I.A.Devyatov, A.V. Burmistrova

Theory of a normal and Josephson current in structures with pnictides

Lomonosov MSU SINP

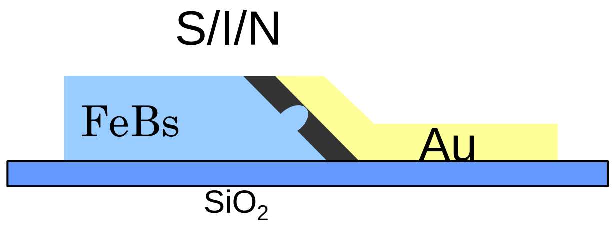
In collaboration with

1. Prof. Yukio Tanaka, Nagoya

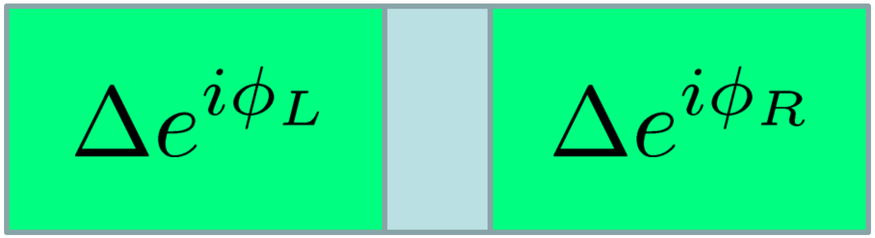
2. Dr. Keiji Yada, Nagoya

3. Dr. Alexander A. Golubov, Twente

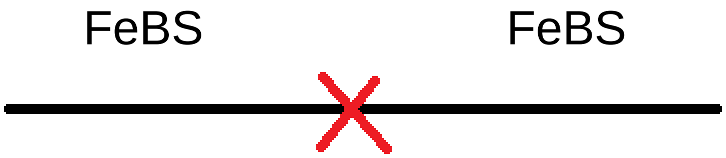
1. SIN junctions



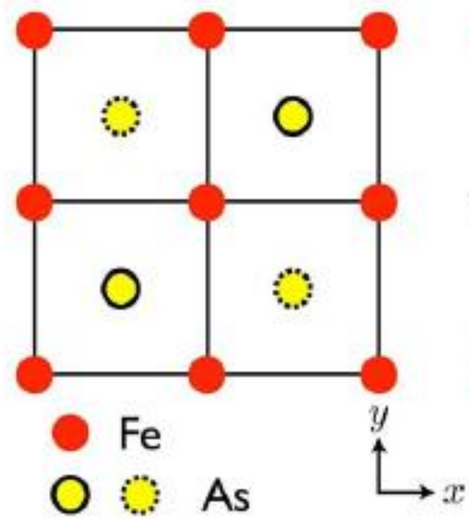
2. Josephson junctions

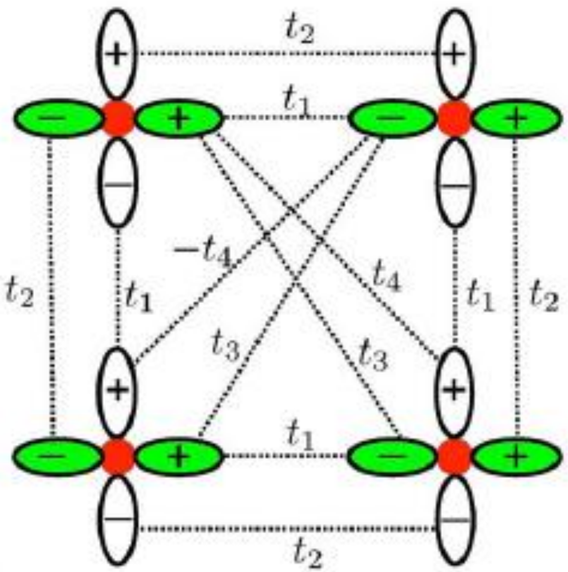


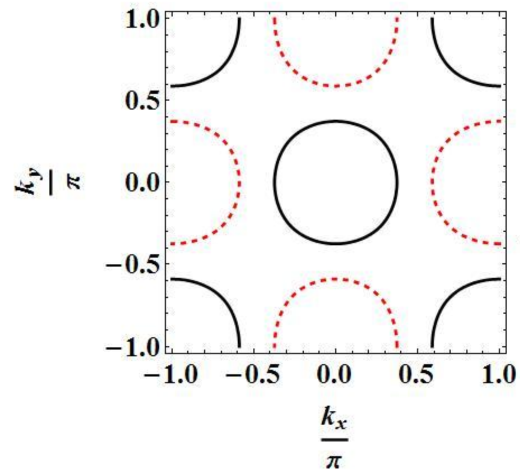
3. Break junctions



The planning of crucial experiment for determination of the order parameter symmetry in iron pnictides.







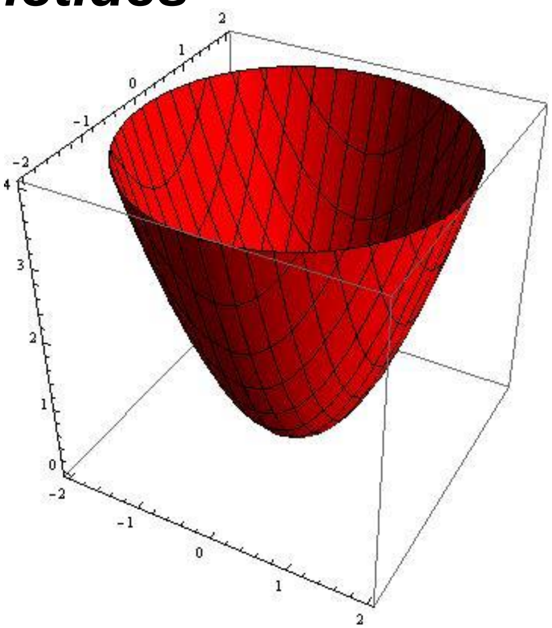
S_{++} $\quad \varphi_1 - \varphi_2 = 0$ $\quad \begin{matrix}\Delta_1 e^{i\varphi_1} \\ \Delta_2 e^{i\varphi_2}\end{matrix}$ $\quad S_{\pm}$ $\quad \varphi_1 - \varphi_2 = \pi$

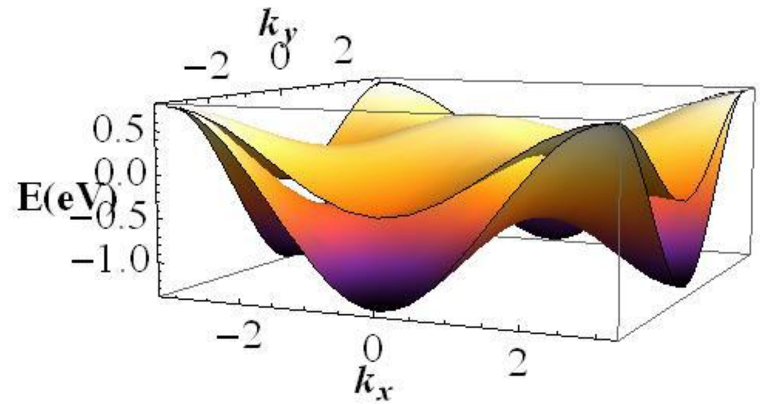
I.I. Mazin, D.J. Singh M. Johannes et al., Phys. Rev. Lett. 101, 057003 (2008)

A. Moreo, M. Daghofer et al., Phys. Rev. B79,134502 (2009).

All previous calculations are phenomenological

<u>The main problem</u>*: we need to coherently match wave functions between normal metal and superconducting pnictides*





This problem have been discussed from 60-s last century and is still unsolved in general case even for normal non superconducting metals

W.A. Harrison, Phys.Rev, 123 , 85 (1961)
B.J.BenDaniel, C.B. Duke, Phys.Rev, 152, 683 (1966)
B. Laikhtman, PRB 46, 4769 (1992)
M. Rontani, L.J. Sham, PRL 94, 186404 (2005)

The main problem of previous attempts

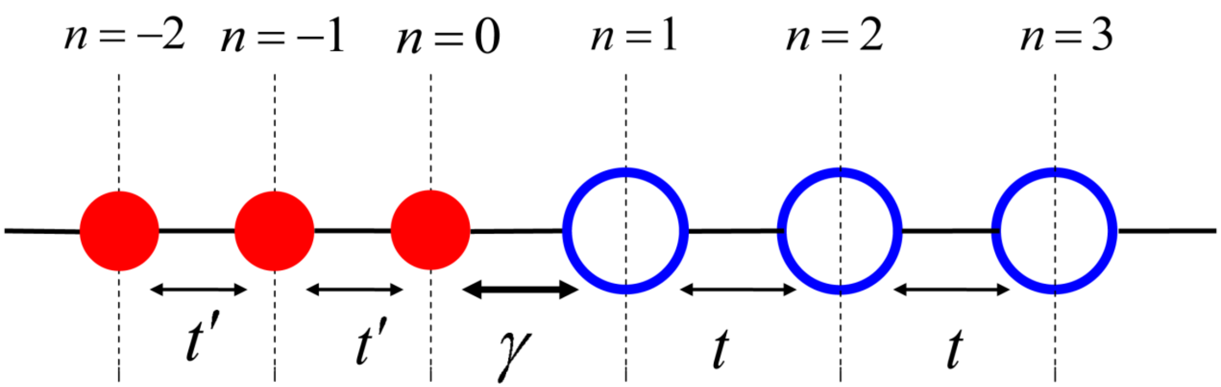
is using the effective mass approximation.

