

Josephson Effect in *d*-Wave Superconductor Junctions in a Lattice Model

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Josephson current between two *d*-wave superconductors is calculated by using a lattice model. Here we consider two types of junctions, i.e., the parallel junction and the mirror-type junction. The maximum Josephson current (J_c) shows a wide variety of temperature (T) dependence depending on the misorientation angles and the types of junctions. When the misorientation angles are not zero, the Josephson current has anomalous temperature dependencies because of a zero energy state (ZES) at the interfaces. In the case of mirror-type junctions, J_c has a non monotonic temperature dependence. These results are consistent with previous results based on the quasiclassical theory [Y. Tanaka and S. Kashiwaya: Phys. Rev. B **56** (1997) 892]. On the other hand, we find that the ZES disappears in several junctions because of the Friedel oscillations of the wave function, which is peculiar to the lattice model. In such junctions, the temperature dependence of J_c is close to the Ambegaokar–Baratoff's relation.

KEYWORDS: zero-energy states, π -junction
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1. Introduction

The Josephson effect is a supercurrent flow between superconductors, where the tunneling effect of Cooper pairs arises the electric current.¹⁾ This effect is quite distinct from other quasiparticle transport phenomena in the sense that the macroscopic phase difference between the two superconductors plays an essential role. So far several expressions of the Josephson current have been derived depending on the transport regimes of a region sandwiched by two superconductors. Ambegaokar and Baratoff first derived a well known expression of the Josephson current in superconductor/insulator/superconductor (SIS) junctions (AB theory).²⁾ Next Kulik and Omelyanchuk presented an expression available for superconductor/orifice/superconductor (SOS) junctions.³⁾ Then Josephson current in superconductor/normal metal/superconductor (SNS) junctions was studied in several papers.^{4–7)} After these works, Furusaki and Tsukada derived a general formula which covers all types of junctions on an equal footing (referred to as FT formula).⁸⁾ The applicability of this work, however, is limited to the conventional *s*-wave superconductor junctions. The FT formula was extended to various directions such as spin-singlet unconventional superconductors⁹⁾ and spin-triplet superconductors.^{10–13)}

The physics of *d*-wave superconductivity has been a hot topic in solid state physics since the discovery of high T_c cuprates. In *d*-wave superconductor junctions, the zero-energy state (ZES)¹⁴⁾ is formed at junction interfaces because of an anomalous interference effect of quasiparticles.^{15–26)} Since the unconventional symmetry of the pair potentials is the essence of the ZES,^{9,27)} the ZES is not expected in conventional *s*-wave superconductors. One of the striking effects of the ZES is the zero-bias conductance peak (ZBCP) in normal-metal/unconventional superconductor junctions.^{9,28)} In hybrid structures consisting of high- T_c

superconductors, a number of experiments observed the ZBCP.^{29–37)} The ZES affects various transport properties through junctions of unconventional superconductors.^{38–43)} The ZES also gives anomalous behaviors of the Josephson current in *d*-wave superconductor junctions.^{44–50)} Tanaka and Kashiwaya developed a general theory of Josephson current (TK theory) in spin-singlet unconventional superconductor junctions.^{44,45)} In the TK theory, following three important points are taken into account: 1) an internal phase of the pair potential which induces π -junction,^{51–54)} 2) the multiple Andreev reflection, and 3) the formation of the ZES.^{44,45)} They have predicted that the current-phase relation in *d*-wave junctions is drastically changed from that in the usual Ambegaokar–Baratoff theory.^{44,45,55–57)} Stimulated by their theory, several related works appear in recent years.^{58,59)} An experiment by Il'ichev *et al.* showed that the current-phase relation of grain boundary YBCO junctions actually exhibit pronounced deviation from a simple sinusoidal current-phase relation.⁶⁰⁾ The experiments accomplished on mirror-type 45° junctions showed a significant amount of $\sin(2\varphi)$ components, which is almost consistent with the TK theory. The anomalous enhancement of the Josephson current in low temperatures and non monotonic temperature dependence of the Josephson current were also predicted by the TK theory. The latter has been also observed in an experiment.⁶¹⁾ Although the TK theory is qualitatively consistent with several experiments, there are still several remaining problems.⁶²⁾ In the TK theory, the quasiclassical approximation^{63–67)} is employed on the derivation of the Josephson current. In high- T_c cuprates, however, the validity of the quasiclassical approximation may be questionable because the coherence length (a few nm) is not much larger than the Fermi wavelength. Thus we must check the validity of the TK theory in a reasonable way. Actually a paper reported that the atomic scale roughness drastically influences the ZES.⁶⁸⁾ In some cases,

the Friedel oscillations of the wave function wash out the zero-energy peak (ZEP) in the local density of states near the interfaces.⁶⁸⁾ So far, however, such effects on the Josephson current have never been studied yet. In order to address these issues, we have developed a theory of Josephson effect where the Bogoliubov–de Gennes equation is solved numerically on a tight-binding lattice.^{49,69–72)} We calculate the current–phase relation and the temperature dependence of the maximum Josephson current, J_c , for various misorientation angles in both the parallel and the mirror-type junctions. We have verified that the main conclusions in the TK theory hold, i.e., the large enhancement of J_c , the anomalous current–phase relation and the non-monotonous temperature dependence of J_c . In addition, we find the absence of the ZES in some junctions. The Fermi wavelength characterizes the oscillations of the wave function. The interference effect of a quasiparticle originating from such rapid oscillations is responsible for the disappearance of the ZES. In these junctions, the current–phase relation and temperature dependence of J_c are explained well by the AB theory. These results may be the guide to fabricate high- T_c junctions with a novel functionality.^{73–77)}

The organization of this theory is as follows. In §2, the model and the formulation are presented. In §3, we show numerical results of the parallel junctions. Corresponding results of the mirror-type junctions are given in §4. In §5, we summarize this paper.

