A tunneling Hamiltonian theory of 0-\(\pi\) transition in \(d\)-wave superconductor/ferromagnetic-insulator heterostructures

Shiro Kawabata\(^1,2\), Satoshi Kashiwaya\(^3\), Yukio Tanaka\(^4\), Alexander A. Golubov\(^5\), Yasuhiro Asano\(^6\)

\(^1\)Nanosystems Research Institute (NRI), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, 305-8568, Japan
\(^2\)CREST, Japan Science and Technology Corporation (JST), Kawaguchi, Saitama 332-0012, Japan
\(^3\)Nanoelectronics Research Institute (NRI), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, 305-8568, Japan
\(^4\)Department of Applied Physics, Nagoya University, Nagoya, 464-8603, Japan
\(^5\)Faculty of Science and Technology and MESA+ Institute of Nanotechnology, University of Twente, 7500 AE, Enschede, The Netherlands
\(^6\)Department of Applied Physics and Center for Topological Science & Technology, Hokkaido University, Sapporo, 060-8628, Japan

E-mail: s-kawabata@aist.go.jp

Abstract. We report a theory of the Josephson transport through ferromagnetic insulators (FIs). Recently the appearance of the atomic scale 0-\(\pi\) transition in such junctions has been predicted based on a numerical simulation. In order to understand the physical mechanism of this anomalous phenomena, we have analytically calculated the Josephson current using the tunneling Hamiltonian method and found that the spin dependent \(\pi\)-phase shift in the FI barrier gives the atomic scale 0-\(\pi\) transition. We also show an experimental setup for observing the atomic-scale 0-\(\pi\) transition based on a \(d\)-wave junction with a LBCO barrier.

1. Introduction
The developing field of superconducting spintronics subsumes many fascinating physical phenomena with potential applications that may complement conventional spintronics devices [1, 2]. Moreover there is an increasing interest in the novel properties of junctions between superconductors and magnetic materials [3, 4]. One of the peculiar phenomena is the Josephson \(\pi\)-junction formation in superconductor/ferromagnetic-metal/superconductor (S/FM/S) heterostructures [5, 6]. In the ground-state phase difference between two coupled superconductors is \(\pi\) instead of 0 as in the ordinary 0-junctions. In terms of the Josephson relationship \(I_J = I_C \sin \phi\), where \(\phi\) is the phase difference between the two superconductor layers, a transition from the 0 to \(\pi\) states implies a change in sign of \(I_C\) from positive to negative. This phenomenon is related with the damping oscillatory behavior of the Cooper pair wave function in a FM. Experimentally the existence of the \(\pi\)-junction in S/FM/S systems has been confirmed by Ryazanov et al. [7] and Kontos et al. [8] Until recently, however, investigations on the \(\pi\) junction have been mainly focused on the S/FM/S systems.
We have predicted a possibility of the $\pi$-junction formation in Josephson junctions through ferromagnetic insulators (FIs) by numerically solving the Bogoliubov-de Genne equation [9, 10] and the Nambu Green’s function [11, 12, 13, 14]. The formation of the $\pi$ junction using such an insulating barrier is very promising for future qubit application [15, 16, 17, 18] because of its low decoherence nature [19, 20]. More interestingly, we found that the ground state of such junction alternates between 0- and $\pi$-states when thickness of FI is increasing by a single atomic layer. In this paper in order to understand the physical mechanism of this atomic scale 0-$\pi$ transition, we analytically calculate the Josephson current based on the tunneling Hamiltonian method and show that the spin-dependent $\pi$-phase shift of the tunneling matrix element of the FI layer is the origin of this anomalous transition.

