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Josephson π State in a Ferromagnetic InsulatorShiro Kawabata,¹ Yasuhiro Asano,² Yukio Tanaka,³ Alexander A. Golubov,⁴ and Satoshi Kashiwaya⁵¹Nanotechnology Research Institute (NRI), National Institute of Advanced Industrial Science and Technology (AIST), and JST-CREST, Tsukuba, Ibaraki, 305-8568, Japan²Department of Applied Physics, Hokkaido University, Sapporo, 060-8628, Japan³Department of Applied Physics, Nagoya University, Nagoya, 464-8603, Japan⁴Faculty of Science and Technology and MESA+ Institute of Nanotechnology, University of Twente, 7500 AE, Enschede, The Netherlands⁵Nanoelectronics Research Institute (NeRI), AIST, Tsukuba, Ibaraki, 305-8568, Japan

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We predict anomalous atomic-scale $0-\pi$ transitions in a Josephson junction with a ferromagnetic-insulator (FI) barrier. The ground state of such junction alternates between 0 and π states when thickness of FI is increasing by a single atomic layer. We find that the mechanism of the $0-\pi$ transition can be attributed to thickness-dependent phase shifts between the wave numbers of electrons and holes in FI. Based on these results, we show that a stable π state can be realized in junctions based on high- T_c superconductors with a $\text{La}_2\text{BaCuO}_5$ barrier.

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The developing field of superconducting spintronics comprises a plenty of fascinating phenomena that may complement nonsuperconducting spintronics devices [1]. Mesoscopic hybrid structures consisting of superconducting and magnetic materials have attracted considerable attention as devices with novel functionalities [2]. One of most interesting effects is the formation of π states in superconductor/ferromagnetic-metal/superconductor (S/FM/S) Josephson junctions [3]. Under appropriate conditions a ferromagnet can become a π phase shifter, providing the phase difference $\phi = \pi$ between two superconductors in the ground state in contrast to $\phi = 0$ in ordinary Josephson junctions. Recently a quiet qubit based on S/FM/S π junction [4] has been suggested as a promising device to realize quantum computation because the spontaneously generated two-level system in this structure is robust against decoherence due to external fluctuations. However, low energy quasiparticle excitations in a FM provide strong dissipation [5]. Therefore Josephson π junctions with a nonmetallic interlayers are highly desired for qubit applications [6]. Moreover, from the fundamental viewpoint, the Josephson transport through a *ferromagnetic insulator* (FI) has been studied based on phenomenological models [7] and not yet been explored explicitly.

In this Letter, we study theoretically the Josephson effect in superconductor/ferromagnetic-insulator/superconductor (S/FI/S) junctions using the tight-binding model. We show that the ground state in such structures alternates between the 0 and π states when the thickness of a FI (L_F) is increasing by a single atomic layer. This remarkable effect originates from the characteristic band structure of a FI. Quasiparticles in the electron and hole branches acquire different phase shifts while propagating across a FI. We will show that the phase difference is exactly πL_F due to the band structure of a FI, thus providing the atomic-scale

$0-\pi$ transition. This mechanism is in striking contrast to the proximity induced $0-\pi$ transition in conventional S/FM/S junctions. On the basis of the obtained results, we predict a stable π state in a Josephson junction based on high- T_c superconductors with a $\text{La}_2\text{BaCuO}_5$ barrier, where electric current flows along the c axis of cuprates.