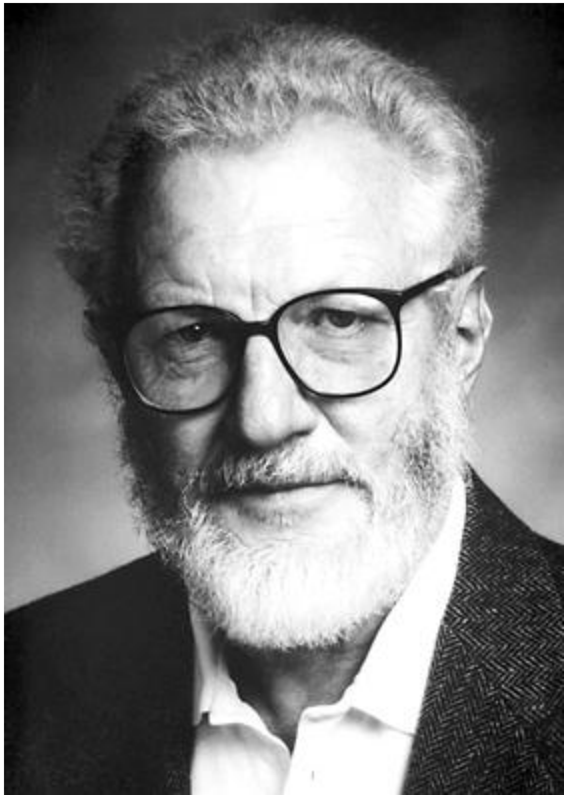
$$E\Phi_0 = -\mu_N \Phi_0 + t'\Phi_{-1} + t'\Phi_1,$$

$$\psi_1' = (\Psi_1 - \Psi_0)/l, \psi_2' = (\Phi_1 - \Phi_0)/l,$$

$$E\Phi_0 = -\mu_N \Phi_0 + t'\Phi_{-1} + \gamma\Psi_1.$$

Herbert Kroemer





$$t'\Phi_1 = \gamma\Psi_1.$$

$$\gamma\Phi_0 = t\Psi_0.$$

Boundary conditions

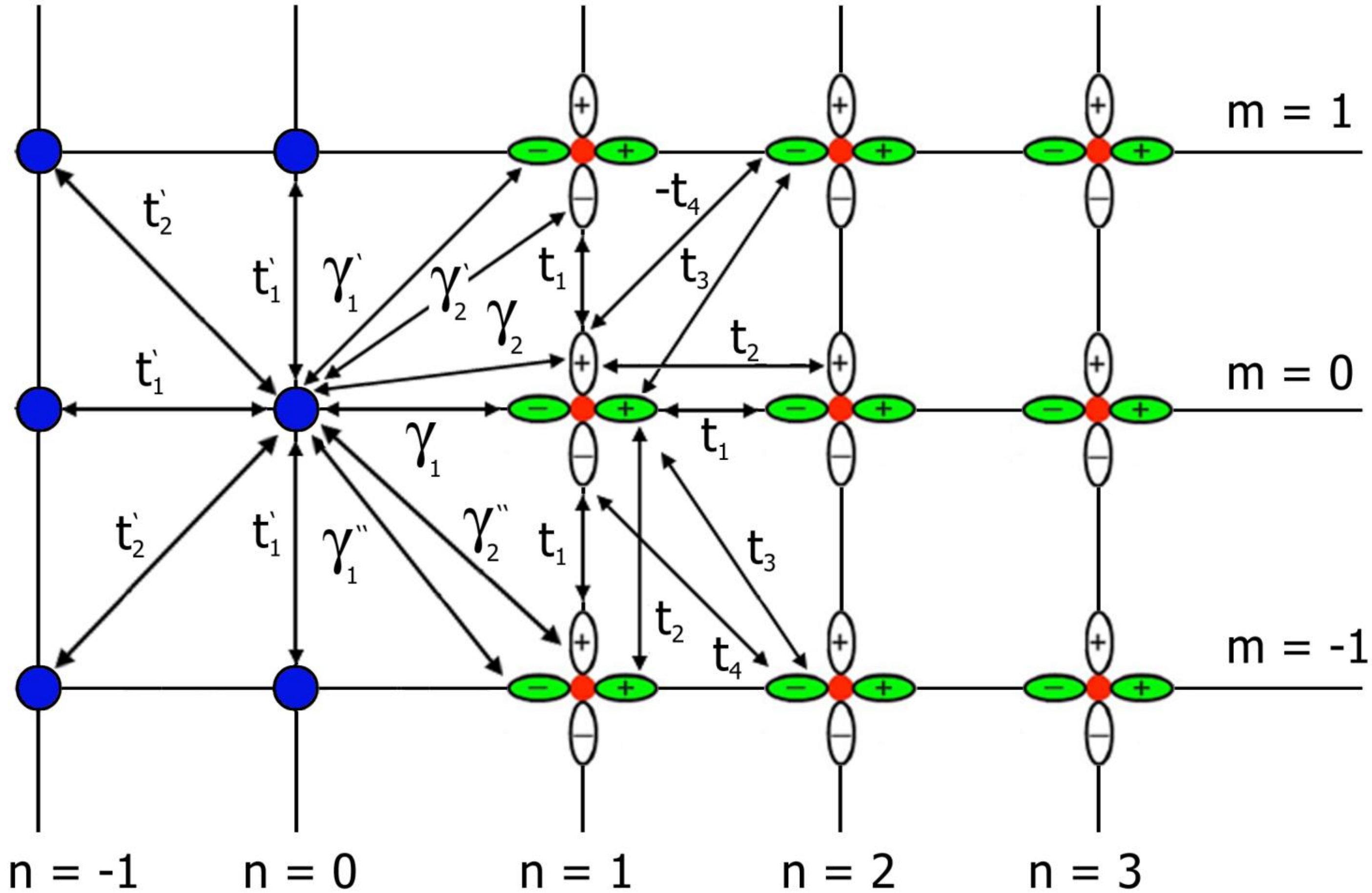
Probability flow

$$J_{n\le -1} = \frac{2t'}{\hbar}\mathrm{Im}(\Phi^*_{n+1}\Phi_n) = J_{n>1} = \frac{2t}{\hbar}\mathrm{Im}(\Psi^*_{n+1}\Psi_n).$$

Q.-G. Zhu and H. Kroemer, Phys. Rev. B 27, 3519 (1983)

1. SIN junctions

Tight-binding model for the contact between s-type normal metal and pnictides: interface is parallel to the