2. Model and Formulation

Let us consider the extended-Hubbard Hamiltonian on two-dimensional tight-binding model,

$$H = - \sum_{\mathbf{r}, \rho, \sigma} t_{\mathbf{r}, \mathbf{r}+\rho} (c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}+\rho, \sigma}) - \mu \sum_{\mathbf{r}, \sigma} c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}, \sigma} - W/2 \sum_{\mathbf{r}, \rho, \sigma, \sigma'} [n_{\mathbf{r}, \sigma} n_{\mathbf{r}+\rho, \sigma'}], \quad (1)$$

where $\mathbf{r} = j\hat{x} + m\hat{y}$ labels a lattice site, $c_{\mathbf{r}, \sigma}^\dagger$ ($c_{\mathbf{r}, \sigma}$) is the creation (annihilation) operator of an electron at \mathbf{r} with spin σ and $n_{\mathbf{r}, \sigma}$ is the number operator. We assume the attractive interaction among the nearest neighbor sites (i.e., $W > 0$). In order to discuss Josephson effect in d -wave superconductivity, we apply the Hartree–Fock–Bogoliubov mean-field approximation. The mean-field Hamiltonian reads,

$$H_{\text{MF}} = - \sum_{\mathbf{r}, \rho, \sigma} \{t_{\mathbf{r}, \mathbf{r}+\rho} - \zeta_{\mathbf{r}, \mathbf{r}+\rho}\} (c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}+\rho, \sigma}) - \tilde{\mu} \sum_{\mathbf{r}, \sigma} c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}, \sigma} + \sum_{\mathbf{r}, \rho} [\Delta_{\mathbf{r}, \mathbf{r}+\rho} c_{\mathbf{r}, \uparrow}^\dagger c_{\mathbf{r}+\rho, \downarrow}^\dagger + \text{h.c.}] + E_0, \quad (2)$$

$$E_0 = W/2 \sum_{\mathbf{r}, \rho, \sigma, \sigma'} \langle n_{\mathbf{r}, \sigma} \rangle \langle n_{\mathbf{r}+\rho, \sigma'} \rangle - W/2 \sum_{\mathbf{r}, \rho, \sigma} \langle c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}+\rho, \sigma} \rangle \langle c_{\mathbf{r}+\rho, \sigma}^\dagger c_{\mathbf{r}, \sigma} \rangle + W \sum_{\mathbf{r}, \rho} \langle c_{\mathbf{r}, \uparrow}^\dagger c_{\mathbf{r}+\rho, \downarrow}^\dagger \rangle \langle c_{\mathbf{r}+\rho, \downarrow} c_{\mathbf{r}, \uparrow} \rangle, \quad (3)$$

$$\tilde{\mu} = \mu + W \sum_{\rho, \sigma} \langle n_{\rho, \sigma} \rangle, \quad (4)$$

$$\zeta_{\mathbf{r}, \mathbf{r}+\rho} = W \langle c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}+\rho, \sigma} \rangle, \quad (5)$$

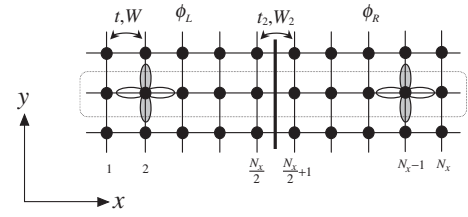


Fig. 1. A schematic figure of the (100) parallel junction. The pair potential is illustrated on the square lattice which represents the CuO_2 plane. The thick solid line is the insulating barrier. The lattice sites surrounded by the dotted line correspond to the unit cell.

In this paper, we take units of $\hbar = k_B = 1$, where k_B is the Boltzmann constant. The vectors ρ represents four vectors connecting nearest neighbor sites. The hopping integral between the nearest neighbor sites is denoted by $t_{\mathbf{r}, \mathbf{r}+\rho}$. We define the pair potential

$$\Delta_{\mathbf{r}, \mathbf{r}+\rho} = -W \langle c_{\mathbf{r}+\rho, \downarrow} c_{\mathbf{r}, \uparrow} \rangle. \quad (6)$$

In the following, we explain the method to calculate the Josephson current in a situation where the a axes of two superconductors are perpendicular to the interface. Such junctions are referred to as the (100) parallel junction in §2. The number of the lattice sites in the x direction is N_x as shown in Fig. 1. The periodic boundary condition is assumed in the y direction. The number of the lattice sites in the y direction is $N_y N_c$, where N_y is the number the lattice sites included in a unit cell and N_c is the number of the unit cells in the y direction. In the case of the (100) parallel junctions, $N_y = 1$. The lattice sites included in the unit cell are surrounded by the dotted line in Fig. 1. The hopping integral in superconductors is taken to be a constant t and that at the potential barrier is $t_2 e^{i\varphi/2}$, where $\varphi = \varphi_L - \varphi_R$ is the phase difference between the two superconductors. We apply the Fourier transformation in the y direction,

$$c_{j\hat{x}+m\hat{y}, \sigma} = \frac{1}{\sqrt{N_c}} \sum_k c_{j, \sigma}(k) e^{ikm}. \quad (7)$$