Let us first consider an S/FI/S junction in the two-dimensional tight-binding model as shown in Fig. 1(a). The vector $\mathbf{r} = j\mathbf{x} + m\mathbf{y}$ points to a lattice site, where

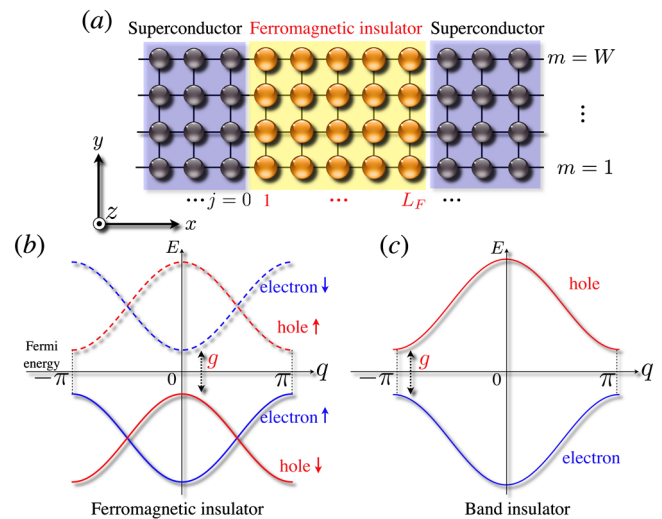


FIG. 1 (color online). (a) The Josephson junction with a ferromagnetic-insulator (FI) barrier on the tight-binding lattice. The magnetic moment in FI is chosen along the z axis in spin space. The band structure of a FI (b) and of standard band insulator (c) in the Bogoliubov–de Gennes picture. The dispersion for a hole with spin σ is obtained as a mirror image of the dispersion for an electron with spin σ with respect to Fermi energy.

x and y are unit vectors in the x and y directions, respectively. The thickness of a FI layer is L_F . In the y direction, we apply the hard wall boundary condition for the number of lattice sites being W . Electronic states in a superconductor are described by the mean-field Hamiltonian, $\mathcal{H} = (1/2)\sum_{r,r' \in S} (\tilde{c}_r^\dagger \hat{h}_{r,r'} \tilde{c}_{r'} - \tilde{c}_r \hat{h}_{r,r'}^* \tilde{c}_r^\dagger) + (1/2)\sum_{r \in S} (\tilde{c}_r^\dagger \hat{\Delta} \tilde{c}_r^\dagger - \tilde{c}_r \hat{\Delta}^* \tilde{c}_r)$ with $\tilde{c}_r = (c_{r,\uparrow}, c_{r,\downarrow})$, where $c_{r,\sigma}^\dagger$ ($c_{r,\sigma}$) is the creation (annihilation) operator of an electron at r with spin σ ($=\uparrow$ or \downarrow), \tilde{c} means the transpose of \tilde{c} , and $\hat{\sigma}_0$ is 2×2 unit matrix. We introduce the hopping integral t among nearest neighbor sites and measure the length in the units of the lattice constant a . In superconductors, the Hamiltonian leads $\hat{h}_{r,r'} = [-t\delta_{|r-r'|,1} + (-\mu_s + 4t)\delta_{r,r'}]\hat{\sigma}_0$, the chemical potential μ_s is measured from the band bottom, and $\hat{\Delta} = i\Delta\hat{\sigma}_2$, where Δ is the amplitude of the pair potential in the s -wave symmetry and $\hat{\sigma}_j$ for $j = 1-3$ are Pauli matrices. We describe a FI by $\hat{h}_{r,r'} = -t\delta_{|r-r'|,1}\hat{\sigma}_0 - (g/2 + 4t)\delta_{r,r'}\hat{\sigma}_3$, where g corresponds to a gap of a FI as shown in Fig. 1(b).

The Hamiltonian is diagonalized by the Bogoliubov transformation. The Andreev bound state consists of sub-gap states whose wave functions decay far from the junction interface. In what follows, we focus on the subspace for spin- \uparrow electron and spin- \downarrow hole [the dispersions shown by solid curves in Fig. 1(b)]. In superconductors, the wave function of a bound state is given by

$$\Psi_L(\mathbf{r}) = \Phi_L \left[\begin{pmatrix} u \\ v \end{pmatrix} A e^{-ikj} + \begin{pmatrix} v \\ u \end{pmatrix} B e^{ik^*j} \right] \chi_l(m), \quad (1)$$

