Microscopic theory of the Josephson current in contacts between Fe-based superconductor and conventional superconductor.

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Microscopic theory of dc Josephson current in contacts between high temperature Fe-based superconductor and spin-singlet s-wave superconductor are presented here. The basis of our method is the construction of a coherent temperature Greens function of the conventional spin-singlet s-wave superconductor/Fe-based superconductor (FeBS) junction in the framework of the tight-binding model. We calculate the phase dependencies of the Josephson current for different directions of current relative to the crystallographic axes of Fe-based superconductor and different length of an insulator layer and temperature dependencies of the critical Josephson current. This proposed method can be applied for calculations of dc Josephson current in contacts with other new unconventional multiorbital superconductors, such as $\text{Sr}_2\text{RuO}_4$ and doped superconducting insulators $\text{Cu}_x\text{Bi}_2\text{Se}_3$.

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I. INTRODUCTION

The type of the symmetry of the order parameter in unconventional superconductors keeps an important information about the mechanism of superconducting pairing in it. Therefore, determination of the symmetry of the order parameter of new unconventional superconductors is one of the first tasks after their discovery. It is well-known that the phase-coherent tunneling experiments with junctions with unusual superconductors provide important information about the symmetry of the order parameter in them. These tunneling experiments may be experiments to study current-voltage characteristics of a junction of a normal metal with a new superconductor or experiments on the Josephson tunneling in superconducting junction with a new superconductor.

Exotic superconducting properties of $\text{Sr}_2\text{RuO}_4$ have provided strong support for an unconventional pairing symmetry. The common property of such new unusual superconductors as $\text{Sr}_2\text{RuO}_4$, Fe-based superconductors (FeBS), doped superconducting insulators $\text{Cu}_x\text{Bi}_2\text{Se}_3$ is that all of them are multibands metals with several bands which intersect a Fermi surface. Also these unconventional superconductors have unusual single-particle excitation spectrum, and one can expect an anisotropic and sign-changing for different directions superconducting order parameters in them. The processes of interband and intervalley scattering are very important at the boundaries of these new multiband unconventional superconductors. A microscopic theory to describe the current of single-particle excitations in junctions of a normal metal with a multiband superconductor, which takes into account these unusual properties of these materials, has been proposed only recently. Other theories devoted to the study of coherent transport in junctions of a FeBS are phenomenological. But there is still no consistent microscopic theory to describe the Josephson tunneling in junctions between multiband superconductor and conventional single-band spin-singlet s-wave superconductor. All previous theories devoted to the investigation of Josephson tunneling in junctions with multiband superconductors are also phenomenological. In this paper we create consistent microscopic description of the Josephson tunneling in junctions with multiband superconductors and applied it to calculation of the Josephson current-phase dependencies in junctions between a s-wave superconductor and a FeBS for different directions of current with respect to the crystallographic axes of a FeBS. We also calculate the temperature dependencies of the Josephson critical current in these junctions. We microscopically confirm one of the recently proposed experiments for determination of the symmetry of the
order parameter in a FeBS.

The organization of our paper is as follows. In Sec. II we discuss the general formulation of our microscopical tight-binding approach for calculation of dc Josephson current in junctions with spin-singlet single-orbital superconductors. We demonstrate that our tight-binding approach reproduce the previous results for the Josephson tunneling both in junctions with only s-wave superconductors and in junctions between s-wave and d-wave superconductor. In Sec. III we discuss the application of our method for calculation of dc Josephson current in junctions between FeBS and conventional spin-singlet s-wave superconductor. We consider FeBS in the framework of the two-band model and describe the procedure of microscopical calculation of the Josephson current for different directions of current with respect to the crystallographic axes of a FeBS. We consider the intra-orbital models of superconducting pairing with the $s_\pm$-wave and the $s_{++}$-wave symmetry. In Sec. IV we present results of numerical calculations of phase dependencies of dc Josephson current for different directions of current with respect to the crystallographic axes of a FeBS and demonstrate that only the investigation of Josephson tunneling in c-direction provides the possibility to distinguish the $s_{\pm}$-wave and the $s_{++}$-wave symmetry in a FeBS. We also present our results for temperature dependencies of the critical Josephson current in this section. We discuss our results and make conclusions in Sec. V.

II. TIGHT-BINDING MODEL OF THE
JOSEPHSON JUNCTIONS WITH
SINGLE-ORBITAL SUPERCONDUCTORS

In this section we demonstrate our microscopical Green’s function tight-binding approach for calculation of dc Josephson current for the case of Josephson junctions, which banks are formed from spin-singlet superconductors. First we consider the procedure of calculation of 1D Josephson transport for $S/I/S$ junctions, where $S$ is usual $s$-wave superconductors ans $I$ is an insulating layer. Then we outline the same procedure for $S/I/S_d$ junctions, where $S_d$ is a spin-singlet single-orbital superconductor with $d$-wave symmetry. We demonstrate that our tight-binding Green’s function approach reproduce the previous results for both $S/I/S$ and $S/I/S_d$ Josephson junctions. In the end of this Section we discuss an alternative plane wave approach for calculation of the Josephson current in superconducting junctions.

A. Model of $S/I/S$ Josephson junction

We consider the tight-binding 1D model of $S/I/S$ Josephson junction as depicted in Fig. 1. In left and right parts of Fig 1 red filled circles represent atoms of $s$-wave spin-singlet superconductor $S$ with hopping $t$ between atoms, in the middle of Fig 1 there are $N$ atoms of an insulator, which we represent as blue circles with hopping $t'$ between atoms. $S/I$ and $I/S$ boundary we describe by equal hopping parameters $\gamma$ in Fig. 1. We assume that superconductors which form $S/I/S$ Josephson junction are the same with equal order parameter $\Delta_0$. For simplicity, we assume that the periods of the crystal lattices in a usual superconductor $S$ and an insulator $I$ are the same and equal to $a = 1$. To calculate the Josephson current across $S/I/S$ junction we should construct coherent Green’s function of the whole system. The simplest way to do it is to construct the Green’s functions of $S$, $I$, $S$ regions and then match them at the boundaries.

We define temperature Green’s functions in the tight-binding approximation in the following form:

$$
G_{n,j}(\tau_1, \tau_2) = -\langle T_\tau c_\tau^\dagger(n, \tau_1) c_\tau(j, \tau_2) \rangle,
$$

$$
F_{n,j}(\tau_1, \tau_2) = \langle T_\tau c_\tau^\dagger(n, \tau_1) c_\tau(j, \tau_2) \rangle,
$$

$$
\tilde{G}_{n,j}(\tau_1, \tau_2) = -\langle T_\tau c_\tau^\dagger(n, \tau_1) c_\sigma(j, \tau_2) \rangle,
$$

$$
\tilde{F}_{n,j}(\tau_1, \tau_2) = \langle T_\tau c_\tau(n, \tau_1) c_\sigma(j, \tau_2) \rangle,
$$

with creation (annihilation) operator $c_\sigma^\dagger(n, \tau_1) (c_\sigma(n, \tau_1))$ of an electron with spin $\sigma$ on n site and imaginary "time" ordering operator $T_\tau$.