The Hamiltonian in eq. (2) results in

$$H_{\text{MF}} = \sum_k \sum_{j, j'=1}^{N_x} \begin{bmatrix} c_{j, \uparrow}^\dagger(k) & c_{j, \downarrow}(-k) \end{bmatrix} \times \begin{bmatrix} h_0(j, j') & h_d(j, j') \\ h_d^*(j, j') & -h_0^*(j, j') \end{bmatrix} \begin{bmatrix} c_{j, \uparrow}(k) \\ c_{j, \downarrow}(-k) \end{bmatrix} + E_0, \quad (8)$$

$$h_0(j, j') = -(t + \zeta_1 + \zeta_2) f(j, j') - \tilde{\mu} \delta_{j, j'} - (t + \zeta_1 - \zeta_2) 2 \cos k - t_2 e^{i\varphi/2} \delta_{j, \frac{N_x}{2}+1} \delta_{j, \frac{N_x}{2}} - t_2 e^{-i\varphi/2} \delta_{j, \frac{N_x}{2}} \delta_{j, \frac{N_x}{2}+1}, \quad (9)$$

$$h_d(j, j') = \Delta f(j, j') - \Delta \delta_{j, j'} 2 \cos k, \quad (10)$$

$$f(j, j') = \delta_{j, j'+1} \left(1 - \delta_{j, \frac{N_x}{2}}\right) \left(1 - \delta_{j', N_x}\right) + \delta_{j, j'-1} \left(1 - \delta_{j, \frac{N_x}{2}-1}\right) \left(1 - \delta_{j', 1}\right), \quad (11)$$

We diagonalize the Hamiltonian in eq. (2) by solving numerically the Bogoliubov–de Gennes (BdG) equation

$$\sum_{j'=1}^{N_x} \begin{bmatrix} h_0(j, j') & h_d(j, j') \\ h_d^*(j, j') & -h_0^*(j, j') \end{bmatrix} \begin{bmatrix} u_{k,\lambda}(j') \\ v_{k,\lambda}(j') \end{bmatrix} = E_{k,\lambda} \begin{bmatrix} u_{k,\lambda}(j) \\ v_{k,\lambda}(j) \end{bmatrix}. \quad (12)$$

Throughout this paper, we assume the *d*-wave symmetry in the pair potential and neglect the spatial dependence of the pair potential. Thus

$$\Delta_{r,r+\rho} = \begin{cases} \Delta & : \rho = \pm \hat{x} \\ -\Delta & : \rho = \pm \hat{y} \end{cases}, \quad (13)$$

where the amplitude of Δ is determined by the gap equation for the bulk superconductor in the *d*-wave symmetry⁷⁸⁾

$$1 = \frac{W}{4} \frac{1}{N} \sum_q \frac{\gamma_q^2}{E_q} \tanh \frac{E_q}{2T}, \quad (14)$$

$$\epsilon_q = -(t + \zeta_1)\eta_q - \zeta_2\gamma_q - (\mu + 8Wn), \quad (15)$$

$$E_q = \sqrt{\epsilon_q^2 + \Delta^2\gamma_q^2}, \quad (16)$$

$$\gamma_q = 2(\cos q_x - \cos q_y), \quad (17)$$

$$\eta_q = 2(\cos q_x + \cos q_y). \quad (18)$$

In the same way, ζ_1 , ζ_2 and n are determined by the self-consistent equations,

$$\zeta_1 = -\frac{W}{8} \frac{1}{N} \sum_q \eta_q \frac{\epsilon_q}{E_q} \tanh \frac{E_q}{2T}, \quad (19)$$

$$\zeta_2 = -\frac{W}{8} \frac{1}{N} \sum_q \gamma_q \frac{\epsilon_q}{E_q} \tanh \frac{E_q}{2T}, \quad (20)$$

$$n = \frac{1}{N} \sum_q \left(1 - \frac{\epsilon_q}{E_q} \tanh \frac{E_q}{2T} \right). \quad (21)$$

We determine the magnitude of Δ , ζ_1 , ζ_2 , and μ for $t = W$ in infinite *d*-wave superconductor so that $n = \langle \sum_{\sigma} n_{r,\sigma} \rangle = 0.85$ is satisfied. For instance, the amplitudes of these parameters at the zero temperature are $\Delta = 0.0799t$, $\zeta_1 = -0.197t$, $\zeta_2 = 0.0t$ and $\mu = -0.2833t$. The coherence length of superconductors and the Fermi wavelength are roughly estimated to be 15 and 2 lattice constant, respectively. The Josephson current is calculated by using these parameters.

The local density of states (LDOS) is defined by

$$N_j(E) = \frac{1}{N_c} \sum_{k,\lambda} \{ |u_{k,\lambda}(j)|^2 \delta(E_{k,\lambda} - E) + |v_{k,\lambda}(j)|^2 \delta(E_{k,\lambda} + E) \}. \quad (22)$$

The bulk density of states is also given in this equation with j being far from both the interface and the edge of superconductors. The free energy of the junction is calculated to be

$$F(\varphi) = -T \ln Z, \quad (23)$$

$$Z = \text{Tr} \exp(-H_{\text{MF}}/T). \quad (24)$$

The Josephson current is determined by an equation

$$J(\varphi) = J = 2e \frac{\partial F(\varphi)}{\partial \varphi}. \quad (25)$$

In the numerical simulation, we first calculate the free energy of the junction as a function of φ . Then we