$$\Psi_R(\mathbf{r}) = \Phi_R \left[\begin{pmatrix} u \\ v \end{pmatrix} C e^{ikj} + \begin{pmatrix} v \\ u \end{pmatrix} D e^{-ik^*j} \right] \chi_l(m), \quad (2)$$

where $\nu = L$ (R) indicates a superconductor in the left-(right-)hand side, ϕ_ν is the phase of a superconductor, $\Phi_\nu = \text{diag}(e^{i\phi_\nu/2}, e^{-i\phi_\nu/2})$, $u(\nu) = [(1 + (-) \times \sqrt{E^2 - \Delta^2}/E)/2]^{1/2}$, and A , B , C , and D are amplitudes of the wave function for an outgoing quasiparticle. The wave function in the y direction is $\chi_l(m) = \sqrt{2/W} \sin[lm\pi/(W+1)]$, where l indicates a transport channel. The energy E is measured from the Fermi energy and $k = \cos^{-1}[2 - \mu_s/2t - \cos\{l\pi/(W+1)\} + i\sqrt{\Delta^2 - E^2}/E]$ is the complex wave number. These wave functions decay as $e^{-(j-L_F)/\xi_0}$ for $j > L_F$ and e^{j/ξ_0} for $j < 0$ with ξ_0 being the coherence length. In a FI, the wave function is given by

$$\Psi_{\text{FI}}(\mathbf{r}) = \left[\begin{pmatrix} f_L e^{-iq_e j} \\ g_L e^{-iq_h j} \end{pmatrix} + \begin{pmatrix} f_R e^{iq_e j} \\ g_R e^{iq_h j} \end{pmatrix} \right] \chi_l(m), \quad (3)$$

$$q_e = \pi + i\beta_\uparrow, \quad (4)$$

$$q_h = 0 + i\beta_\downarrow, \quad (5)$$

where $\cosh\beta_\uparrow = 1 + E/2t + g/4t + \cos[l\pi/(W+1)] -$

$\cos[W\pi/(W+1)]$, $\cosh\beta_\downarrow = 1 + E/2t + g/4t - \cos[l\pi/(W+1)] - \cos[\pi/(W+1)]$, and f_L, f_R, g_L and g_R are amplitudes of wave function in a FI. The Andreev levels $\varepsilon_{n,l}(\phi = \phi_L - \phi_R)$ [$n = 1, \dots, 4$] can be calculated from boundary conditions $\Psi_L(\lambda, m) = \Psi_{\text{FI}}(\lambda, m)$ and $\Psi_R(L_F + \lambda, m) = \Psi_{\text{FI}}(L_F + \lambda, m)$ for $\lambda = 0$ and 1 . The Josephson current is related to $\varepsilon_{n,l}$ via $I_J(\phi) = (2e/\hbar)\sum_{n,l} [\partial \varepsilon_{n,l}(\phi)/\partial \phi] f(\varepsilon_{n,l}(\phi))$, where $f(\varepsilon)$ is the Fermi-Dirac distribution function. The Josephson critical current I_C is defined by $I_C = I_J(\pi/2)$.

In Fig. 2(a), we first show the Andreev levels $\varepsilon_{n,1} \equiv \varepsilon_n$ for odd L_F ($=3$ and 5) and even L_F ($=4$ and 6) with $W = 1$, $\mu_s = 2t$, and $\Delta = 0.01t$. The results show that the ground state for odd L_F is at $\phi = \pi$, whereas that for even L_F is at $\phi = 0$. This atomic-scale $0-\pi$ transition persists even if we increase L_F and W . In Fig. 2(b), we show the Josephson critical current as a function of L_F for $W = 1$. Temperature T is set to be $0.01T_c \ll T_c$, where T_c is the transition temperature of a superconductor. The $\pi(0)$ state is always more stable than the $0(\pi)$ state when the thickness of FI is an odd(even) integer. The reason is as follows. At low temperatures, only the Andreev levels below the Fermi energy, i.e., ε_1 and ε_2 , contribute to I_C [see Fig. 2(a)]. In the odd (even) L_F cases, the π - (0 -) state is stable because of $\partial_\phi \varepsilon_1|_{\phi=\pi/2} > (<)0$, $\partial_\phi \varepsilon_2|_{\phi=\pi/2} < (>)0$, and $|\partial_\phi \varepsilon_2|_{\phi=\pi/2}| > |\partial_\phi \varepsilon_1|_{\phi=\pi/2}|$. The atomic-scale $0-\pi$ transition is insensitive to W and material parameters