2. Electronic properties of a ferromagnetic insulator

In this section, we briefly describe the electronic structure of a representative of FI materials, i.e., La$_2$BaCuO$_5$ (LBCO) [21, 22, 23]. The typical DOS of LBCO for each spin direction is shown schematically in Fig. 1(a). The exchange splitting $V_{ex}$ is estimated to be 0.34 eV by a first-principle band calculation using the spin-polarized local density approximation [24]. Since the exchange splitting is large and the bands are originally half-filled, the system becomes FI. Based on the band structure [Fig. 1(a)], the spin-dependent transmission coefficient $T_\sigma$ for the FI barrier can be calculated as [9]

$$T_\sigma = \alpha_{L_F} \left( \frac{\rho_\sigma t}{g} \right)^{L_F},$$

by using the transfer matrix method, where $\rho_{\uparrow(\downarrow)} = -(+)1$ and $\alpha_{L_F}$ is a spin-independent complex constant, $t$ is the hopping integral in the FI, $g$ is the gap between the up- and down-

![Figure 1](image)

Figure 1. (a) The density of states for each spin direction for a ferromagnetic insulator, e.g., LBCO, and (b) schematic picture of c-axis stack high-$T_c$ d-wave superconductor/LBCO/high-$T_c$ d-wave superconductor Josephson junction.
spin band, and \( L_F \) is the layer number of the FI. We immediately find
\[
\frac{T_\uparrow}{T_\downarrow} = (-1)^{L_F},
\]
so the relative phase of \( T_\sigma \) between spin up and down is \( \pi (0) \) for the odd (even) number of \( L_F \).

Next section, we will calculate the Josephson current through such a FI analytically.

It is important to note that the usage of high-\( T_c \) cuprate superconductors, e.g., \( \text{YBa}_2\text{Cu}_3\text{O}_{7-\delta} \) and \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) is desirable from the perspectives of the high-temperature device-operation. Moreover, recent development of the pulsed laser deposition technique enables layer-by-layer epitaxial-growth of such oxide superlattices [25]. Thus in this paper we mainly focused on the high-\( T_C \) \( d \)-wave junction with a FI barrier [Fig. 1(b)]. We note that the qualitatively same result can be obtained for the case of \( s \)-wave junctions.

3. Theory
In this section, we develop a analytical calculation method for the Josephson current of S/FI/S junctions based on the tunneling Hamiltonian approach. Let us consider a three-dimensional S/FI/S junction as shown in Fig. 1(b). The Hamiltonian of the system is given by
\[
\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_T + \mathcal{H}_Q,
\]
where \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) are Hamiltonians describing the \( d \)-wave superconductors:
\[
\mathcal{H}_1 = \sum_\sigma \int dr \psi_{1\sigma}^\dagger (r) \left( -\frac{\hbar^2 \nabla^2}{2m} - \mu \right) \psi_{1\sigma} (r) - \frac{1}{2} \sum_{\sigma,\sigma'} \int dr \int dr' \psi_{1\sigma}^\dagger (r) \psi_{1\sigma'}^\dagger (r') g_1 (r - r') \psi_{1\sigma'} (r') \psi_{1\sigma} (r),
\]
where \( \mu \) is the chemical potential and \( \psi \) (\( \psi^\dagger \)) is the fermion field operator and \( g (r - r') \) is the attractive interaction. The tunneling Hamiltonian with a spin-dependent tunneling matrix element \( t_\sigma \) of the FI barrier is given by
\[
\mathcal{H}_T = \sum_\sigma \int dr \int dr' \left[ t_\sigma (r, r') \psi_{1\sigma}^\dagger (r) \psi_{2\sigma} (r') + \text{h.c.} \right],
\]
and
\[
\mathcal{H}_Q = \frac{(Q_1 - Q_2)^2}{8C}
\]
is the charging Hamiltonian, where \( C \) is the capacitance of the junction and \( Q_1(2) \) is the operator for the charge on the superconductor 1 (2), which can be written as
\[
Q_1 = e \sum_\sigma \int dr \psi_{1\sigma}^\dagger (r) \psi_{1\sigma} (r).
\]