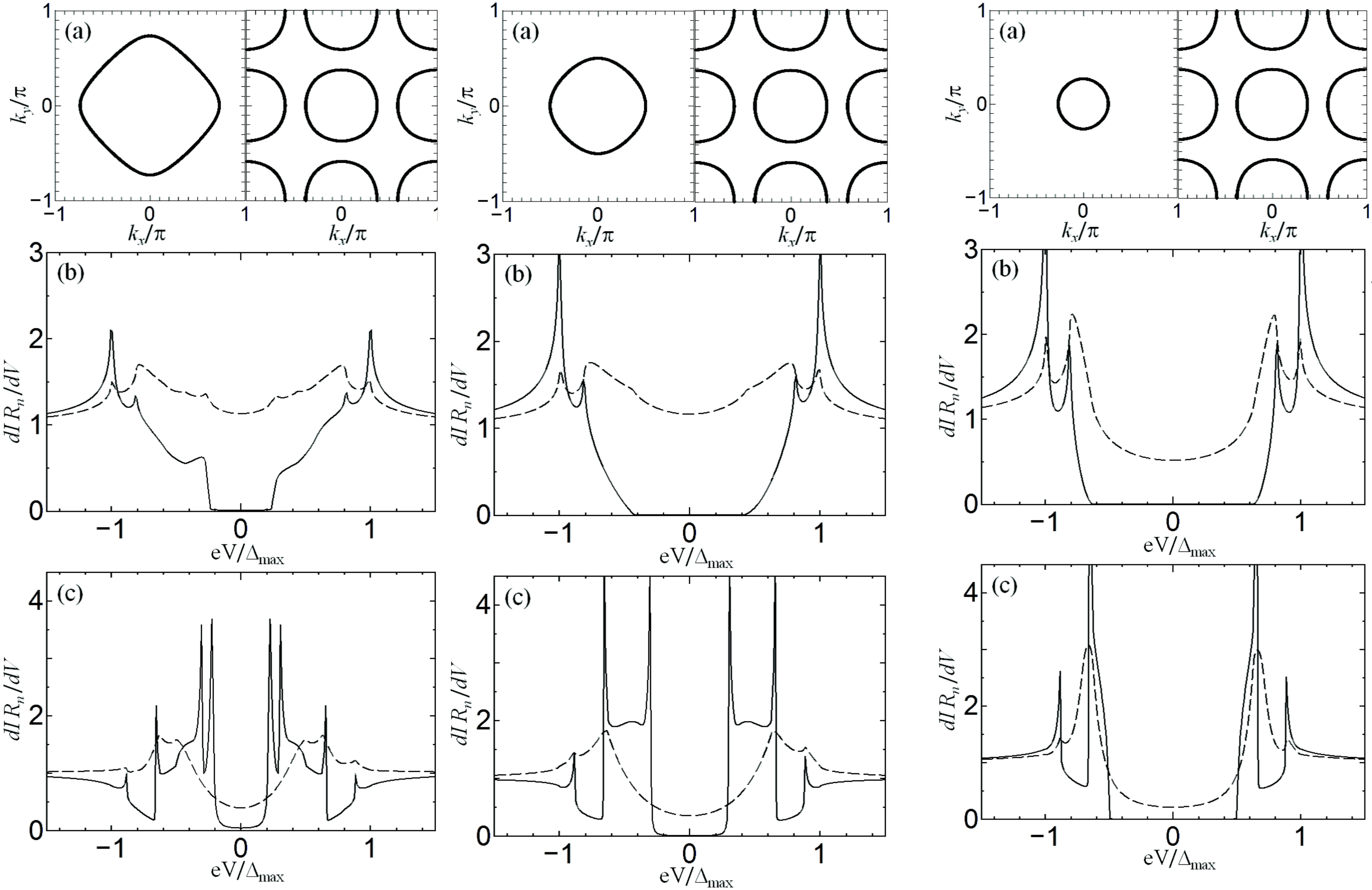
Boundary conditions for zero misorientation angle

$$\begin{cases} t_1'\Phi_1 = \gamma_1\Psi_1^{\alpha} + \gamma_2\Psi_1^{\beta}, \\ t_1'\bar{\Phi}_1 = \gamma_1\bar{\Psi}_1^{\alpha} + \gamma_2,\bar{\Psi}_1^{\beta}, \\ \gamma_1\Phi_0 = (t_1 + 2t_3\cos k_y)\Psi_0^{\alpha} + 2it_4\sin k_y\Psi_0^{\beta} \\ \; + 2\Delta_0\zeta(k_y)\bar{\Psi}_0^{\alpha}, \\ \gamma_1\bar{\Phi}_0 = (t_1 + 2t_3\cos k_y)\bar{\Psi}_0^{\alpha} + 2it_4\sin k_y\bar{\Psi}_0^{\beta} \\ \; - 2\Delta_0\zeta(k_y)\Psi_0^{\alpha}, \\ \gamma_2\Phi_0 = (t_2 + 2t_3\cos k_y)\Psi_0^{\beta} + 2it_4\sin k_y\Psi_0^{\alpha} \\ \; + 2\Delta_0\zeta(k_y)\bar{\Psi}_0^{\beta}, \\ \gamma_2\bar{\Phi}_0 = (t_2 + 2t_3\cos k_y)\bar{\Psi}_0^{\beta} + 2it_4\sin k_y\bar{\Psi}_0^{\alpha} \\ \; - 2\Delta_0\zeta(k_y)\Psi_0^{\beta}, \end{cases}$$