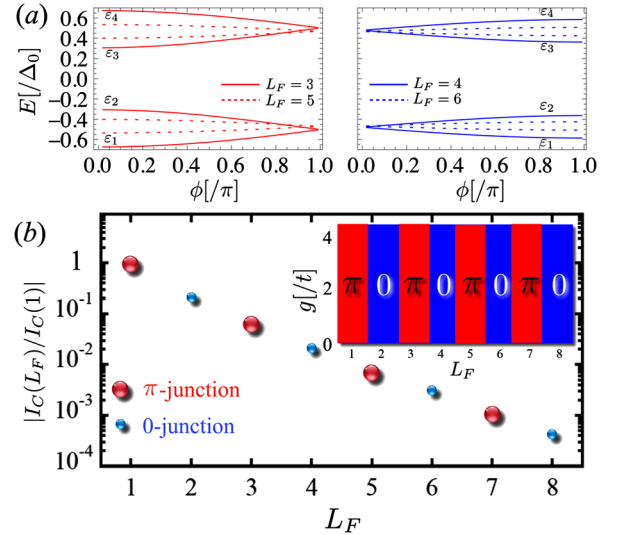


FIG. 2 (color online). (a) The Andreev levels $\varepsilon_i \equiv \varepsilon_{i,1}$ are plotted as functions of ϕ for an one-dimensional S/FI/S junction with $W = 1$. Left (right) panel shows the results for odd L_F (even L_F) with $g = 0.5t$. (b) Josephson critical current I_C at $T = 0.01T_c$ as a function of the thickness L_F for $W = 1$ and $g = 0.5t$. The large red (small blue) circles indicate the $\pi(0)$ junction. In the inset, the $0-\pi$ phase diagram on the $g-L_F$ plane is shown for a two-dimensional S/FI/S junction with $W = 10$ at $T = 0.01T_c$, where the red and blue regimes correspond to the π and 0 states, respectively.

such as μ_s , g , and Δ . As an example, inset of Fig. 2(b) shows the phase diagram on the g - L_F plane for $W = 10$.

The mechanism of the 0 - π transition in a FI is very different from that in a FM. The key feature is expressed by the wave number of a quasiparticle in a FI as shown in Eqs. (4) and (5), where q_e and q_h are the wave numbers for an electron spin- \uparrow and a hole spin- \downarrow , respectively. The real parts of q_e and q_h reflect the wave number at the q points, where energy is closest to the Fermi energy, and differ by π from each other. As shown in Fig. 1(b), the real part of q_e is π because the top of the electron band is located at $q = \pi$. On the other hand, the real part of q_h is 0 because the top of the hole band is at $q = 0$. This is the origin of the difference between q_e and q_h which accounts the atomic-scale 0 - π transition. When we consider a usual band insulator as shown in Fig. 1(c), we always obtain $q_e = q_h$ and their real parts equal π because both the top of the electron band and the bottom of the hole band are located at $q = \pi$. As a consequence, 0 -state is always stable in usual band insulators. Thus we conclude that the characteristic band structure of a FI is the origin of atomic-scale 0 - π transitions. These features basically remain unchanged even when we consider Josephson junctions in higher dimensions. In such junctions, however, the appearance of 0 - π transitions depends on relative directions between the current and the crystalline axis. We will address this issue below. It should be emphasized that peculiar results presented above cannot be described by the standard quasiclassical Green's function method [8] where band structure far from the Fermi energy is ignored.