By using the functional integral method [19, 26, 27, 28, 29, 30] and taking into account the spin dependence of \( t_\sigma \) explicitly, the ground partition function for the system can be written as follows
\[
Z = \int \mathcal{D}\bar{\psi}_1 \mathcal{D}\psi_1 \mathcal{D}\bar{\psi}_2 \mathcal{D}\psi_2 \exp \left[ -\frac{1}{\hbar} \int_0^{\hbar \beta} d\tau \mathcal{L}(\tau) \right],
\]
where $\beta = 1/k_B T$, $\psi(\bar{\psi})$ is the Grassmann field which corresponds to the fermionic field operator $[\psi(\psi^\dagger)]$ in Eq. (2), and the Lagrangian $\mathcal{L}$ is given by

$$\mathcal{L}(\tau) = \sum_\sigma \sum_{i=1,2} \int dr \bar{\psi}_{i\sigma} (r, \tau) \partial_\tau \psi_{i\sigma} (r, \tau) + \mathcal{H}(\tau).$$

In order to remove the $\psi^4$ term in the Hamiltonian $\mathcal{H}(\tau)$, we will use the Hubbard-Stratonovich transformation,

$$\exp \left[ -\frac{1}{\hbar} \int_0^{\hbar} d\tau \int dr \int dr' \bar{\psi}_1 (r', \tau) \bar{\psi}_1 (r, \tau) g (r-r') \psi_1 (r, \tau) \psi_1 (r', \tau) \right]$$

$$= \int D\Delta (r, r'; \tau) \int D\Delta (r, r'; \tau) \exp \left[ -\frac{1}{\hbar} \int_0^{\hbar} d\tau \int dr \int dr' \left\{ -\frac{|\Delta (r, r'; \tau)|^2}{g (r-r')} + \Delta (r, r'; \tau) \psi_1 (r, \tau) \psi_1 (r', \tau) + \bar{\psi}_1 (r, \tau) \bar{\psi}_1 (r', \tau) \Delta (r, r'; \tau) \right\} \right].$$

This introduces a complex pair potential field

$$\Delta (r, r'; \tau) = |\Delta (r, r'; \tau)| \exp \left[ i \phi (r, r'; \tau) \right].$$

The resulting action is only quadratic in the Grassmann field, so that the functional integral over this number can readily be performed explicitly. The functional integral over the modulus of the pair potential field is taken by the saddle-point method. Then the partition function is reduced to a single functional integral over the phase difference $\phi = \phi_1 - \phi_2$. To second order in the tunneling matrix element, one finds

$$Z = \int D\phi (\tau) \exp \left[ -\frac{\mathcal{S}_{\text{eff}} [\phi]}{\hbar} \right],$$

where the effective action is given by

$$\mathcal{S}_{\text{eff}} [\phi] = \int_0^{\hbar} d\tau \left[ \frac{C}{2} \left( \frac{\hbar}{2e} \frac{\partial \phi (\tau)}{\partial \tau} \right)^2 - \frac{\hbar}{2e} I_C \cos \phi (\tau) \right].$$

In the calculation we have ignored the irrelevant quasiparticle tunneling term for simplicity. Here

$$I_C = -\frac{2e}{\hbar} \int_0^{\hbar} d\tau \beta (\tau)$$

is the Josephson critical current, and then the Josephson current is given by

$$I_J (\phi) = I_C \sin \phi,$$

where the negative (positive) $I_C$ corresponds to the $\pi$ ($0$) junction. The Josephson kernel $\beta (\tau)$ is given in terms of the off-diagonal Nambu Green’s function for two superconductor $F_i$ ($i = 1, 2$), i.e.,