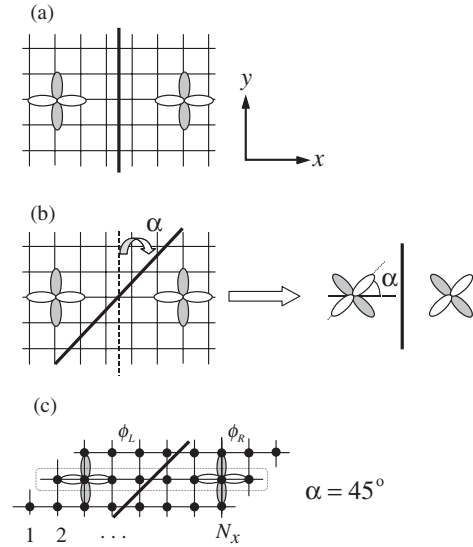


Fig. 2. Schematic figures of the parallel junctions. The pair potential is illustrated on the square lattice which represents the CuO_2 plane. The thick solid line is the insulating barrier introduced on the CuO_2 plane, where α is the orientation angle between the insulating layer and the a axis of high- T_c materials.

decompose the resulting free energy into the Fourier series. Finally, we carry out the derivative with respect to φ in eq. (25) analytically. The application of the method to other parallel junctions and mirror-type junctions is straightforward.

3. Numerical Results in Parallel Junctions

The parallel junctions can be fabricated by introducing an insulating barrier onto the CuO_2 plane as shown in Fig. 2. When the insulating barrier is parallel to the y direction, we obtain the (100) parallel junctions as shown in Fig. 2(a). The angle between the insulating layer and the y direction is the orientation angle α as shown in Fig. 2(b). Effects of the insulating barrier is taken into account through the hopping integral across the barrier, $t_2 = 0.05t$. When we calculate the free energy, the size of the unit cell in the x direction is taken to be $N_x = 100$ for all junctions in this paper. The size of the unit cell in the y direction, N_y , depends on α . In the case of $\alpha = 45^\circ$, for instance, $N_y = 1$ as shown in Fig. 2(c), where the lattice sites surrounded by the dotted line correspond to the unit cell. The number of unit cells in the y direction is fixed at $N_c = 200$ which corresponds to the number of k in the summation of eq. (7). In the following, we show the calculated results in (100), (110), (120) and (130) parallel junctions, where $\alpha = 0^\circ, 45^\circ, 26.5^\circ$ and 18.4° , respectively.

In Fig. 3(a), we illustrate the (100) parallel junction, where $\alpha = 0^\circ$ and the unit cell used in the calculation is indicated by the dotted line. In Fig. 3(b), we show the LDOS at the lattice site A and the bulk density of states. The energy of a quasiparticle measured from the Fermi energy is plotted in the horizontal axis, where Δ_0 is the amplitude of the pair potential at the zero temperature. Since we confirmed in the actual calculation that the density of states are insensitive to φ , hereafter we calculate the density of states at $\varphi = \pi$ and $T = 0$. There is no peak at the zero-energy in the LDOS. The results indicate no ZES at the interface, which are consistent with that of TK theory. In Figs. 3(c) and 3(d), we show the

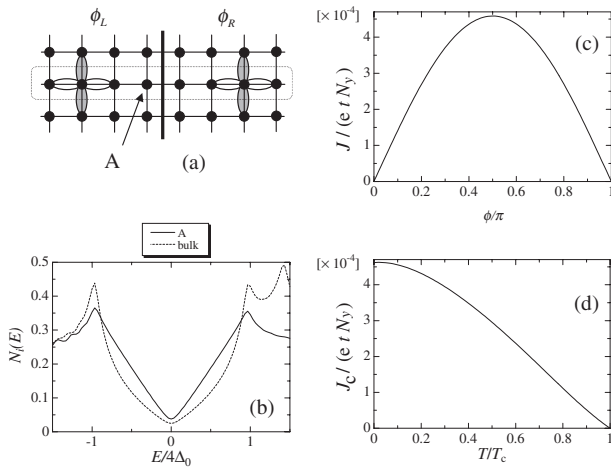


Fig. 3. The (100) parallel junction is illustrated in (a). The local density of states at a lattice site A and the bulk density of states are shown in (b). The current–phase relation at $T = 0$ and the temperature dependence of J_c are shown in (c) and (d), respectively.

current–phase relation at $T = 0$ and the maximum Josephson current as a function of temperatures, respectively. The Josephson current is proportional to $\sin \varphi$ and takes its maximum at $\varphi = 0.5\pi$ as shown in (c). As shown in (d), J_c saturates at low temperatures as that in the AB theory.

In Fig. 4, we illustrate the (110) parallel junction in (a), where $\alpha = 45^\circ$, $N_y = 1$ and the unit cell used in the calculation is indicated by the dotted line. In Fig. 4(b), we show the LDOS at the lattice site A and the bulk density of states. There is a large zero-energy peak (ZEP) in the LDOS at A, whereas there is no ZEP in the bulk density of states. The results indicate the presence of the ZES near the interface, which affects the Josephson current. In Figs. 4(c) and 4(d), we show the current–phase relation for several T and J_c as a function of temperatures, respectively. In low temperatures, the current phase relation of the Josephson current deviates from the sinusoidal function of φ because the resonant tunneling via the ZES enhances the transmission of Cooper pairs, which results in the multiple