t_1', t_2' t_1, t_2, t_3, t_4 - hopping amplitudes

γ_1 γ_2 -hopping amplitudes across the interface

Angle averaged conductance for different size of normal metal Fermi surface



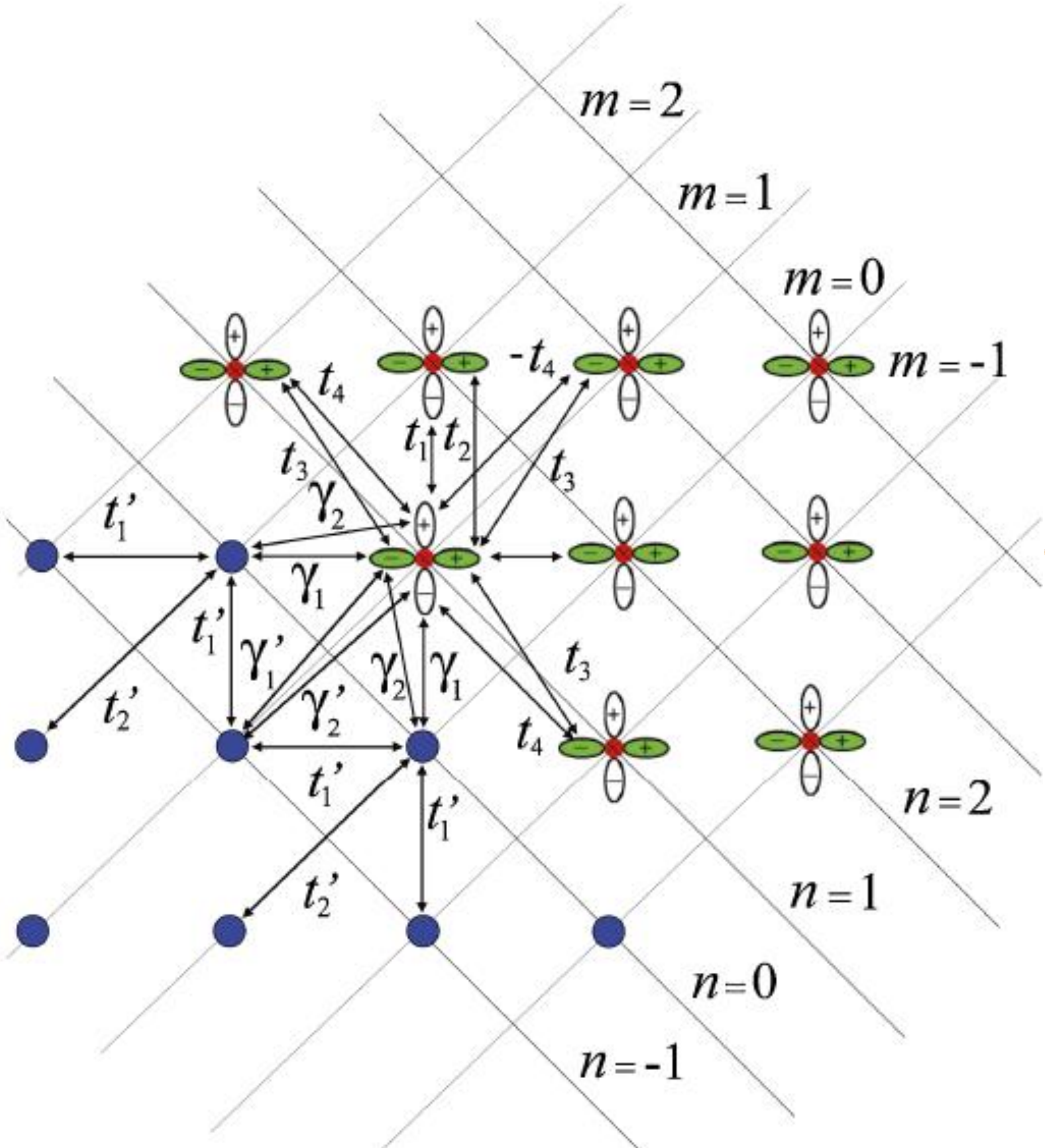
Fermi surface

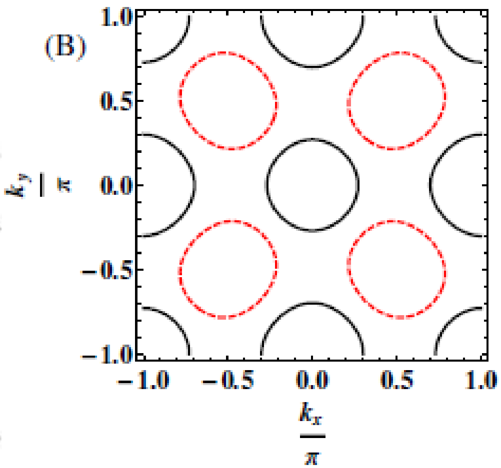
s_{++}

$s_{\pm}$

A. V. Burmistrova, I. A.D., A. A. Golubov, K. Yada, Y. Tanaka, JPSJ, **82**, 034716 (2013).

SIN, Non-zero misorientation angle

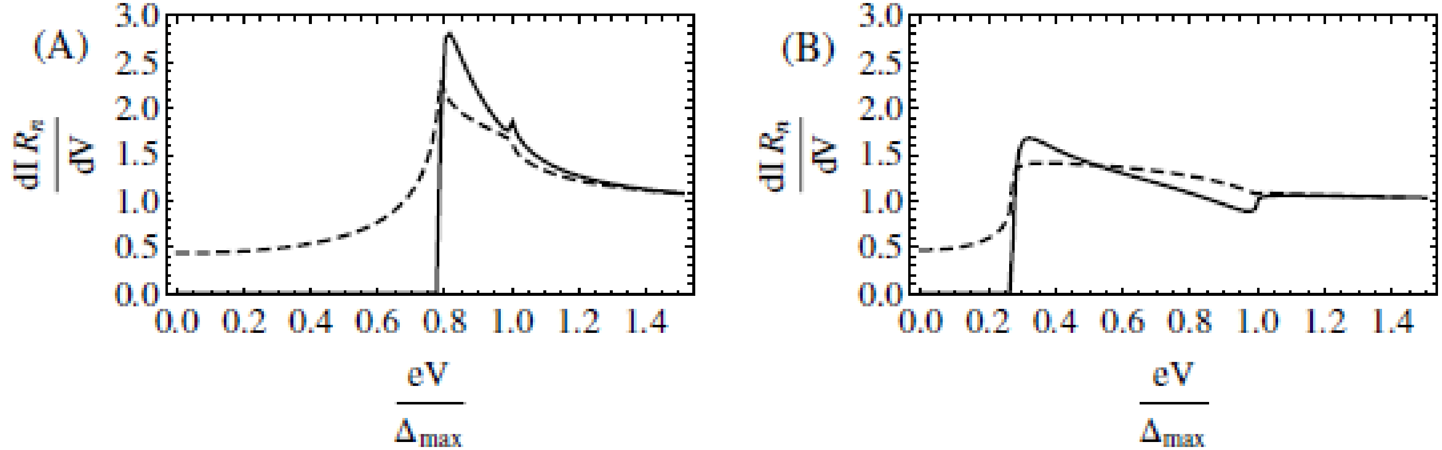


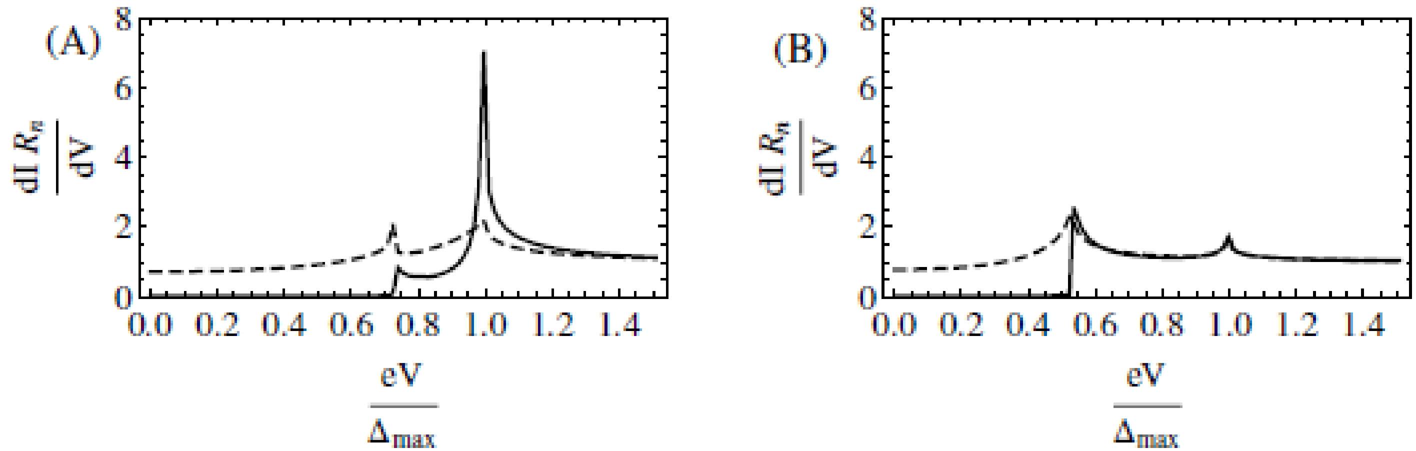


Nonzero misorientation angle. Boundary conditions.

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

The conductivities of the Sp-I-N junction for the $s_{\pm}$, s_{++} models for nonzero misorientation angle



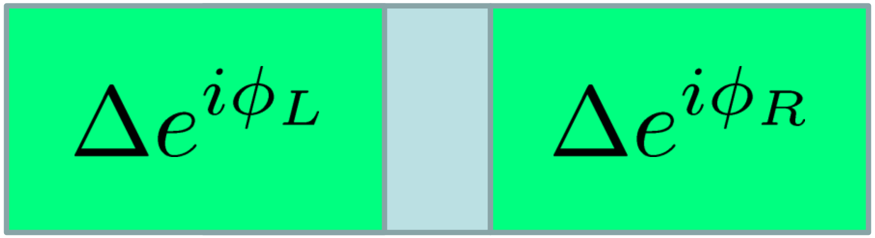


A.V. Burmistrova, I.A. Devyatov, JETPh Letters, **96**, 391 (2012).
A. V. Burmistrova, I. A.D., A. A. Golubov, K. Yada, Y. Tanaka, JPSJ, **82**, 034716 (2013).

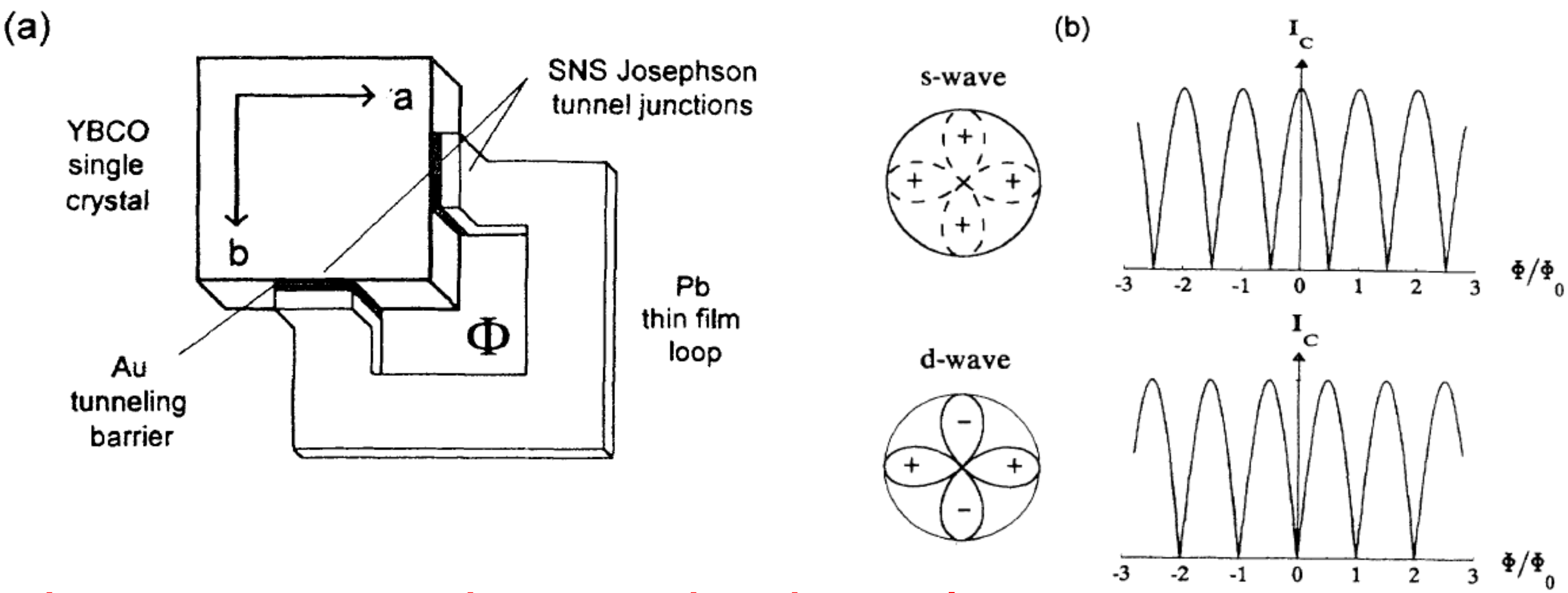
Conclusion for SIN part.

