},\\
\gamma_2'\bar{\Phi}_0=t_3\bar{\Psi}_0^{\beta}-t_4\bar{\Psi}_0^{\alpha}-\Delta_0\Psi_0^{\beta},\\
t_2'\Phi_1=\gamma_1'\Psi_1^{\alpha}+\gamma_2'\Psi_1^{\beta},\\
t_2'\bar{\Phi}_1=\gamma_1'\bar{\Psi}_1^{\alpha}+\gamma_2'\bar{\Psi}_1^{\beta}.
\end{cases}
\tag{10}
$$

Due to the translational symmetry in the direction parallel to the boundary in electron (hole) wave functions $\Psi_{n,m}^{\alpha(\beta)}$ ($\bar{\Psi}_{n,m}^{\alpha(\beta)}$) second subscript (m) corresponding to the coordinate of an atom in a direction parallel to the boundary is omitted.

The wave functions of the $N-S_p$ contact in the case of misorientation angle between crystallographic axes of pnictides and the interface which is equal to $\pi/4$ are defined by 8 plane waves with amplitudes $a_1, a_2, b_1, b_2, c_1, c_2, d_1, d_2, f_1, f_2, g_1, g_2$: a_1, a_2, b_1, b_2 describe the Andreev and normal reflected at normal metal waves, and $c_1, c_2, d_1, d_2, f_1, f_2, g_1, g_2$ describe 8 transmitted in the two-band superconducting pnictides waves:

$$
\begin{cases}
\Phi_n=\exp(iq_1nl)+b_1\ \exp(-iq_1nl)+b_2\ \exp(-iq_2nl),\\
\bar{\Phi}_n=a_1\ \exp(iq_3nl)+a_2\ \exp(iq_4nl),\\
\Psi_n^{\alpha}=c_1u_1(k_1)\exp(ik_1nl)+c_2u_1(k_2)\exp(ik_2nl)\\
+d_1u_1(k_3)\exp(ik_3nl)+d_2u_1(k_4)\exp(ik_4nl)\\
+f_1u_1(k_5)\exp(ik_5nl)+f_2u_1(k_6)\exp(ik_6nl)\\
+g_1u_1(k_7)\exp(ik_7nl)+g_2u_1(k_8)\exp(ik_8nl),\\
\Psi_n^{\beta}=c_1u_2(k_1)\exp(ik_1nl)+c_2u_2(k_2)\exp(ik_2nl)\\
+d_1u_2(k_3)\exp(ik_3nl)+d_2u_2(k_4)\exp(ik_4nl)\\
+f_1u_2(k_5)\exp(ik_5nl)+f_2u_2(k_6)\exp(ik_6nl)\\
+g_1u_2(k_7)\exp(ik_7nl)+g_2u_2(k_8)\exp(ik_8nl),\\
\bar{\Psi}_n^{\alpha}=c_1v_1(k_1)\exp(ik_1nl)+c_2v_1(k_2)\exp(ik_2nl)\\
+d_1v_1(k_3)\exp(ik_3nl)+d_2v_1(k_4)\exp(ik_4nl)\\
+f_1v_1(k_5)\exp(ik_5nl)+f_2v_1(k_6)\exp(ik_6nl)\\
+g_1v_1(k_7)\exp(ik_7nl)+g_2v_1(k_8)\exp(ik_8nl),\\
\bar{\Psi}_n^{\beta}=c_1v_2(k_1)\exp(ik_1nl)+c_2v_2(k_2)\exp(ik_2nl)\\
+d_1v_2(k_3)\exp(ik_3nl)+d_2v_2(k_4)\exp(ik_4nl)\\
+f_1v_2(k_5)\exp(ik_5nl)+f_2v_2(k_6)\exp(ik_6nl)\\
+g_1v_2(k_7)\exp(ik_7nl)+g_2v_2(k_8)\exp(ik_8nl).
\end{cases}
\tag{11}
$$

Four transmitted waves with amplitudes c_1, c_2, d_1, d_2 correspond to the pnictides lower band. These four waves on energy scales of order Δ are propagating waves, except the region under the superconducting gaps. Four plane waves with amplitudes f_1, f_2, g_1, g_2 correspond to the pnictides upper band. These four waves on scales of order Δ are evanescent waves.