$$\beta (\tau) = -\frac{2}{\hbar} \sum_{k,k'} t_i^* (k, k') t_i (k, k') F_1 (k, \tau) F_2^\dagger (k', -\tau).$$
The Nambu Green functions is given by
\[
\mathcal{F}_i(k, \omega_n) = \frac{\hbar \Delta_i(k)}{(\hbar \omega_n)^2 + \xi_k^2 + \Delta_i(k)^2},
\] (17)
where \(\xi_k = \hbar^2 k^2 / 2m - \mu\) is the single particle energy relative to the Fermi energy and \(\hbar \omega_n = (2n + 1)\pi / \beta\) is the fermionic Matsubara frequency (\(n\) is an integer). In the case of the cuprate high-\(T_c\) superconductors (the \(d_{x^2-y^2}\) symmetry) \[31\], the order parameter is given by
\[
\Delta_i(k) = \Delta_0 \cos 2\theta.
\] (18)

Below we will calculate the Josephson critical current \(I_C\) analytically and discuss the possibility of the atomic scale 0-\(\pi\) transition.

4. Josephson critical current

The Josephson critical current \(I_C\) for a \(c\)-axis \(d\)-wave junction through the ferromagnetic insulator [Fig. 1(b)] can be expressed as
\[
I_C = \frac{2e^2}{\hbar \beta} \sum_{k, k', \omega_n} t_+^*(k, k') t_+^*(k, k') \mathcal{F}(k, \omega_n) \mathcal{F}(k', \omega_n)
\] (19)
by assuming \(\Delta_1 = \Delta_2 = \Delta_0 \cos 2\theta\) and thus \(\mathcal{F}_1 = \mathcal{F}_2 = \mathcal{F}\). We also assume that the tunneling matrix element \(t_\sigma(k, k')\) is given in terms of the coherent tunneling in which the momentum \(k_\parallel\) parallel to the layer is conserved \[26, 29\] and has the same \(L_F\) dependence on the transmission coefficient \(T_\sigma\) as Eq. (1) \[9\], i.e.,
\[
t_+^*(k, k') t_+^*(k, k') = |t_0|^2 (-1)^{L_F} \delta_{k_\parallel k'_\parallel},
\] (20)
we obtain an analytical expression of \(I_C\) for \(T = 0\) K as
\[
I_C = (-1)^{L_F} \frac{\Delta_0 G_N}{2\pi e},
\] (21)
where
\[
G_N = \frac{4\pi e^2}{\hbar} |t_0|^2 N_0^2,
\] (22)
is the normal conductance with \(N_0\) being the density of states at \(E_F\). The sign of \(I_C\) becomes negative for the odd number of \(L_F\) and positive for the even number of \(L_F\) as was numerically found in \[9, 10, 11, 12, 13, 14\]. Therefore, the spin dependent \(\pi\)-phase shift of the tunneling matrix element \(t_\sigma\) in the FI barrier gives rise to the atomic scale 0-\(\pi\) transition.

Finally would like to show an experimental set-up for observing the \(\pi\)-junction using LBCO. The experimental detection of the \(\pi\)-junction is possible by using a superconducting ring which contains two Josephson junctions as shown in Fig. 2. When both junctions are in 0- (or \(\pi\)-) state at the same time, the critical current of the ring reaches its maximum at zero external magnetic flux. On the other hand, the critical current reaches its minimum at zero magnetic flux when the 0 state is stable in one junction and \(\pi\) is stable in the other \[32\]. Experimentally, the half-periodic shifts in the interference patterns of the HTSC ring can be used as a strong evidence of the \(\pi\)-junction. Such a half flux quantum shifts have been observed in a \(s\)-wave ring made with a S/FM/S \[33\] and a S/quantum dot/S junction. \[34\]
Figure 2. Schematic picture of a superconductor ring with high-$T_c$ superconductor/LBCO/high-$T_c$ superconductor Josephson junctions which can be used in experimental observations of the $\pi$-junction.