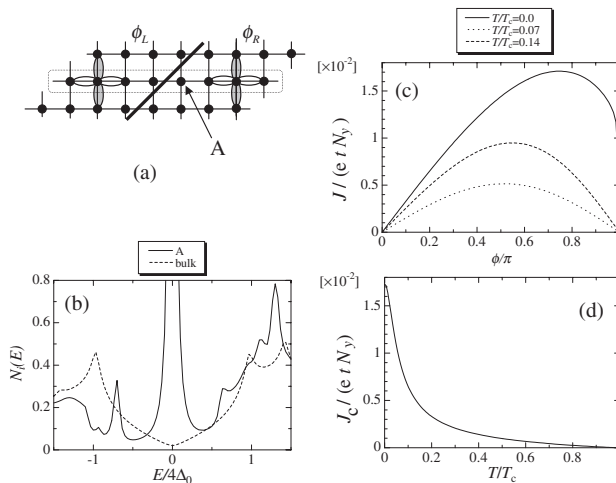


Fig. 4. The (110) parallel junction is illustrated in (a). The local density of states at a lattice site A and the bulk density of states are shown in (b). The current–phase relation and the temperature dependence of J_c are shown in (c) and (d), respectively.

Andreev reflection. The obtained current–phase relation becomes similar to that in SOS junctions.⁴⁾ The Josephson current takes its maximum at $\varphi = 0.75\pi$ at $T = 0$. In Fig. 4(d), J_c increases rapidly with decreasing temperatures, which is called the low-temperature anomaly. The ZES is responsible for the low-temperature anomaly in the Josephson current. These results are consistent with the TK theory.

In Fig. 5, we illustrate the (120) parallel junction in (a), where $\alpha = 26.5^\circ$, $N_y = 2$ and the unit cell used in the calculation is indicated by the dotted line. There are two different lattice sites at the interface. A quasiparticle on site A moves beyond the insulating barrier by hopping into the $-x$ direction. On the other hand, a quasiparticle on site B moves beyond the insulating barrier by hopping into the $-x$ and $+y$ directions as shown in Fig. 5(a). In Fig. 5(b), we show the LDOS at the lattice sites A and B. For comparison, we also show the bulk density of states. According to the TK theory, a peak at the zero-energy is expected in the LDOS at both A and B. However as shown in Fig. 5(b), the resulting LDOS does not have the ZEP, which contradicts to the TK theory. The disappearance of the ZES can be explained in terms of the Friedel oscillations of the wave function. The period in the spatial oscillations of the wave function is characterized by the Fermi wave length. The Fermi surface near the half-filling has almost the square shape and the Fermi wave length corresponds to two lattice constants. Then the wave functions of the ZES at A and B site interfere destructively each other and the resulting LDOS does not have the ZEP. The origin of the absence of the ZEP was also reported in the LDOS at the (120) surface in the extended Hubbard model⁶⁸⁾ and t - J model.^{95,96)} In Figs. 5(c) and 5(d), we show the current–phase relation at $T = 0$ and J_c as a function of temperatures, respectively, where the results are normalized by $N_y = 2$. The Josephson current shows the sinusoidal current–phase relation even at $T = 0$. This is because the resonant transmission of Cooper pairs is suppressed due to the absence of the ZES. In Fig. 5(d), the magnitude of J_c is nearly constant with the decrease of temperatures for $T < 0.15T_c$, which is qualitatively same with those in the AB theory. At the zero temperature, the

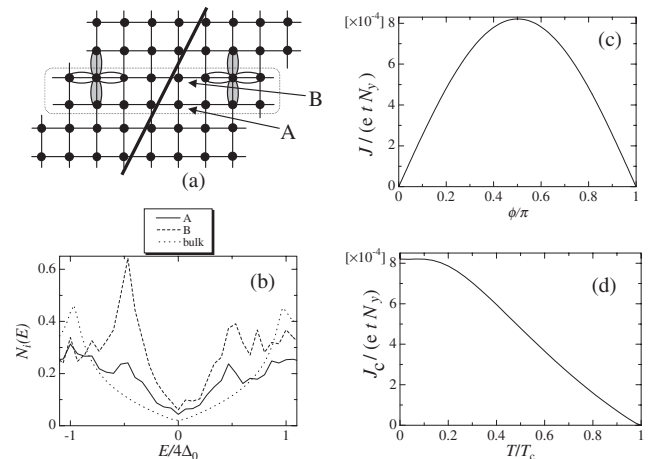


Fig. 5. The (120) parallel junction is illustrated in (a). The local density of states at A and B, and the bulk density of states are shown in (b). The current–phase relation and the temperature dependence of J_c are shown in (c) and (d), respectively.

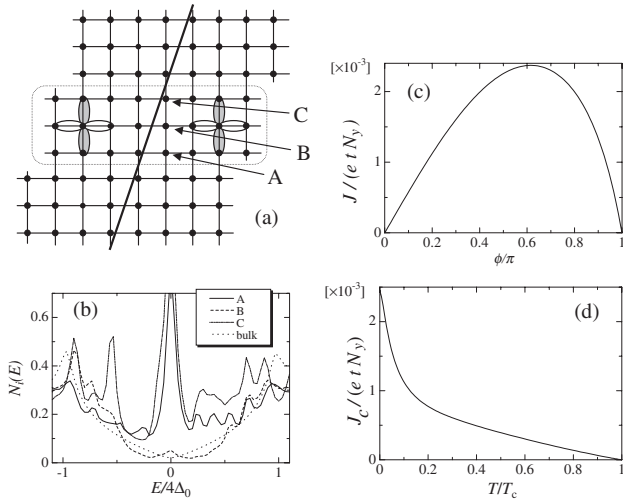


Fig. 6. The (130) parallel junction is illustrated in (a). The local density of states at lattice sites A , B and C are shown in (b). The current–phase relation and the temperature dependence of J_c are shown in (c) and (d), respectively.

magnitude of J_c is as large as 1.8 times as that in the (100) junction. This is because three hopping paths go over the barrier in the unit cell of the (120) junction, whereas the two superconductors are connected by only one hopping path in the unit cell of the (100) junction. In the (120) junction, the ZES disappears because of the interference effect of a quasiparticle. This is a direct consequence of the electronic structures in the lattice model near the half-filling.