After the differentiation of Green’s functions with respect to $\tau_1$, the expansion them in Fourier series and using Hamiltonian for 1D model of a $s$-wave single-band superconductor in the tight-binding approximation one can obtain the following Gorkov’s equations for the bulk of superconductor $S$, which are the generalization of the usual Gorkov’s equations for the discrete case:

$$
\begin{align}
(i\omega_n - \mu)G_{n,j}^{\omega} - \sum_l t_{n,l} G_{l,j}^{\omega} + \Delta_n F_{n,j}^{\omega} &= \delta_{n,j},
(i\omega_n + \mu)F_{n,j}^{\omega} + \sum_l t_{n,l} F_{l,j}^{\omega} + \Delta_n^* G_{n,j}^{\omega} &= 0,
(i\omega_n - \mu)\tilde{G}_{n,j}^{\omega} - \sum_l t_{n,l} \tilde{G}_{l,j}^{\omega} + \Delta_n^* \tilde{F}_{n,j}^{\omega} &= 0,
(i\omega_n + \mu)\tilde{F}_{n,j}^{\omega} + \sum_l t_{n,l} \tilde{F}_{l,j}^{\omega} + \Delta_n G_{n,j}^{\omega} &= 0,
\end{align}
$$

where $t_{n,l} = t$ for $l = n \pm 1$ and $t_{n,l} = 0$ for another values of $l$, $\omega_n = \pi T(2m + 1)$, $m$ is integer value, $T$

![FIG. 1. Schematic illustration of 1D model of the S/I/S Josephson junction.](image-url)
is the temperature. Discrete Gorkov’s equations for the Green’s function of the bulk an insulator $I$ have the same form in Eq. (2), but without the last term in the left side of Eqs. (3).

One can find exact solutions of discrete Eqs. (2). In the case when right side (source term $\delta_{n,j}$) is not equal to zero in the insulator $I$ layer, these solutions have a particularly simple form:

$$ \begin{align*}
(G_{n,j}^{\omega,S_L} & \quad F_{n,j}^{\omega,S_L}) = a_1 \left( \beta e^{i\phi} \right) e^{-ikn} + a_2 \left( \beta^{-1} e^{i\phi} \right) e^{ikn} \quad (3) \\
(G_{n,j}^{\omega,S_R} & \quad F_{n,j}^{\omega,S_R}) = b_1 \left( \beta \right) e^{ikn} + b_2 \left( 1 \right) e^{-ikn} \quad (4)
\end{align*}$$

in the left superconductor,

$$ \begin{align*}
(G_{n,j}^{\omega,I} & \quad F_{n,j}^{\omega,I}) = c_1 \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) e^{qn} + c_2 \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) e^{-qn} \\
& + c_3 \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) e^{qn} + c_4 \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) e^{-qn} - \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \frac{e^{-q(n-j)}}{2t \sin q} \quad (5)
\end{align*}$$

in the insulator. In Eqs. (3) - (5) $\varphi = \varphi_R - \varphi_L$ is the phase difference between left and right superconductor, $\beta = -i(\sqrt{\omega^2 + |\Delta|^2} + \omega)/|\Delta|$ and $k (q)$ - quasimomentum in superconductor (insulator), respectively. We assumed also, that in Eqs. (3) - (5) the quasiclassical approximation ($\Delta << \mu, t, t'$) is fulfilled.

Unknown coefficients $a_1, a_2, b_1, b_2, c_1, c_2, c_3, c_4$ in Eqs. (3) - (5) can be obtained from matching the Green’s functions $\varphi = \varphi_R - \varphi_L$ at the S/I and I/S interfaces. The boundary conditions for matching of wave functions in multiorbital metals in tight-binding approximation were proposed in [22]. For temperature Green’s functions these boundary conditions in the quasiclassical approximation ($\Delta_0 << \mu, t, t'$) at S/I boundary have the form:

$$ \begin{align*}
tG_{1,j}^{\omega,S_L} = \gamma G_{1,j}^{\omega,I}, \\
tF_{1,j}^{\omega,S_L} = \gamma F_{1,j}^{\omega,I}, \\
\gamma G_{0,j}^{\omega,S_L} = t'G_{0,j}^{\omega,I}, \\
\gamma F_{0,j}^{\omega,S_L} = t'F_{0,j}^{\omega,I},
\end{align*}$$

and the following at I/S boundary:

$$ \begin{align*}
t'G_{N+1,j}^{\omega,I} = \gamma G_{N+1,j}^{\omega,S_R}, \\
t'F_{N+1,j}^{\omega,I} = \gamma F_{N+1,j}^{\omega,S_R}, \\
\gamma G_{N,j}^{\omega,I} = tG_{N,j}^{\omega,S_R}, \\
\gamma F_{N,j}^{\omega,I} = tF_{N,j}^{\omega,S_R}.
\end{align*}$$

In the same way one can find the other pair of Green’s functions $G_{n,j}^{\omega}, F_{n,j}^{\omega}$ from Eq. (6).

The Josephson current across 1D $S/I/S$ junction in the tight-binding model are given by the following expression:

$$ I(\varphi) = \frac{eTt}{i\hbar} \sum_{\omega_m} (G_{j,j+1}^{\omega} - G_{j+1,j}^{\omega} + G_{j,j+1}^{\omega} - G_{j+1,j}^{\omega}). \quad (8) $$

The Eq. (8) is the generalization for discrete case of the usual expression for calculation of a current in the framework of Green’s function approach.

Using Eqs. (3) - (7) it is possible to demonstrate analytically, that previous results [18, 22] for Josephson tunneling across S/I/S constriction for equal hopping parameters in S and I $t = t'$ are reproduced by our tight-binding approach with generalized definition of the normal state conductance:

$$ I(\varphi) = \frac{e\Delta_0 \sigma_N \sin \varphi}{2\sqrt{1 - \sigma_N \sin^2(\frac{\varphi}{2})}} \tanh \frac{\theta_0}{2T}, \quad \text{Eq. (9)} $$

where $\sigma_N$ is the transparency of the S/I/S junction at the normal state. The transparency $\sigma_N$ is equal to unity in the case of atomically sharp boundary ($N = 0$ layers of insulator atoms) and equal hopping parameters in the bulk and across interface: $\gamma = t$. For atomically sharp boundary the relation for normal state transparency of the S/I/S junction has the following form:

$$ \sigma_N = \frac{2\sigma_1^2(1 - \cos 2k)}{1 - 2\sigma_1^2 \cos 2k + 1}. \quad \text{Eq. (10)} $$

where $\sigma_1 = t^2/\gamma^2$. In the case of $\gamma = t$ but nonzero length of an insulating region $N \neq 0$ transparency $\sigma_N$ of the S/I/S junction has the following form:

$$ \sigma_N = \frac{4 \sin^2 k \sin^2 q}{(\sigma_2^2 + \sigma_3^2 - 2\sigma_2 \sigma_3 \cos(2qN))^2}. \quad \text{Eq. (11)} $$

where $\sigma_2 = 1 - \cos(k + q)$, $\sigma_3 = 1 - \cos(k + q)$.

So one can conclude that our Green’s functions tight-binding approach for calculation of the Josephson current across S/I/S constriction leads to well-known previous results [18, 22] Eq. (10), but with generalized definition of the normal state transparency Eqs. (10), (11).

**B. Model of S/I/S Josephson junction**

Now we extend this tight-binding Green’s functions approach for calculation of the Josephson current in junctions with unconventional single-orbital superconductors
with d-wave symmetry of the order parameter ($S_d$). We consider 2D model of $S/I/S_d$ planar junction, where order parameter in d-wave superconductor has the form $\Delta = 2\Delta_d (\cos k_x - \cos k_y)$ for zero misorientation angle and $\Delta = 4\Delta_d \sin k_x \sin k_y$ for $\pi/4$ misorientation angle of crystallographic axes of $S_d$ with respect to the interface. We assume that the normal excitation spectrum in both superconductors has the form $\varepsilon_N = 2t (\cos k_x + \cos k_y) + \mu_N$ and the excitation spectrum in an insulating region has the form $\varepsilon_I = 2t (\cos k_x + \cos k_y) + \mu_I$ with $\mu_I > \mu_N$, so a wave number $q$ in an insulator is the imaginary number. We should note that changing the value of $k_y$ leads to raising of the bottom of the conduction band in an insulating region and, consequently, increasing the attenuation of the transmitted in an insulator waves. It means that on averaging over all possible values of $k_y$ the presence of an insulating region with nonzero length suppresses the contributions to the total Josephson current from the regions with large values of $k_y$.