Expression for the probability flow in the case of misorientation angle between crystallographic axes of pnictides and the interface which is equal to $\pi/4$ differs from the corresponding relation for the case of zero misorientation angle and has the following form:

$$
\begin{aligned}
J = \frac{2}{\hbar}(t_1 Im\{(\Psi^{\alpha}_{n+1})^* \Psi^{\alpha}_n e^{ik_y l}\} + \\
+t_2 Im\{(\Psi^{\alpha}_{n+1})^* \Psi^{\alpha}_n e^{-ik_y l}\} + \\
+t_3 Im\{(\Psi^{\alpha}_{n+1})^* \Psi^{\alpha}_{n-1} + (\Psi^{\alpha}_{n+2})^* \Psi^{\alpha}_n\} + \\
+t_1 Im\{(\Psi^{\beta}_{n+1})^* \Psi^{\beta}_n e^{-ik_y l}\} + t_2 Im\{(\Psi^{\beta}_{n+1})^* \Psi^{\beta}_n e^{ik_y l}\} + \\
+t_3 Im\{(\Psi^{\beta}_{n+1})^* \Psi^{\beta}_{n-1} + (\Psi^{\beta}_{n+2})^* \Psi^{\beta}_n\} - \\
-t4(Im\{(\Psi^{\alpha}_{n+1})^* \Psi^{\beta}_{n-1}\} + Im\{(\Psi^{\beta}_{n+1})^* \Psi^{\alpha}_{n-1}\} + \\
+Im\{(\Psi^{\alpha}_{n+2})^* \Psi^{\beta}_n\} + Im\{(\Psi^{\beta}_{n+2})^* \Psi^{\alpha}_n\}) \\
-t_1 Im\{(\bar{\Psi}^{\alpha}_{n+1})^* \bar{\Psi}^{\alpha}_n e^{ik_y l}\} - t_2 Im\{(\bar{\Psi}^{\alpha}_{n+1})^* \bar{\Psi}^{\alpha}_n e^{-ik_y l}\} - \\
-t_3 Im\{(\bar{\Psi}^{\alpha}_{n+1})^* \bar{\Psi}^{\alpha}_{n-1} + (\bar{\Psi}^{\alpha}_{n+2})^* \bar{\Psi}^{\alpha}_n\} - \\
-t_1 Im\{(\bar{\Psi}^{\beta}_{n+1})^* \bar{\Psi}^{\beta}_n e^{-ik_y l}\} - t_2 Im\{(\bar{\Psi}^{\beta}_{n+1})^* \bar{\Psi}^{\beta}_n e^{ik_y l} - \\
-t_3 Im\{(\bar{\Psi}^{\beta}_{n+1})^* \bar{\Psi}^{\beta}_{n-1} + (\bar{\Psi}^{\beta}_{n+2})^* \bar{\Psi}^{\beta}_n\} \\
+t4(Im\{(\bar{\Psi}^{\alpha}_{n+1})^* \bar{\Psi}^{\beta}_{n-1}\} + Im\{(\bar{\Psi}^{\beta}_{n+1})^* \bar{\Psi}^{\alpha}_{n-1}\} + \\
+Im\{(\bar{\Psi}^{\alpha}_{n+2})^* \bar{\Psi}^{\beta}_n\} + Im\{(\bar{\Psi}^{\beta}_{n+2})^* \bar{\Psi}^{\alpha}_n\}) \\
+\Delta_0 Im\{(\Psi^{\alpha}_{n+1})^* \bar{\Psi}^{\alpha}_{n-1} + (\bar{\Psi}^{\alpha}_{n+1})^* \Psi^{\alpha}_{n-1} + \\
+(\Psi^{\beta}_{n+1})^* \bar{\Psi}^{\beta}_{n-1} + (\bar{\Psi}^{\beta}_{n+1})^* \Psi^{\beta}_{n-1} + (\Psi^{\alpha}_{n+2})^* \bar{\Psi}^{\alpha}_n + \\
+(\bar{\Psi}^{\alpha}_{n+2})^* \Psi^{\alpha}_n + (\Psi^{\beta}_{n+2})^* \bar{\Psi}^{\beta}_n + (\bar{\Psi}^{\beta}_{n+2})^* \Psi^{\beta}_n\}). \qquad (12)
\end{aligned}
$$

The wave functions Eq. (11) and the relation for probability flow (12) take into account not only the electron transport in two energy bands, but also in two valleys in these bands.

Fig. 1 $1D$ chain of atoms. Left region (red filled circles) corresponds to the region of normal metal with hopping parameter $t^{'}$, right region (blue circles) corresponds to the region of superconducting metal with hopping parameter t, $N-S$ boundary is described by hopping parameter γ

Fig.2 $2D$ $N-S_p$ boundary. Angle between crystallographic axes of the pnictides and a normal metal is equal to $\pi/4$. The lower left region (orange circles) corresponds to the region of normal metal with hopping parameters t_1', t_2', right region (sites with two d-orbitals) corresponds to the region of superconducting pnictides with hopping parameters t_1, t_2, t_3, t_4. Boundary is described by hopping parameters $\gamma_1, \gamma_2, \gamma_1', \gamma_2'$