In order to distinguish s++ and s+- models in pnictide one should use SIN contacts with zero misorientation angle and large Fermi surface of normal metal.

2. Josephson Junction



$$J \propto \sin(\phi_L - \phi_R)$$

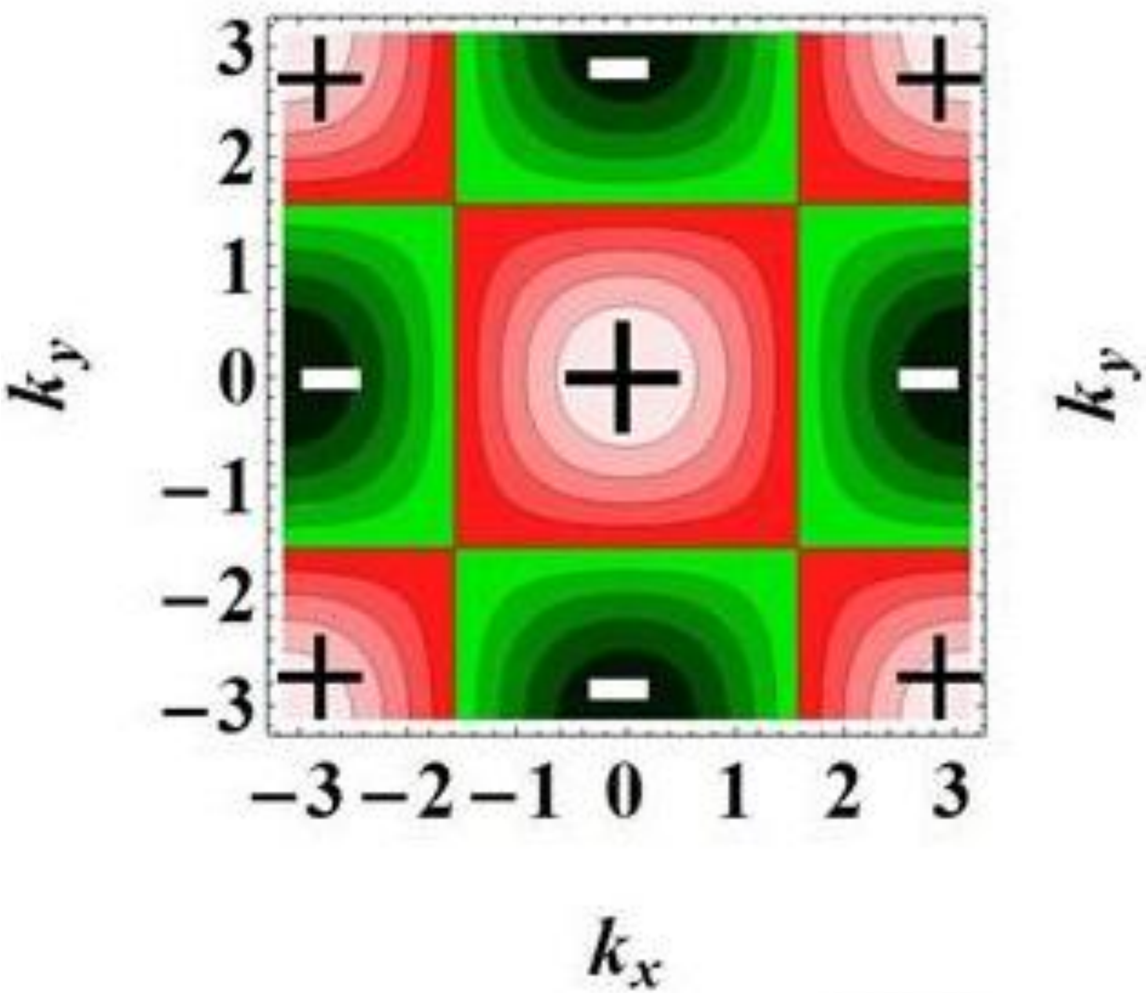


Order parameter change sign in real space

d-I-d

D. A. Wollman, et al., Phys. Rev. B **27**, 3519 (1983)

Pnictide –order parameter change sign in k-space!



Josephson current in S/I/S_p structure in x-y plane.

$$\Delta = 4\Delta_p \cos k_x \cos k_y$$

Green's functions

$$G_{\{n\},\{j\}}(\tau_1,\tau_2) = \begin{pmatrix} G^{\alpha}_{\{n\},\{j\}}(\tau_1,\tau_2) & G^{\alpha\beta}_{\{n\},\{j\}}(\tau_1,\tau_2) \\ G^{\beta\alpha}_{\{n\},\{j\}}(\tau_1,\tau_2) & G^{\beta}_{\{n\},\{j\}}(\tau_1,\tau_2) \end{pmatrix} = \begin{pmatrix} -\langle T_\tau c_\uparrow(\{n\},\tau_1) c^+_\uparrow(\{j\},\tau_2)\rangle & -\langle T_\tau c_\uparrow(\{n\},\tau_1) d^+_\uparrow(\{j\},\tau_2)\rangle \\ -\langle T_\tau d_\uparrow(\{n\},\tau_1) c^+_\uparrow(\{j\},\tau_2)\rangle & -\langle T_\tau d_\uparrow(\{n\},\tau_1) d^+_\uparrow(\{j\},\tau_2)\rangle \end{pmatrix}$$

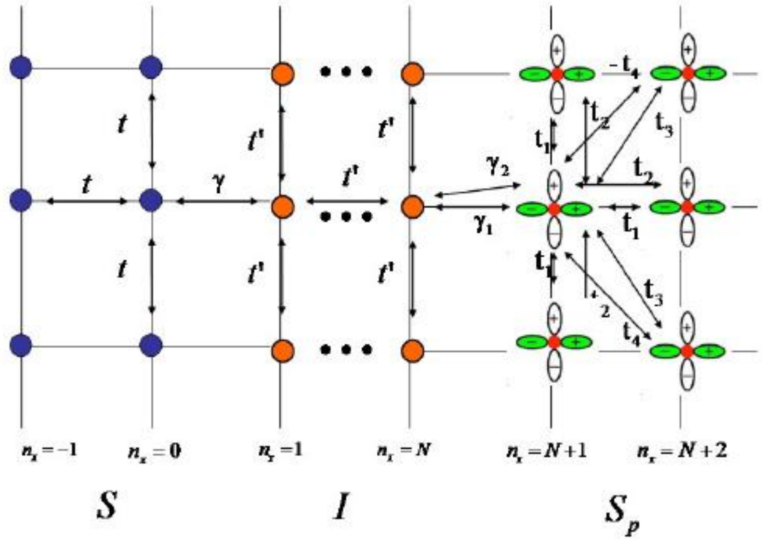
$$F_{\{n\},\{j\}}(\tau_1,\tau_2) = \begin{pmatrix} F^{\alpha}_{\{n\},\{j\}}(\tau_1,\tau_2) & F^{\alpha\beta}_{\{n\},\{j\}}(\tau_1,\tau_2) \\ F^{\beta\alpha}_{\{n\},\{j\}}(\tau_1,\tau_2) & F^{\beta}_{\{n\},\{j\}}(\tau_1,\tau_2) \end{pmatrix} = \begin{pmatrix} -\langle T_\tau c^+_\downarrow(\{n\},\tau_1) c^+_\uparrow(\{j\},\tau_2)\rangle & -\langle T_\tau c^+_\downarrow(\{n\},\tau_1) d^+_\uparrow(\{j\},\tau_2)\rangle \\ -\langle T_\tau d^+_\downarrow(\{n\},\tau_1) c^+_\uparrow(\{j\},\tau_2)\rangle & -\langle T_\tau d^+_\downarrow(\{n\},\tau_1) d^+_\uparrow(\{j\},\tau_2)\rangle \end{pmatrix}$$