Note that in the case of $c$-axis stack high-$T_c$ Josephson junction [35], no zero-energy Andreev bound-states [31] which give a strong Ohmic dissipation [27, 28, 36] are formed. Moreover, the influence of nodal-quasiparticles due to the $d$-wave order-parameter symmetry on the macroscopic quantum dynamics in such junctions is found to be week both theoretically [26, 37, 38, 39] and experimentally [40, 41, 42, 43, 44]. Therefore we can safely apply such high-$T_c$ superconductor/LBCO/high-$T_c$ superconductor $\pi$-junctions to qubits.

5. Summary
To summarize, we have studied the Josephson effect in S/FI/S junction by use of the tunneling Hamiltonian method. We have analytically calculated the Josephson current and showed the possibility of the formation of the atomic scale 0-$\pi$ transition in such systems. This observation is consistent with previous numerically results. We hop that such FI based $\pi$-junctions become an element in the architecture of quantum information devices.

Acknowledgements
This work was supported by CREST-JST, and a Grant-in-Aid for Scientific Research from the Ministry of Education, Science, Sports and Culture of Japan (Grant No. 19710085).

[1] I. Zutic, J. Fabian, and S. D. Sarma, Rev. Mod. Phys. 76, 323 (2004).
[2] J. Fabian, A. Matos-Abiague, C. Ertlera, P Stanoa, and I. Zutic, Acta Phys. Slov. 57, 565 (2007).
[3] A. A. Golubov, M. Y. Kupriyanov, and E. Il’ichev, Rev. Mod. Phys. 76, 411 (2004).
[4] A. I. Buzdin, Rev. Mod. Phys. 77, 935 (2005).
[5] L. N. Bulaevskii, V. V. Kuzii, and A. A. Sobyanin, JETP Lett. 25, 291 (1977).
[6] A. I. Buzdin, L. N. Bulaevskii, and S. V. Panyukov, JETP Lett. 35, 179 (1982).
[7] V. V. Ryazanov, V. A. Obozov, A. Y. Rusov, A. V. Veretennikov, A. A. Golubov, and J. Aarts, Phys. Rev. Lett. 86, 2427 (2001).
[8] T. Kontos, M. Aprili, J. Lesueur, F. Genêt, B. Stephanidis, and R. Boursier, Phys. Rev. Lett. 89, 137007 (2002).
[9] S. Kawabata, Y. Asano, Y. Tanaka, A. A. Golubov, and S. Kashiwaya, Phys. Rev. Lett. 104, 117002 (2010).
[10] S. Kawabata, Y. Tanaka, and Y. Asano, Physica E (2010) in press.
[11] S. Kawabata, Y. Asano, Int. J. Mod. Phys. B 23 (2009) 4329.
[12] S. Kawabata, Y. Asano, Y. Tanaka, S. Kashiwaya, Physica C 469 (2009) 1621.
[13] S. Kawabata, Y. Asano, Y. Tanaka, S. Kashiwaya, Physica E 42 (2010) 1010.
[14] S. Kawabata, Y. Asano, Low Temp. Phys. (2010) in press.
[15] S. Kawabata, S. Kashiwaya, Y. Asano, Y. Tanaka, Physica C 437-438 (2006) 136.
[16] S. Kawabata, S. Kashiwaya, Y. Asano, Y. Tanaka, A. A. Golubov, Phys. Rev. B 74 (2006) 180502(R).
[17] S. Kawabata, S. Kashiwaya, Y. Asano, Y. Tanaka, S. Kashiwaya, Physica C 468 (2009) 1621.