For zero misorientation angle of crystallographic axes of $S_d$ with respect to the interface the phase dependence of the averaged over all possible values of $k_y$ Josephson current across the $S/I/S_d$ junction has equilibrium state at phase difference $\varphi$ ($-\pi \leq \varphi \leq \pi$). The origin of $\varphi$-contact is explained by presence in the Brillouin zone of areas with relatively small values of $k_y$, at which 0-contacts arise, and areas with relatively large values of $k_y$, at which $\pi$-contacts arise. Our calculations demonstrate that increasing the length of an insulating region to $N = 3$ layers of an insulator atoms after averaging over all values of $k_y$ leads to appearance 0-junction, because in this case contributions to the averaged Josephson current from the regions with relatively large $k_y$ are suppressed and contributions from the regions with relatively small $k_y$ prevail. This results obtained in the framework of our Green’s function tight-binding approach coincide qualitatively with the previous results derived in\textsuperscript{24} (Fig. 3 of \textsuperscript{24}).

In the case of $\pi/4$ misorientation angle of crystallographic axes of $S_d$ with respect to the interface the regions with positive and negative values of $k_y$ give rise to different phase dependencies of the Josephson current for fixed $k_y$ (positive values of $k_y$ correspond to $0$-contact and negative - to $\pi$-contact). So, the phase dependence of the averaged Josephson current across the $S/I/S_d$ junction for the case of $\pi/4$ misorientation angle of crystallographic axes of $S_d$ with respect to the interface and for atomically sharp boundary has equilibrium state at phase difference $\varphi$ ($-\pi \leq \varphi \leq \pi$). Our calculations demonstrate that with increasing of the length of an insulating region to $N = 4$ layers of an insulator atoms one again has $\varphi$-contact despite the suppression of the contributions to the averaged current from regions with large $k_y$, because at this angle as mentioned above the regions with positive and negative values of $k_y$ give rise to different phase dependencies of the Josephson current for fixed $k_y$. These results obtained in the framework of our Green’s function tight-binding approach coincide qualitatively with the previous results derived in\textsuperscript{24} (Fig. 3 of \textsuperscript{24}).

It is necessary to note that the same results as described above can be obtained not only in terms of Green’s functions but also in terms of wave functions. For this purpose one should solve Bogoliubov-de Gennes equations and find wave functions for a s-wave superconductor, an insulating region and a d-wave superconductor on the sites of the discrete lattice. Then one should match these wave functions at the interfaces, using boundary-conditions in the tight-binding approximation\textsuperscript{24}. Knowledge of wave functions allows to calculate the contribution to the total Josephson current from continuous spectrum using the following equation:

$$I_c(\varphi) = \frac{e}{\pi \hbar} \left( \int_{-\infty}^{-\Delta_0} + \int_{\Delta_0}^{\infty} \right) J(E, \varphi) f_0(E) dE.$$ \hspace{1cm} (12)

It is should be noted that the current from continuous spectrum considerably contributes to the total Josephson current when the order parameters in superconductors which form the Josephson junction differ greatly\textsuperscript{25}. Also it is possible to calculate the contribution to the total Josephson current from discrete Andreev’s levels which is given by the following formula

$$I_d(\varphi) = \sum_n \{ I_n^+(\varphi) f_0(E_n^+(\varphi)) + I_n^-(\varphi) f_0(E_n^-(\varphi)) \},$$ \hspace{1cm} (13)

where

$$I_n^\pm = \frac{2e}{\hbar} \frac{dE_n^\pm}{d\varphi}.$$ \hspace{1cm} (14)

The total Josephson current $I_s$ between two superconductors in equilibrium consists of current $I_d(\varphi)$ carried by quasiparticles occupying discrete Andreev’s levels and current $I_c(\varphi)$ carried by quasiparticles flowing in continuum levels\textsuperscript{18,23}, that is,

$$I_s(\varphi) = I_d(\varphi) + I_c(\varphi).$$ \hspace{1cm} (15)

But calculations of the total Josephson current in terms of wave functions are more cumbersome and inconvenient for the averaging of the Josephson current over all possible values of $k_y$ than in terms of Green’s functions and lead to numerical errors. Therefore, in the following sections we use the tight-binding Green’s functions approach for calculating of the averaged Josephson current in structures with a FeBS.

III. MODEL FOR THE CONTACT BETWEEN S-WAVE SUPERCONDUCTOR AND A FEBS

In this section we consider Josephson transport across the $S/I/S_p$ junctions, where $S$ is a usual s-wave spin-singlet superconductor, $I$ is an insulating layer and $S_p$
is a FeBS. First we consider in detail the procedure of calculation of 2D Josephson transport for (100) oriented S/I/S_p junctions for zero misorientation angle of crystallographic axes of a FeBS with respect to the interface. Then we describe the same procedure for c-oriented S/I/S_p junctions.

Consider a FeBS in this model. There are four hopping parameters \( t_1, t_2, t_3 \) and \( t_4 \) in this model, as shown in Fig. 2. The Fermi surface of a FeBS in unfolded Brillouin zone is shown in Fig. 3a.

FIG. 2. 2D tight-binding model of the (100) oriented S/I/S_p junction.

**A. 2D model of the S/I/S_p Josephson junction with a (100) oriented FeBS**

In Fig. 2 a two-dimensional crystallographic plane of a usual s-wave spin-singlet superconductor S (blue filled circles on left side of Fig. 2), N atomic layers of an insulator (circles in the middle of Fig. 2) and a FeBS in the right part of Fig. 2 is presented. The minimal model to reproduce Fermi surfaces in a FeBS is a two-orbital model considering \( d_{xz} \) and \( d_{yz} \) orbitals in iron, so we consider a FeBS in this model. There are four hopping parameters \( t_1, t_2, t_3 \) and \( t_4 \) in this model, as shown in Fig. 2. The Fermi surface of a FeBS in unfolded Brillouin zone is shown in Fig. 3a.

For the pair potential the intra-orbital \( s_\pm \) and \( s_{\pm \pm} \) models are considered. The hopping between sites of a usual superconductor S and an insulator I is described by parameters \( t \) and \( t' \), respectively. The hopping parameter across the interface between of a usual superconductor S and an insulator I is described by \( \gamma \) and the hopping parameters across the interface between an insulator I and \( d_{xz} \) (or \( d_{yz} \))-orbitals of a FeBS are described by \( \gamma_1 \) (or \( \gamma_2 \)). For simplicity, we assume that the periods of the crystal lattices in S, I and FeBSs are the same and equal to \( a = 1 \). To calculate the Josephson current across S/I/S_p junction we should construct coherent Green’s function of the whole system. The simplest way to do it is to construct the Green’s functions of S, I, S_p regions and then match them at the boundaries. The Green’s function in S, I regions are presented in section A (Eqs. (3), (5)). We define the temperature matrix Green’s function of a FeBS in the tight-binding approximation in the framework of the two-orbital model in the following form:

\[
\begin{align*}
G_{(n),(j)}(\tau_1, \tau_2) &= \begin{pmatrix}
G^{\alpha\alpha}_{(n),(j)}(\tau_1, \tau_2) & G^{\alpha\beta}_{(n),(j)}(\tau_1, \tau_2) \\
G^{\beta\alpha}_{(n),(j)}(\tau_1, \tau_2) & G^{\beta\beta}_{(n),(j)}(\tau_1, \tau_2)
\end{pmatrix} = \begin{pmatrix}
-\langle T, c^\dagger_1(\{n\}, \tau_1) c^\dagger_1(\{j\}, \tau_2) \rangle - \langle T, d^\dagger_1(\{n\}, \tau_1) d^\dagger_1(\{j\}, \tau_2) \rangle \\
-\langle T, d^\dagger_1(\{n\}, \tau_1) c^\dagger_1(\{j\}, \tau_2) \rangle - \langle T, d^\dagger_1(\{n\}, \tau_1) d^\dagger_1(\{j\}, \tau_2) \rangle
\end{pmatrix}, \\
F_{(n),(j)}(\tau_1, \tau_2) &= \begin{pmatrix}
F^{\alpha\alpha}_{(n),(j)}(\tau_1, \tau_2) & F^{\alpha\beta}_{(n),(j)}(\tau_1, \tau_2) \\
F^{\beta\alpha}_{(n),(j)}(\tau_1, \tau_2) & F^{\beta\beta}_{(n),(j)}(\tau_1, \tau_2)
\end{pmatrix} = \begin{pmatrix}
\langle T, c^\dagger_1(\{n\}, \tau_1) c^\dagger_1(\{j\}, \tau_2) \rangle + \langle T, c^\dagger_1(\{n\}, \tau_1) d^\dagger_1(\{j\}, \tau_2) \rangle \\
\langle T, d^\dagger_1(\{n\}, \tau_1) c^\dagger_1(\{j\}, \tau_2) \rangle + \langle T, d^\dagger_1(\{n\}, \tau_1) d^\dagger_1(\{j\}, \tau_2) \rangle
\end{pmatrix}, \\
\tilde{G}_{(n),(j)}(\tau_1, \tau_2) &= \begin{pmatrix}
\tilde{G}^{\alpha\alpha}_{(n),(j)}(\tau_1, \tau_2) & \tilde{G}^{\alpha\beta}_{(n),(j)}(\tau_1, \tau_2) \\
\tilde{G}^{\beta\alpha}_{(n),(j)}(\tau_1, \tau_2) & \tilde{G}^{\beta\beta}_{(n),(j)}(\tau_1, \tau_2)
\end{pmatrix} = \begin{pmatrix}
-\langle T, c^\dagger_1(\{n\}, \tau_1) c^\dagger_1(\{j\}, \tau_2) \rangle - \langle T, c^\dagger_1(\{n\}, \tau_1) d^\dagger_1(\{j\}, \tau_2) \rangle \\
-\langle T, d^\dagger_1(\{n\}, \tau_1) c^\dagger_1(\{j\}, \tau_2) \rangle - \langle T, d^\dagger_1(\{n\}, \tau_1) d^\dagger_1(\{j\}, \tau_2) \rangle
\end{pmatrix}, \\
\tilde{F}_{(n),(j)}(\tau_1, \tau_2) &= \begin{pmatrix}
\tilde{F}^{\alpha\alpha}_{(n),(j)}(\tau_1, \tau_2) & \tilde{F}^{\alpha\beta}_{(n),(j)}(\tau_1, \tau_2) \\
\tilde{F}^{\beta\alpha}_{(n),(j)}(\tau_1, \tau_2) & \tilde{F}^{\beta\beta}_{(n),(j)}(\tau_1, \tau_2)
\end{pmatrix} = \begin{pmatrix}
\langle T, c^\dagger_1(\{n\}, \tau_1) c^\dagger_1(\{j\}, \tau_2) \rangle + \langle T, c^\dagger_1(\{n\}, \tau_1) d^\dagger_1(\{j\}, \tau_2) \rangle \\
\langle T, d^\dagger_1(\{n\}, \tau_1) c^\dagger_1(\{j\}, \tau_2) \rangle + \langle T, d^\dagger_1(\{n\}, \tau_1) d^\dagger_1(\{j\}, \tau_2) \rangle
\end{pmatrix},
\end{align*}
\]

with creation (annihilation) operator \( c^+_\sigma(\{n\}, \tau_1) (c_\sigma(\{n\}, \tau_1)) \) of an electron belonging to the \( d_{xx} \) orbital with spin \( \sigma \) on \( \{n\} = (n_x, n_y) \), creation (annihilation) operator \( d^+_\sigma(\{n\}, \tau_1) (d_\sigma(\{n\}, \tau_1)) \) of an
electron belonging to the $d_{xz}$ orbital with spin $\sigma$ on \( \{n\} = (n_x, n_y) \) site and imaginary "time" ordering operator $T_{\tau}$. Upper superscript $\alpha(\beta)$ corresponds to the $d_{xz}(d_{yz})$ orbital, respectively.

After the differentiation of Green’s functions \[ (\text{10}) \] with respect to $\tau$, the expansion them in Fourier series and using Hamiltonian for 2D two-orbital model of a FeBS in the tight-binding approximation\[18\] one can obtain the following Gorkov’s equations in the discrete case for arbitrary model of the intraorbital superconducting pairing:

\[
\begin{align*}
(\omega_m - \mu)G^{\alpha\alpha,\omega}_{\{n\},\{l\}} &= \sum_{\{l\}} t^{\alpha}_{\{n\},\{l\}} G^{\alpha\alpha,\omega}_{\{l\},\{l\}} - \sum_{\{l\}} t^{\beta}_{\{n\},\{l\}} G^{\beta\alpha,\omega}_{\{l\},\{l\}} + \sum_{\{l\}} \Delta_{\{n\},\{l\}} F^{\alpha\alpha,\omega}_{\{l\},\{l\}} = \delta_{\{n\},\{l\}}, \\
(\omega_m - \mu)G^{\beta\beta,\omega}_{\{n\},\{l\}} &= \sum_{\{l\}} t^{\beta}_{\{n\},\{l\}} G^{\beta\beta,\omega}_{\{l\},\{l\}} - \sum_{\{l\}} t^{\alpha}_{\{n\},\{l\}} G^{\alpha\beta,\omega}_{\{l\},\{l\}} + \sum_{\{l\}} \Delta_{\{n\},\{l\}} F^{\beta\beta,\omega}_{\{l\},\{l\}} = 0, \\
(\omega_m + \mu)F^{\alpha\alpha,\omega}_{\{n\},\{l\}} &= \sum_{\{l\}} t^{\alpha}_{\{n\},\{l\}} F^{\alpha\alpha,\omega}_{\{l\},\{l\}} + \sum_{\{l\}} t^{\beta}_{\{n\},\{l\}} F^{\beta\alpha,\omega}_{\{l\},\{l\}} + \sum_{\{l\}} \Delta^*_{\{n\},\{l\}} G^{\alpha\alpha,\omega}_{\{l\},\{l\}} = 0, \\
(\omega_m + \mu)F^{\beta\beta,\omega}_{\{n\},\{l\}} &= \sum_{\{l\}} t^{\beta}_{\{n\},\{l\}} F^{\beta\beta,\omega}_{\{l\},\{l\}} + \sum_{\{l\}} t^{\alpha}_{\{n\},\{l\}} F^{\alpha\beta,\omega}_{\{l\},\{l\}} + \sum_{\{l\}} \Delta^*_{\{n\},\{l\}} G^{\beta\beta,\omega}_{\{l\},\{l\}} = 0, \\
\end{align*}
\]

where $t^{\alpha}_{\{n\},\{l\}}$, $t^{\beta}_{\{n\},\{l\}}$ are the hopping parameters between the same $d_{xz}(d_{yz})$ orbitals, respectively, and $\Delta_{\{n\},\{l\}}$, $\Delta^*_{\{n\},\{l\}}$ are the hopping parameters between the different orbitals, which have the following form:

\[
\begin{align*}
& t^{(11)}_{\{n_x, n_y\}, \{l_x, l_y\}} = t_1 \text{ for } l_x = n_x \pm 1, l_y = n_y, \\
& t^{(11)}_{\{n_x, n_y\}, \{l_x, l_y\}} = t_2 \text{ for } l_x = n_x, l_y = n_y \pm 1, \\
& t^{(22)}_{\{n_x, n_y\}, \{l_x, l_y\}} = t_3 \text{ for } l_x = n_x \pm 1, l_y = n_y \pm 1, \\
& t^{(11)}_{\{n_x, n_y\}, \{l_x, l_y\}} = 0 \text{ for the other conditions on the variables } l_x, n_x, l_y, n_y; \\
& t^{(22)}_{\{n_x, n_y\}, \{l_x, l_y\}} = t_2 \text{ for } l_x = n_x \pm 1, l_y = n_y, \\
& t^{(22)}_{\{n_x, n_y\}, \{l_x, l_y\}} = t_3 \text{ for } l_x = n_x \pm 1, l_y = n_y \pm 1, \\
& t^{(22)}_{\{n_x, n_y\}, \{l_x, l_y\}} = 0 \text{ for the other conditions on the variables } l_x, n_x, l_y, n_y; \\
& t^{(21)}_{\{n_x, n_y\}, \{l_x, l_y\}} = t_4 \text{ for } l_x = n_x \pm 1, l_y = n_y \pm 1, \\
& t^{(21)}_{\{n_x, n_y\}, \{l_x, l_y\}} = 0 \text{ for the other conditions on the variables } l_x, n_x, l_y, n_y.
\end{align*}
\]