$$\tilde{G}_{\{n\},\{j\}}(\tau_1,\tau_2) = \begin{pmatrix} \tilde{G}^{\alpha}_{\{n\},\{j\}}(\tau_1,\tau_2) & \tilde{G}^{\alpha\beta}_{\{n\},\{j\}}(\tau_1,\tau_2) \\ \tilde{G}^{\beta\alpha}_{\{n\},\{j\}}(\tau_1,\tau_2) & \tilde{G}^{\beta}_{\{n\},\{j\}}(\tau_1,\tau_2) \end{pmatrix} = \begin{pmatrix} -\langle T_\tau c^+_\downarrow(\{n\},\tau_1) c_\downarrow(\{j\},\tau_2)\rangle & -\langle T_\tau c^+_\downarrow(\{n\},\tau_1) d_\downarrow(\{j\},\tau_2)\rangle \\ -\langle T_\tau d^+_\downarrow(\{n\},\tau_1) c_\downarrow(\{j\},\tau_2)\rangle & -\langle T_\tau d^+_\downarrow(\{n\},\tau_1) d_\downarrow(\{j\},\tau_2)\rangle \end{pmatrix}$$

$$\tilde{F}_{\{n\},\{j\}}(\tau_1,\tau_2) = \begin{pmatrix} \tilde{F}^{\alpha}_{\{n\},\{j\}}(\tau_1,\tau_2) & \tilde{F}^{\alpha\beta}_{\{n\},\{j\}}(\tau_1,\tau_2) \\ \tilde{F}^{\beta\alpha}_{\{n\},\{j\}}(\tau_1,\tau_2) & \tilde{F}^{\beta}_{\{n\},\{j\}}(\tau_1,\tau_2) \end{pmatrix} = \begin{pmatrix} -\langle T_\tau c_\uparrow(\{n\},\tau_1) c_\downarrow(\{j\},\tau_2)\rangle & -\langle T_\tau c_\uparrow(\{n\},\tau_1) d_\downarrow(\{j\},\tau_2)\rangle \\ -\langle T_\tau d_\uparrow(\{n\},\tau_1) c_\downarrow(\{j\},\tau_2)\rangle & -\langle T_\tau d_\uparrow(\{n\},\tau_1) d_\downarrow(\{j\},\tau_2)\rangle \end{pmatrix},$$

Gorkov equations

$$\begin{cases} (i\omega - \varepsilon_n^{(\alpha)} + \mu) G^{(\alpha\alpha),\omega}_{\{n\},\{j\}} - \sum\limits_{\{l\}} t^{(\alpha)}_{\{n\},\{l\}} G^{(\alpha\alpha),\omega}_{\{l\},\{j\}} - \sum\limits_{\{l\}} t^{(\alpha\beta)}_{\{n\},\{l\}} G^{(\alpha\beta),\omega}_{\{l\},\{j\}} + \sum\limits_{\{l\}} \Delta_{\{n\},\{l\}} F^{(\alpha\alpha),\omega}_{\{l\},\{j\}} = \delta_{\{n\},\{j\}}, \\ (i\omega - \varepsilon_n^{(\beta)} + \mu) G^{(\alpha\beta),\omega}_{\{n\},\{j\}} - \sum\limits_{\{l\}} t^{(\beta)}_{\{n\},\{l\}} G^{(\alpha\beta),\omega}_{\{l\},\{j\}} - \sum\limits_{\{l\}} t^{(\beta\alpha)}_{\{n\},\{l\}} G^{(\alpha\alpha),\omega}_{\{l\},\{j\}} + \sum\limits_{\{l\}} \Delta_{\{n\},\{l\}} F^{(\alpha\beta),\omega}_{\{l\},\{j\}} = 0, \\ (i\omega + \varepsilon_n^{(\alpha)} - \mu) F^{(\alpha\alpha),\omega}_{\{n\},\{j\}} + \sum\limits_{\{l\}} t^{(\alpha)}_{\{n\},\{l\}} F^{(\alpha\alpha),\omega}_{\{l\},\{j\}} + \sum\limits_{\{l\}} t^{(\alpha\beta)}_{\{n\},\{l\}} F^{(\alpha\beta),\omega}_{\{l\},\{j\}} + \sum\limits_{\{l\}} \Delta^*_{\{n\},\{l\}} G^{(\alpha\alpha),\omega}_{\{l\},\{j\}} = 0, \\ (i\omega + \varepsilon_n^{(\beta)} - \mu) F^{(\alpha\beta),\omega}_{\{n\},\{j\}} + \sum\limits_{\{l\}} t^{(\beta)}_{\{n\},\{l\}} F^{(\alpha\beta),\omega}_{\{l\},\{j\}} + \sum\limits_{\{l\}} t^{(\beta\alpha)}_{\{n\},\{l\}} F^{(\alpha\alpha),\omega}_{\{l\},\{j\}} + \sum\limits_{\{l\}} \Delta^*_{\{n\},\{l\}} G^{(\alpha\beta),\omega}_{\{l\},\{j\}} = 0. \end{cases}$$



S/I/S_p structure

boundary conditions in the quasiclassical approximation $(\Delta_0, \Delta_p << \mu_I, \mu_p, \mu_s, t, t_1, t_2, t_3, t_4)$

$$
\begin{cases}
tG^{S}_{1,j} = \gamma G^{I}_{1,j}, \\
tF^{S_L}_{1,j} = \gamma F^{I}_{1,j}, \\
\gamma G^{S}_{0,j} = t' G^{I}_{0,j}, \\
\gamma F^{S}_{0,j} = t' F^{I}_{0,j}
\end{cases}
$$

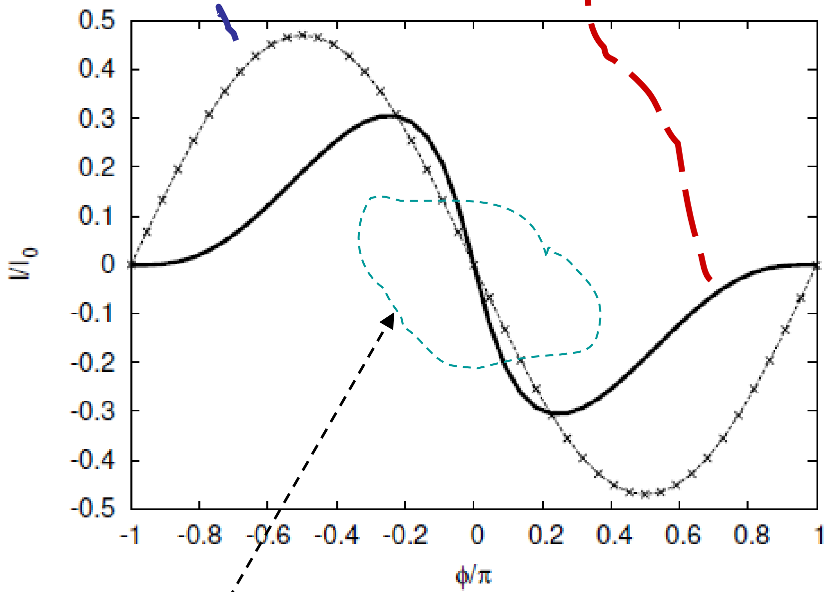
$$
\begin{cases}
t_1 G^{(\alpha\alpha)}_{N,j} + 2t_3 \cos k_y G^{(\alpha\alpha)}_{N,j} + 2it_4 \sin k_y G^{(\alpha\beta)}_{N,j} = \gamma_1 G^{I}_{N,j}, \\
t_1 F^{(\alpha\alpha)}_{N,j} + 2t_3 \cos k_y F^{(\alpha\alpha)}_{N,j} + 2it_4 \sin k_y F^{(\alpha\beta)}_{N,j} = \gamma_1 F^{I}_{N,j}, \\
t_2 G^{(\alpha\beta)}_{N,j} + 2t_3 \cos k_y G^{(\alpha\beta)}_{N,j} + 2it_4 \sin k_y G^{(\alpha\alpha)}_{N,j} = \gamma_2 G^{I}_{N,j}, \\
t_2 F^{(\alpha\beta)}_{N,j} + 2t_3 \cos k_y F^{(\alpha\beta)}_{N,j} + 2it_4 \sin k_y F^{(\alpha\alpha)}_{N,j} = \gamma_2 F^{I}_{N,j}, \\
\gamma_1 G^{(\alpha\alpha)}_{N+1,j} + \gamma_2 G^{(\alpha\beta)}_{N+1,j} = tG^{I}_{N+1,j}, \\
\gamma_1 F^{(\alpha\alpha)}_{N+1,j} + \gamma_2 F^{(\alpha\beta)}_{N+1,j} = tF^{I}_{N+1,j},
\end{cases}
$$