In Fig. 6, we illustrate the (130) parallel junction in (a), where $\alpha = 18.4^\circ$, $N_y = 3$ and the unit cell used in the calculation is indicated by the dotted line. There are three different lattice sites at the interface as indicated by A , B and C . In Fig. 6(b), we show the bulk density of states and the LDOS at A , B and C , where $\varphi = \pi$ and $T = 0$. The LDOS at A and C show a large peak at the zero-energy, whereas there is no ZEP in the density of states at B . The absence of the ZES at B can be also explained by the Friedel oscillations of the wave function. As shown in the LDOS in the (120) and the (130) junctions, the number of columns in the y direction included in the unit cell, N_y , dominates the presence or the absence of the ZES. When N_y is odd integers, the ZES appears at the interface. In the case of even integers, on the other hand, we find no ZES. In Figs. 6(c) and 6(d), we show the current–phase relation at $T = 0$ and J_c as a function of temperatures, respectively. The current phase relation of the Josephson current deviates from $\sin \varphi$ because of the resonant transmission of Cooper pairs through the ZES's at A and C . The degree of the deviation is rather small when we compare the results in Fig. 6(c) with those in Fig. 4(c). This is because the ZES is absent at B and the degree of the resonance in the (130) junction is weaker than that in the (110) junction. Actually, the Josephson current takes its maximum at $\varphi = 0.61\pi$ in the (130) junction, whereas $\varphi = 0.75\pi$ characterizes the maximum value in the (110) junction. In Fig. 6(d), J_c shows the low-temperature anomaly as well as that in the (110) junctions.

4. Numerical Results in Mirror-Type Junctions

To fabricate the mirror-type junctions, we first cut the two

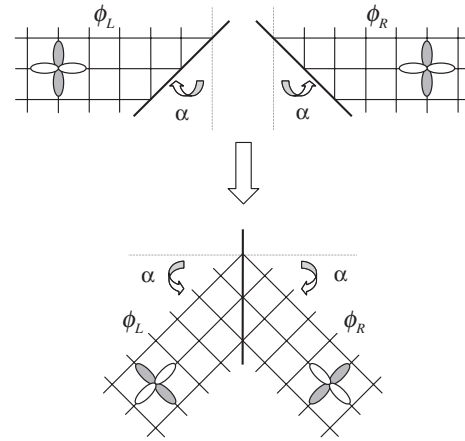


Fig. 7. Schematic figures of the mirror-type junctions.

CuO₂ planes along the line oriented by α from the a axis as shown in Fig. 7, where the thick solid lines indicate the cutting lines. Then we attach one cutting line to the other. The cutting line corresponds to the insulating barrier as shown in Fig. 7(b). In actual experiments, the mirror-type junctions can be fabricated on bicrystal substrates, where the grain boundary formed between the two superconductors behaves as an insulating barrier. In the following, we show the calculated results in the (110), (120) and (130) junctions as well as those in the parallel junctions. We note that the (100) mirror-type junction is essentially the same with the (100) parallel junction.

In Fig. 8, we illustrate the (110) mirror-type junction in (a), where $\alpha = 45^\circ$, $N_y = 1$ and the unit cell used in the calculation is indicated by the dotted line. In Fig. 8(b), we show the LDOS at the lattice site A and the bulk density of states. In addition to the hopping between A and B , (t_2), we also consider the hopping between A and C , ($t_3 = 1/\sqrt{2}t_2$). The LDOS show a large ZEP as show in the solid line. These results are qualitatively the same with those in the (110) parallel junctions. As a comparison, we show the density of states at A in the absence of the hopping between A and C ,

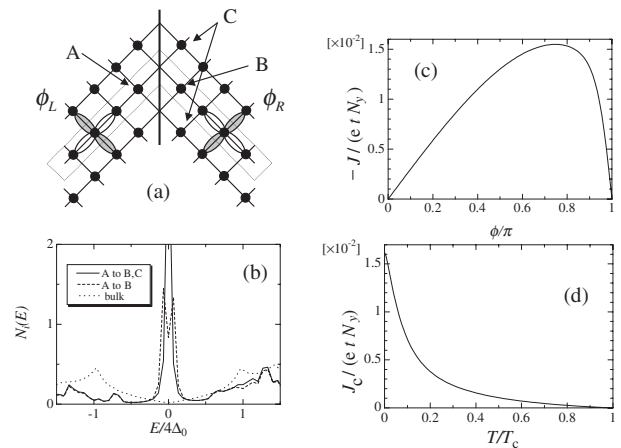


Fig. 8. The (110) mirror-type junction is illustrated in (a). The local density of states at a lattice site A and the bulk density of states are shown in (b). We consider the hopping between A and C (t_3) in the solid line and t_3 is set to be zero in the broken line. The current–phase relation and the temperature dependence of J_c are shown in (c) and (d), respectively.