Last upper index "ω" at Green’s functions in Eq. \[ (17) \] denote that this Green’s function is the Fourier component of Green’s function Eq. \[ (10) \]. In a similar way one can obtain the equations for components of the Green’s functions $\tilde{G}^{\alpha\alpha,\omega}_{\{n\},\{l\}}$, $\tilde{G}^{\beta\beta,\omega}_{\{n\},\{l\}}$, $\tilde{G}^{\alpha\beta,\omega}_{\{n\},\{l\}}$, $\tilde{G}^{\beta\alpha,\omega}_{\{n\},\{l\}}$ and $\tilde{F}^{\alpha\alpha,\omega}_{\{n\},\{l\}}$, $\tilde{F}^{\beta\beta,\omega}_{\{n\},\{l\}}$, $\tilde{F}^{\alpha\beta,\omega}_{\{n\},\{l\}}$, $\tilde{F}^{\beta\alpha,\omega}_{\{n\},\{l\}}$.

The simplest way to build the coherent Green’s function of the whole system is to assume that the source terms $\delta_{\{n\},\{l\}}$ in right part of Eqs. \[ (2) \], \[ (17) \] is nonzero in the insulating region $J$ and is equal to zero in the $S_{\tau}$ and the $S_{\rho}$ regions. In this case one can note from analyzing the equations \[ (17) \] that four upper and four lower
equations (17) coincide, if we denote \(G^{\alpha,\omega}_{n,(j)}\) as \(G^{\alpha,\omega}_{n,(j)}\), \(G^{\beta,\omega}_{n,(j)}\) as \(G^{\beta,\omega}_{n,(j)}\), \(F^{\beta,\omega}_{n,(j)}\) as \(F^{\beta,\omega}_{n,(j)}\) and \(F^{\beta,\omega}_{n,(j)}\) as \(F^{\beta,\omega}_{n,(j)}\). Therefore, in order to calculate the Josephson current across this \(S/I/S_p\) junction it is enough to solve only first or second four equations (17), because the remaining system of the equations gives the same result.

Solving four first Gorkov’s equations (17) for a FeBS we obtain the following components of Green’s functions in the quasi-classical approximation (\(\Delta_p << \mu, t_1, t_2, t_3, t_4\)):

\[
\begin{align*}
(G^{\alpha,\omega}_{n,(j)} & )_n = a_1 \left( \begin{array}{c}
\begin{array}{} 
  & u_0(-k_F) \\
  & v_0(-k_F) \\
\end{array} \right) e^{-ik_F n_x + i k_y n_y} + a_2 \\
& \left( \begin{array}{c}
\begin{array}{} 
  & u_0(k_F) \\
  & v_0(k_F) \\
\end{array} \right) e^{ik_F n_x + i k_y n_y}
\end{align*}
\]

\[+
\begin{align*}
& a_3 \left( \begin{array}{c}
\begin{array}{} 
  & u_0(-k_F) \\
  & v_0(-k_F) \\
\end{array} \right) e^{-ik_F n_x + i k_y n_y} + a_4 \\
& \left( \begin{array}{c}
\begin{array}{} 
  & u_0(k_F) \\
  & v_0(k_F) \\
\end{array} \right) e^{ik_F n_x + i k_y n_y}
\end{align*}\]

\[(18)\]

where

\[u_0(k_x, k_y) = \left( \begin{array}{c}
\begin{array}{} 
  1 \\
  -\xi_{xx}(k_F)/\xi_{xy}(k_F) \\
\end{array} \right) \]

and

\[
\beta^{1,2}_p = i e^{i \phi} \left[ \frac{\Delta_p (-k_F^{(1,2)}, k_y)}{\sqrt{\omega_m^2 + |\Delta_p (-k_F^{(1,2)}, k_y)|^2 + \omega_m}}, \frac{\Delta_p (k_F^{(1,2)}, k_y)}{\sqrt{\omega_m^2 + |\Delta_p (k_F^{(1,2)}, k_y)|^2}} \right],
\]

with \(\xi_{xx} = 2t_1 \cos(k_x) + 2t_2 \cos(k_y) + \mu, \mu\) is a chemical potential in a FeBS, and \(\xi_{xy} = 4t_4 \sin(k_x) \sin(k_y)\) - dispersion relation of the \(d_{xz}\) orbital and hybridization term, respectively, \(k_F^{(1,2)}\) - quasimomentum of the first (second) band in a FeBS. In the similar way one can obtain the expressions for components of the Green’s functions \(G^{\alpha,\omega}_{n,(j)}, G^{\beta,\omega}_{n,(j)}\) and \(F^{\alpha,\omega}_{n,(j)}, F^{\beta,\omega}_{n,(j)}\).

To build the coherent Green’s function of whole S/I/S_p junction one should match Green’s functions of S, I and S_p regions (Eqs. (8), (9), (13)) at the both S/I and I/S_p interfaces. The boundary conditions for the Green’s functions in the tight-binding approximation can be found in the similar way as in (15). Due to the translational invariance of the structure in the direction parallel to the interface, \(k_y\) component of the quasimomentum is conserved. Further, due to the translational invariance of considered structure the subscript with index \((y)\) corresponding to the coordinate of an atom in a direction parallel to the boundary is omitted. Thus, boundary conditions on the first S/I boundary coincide with Eq. (9). For second I/S_p boundary in the quasi-classical approximation (\(\Delta_0, \Delta_p, \Delta_p' << \mu_1, \mu, \mu_N, t, t', t_1, t_2, t_3, t_4\)) boundary conditions have the following form (12):

B. 3D model of the S/I/S_p Josephson junction with a c-oriented FeBS

Now we consider Josephson transport across S/I/S_p junction in direction parallel to \(z\) crystallographic axes of a FeBS, where \(S\) is a usual s-wave spin-singlet superconductor, \(I\) is an insulating layer and \(S_p\) is a FeBS.

In Fig. (4) a 3D crystallographic plane of a usual s-wave spin-singlet superconductor \(S\) (red filled circles on left side of Fig. (4), \(N\) atomic layers of an insulator (blue circles in the middle of Fig. (4)) and a FeBS in \(z\)-direction in the right part of Fig. (4) is presented. For 3D tight-binding model of a FeBS in addition to hopping parameter \(t_1, t_2, t_3, t_4\) in \(x - y\) plane hopping parameter \(t_z\) between the same orbitals on the nearest neighbor sites in \(z\)-direction should be taking into account. The existence of this hopping parameter \(t_z\) leads to the light periodic changes of cylindrical Fermi surface sheets in this direction. The main property of excitation spectrum of
a FeBS as a function of $k_z$ is that for each fixed value of $k || = (k_x, k_y)$ only one band crosses the Fermi level and the second band is located sufficiently far from it (Fig. 3). This means that for each value of $k ||$ an effective contribution to the transport properties of a FeBS is only from one of the bands of a FeBS. Hopping across $S/I$ interface we describe by parameter $\gamma$, hopping across $I/S_p$ interface we describe by parameters $\gamma_{1z}, \gamma_{2z}$ (Fig. 4).