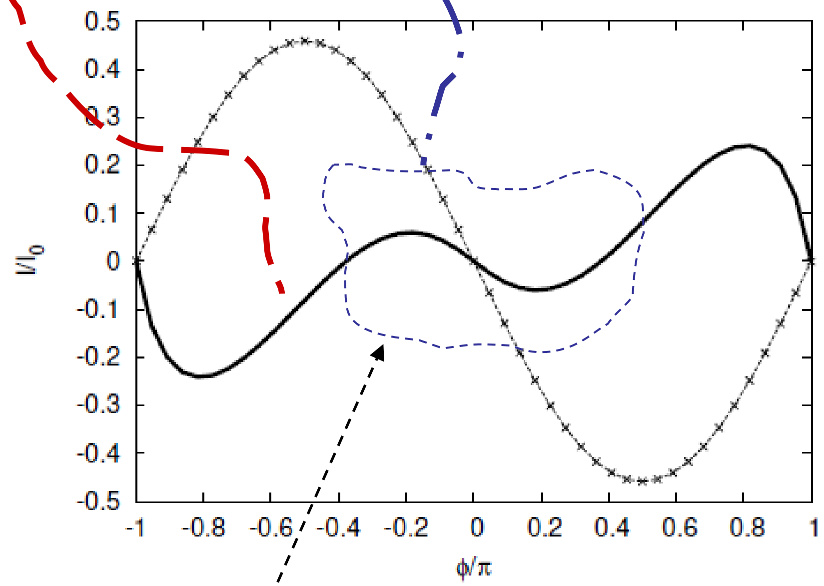
Josephson current in S/I/S_p structure.

The phase dependence of Josephson current in the $S_d/I/S$ structure for zero misorientation angle of crystallographic axes of pnictide with respect to the interface,

N=0

N=3



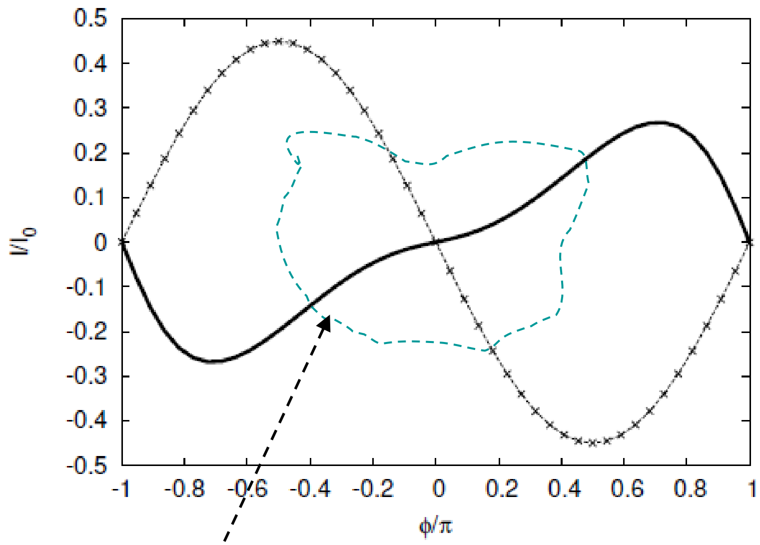


π-contact

ϕ-contact

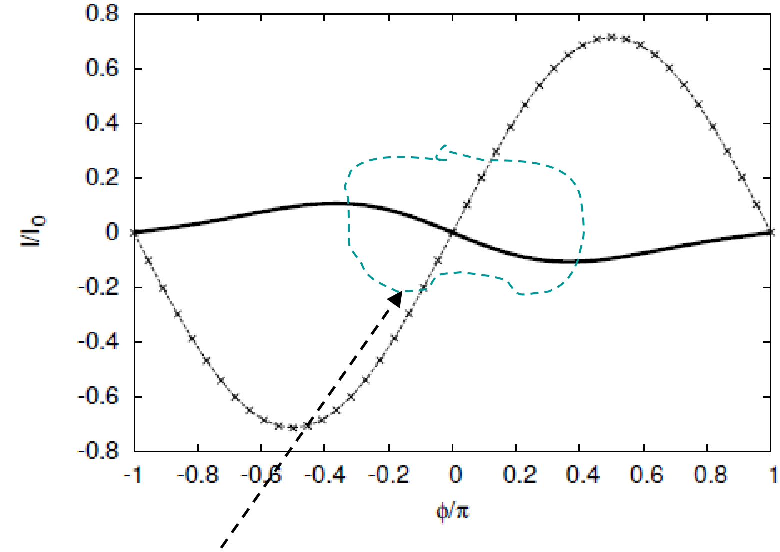
$\gamma_1 = 0.02, \gamma_2 = 0.2,$

$\gamma_1 = 0.02, \gamma_2 = 0.3$



0-contact

$\gamma_1 = 0.02, \gamma_2 = 0.4$



π-contact

$\gamma_1 = 0.2, \gamma_2 = 0.02$

Thus changing hopping parameters at the interface for zero length of an insulator for the case of the $s_\pm$ model of the superconducting pairing one can obtain in the considered $S/I/S_p$ structure after averaging over all possible values of k_y 0-, π- or ϕ-contact.

$S/I/S_p$ sctructure with the sufficiently long insulating region has the ground state either at 0 or π phase difference depending on the values of the hopping parameters at the interface and the size of the Fermi surface in s-wave superconductor.

Conclusion for Josephson current in S-I-Sp structure for tunneling in x-y plane

For s+- symmetry of the order parameter it is possible the existence 0, π, and φ contacts for junctions with atomically sharp boundaries,
for long barriers it is possible only 0 and π contacts.
For s++ symmetry it is possible only 0 contacts.

3. Break Sp-I-Sp junctions

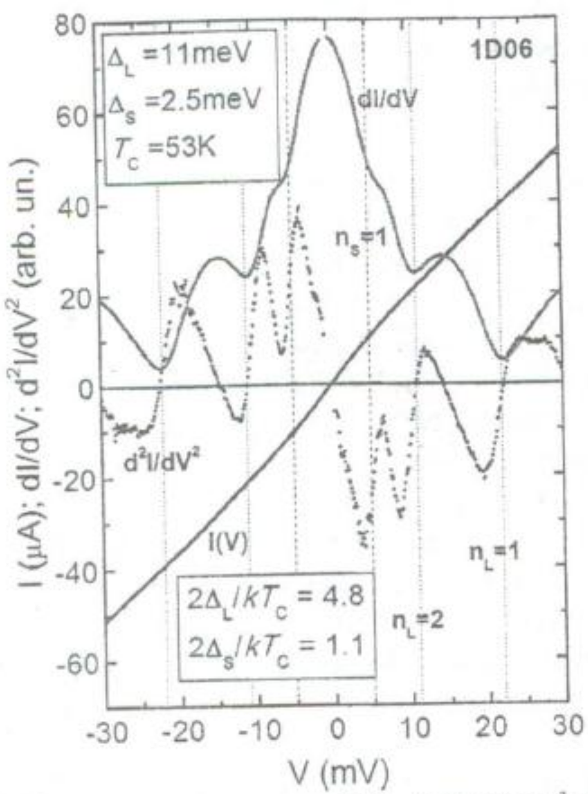
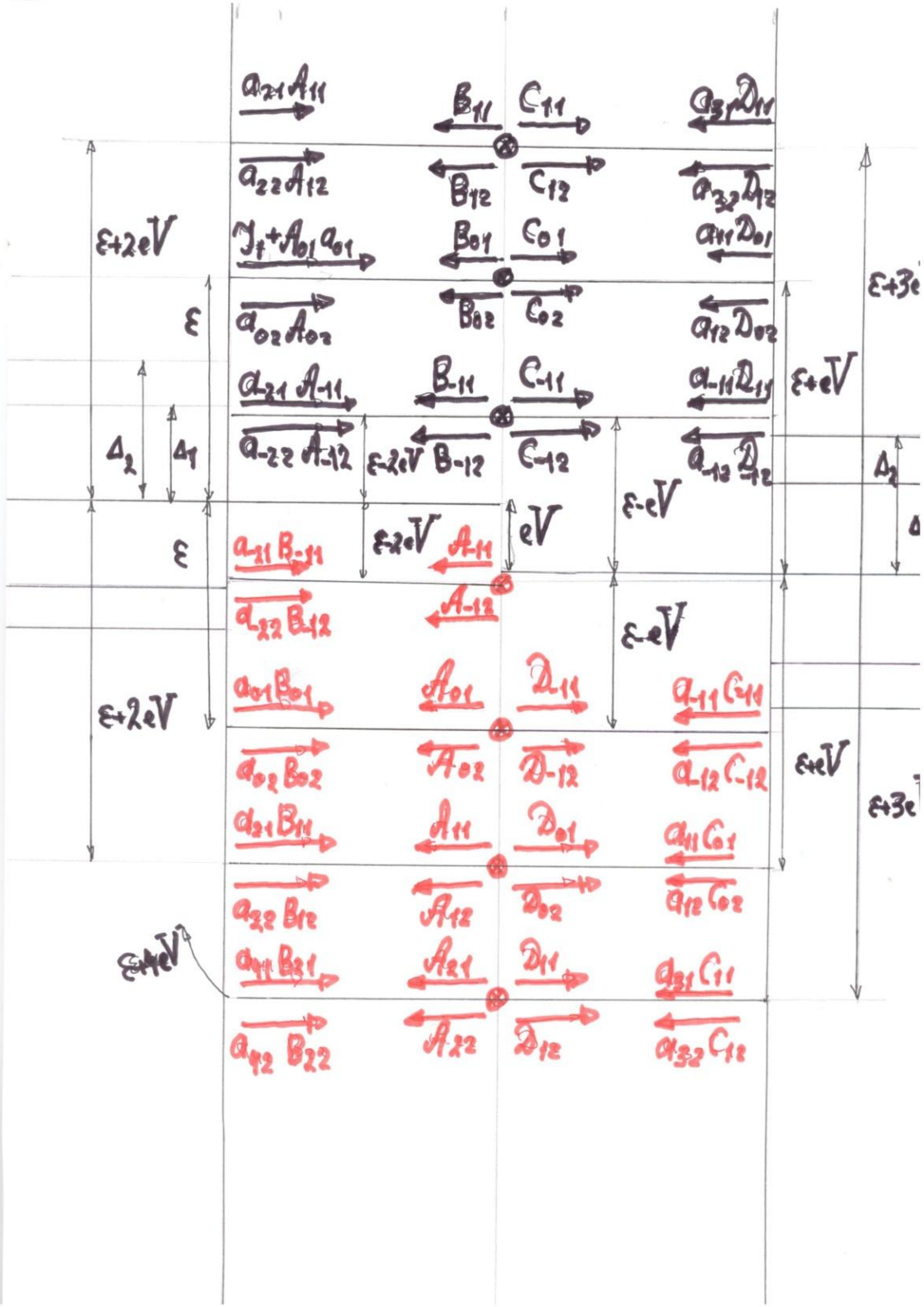