(i.e., $t_3 = 0$). In this case, the ZEP splits into two peaks as shown with the broken line. This result is consistent with the fact that random potential by impurity near the interface can split the ZBCP.⁸⁸⁾ Since the absence of t_3 is considered to be an imperfection at the interface, the origin of the splitting in Fig. 8(b) can be explained in the same way with that found in the disordered junctions.⁸⁸⁾ In Figs. 8(c) and 8(d), we show the current–phase relation at $T = 0$ and the maximum Josephson current as a function of temperatures, respectively. At $T = 0$, the current phase relation of the Josephson current deviates from $\sin \varphi$ because the resonant tunneling via the ZES enhances the transmission of Cooper pairs. The Josephson current at $T = 0$ takes its maximum value at $\varphi = 0.75\pi$ as well as that in the (110) parallel junction. In Fig. 8(d), J_c shows the low-temperature anomaly because of the ZES. We note that the (110) mirror-type junction is always the π -junction. These results are consistent with the TK theory.

In Fig. 9, we illustrate the (120) mirror-type junction in (a), where $\alpha = 26.5^\circ$, $N_y = 2$ and the unit cell used in the calculation is indicated by the dotted line. There are four different lattice sites near the interface as indicated by A , B , C and D . In addition to the hopping integral between A and C (t_2), we also consider the hopping between B and D , where we assume $t_3 = t_2/2$. In Fig. 9(b), we show the LDOS at A and B . As a reference, we also show the bulk density of states. The results show the absence of the ZEP, which contradicts to the TK theory. The disappearance of the ZES in this case can be also explained in the same way as that found in the (120) parallel junction. Since the Fermi wavelength corresponds to two lattice constants, the wave functions of the ZES at A and B interfere destructively for the formation of ZES with each other. In Figs. 9(c) and 9(d), we show the current–phase relation at $T = 0$ and the maximum Josephson current as a function of temperatures, respectively. The Josephson current shows the sinusoidal current–phase relation even at $T = 0$ because the resonant transmission of Cooper pairs is suppressed in the absence of the ZES. In Fig. 9(d), J_c does not show the low-temperature anomaly. In (120) mirror-type junctions, the ZES also disappears because of the interference effect of a quasipar-

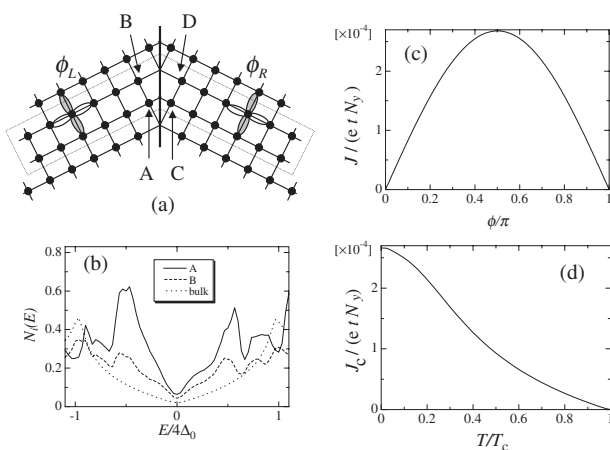


Fig. 9. The (120) mirror-type junction is illustrated in (a). The local density of states at A and B , and the bulk density of states are shown in (b). The current–phase relation and the temperature dependence of J_c are shown in (c) and (d), respectively.

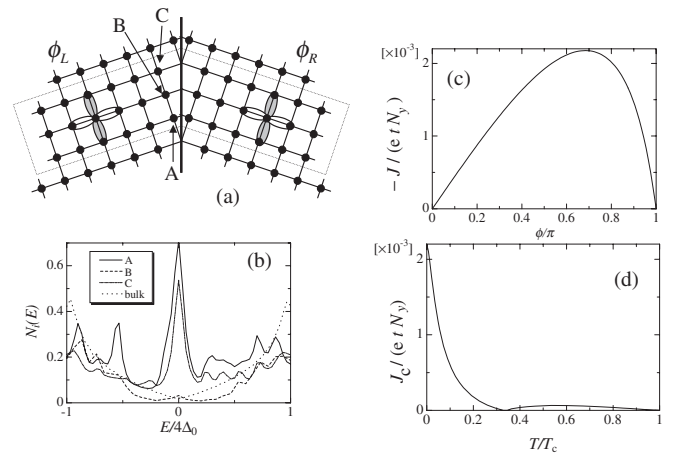


Fig. 10. The (130) mirror-type junction is illustrated in (a). The local density of states at lattice sites A , B and C are shown in (b). The current–phase relation and the temperature dependence of J_c are shown in (c) and (d), respectively.

article, which is one of characteristic features in the lattice model.

In Fig. 10, we illustrate the (130) mirror-type junction in (a), where $\alpha = 18.4^\circ$, $N_y = 3$ and the unit cell used in the calculation is indicated by the dotted line. There are three different lattice sites at the interface as indicated by A , B and C . In addition to the hopping in the $+x$ direction from A (t_2), we consider the hopping from B ($t_3 = t_2/2$) and from C ($t_4 = t_2/3$) across the insulating barrier. In Fig. 10(b), we show the bulk density of states and the LDOS at A , B and C . The LDOS at A and C show a large ZEP, whereas there is no ZEP in the density of states at B . The absence of the ZEP at B is also explained by the Friedel oscillations of the wave functions. In Figs. 10(c) and 10(d), we show the current–phase relation at $T = 0$ and J_c as a function of temperatures, respectively. The Josephson current deviates the sinusoidal function of φ because of the resonant tunneling of Cooper pairs via the ZES. In Fig. 10(d), J_c vanishes at $T = 0.33T_c$. Then J_c rapidly increases with the decrease of temperatures. The minimum point of $F(\varphi)$ is changed from $\varphi = 0$ to $\varphi = \pi$, when temperatures decrease across $0.33T_c$. Thus the junction becomes the 0-junction for $T > 0.33T_c$ and the π -junction for $T < 0.33T_c$. In order to understand this crossover, we focus on the sign of the Josephson current which can be understood by a simple argument within the quasiclassical approximation as follows. Since the transparency of the junction is low, the Josephson current can be approximated to be