Let us reconsider atomic-scale 0 - π transitions from a different view point of quasiparticle transmission coefficient. In the high barrier limit ($g \gg t$), the Josephson critical current is perturbatively given by $I_C \propto T_{\downarrow}^* T_{\uparrow}$ [6]. Here $T_{\uparrow(\downarrow)}$ is a transmission coefficient of a FI for an electron with spin- \uparrow (\downarrow). By using the transfer-matrix method [9], T_{σ} for one-dimensional junctions can be obtained analytically $T_{\sigma} \approx \alpha_{L_F} (\rho_{\sigma} t / g)^{L_F}$. Here $\rho_{\uparrow(\downarrow)} = -(+)1$ and α_{L_F} is a spin-independent complex constant. We immediately find $T_{\uparrow}/T_{\downarrow} = (-1)^{L_F}$. Thus the relative phase of T_{σ} between spin- \uparrow and spin- \downarrow is π (0) for the odd (even) number of L_F . As a consequence, the sign of $I_C \propto (-1)^{L_F}$ becomes negative for odd L_F and positive for even L_F . In other words, a FI acts as a π phase shifter for the spin- \uparrow electron for odd L_F .

The transfer-matrix method in real space also enables us to extend the calculations to another magnetic materials. Up to now, we have considered uniform magnetic moment in FI, which can be schematically expressed by $S/\uparrow_1\uparrow_2 \cdots \uparrow_{L_F}/S$ or $S/\downarrow_1\downarrow_2 \cdots \downarrow_{L_F}/S$. The arrows \uparrow_j and \downarrow_j indicate the z -axis magnetization at j . We can extend the above simple analysis to the arbitrary magnetization configuration, e.g., a random alignment described by $S/\downarrow_1\uparrow_2\downarrow_3 \cdots \uparrow_{L_F-2}\uparrow_{L_F-1}\downarrow_{L_F}/S$. In such junctions, we find $I_C \sim \prod_{i=1, L_F} T_{i, \downarrow}^* T_{i, \uparrow} = \prod_{i=1, L_F} (-1) = (-1)^{L_F}$, where $T_{i, \sigma}$ is

the transmission coefficient of an FI layer at i . Therefore we obtain a noticeable result, i.e., the sign of I_C is independent of magnetization configurations and is negative (positive) for odd (even) L_F . The appearance of the atomic-scale 0 - π transition has been also predicted in S/antiferromagnetic-interlayer/S junctions [10]. In their theory, however, the antiferromagnetic configuration is found to be essential for the atomic-scale transition. On the other hand, we conclude that the magnetization symmetry is not necessary and that the π -phase difference between T_{\uparrow} and T_{\downarrow} is an essential feature for the atomic-scale transition. Therefore, our analysis provides a more general view for the physics of the atomic-scale 0 - π transition.

Finally, we show the possibility of the atomic-scale 0 - π transition in a three-dimensional junction using realistic materials. Here we focus on $\text{La}_2\text{BaCuO}_5$ (LBCO) [11], which is an important representative FI in spintronics. According to a first-principle band calculation [12], the bottom of the minority spin band is at the Γ point whose wave number is $(k_a, k_b, k_c) = (0, 0, 0)$, where k_j for $j = a, b$, and c is the wave number along the j axis (see Fig. 6 in Ref. [12]). The mirror image of the minority spin band with respect to the Fermi energy corresponds to the hole band with minority spin in the Bogoliubov-de Gennes picture. Thus the top of the minority spin hole band is at the Γ point. On the other hand, top of the majority spin band is at the Z point with $(k_a, k_b, k_c) = (0, 0, \pi)$. Thus we can predict that the π state would be possible if one fabricates a Josephson junction along the c axis as shown in Fig. 3(a). Note that it is impossible to realize the π state if current flows in the ab plane. This is because wave numbers in the ab plane at the bottom of the minority spin band and those at the top of the majority spin band are given by the same wave number $(k_a, k_b) = (0, 0)$ [12].