\[
\begin{align*}
(t^{(1)}_{(n_x,n_y,n_z),\{l_x,l_y,l_z\}}) &= t_1 \quad \text{for} \quad l_x = n_x \pm 1, l_y = n_y, l_z = n_z, \\
(t^{(1)}_{(n_x,n_y,n_z),\{l_x,l_y,l_z\}}) &= t_2 \quad \text{for} \quad l_x = n_x, l_y = n_y \pm 1, l_z = n_z, \\
(t^{(1)}_{(n_x,n_y,n_z),\{l_x,l_y,l_z\}}) &= t_3 \quad \text{for} \quad l_x = n_x \pm 1, l_y = n_y \pm 1, l_z = n_z, \\
(t^{(1)}_{(n_x,n_y,n_z),\{l_x,l_y,l_z\}}) &= t_4 \quad \text{for} \quad l_x = n_x \pm 1, l_y = n_y \pm 1, l_z = n_z,
\end{align*}
\]

For calculation of the Josephson current across $S/I/S_p$ junction along $z$-axes of a FeBS one can define the temperature Green’s function of a FeBS in the same way as in Eq. (10). One can obtain the same Gorkov’s equations Eq. (11) as in the previously considered case of the Josephson transport in $x-y$ plane of a FeBS, but with different definition of the hopping parameters:

\[
(t^{(1)}_{\{n_x,n_y\},\{l_x,l_y\}}), (t^{(2)}_{\{n_x,n_y\},\{l_x,l_y\}}), (t^{(12)}_{\{n_x,n_y\},\{l_x,l_y\}}) = 0 \quad \text{for} \quad l_x = n_x \pm 1, l_y = n_y \pm 1, l_z = n_z.
\]

Solving Gorkov’s equations for this 3D model of a FeBS one can obtain the Green’s function in $S_p$ region, which has the same form as Eq. (13) in the case of 2D model of a FeBS, but with another definition of the dispersion relation of the $d_{xz}$ orbital $\xi_{xz}$ in Eq. (10): $\xi_{xz} = 2t_1 \cos(k_x) + 2t_2 \cos(k_y) + 2t_z \cos(k_z) + \mu$. In the similar way one can obtain the expressions for components of Green’s functions $\tilde{G}^{(n\alpha\omega)}_{\{n\},\{l\}}, \tilde{G}^{(n\beta\omega)}_{\{n\},\{l\}}$ and $\tilde{F}^{(n\alpha\omega)}_{\{n\},\{l\}}, \tilde{F}^{(n\beta\omega)}_{\{n\},\{l\}}$ for 3D model of a FeBS.

\[
\begin{align*}
\tilde{G}^{(n\alpha\omega)}_{\{n\},\{l\}}, \tilde{G}^{(n\beta\omega)}_{\{n\},\{l\}}, \tilde{G}^{(n\gamma\omega)}_{\{n\},\{l\}}, \tilde{G}^{(n\delta\omega)}_{\{n\},\{l\}} \\
\tilde{F}^{(n\alpha\omega)}_{\{n\},\{l\}}, \tilde{F}^{(n\beta\omega)}_{\{n\},\{l\}}, \tilde{F}^{(n\gamma\omega)}_{\{n\},\{l\}}, \tilde{F}^{(n\delta\omega)}_{\{n\},\{l\}}
\end{align*}
\]

in the similar way as in section IIIA.

The boundary conditions for Green’s functions in the tight-binding approximation for transport along $z$-axes can be found in the similar way as in section IIIA and they have a simpler form than in the case of transport in $x-y$ plane. Due to the translational invariance of the structure in the direction parallel to the interface, $k || = (k_x, k_y)$ component of the quasimomentum is conserved. Further, due to the translational invariance of considered structure the subscripts with indices $(x, y)$ corresponding to the coordinate of an atom in a direction parallel to the
boundary is omitted. Thus, boundary conditions on the first $S/I$ boundary coincide with Eq. (8). For second $I/S_p$ boundary we obtained the following boundary conditions in $z$-direction in the quasiclassical approximation ($\Delta_0, \Delta_p, \Delta'_p << \mu_I, \mu, \mu_N, t, t', t_1, t_2, t_3, t_4, t_5$):

$$
\begin{aligned}
& t_2G^{\alpha\alpha}_{N+1,j} = \gamma_{1z}G^I_{N+1,j}, \\
& t_2F^{\alpha\alpha}_{1,j} = \gamma_{1z}F^I_{1,j}, \\
& t_2G^{\alpha\beta}_{N+1,j} = \gamma_{2z}G^I_{N+1,j}, \\
& t_2F^{\alpha\beta}_{N+1,j} = \gamma_{2z}F^I_{N+1,j}, \\
& \gamma_{1z}G^{\alpha\alpha}_{N,j} + \gamma_{2z}G^{\alpha\beta}_{N,j} = tG^I_{N,j}, \\
& \gamma_{1z}F^{\alpha\alpha}_{N,j} + \gamma_{2z}F^{\alpha\beta}_{N,j} = tF^I_{N,j}.
\end{aligned}
$$

(22)

The Josephson current across $S/I/S_p$ junction is described by the sum over all possible values of $k_\parallel$ of Eq. (5) where $k_\parallel = (k_x, k_y)$ in the case of transport in $c$-direction and $k_\parallel = k_y$ in the case of transport in $x - y$ plane.

IV. NUMERICAL RESULTS

In this section we present the results of numerical calculations of the Josephson current across $S/I/S_p$ junction. We calculate the averaged over all possible values of $k_\parallel$ Josephson current for two the most popular models of superconducting pairing in a FeBS: the $s_\pm$ model with order parameter $\Delta = 4\Delta_p \cos k_x \cos k_y$ with $\Delta_p = 0.008$ (eV) and the $s_+ \pm$ model with order parameter $\Delta = 2\Delta_p (\cos k_x + \cos k_y) + \Delta'_p$ with $\Delta_p = 0.001, \Delta'_p = 0.0042$ (eV). We choose the magnitude of the order parameter in $S$ $\Delta_0 = 0.002$ (eV).

After averaging over all possible values of $k_\parallel$ the Josephson current across $S/I/S_p$ junction depend on the following factors:

1. the values of the hopping parameters at the $I/S_p$ interface $\gamma_1$ and $\gamma_2$;
2. the size of the Fermi surface of a s-wave superconductor, because the Josephson current strongly depends on the values of $k_\parallel$, and varying the size of the Fermi surface in $S$ we change the contributions to the averaged Josephson current from regions with different values of $k_\parallel$; consequently, we obtain different values of the total Josephson current.
3. the length of an insulating layer, because increasing the length of this layer leads to the suppression of the contributions to the averaged Josephson current from regions with large $k_\parallel$.

A. Phase dependencies of the Josephson current in $S/I/S_p$ junctions

First we present the results of numerical calculations of phase dependence of the Josephson current in (100) oriented $S/I/S_p$ junctions, when charge transport occurs in

FIG. 6. The phase dependence of the Josephson current for the (100) oriented $S/I/S_p$ junction for zero misorientation angle of crystallographic axes of a FeBS with respect to the interface, $\gamma_1 = 0.02, \gamma_2 = 0.2, T/T_c \approx 0.02$. Solid line corresponds to the total Josephson current, dotted line corresponds to the averaged over all $k_y < \pi/2$ Josephson current (over bands of a FeBS near $(k_x, k_y) = (0, 0)$ and $(\pm \pi, 0)$), line with crosses corresponds to the averaged over all $k_y > \pi/2$ Josephson current (over bands of a FeBS near $(k_x, k_y) = (0, \pi)$ and $(\pm \pi, \pi)$), $I_0 = e\Delta_0/h$. Fig. 6(a) corresponds to atomically sharp boundary, Fig. 6(b) corresponds to $N = 3$ layers of the insulator atoms.

FIG. 7. The same as in Fig. 6 but $\gamma_1 = 0.02, \gamma_2 = 0.3$.

FIG. 8. The same as in Fig. 6 but $\gamma_1 = 0.02, \gamma_2 = 0.4$.