[18] S. Kawabata, Y. Asano, Y. Tanaka, S. Kashiwaya, A. A. Golubov, Physica C 469 (2009) 1621.
[19] G. Schön, A. D. Zaikin, Phys. Reports 198 (1990) 237.
[20] T. Kato, A. A. Golubov, Y. Nakamura, Phys. Rev. B 76 (2007) 172502.
[21] F. Mizuno, H. Masuda, I. Hirabayashi, S. Tanaka, M. Hasegawa, and U. Mizutani, Nature 345, 788 (1990).
[22] H. Masuda, F. Mizuno, I. Hirabayashi, and S. Tanaka, Phys. Rev. B 43, 7881 (1991).
[23] W. Ku, H. Rosner, W. E. Pickett, and R. T. Scalettar, Phys. Rev. Lett. 89, 167204 (2002).
[24] V. Eyert, K. H. Hoc, and P. S. Riseborough, Europhys. Lett. 31, 385 (1995).
[25] W. Prellier, P. Lecoeur and B. Mercey, J. Phys.: Cond. Matter 13, R915 (2001).
[26] S. Kawabata, S. Kashiwaya, Y. Asano, and Y. Tanaka, Phys. Rev. B 70, 132505 (2004).
[27] S. Kawabata, S. Kashiwaya, Y. Asano, and Y. Tanaka, Phys. Rev. B 72, 052506 (2005).
[28] S. Kawabata, A. A. Golubov, Ariando, C. J. M. Verwijs, H. Hilgenkamp, and J. R. Kirtley, Phys. Rev. B 76, 064505 (2007).
[29] T. Yokoyama, S. Kawabata, T. Kato, and Y. Tanaka, Phys. Rev. B 76, 134501 (2007).
[30] S. Kawabata, A. A. Golubov, Ariando, C. J. M. Verwijs, H. Hilgenkamp, and J. R. Kirtley, Phys. Rev. B 76, 064505 (2007).
[31] S. Kashiwaya and Y. Tanaka, Rep. Prog. Phys. 63, 1641 (2000).
[32] M. Sigrist and T. M. Rice, J. Phys. Soc. Jpn. 61, 4283 (1992).
[33] W. Guichard, M. Aprili, O. Bourgeois, T. Kontos, J. Lesueur, and P. Gandit, Phys. Rev. Lett. 90, 167001 (2003).
[34] J. A. van Dam, Y. V. Nazarov, E. P. A. M. Bakkers, S. De Franceschi, and L. P. Kouwenhoven, Nature 442, 667 (2006).
[35] R. Kleiner, F. Steinmeyer, G. Kunkel, and P. Müller, Phys. Rev. Lett. 68, 2394 (1992).
[36] S. Kawabata, S. Kashiwaya, Y. Asano, Y. Tanaka, T. Kato, and A. A. Golubov, Supercond. Sci. Technol. 20, S6 (2007).
[37] Y. V. Fominov, A. A. Golubov, and M. Kupriyanov, JETP Lett. 77, 587 (2003).
[38] M. H. S. Amin and A. Y. Smirnov, Phys. Rev. Lett. 92, 017001 (2004).
[39] T. Umeki, T. Kato, T. Yokoyama, Y. Tanaka, S. Kawabata, and S. Kashiwaya, Physica C 463-465, 157 (2007).
[40] K. Inomata, S. Sato, K. Nakajima, A. Tanaka, Y. Takano, H. B. Wang, M. Nagao, H. Hatano, and S. Kawabata, Phys. Rev. Lett. 95, 107005 (2005).
[41] X. Y. Jin, J. Lisenfeld, Y. Koval, A. Lukashenko, A. V. Ustinov, P. Müller, Phys. Rev. Lett. 96, 177003 (2006).
[42] T. Matsumoto, H. Kashiwaya, H. Shibata, S. Kashiwaya, S. Kawabata, H. Eisaki, Y. Yoshida, and Y. Tanaka, Supercond. Sci. Technol. 20, S10 (2007).
[43] H. Kashiwaya, T. Matsumoto, H. Shibata, S. Kashiwaya, H. Eisaki, Y. Yoshida, S. Kawabata, and Y. Tanaka, J. Phys. Soc. Jpn. 77, 104718 (2008).
[44] H. Kashiwaya, T. Matsumoto, H. Shibata, H. Eisaki, Y. Yoshida, S. Kawabata, and S. Kashiwaya, Appl. Phys. Exp. 3, 043101 (2010).