From the perspectives of the S/FI interface matching and the high-temperature device operation, the usage of high- T_c cuprate superconductors (HTSC), e.g., $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ and $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) is desirable. Recent development of the pulsed laser deposition technique enables layer-by-layer epitaxial growth of oxide superlattices [13]. In order to show the possibility of π coupling in such realistic HTSC junctions, we have calculated the c -axis Josephson critical current I_C based on a three-dimensional tight-binding model with L_a and L_b being the numbers of lattice sites in the a and b directions [Fig. 3(a)]. In the calculation we have taken into account the d -wave order-parameter symmetry in HTSC, i.e., $\Delta = \Delta_d(\cos k_x a - \cos k_y a)/2$. The tight-binding parameters t and g have been determined by fitting to the first-principle band structure calculations along the line from the Γ to Z point [12]. Figure 3(c) shows the thickness L_F dependence of I_C at $T = 0.01T_c$ for a LSCO/LBCO/LSCO junction with $g/t = 20$, $\Delta_d/t = 0.6$, and $L_a = L_b = 100$. As expected, the atomic-scale 0 - π transitions can be realized in such oxide-based c -axis stack junctions.

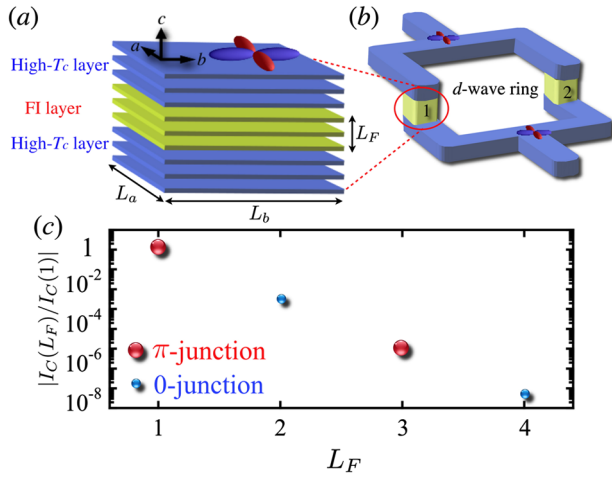


FIG. 3 (color online). (a) Schematic picture of a c -axis stack high- T_c superconductor/FI/high- T_c superconductor Josephson junction and (b) a d -wave ring to detect the π -junction behavior experimentally. (c) The Josephson critical current I_C as a function of the FI thickness L_F at $T = 0.01T_c$ for a c -axis stack LSCO/LBCO/LSCO junction with $g/t = 20$, $\Delta_d/t = 0.6$, and $L_a = L_b = 100$. The large red (small blue) circles indicate the $\pi(0)$ junction.

The experimental detection of the π junction is possible by using a superconducting ring which contains two Josephson junctions as shown in Fig. 3(b). When both junctions are in the 0 (or π) 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 π is stable in the other [14].

From the viewpoint of qubit applications, it is important to note that the harmful influence of midgap Andreev resonant states [15,16] and nodal quasiparticles due to the d -wave symmetry on the macroscopic quantum dynamics in HTSC c -axis junctions [17] is found to be weak, both theoretically [18] and experimentally [19]. Therefore, we conclude that HTSC/LBCO/HTSC π junctions would be promising candidates as basic elements for quiet qubits.

In summary, we have studied the Josephson effect in S/FI/S junctions based on the tight-binding model. We predict the formation of the atomic-scale 0- π transitions in such junctions. This result is insensitive to the material parameters such as the gap g of the FI and the superconducting gap Δ , indicating that it is a robust and universal phenomenon. Our findings suggest the way of realizing *ideal quiet qubits*, which possess both the quietness and the weak quasiparticle-dissipation nature.

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