$$J = \int_{-k_F}^{k_F} dk_y C(k_x, k_y) \Delta^L(k_x, k_y) \Delta^R(k_x, k_y) \times \Xi^L(k_y) \Xi^R(k_y) \sin \varphi, \quad (26)$$

where $\Delta^L(k_x, k_y)$ and $\Delta^R(k_x, k_y)$ are the pair potential of the left and the right superconductors, respectively. In the above, we can choose positive functions Ξ^L and Ξ^R which describe the temperature dependence of the Josephson current. A function $C(k_x, k_y)$ symbolically represents the transmission probability of the junctions. The wave number in the directions perpendicular and parallel to the junction interface are k_x and k_y , respectively. The integration of k_y can be

separated into two regions: (i) a region where the ZES does not appear at the interface and (ii) a region where the ZES appears. The contribution from the region (i) saturates in low temperatures, whereas that from (ii) rapidly increases with decreasing temperatures because of the existence of ZES. The sign of J for fixed φ is determined by the sign of $\Delta^L(k_x, k_y)\Delta^R(k_x, k_y)$. In the mirror-type junctions, $\Delta^L(k_x, k_y)\Delta^R(k_x, k_y)$ is always positive [negative] for the region (i) [(ii)]. For high temperatures, the contribution from (i) is rather dominant and the magnitude of J takes a positive (negative) value for $0 < \varphi < \pi$ ($-\pi < \varphi < 0$) and has a maximum at $\varphi = \varphi_m = \pi/2$. On the other hand in low temperatures, the contribution from (ii) becomes much larger than that in (i). The resulting J takes a negative (positive) value for $0 < \varphi < \pi$ ($-\pi < \varphi < 0$) and has a maximum at $\varphi = \varphi_m = -\pi/2$. At $T = 0.33T_c$, φ_m jumps from $\pi/2$ to $-\pi/2$ with the decrease of the temperatures. The jump of φ_m is a characteristic feature of unconventional superconductor junctions and most prominently appears in the mirror-type junctions. Details of the microscopic calculation are given in the previous papers by Tanaka and Kashiwaya.^{44,45)}

5. Conclusions

In this paper, the Josephson current in d -wave superconductor/ d -wave superconductor junctions is calculated based on a lattice model. Here we consider two types of junctions, i.e., the parallel junction and the mirror-type junction, with several misorientation angles. In both types of junctions, J_c shows the low-temperature anomaly in the presence of the ZES at the junction interface. In such situation, the current–phase relation deviates significantly from a sinusoidal function of φ . We find the ZES in the (110) and (130) junctions. But no ZES is found in (100) and (120) junctions. The absence of the ZES in the (120) junction contradicts to the theory by Tanaka and Kashiwaya (TK theory). In the TK theory, the quasichlassical approximation is employed to derive the Josephson current formula. The approximation is justified when the coherence length is much larger than the Fermi wave length. The electronic structures in high- T_c superconductors may be described by those in the two-dimensional tight-binding model near the half-filling. The coherence length is considered to be comparable to the Fermi wavelength. Indeed, the wave function of a quasiparticle at the zero-energy interferes destructively near the interface of the (120) junctions, which leads to the absence of the ZES. This interference effect is peculiar to the tight-binding model near the half-filling. Since there is no ZES at the interface, the current–phase relation becomes the sinusoidal function of φ and the temperature dependence of the maximum Josephson current is close to the results in the Ambegaokar–Baratoff theory. However, when the electron density deviates far away from the half-filling, such destructive interference effect does not happen and ZES recovers.⁶⁸⁾ In this case, the Josephson current is expected to be consistent with the TK theory. The characteristic behavior of the Josephson current in two types of junctions is qualitatively different from each other. The extreme case is (130) junctions, where we have found non-monotonic temperature dependence of J_c . This result is consistent with the TK theory. In this study, we have

confirmed that main conclusions of the TK theory: i) the enhancement of J_c at low temperatures and ii) the non monotonous temperature dependence of J_c , are valid even if we consider more realistic electronic structures in high- T_c materials.

There are several remaining problems. In the present study, flat interfaces are assumed for the simplicity. Since random potentials by impurity scatterings near the interface suppress the ZES,^{49,50,79–89)} it may be important to clarify effects of the atomic scale roughness on the Josephson current.

In the present paper, the spatial depletion of the pair potential is not taken into account for simplicity. To our knowledge, this treatment would not seriously modify the conclusion of this paper unless subdominant components of the pair potential do not break the time reversal symmetry.⁹⁾ When subdominant s or d_{xy} component breaks the time reversal symmetry near the interface, the temperature dependence of J_c would be seriously changed by the broken time reversal symmetry state (BTRSS).⁴⁶⁾ Although there are several works about the BTRSS,^{90–104)} it has not been established yet whether such state is really realized at the interface.^{105–110)} However, from the theoretical view point, the extension of the present theory in this direction is a challenging future problem.

In the present paper, we only focus on the dc Josephson effect at the zero bias-voltage across the junctions. It is also interesting to study the quasiparticle current and the ac Josephson effect^{111–113)} in the present approach.

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