FIG. 9. The same as in Fig. 6 but $\gamma_1 = 0.2, \gamma_2 = 0.02$. 
parameters across this boundary. Consequently, areas with large $k_y$ in a FeBS contribute to the current (Fig. 3). We use the following values of the hopping parameters and chemical potential in a FeBS: $t_1 = -0.1051$, $t_2 = 0.1472$, $t_3 = -0.1909$, $t_4 = -0.0874$ and $\mu = -0.0811$ (eV), according to 28, and suppose relatively low temperature $T/T^* \approx 0.02$, where $T^*$ is the critical temperature of the usual $s$-wave superconductor. In the insulating region we choose the normal excitation spectrum in the form of $\varepsilon_{\ell} = 2t'(\cos k_x + \cos k_y) + \mu_{\ell}$ with hopping parameter $t' = -0.3$ (eV) and chemical potential $\mu_{\ell} = 1.2$ (eV).

The phase dependence of the averaged over $k_y = k_y$ Josephson current across the $S/I/S_p$ junction for atomically sharp boundary is depicted in Fig. 6a for hopping parameters across this boundary $\gamma_1 = 0.02, \gamma_2 = 0.2$. Solid line corresponds to the total Josephson current, dotted line corresponds to the averaged Josephson current over all $k_y < \pi/2$ (over values of $k_y$ belonging to the hole and electron pockets of a FeBS near $(k_x, k_y) = (0, 0)$ and $(\pm \pi, 0)$, respectively (Fig. 3a)). Line with crosses corresponds to the averaged Josephson current over all values of $k_y > \pi/2$ (over values of $k_y$ belonging to the electron and hole pockets of a FeBS near $(k_x, k_y) = (0, \pi)$ and $(\pm \pi, \pi)$ (Fig. 3a)). Contributions to the Josephson current from small $k_y$ lead to appearance of the $\pi$-contact, contributions from large values of $k_y$ - to 0-contact, but the sum of this contributions leads to the appearance of the resulting $\pi$-contact. The increasing of the length of an insulating layer to $N = 3$ atom layers leads to the suppression of the contributions to the averaged Josephson current from regions with large values of $k_y$, therefore the regions with small values of $k_y$ dominate and this contact remains to be the $\pi$-contact for nonzero length of an insulator (Fig. 6b).

The phase dependence of the averaged over $k_y$ Josephson current across the $S/I/S_p$ junction for atomically sharp boundary is depicted in Fig. 7a for another value of $\gamma_2$ ($\gamma_1 = 0.02, \gamma_2 = 0.3$). For these values of hopping parameters for atomically sharp boundary we obtain the total averaged Josephson current with the stable equilibrium phase difference at $\phi = 0$ (0-contact). But the increasing of the length of an insulator to $N = 3$ atom layers leads to the suppression of the contributions to the averaged Josephson current from regions with large values of $k_y$ and this Josephson junction become $\pi$-contact (Fig. 7b).

The phase dependence of the averaged over $k_y$ Josephson current across the $S/I/S_p$ junction for atomically sharp boundary is depicted in Fig. 8a for another set of hopping parameters across this boundary $\gamma_1 = 0.2, \gamma_2 = 0.02$. For these values of hopping parameters we come to the opposite situation in comparison with the previous cases with another sets of hopping amplitudes (Figs. 3-5), because now contributions to the averaged Josephson current from small values of $k_y$ lead to appearance of the 0-contact, contributions from large values of $k_y$ - to $\pi$-contact. But as in the case with $\gamma_1 = 0.02, \gamma_2 = 0.2$ (Fig. 3a) the sum of these contributions leads to the appearance of the resulting $\pi$-contact, because the contribution to the total Josephson current from regions with large values of $k_y$ prevails over the contribution to the total Josephson current from regions with small values of $k_y$. But increasing of the length of an insulator to $N = 3$ atom layers leads to the suppression of the contributions to the averaged Josephson current from regions with large values of $k_y$ and this Josephson junction become 0-contact (Fig. 3b).

In the case of $s++$ model of the superconducting pairing in a FeBS the order parameter has constant sign “+” on each pocket at Fermi surface (Fig. 3a). Hence, for each value of $k_y$ and for any set of hopping amplitudes across the $I/S_p$ interface $\gamma_1$ and $\gamma_2$ we always obtain 0-contact. So, after averaging over all possible values of $k_y$ this $S/I/S_p$ junction has equilibrium phase which is equal to zero. The increasing the length of an insulating layer leads to the suppression of the contributions to averaged Josephson current from regions with large values of $k_y$, but does not change the situation and averaged Josephson current still has equilibrium state at zero phase difference.

So, changing hopping parameters at the interface, size of the Fermi surface in s-wave superconductor and length $x - y$ planes of a FeBS. We choose the normal excitation spectrum in $S$ in the form $\varepsilon_N = 2t(\cos k_x + \cos k_y) + \mu_N$, where $t = -0.3$ and $\mu_N = 0.05$ in order to provide large size of the Fermi surface in $S$. Consequently, areas with large $k_y$ in a FeBS contribute to the current (Fig. 3). We use the following values of the hopping parameters and chemical potential in a FeBS: $t_1 = -0.1051$, $t_2 = 0.1472$, $t_3 = -0.1909$, $t_4 = -0.0874$ and $\mu = -0.0811$ (eV), according to 28, and suppose relatively low temperature $T/T^* \approx 0.02$, where $T^*$ is the critical temperature of the usual $s$-wave superconductor. In the insulating region we choose the normal excitation spectrum in the form of $\varepsilon_{\ell} = 2t'(\cos k_x + \cos k_y) + \mu_{\ell}$ with hopping parameter $t' = -0.3$ (eV) and chemical potential $\mu_{\ell} = 1.2$ (eV).

The phase dependence of the averaged over $k_y = k_y$ Josephson current across the $S/I/S_p$ junction for atomically sharp boundary is depicted in Fig. 6a for hopping parameters across this boundary $\gamma_1 = 0.02, \gamma_2 = 0.2$. Solid line corresponds to the total Josephson current, dotted line corresponds to the averaged Josephson current over all $k_y < \pi/2$ (over values of $k_y$ belonging to the hole and electron pockets of a FeBS near $(k_x, k_y) = (0, 0)$ and $(\pm \pi, 0)$, respectively (Fig. 3a)). Line with crosses corresponds to the averaged Josephson current over all values of $k_y > \pi/2$ (over values of $k_y$ belonging to the electron and hole pockets of a FeBS near $(k_x, k_y) = (0, \pi)$ and $(\pm \pi, \pi)$ (Fig. 3a)). Contributions to the Josephson current from small $k_y$ lead to appearance of the $\pi$-contact, contributions from large values of $k_y$ - to 0-contact, but the sum of this contributions leads to the appearance of the resulting $\pi$-contact. The increasing of the length of an insulating layer to $N = 3$ atom layers leads to the suppression of the contributions to the averaged Josephson current from regions with large values of $k_y$, therefore the regions with small values of $k_y$ dominate and this contact remains to be the $\pi$-contact for nonzero length of an insulator (Fig. 6b).

The phase dependence of the averaged over $k_y$ Josephson current across the $S/I/S_p$ junction for atomically sharp boundary is depicted in Fig. 7a for another value of $\gamma_2$ ($\gamma_1 = 0.02, \gamma_2 = 0.3$). For these values of hopping parameters for atomically sharp boundary we obtain the total averaged Josephson current with the stable equilibrium phase at $\phi = 0$ ($0 - \phi$ - contact). But the increasing of the length of an insulator to $N = 3$ atom layers leads to the suppression of the contributions to the averaged Josephson current from regions with large values of $k_y$ and this Josephson junction become $\pi$-contact (Fig. 7b).