Рис. 2. Типичные зависимости $I(V)$, $dI(V)/dV$ и $d^2I(V)/dV^2$ для одиночного SNS-контакта 1D06 при T = 4.2 K. Отмечены особенности, соответствующие большой щели n_L=1, n_L=2 и малой щели n_S=1

Experiment of Pudalov's group: usual $2\Delta/n$ pecularities.

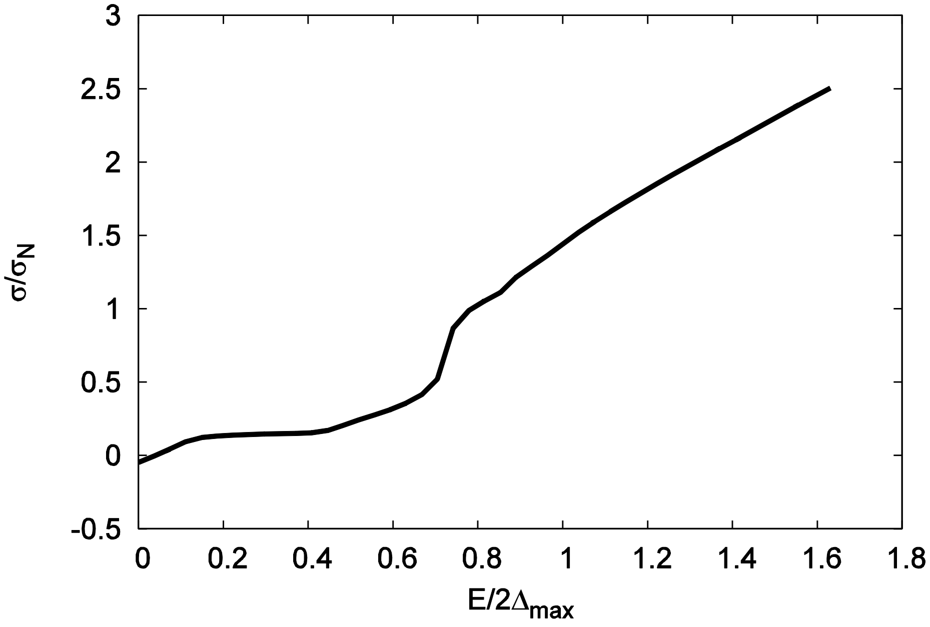
$$\begin{bmatrix}B_{01}\\C_{01}\\B_{02}\\C_{02}\end{bmatrix} = \begin{bmatrix}S_{11}&S_{12}&S_{13}&S_{14}\\S_{21}&S_{22}&S_{23}&S_{24}\\S_{31}&S_{32}&S_{33}&S_{34}\\S_{41}&S_{42}&S_{43}&S_{44}\end{bmatrix}\begin{bmatrix}J_1+a_{01}A_{01}\\a_{11}D_{01}\\a_{02}A_{02}\\a_{12}D_{02}\end{bmatrix}$$

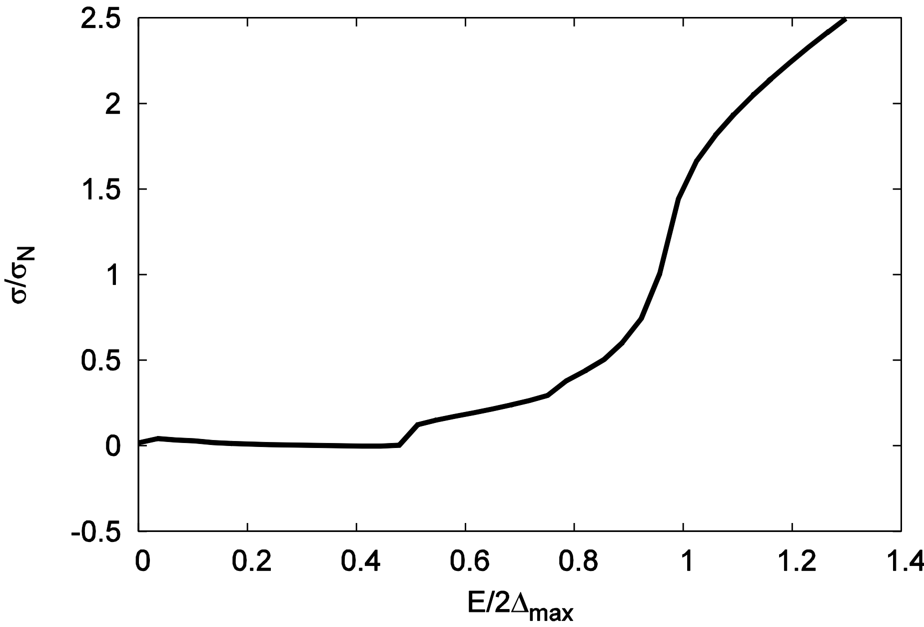


There are no exact continued fraction solutions for 4x4 scattering Matrixes!

$$\begin{bmatrix}A_{01}\\D_{-11}\\A_{02}\\D_{-12}\end{bmatrix} = \begin{bmatrix}S^*_{11}&S^*_{21}&S^*_{31}&S^*_{41}\\S^*_{12}&S^*_{22}&S^*_{32}&S^*_{42}\\S^*_{13}&S^*_{23}&S^*_{33}&S^*_{43}\\S^*_{14}&S^*_{24}&S^*_{34}&S^*_{44}\end{bmatrix}\begin{bmatrix}a_{01}B_{01}\\a_{-11}C_{-11}\\a_{02}B_{02}\\a_{-12}C_{-12}\end{bmatrix}$$

Results of calculations – not angle averaged CVC





S+- model

S++ model

Conclusion for break junctions part.

Comparison existing experimental results
with our preliminary not angle averaged calculations
confirm s++ model

Conclusions.

1. We have proposed consistent tight-binding model for the coherent charge transport in the structures, containing multiband superconductors with complex non-parabolic excitation spectrum and anisotropic order parameter.

2. In order to distinguish s++ and s+- models in pnictide one should use SIN contacts with zero misorientation angle and large Fermi surface of normal metal

3. For s+- symmetry of the order parameter it is possible the existence 0, π, and φ S-I-Sp Josephson contacts for junctions with atomically sharp boundaries, for long barriers it is possible only 0 and π contacts.
For s++ symmetry it is possible only 0 contacts.

4. Comparison existing experimental results for Sp-Sp break junctions with our preliminary not angle averaged calculations confirm s++ model.

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Thank you for your attention