The phase dependence of the averaged over $k_y$ Josephson current across the $S/I/S_p$ junction for atomically sharp boundary is depicted in Fig. 8a for another set of hopping parameters across this boundary $\gamma_1 = 0.2, \gamma_2 = 0.02$. For these values of hopping parameters we come to the opposite situation in comparison with the previous cases with another sets of hopping amplitudes (Figs. 3-5), because now contributions to the averaged Josephson current from small values of $k_y$ lead to appearance of the 0-contact, contributions from large values of $k_y$ - to $\pi$-contact. But as in the case with $\gamma_1 = 0.02, \gamma_2 = 0.2$ (Fig. 3a) the sum of these contributions leads to the appearance of the resulting $\pi$-contact, because the contribution to the total Josephson current from regions with large values of $k_y$ prevails over the contribution to the total Josephson current from regions with small values of $k_y$. But increasing of the length of an insulator to $N = 3$ atom layers leads to the suppression of the contributions to the averaged Josephson current from regions with large values of $k_y$ and this Josephson junction become 0-contact (Fig. 8b).

In the case of $s++$ model of the superconducting pairing in a FeBS the order parameter has constant sign “+” on each pocket at Fermi surface (Fig. 3a). Hence, for each value of $k_y$ and for any set of hopping amplitudes across the $I/S_p$ interface $\gamma_1$ and $\gamma_2$ we always obtain 0-contact. So, after averaging over all possible values of $k_y$ this $S/I/S_p$ junction has equilibrium phase which is equal to zero. The increasing the length of an insulating layer leads to the suppression of the contributions to averaged Josephson current from regions with large values of $k_y$, but does not change the situation and averaged Josephson current still has equilibrium state at zero phase difference.

So, changing hopping parameters at the interface, size of the Fermi surface in s-wave superconductor and length $x - y$ planes of a FeBS.
of an insulator for the case of the $s_\pm$ model of the superconducting pairing we can obtain in (100) oriented $S/I/S_p$ Josephson junction 0-, $\pi$- or $\phi$-contact, but for the case of the $s_{\pm}$ model of the superconducting pairing we always obtain in (100) oriented $S/I/S_p$ Josephson junction 0-contact only.

We also calculate the Josephson current in $S/I/S_p$ junction with transport in a FeBS along $z$-axis using the tight-binding Green’s function as described in Sec. III B. In these calculations we assume that the normal excitation spectrum in $S$ has the form $\varepsilon_N = 2t(\cos k_x + \cos k_y + \cos k_z) + \mu_N$ with hopping parameter $t = -0.3$ (eV) and chemical potential $\mu_N = 0.6$ (eV). For such values of hopping parameters and chemical potential the size of Fermi surface in $S$ is sufficiently large, so both electronic and hole packets in a FeBS participate in the Josephson transport. For a FeBS along $z$-axis hopping $t_z = -0.1$ (eV) between the same orbitals on the nearest neighbor sites is taken into account. We assume that the $S/I$ interface is completely transparent and the $I/S_p$ interface is characterized by the following set of hopping amplitudes: $\gamma_{1z} = \gamma_{2z} = 0.17$. As in the previous case we assume that the temperature is relatively low: $T/T^* = 0.02$. In contrast to the previously considered case of (100) oriented $S/I/S_p$ Josephson junction in the case of the Josephson transport along $z$-axis of a FeBS at each fixed $k_\parallel = (k_x, k_y)$ only one of a FeBS bands participates in the Josephson transport, since the second band is significantly far from the Fermi level (Fig. 11). The phase dependencies of the averaged over $k_\parallel$ = $(k_x, k_y)$ Josephson current in $z$-direction across the $S/I/S_p$ junction are depicted in Fig. 11. In Fig. 11a one can see the phase dependence of the Josephson current for atomically sharp boundary and in Fig. 11b - the phase dependence of the Josephson current for $N = 3$ layers of an insulator atoms. In the case of atomically sharp boundary the main contribution to the total Josephson current stems from electron pockets. So in this case the $S/I/S_p$ Josephson junction has ground state at $\pi$ phase difference (Fig. 11a). In the presence of the insulating layer due to the suppression of the contributions to the total Josephson current from regions with large $k_\parallel$ the main contribution to the Josephson current stems from hole pockets, so, in this case the $S/I/S_p$ Josephson junction has ground state at phase difference equal to zero (Fig. 11b). Modern technology permit to create the loop of the normal superconductor, one end of which is oxidized and other is not, connect it with a c-oriented FeBS and create dc SQUID. If one observes in this experiment $\pi$ phase shift, it will be the crucial evidence in favor of the presence of the $s_\pm$ symmetry in a FeBS. The same experiment was suggested recently in[29]. The important feature of c-oriented $S/I/S_p$ Josephson junction is the significant suppression of the magnitude of the Josephson current in the case of long insulator layer (Fig. 11b) compare to atomically sharp boundary (Fig. 11a). The Josephson critical current suppression have been observed in recent Josephson tunneling experiments in a FeBS[30].

![Image](image.png)  
**FIG. 11.** The temperature dependence of the critical Josephson current of the (100) oriented $S/I/S_p$ junction for zero misorientation angle of crystallographic axes of a FeBS with respect to the interface with hopping parameters at the interface $\gamma_1 = 0.02, \gamma_2 = 0.2$. Solid line corresponds to atomically sharp boundary and line with crosses corresponds to $N = 3$ layers of the insulator atoms. Dashed line corresponds to the Ambegaokar, Baratoff temperature dependence of the critical current of the $S/I/S$ junction.

![Image](image.png)  
**FIG. 12.** The same as in Fig. 11 but with $\gamma_1 = 0.02, \gamma_2 = 0.3$.

![Image](image.png)  
**FIG. 13.** The same as in Fig. 11 but with $\gamma_1 = 0.02, \gamma_2 = 0.4$. 
critical current of the $S/I/S$ junction. One can observe in Fig[11]-Fig[14] that decreasing of the critical current with increasing of the temperature proceeds more slowly in the case of the $S/I/S_p$ structure with long insulating layer than in the case of $S/I/S$ structure for all considered sets of hopping parameters $\gamma_1, \gamma_2$ across the $I/S_p$ interface. The behavior of the temperature dependence of the critical current of the $S/I/S_p$ junction with atomically sharp boundary varies with changing of the sets of the hopping parameters at the $I/S_p$ interface. The most significant difference in the behavior of the temperature dependence of the critical current in $S/I/S_p$ junction with atomically sharp boundary in comparison with the one in $S/I/S$ junction (the Ambegaokar, Baratoff temperature dependence of the critical current\cite{24}) is observed in the case of hopping parameters $\gamma_1 = 0.02, \gamma_2 = 0.3$ (Fig[12]). This set of hopping parameters corresponds to the case of nontrivial phase dependence of the Josephson current with phase difference in the ground state at $\phi (0 < \phi < \pi)$ (Fig[14a]). For the Josephson transport in $z$-direction the temperature dependence of the critical current of the $S/I/S_p$ junction with atomically sharp boundary and $N = 3$ layers of the insulator atoms are rather close to each other, and the decreasing of these dependencies with increasing of the temperature proceeds a little slowly than in the case of $S/I/S$ junction (Fig[13]).

V. CONCLUSION

In this paper in the framework of tight-binding model we have proposed a microscopic theory describing Josephson tunneling in junctions with unusual multiband superconductors. Our theory takes into account not only the complex excitation spectrum of these superconductors, their multiband Fermi surface, interband and intervalley scattering at the boundaries, but also anisotropy and possible sign-changing of the order parameter in them. This theory has been applied to the calculation of the Josephson current-phase relations and critical current temperature dependencies in junctions of a FeBS with a spin-singlet $s$-wave single-orbital superconductor for different directions of current relative to the crystallographic axes of a FeBS and different length of an insulator layer. We have demonstrated theoretically that investigation of the Josephson transport in the direction parallel to $z$ crystallographic axes of a FeBS allows to distinguish the $s_{\pm}$-wave and the $s_{\mp}$-wave symmetry of the superconducting order parameter in a FeBS. Using our microscopic theory the recently proposed experimental scheme to determine the symmetry of the order parameter in a FeBS\cite{29} has been confirmed microscopically. It is interesting to note that our proposed in the framework of tight-binding model technique can be used for calculations of the charge transport in structures with different unusual materials, such as other multiband superconductors, topological insulators and superconductors and superconducting topological insulators.
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