Effect of zero-energy bound states on macroscopic quantum tunneling in high-T_c superconductor junctions

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The macroscopic quantum tunneling (MQT) in the current biased high-T_c superconductor Josephson junctions and the effect of the zero-energy bound states (ZES) on the MQT are theoretically investigated. We obtained the analytical formula of the MQT rate and showed that the presence of the ZES at the normal/superconductor interface leads to a strong ohmic quasiparticle dissipation. Therefore the MQT rate is noticeably inhibited compared with the c-axis junctions in which the ZES are completely absent.

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Great attention has been attracted to theoretical and experimental studies of the effect of the dissipation on the macroscopic quantum tunneling (MQT) in superconductor Josephson junctions.[1] In current-biased Josephson junctions, the macroscopic variable is the phase difference ϕ between two superconductors and measurements of the MQT are performed by switching the junction from its metastable zero-voltage state to a nonzero-voltage state [see Fig. 1(c)]. Heretofore, experimental tests of the MQT have been focused on s-wave (low-T_c) junctions.[2,3] This fact is due to the naive preconception that the existence of the low energy nodal-quasiparticle in the d-wave order parameter of a high-T_c cuprate superconductor[4,5] may preclude the possibility of observing the MQT.

Recently we have theoretically investigated the effect of the nodal-quasiparticle on the MQT in the d-wave c-axis junctions[6] (e.g., the Bi2212 intrinsic junction[7] and the cross-whisker junctions[8]). We have shown that the effect of the nodal-quasiparticle gives rise to a superohmic dissipation[9,10] and the suppression of the MQT due to the nodal-quasiparticle is very weak. In fact, recently, Inomata *et al.* have experimentally observed the MQT in the Bi2212 intrinsic junctions.[11] They have reported that the effect of the nodal-quasiparticle on the MQT is negligibly small and the thermal-to-quantum crossover temperature T_{co} is relatively high ($\sim$1 K) compared with the case of s-wave junctions in which T_{co} is at most around 300 mK.

In this paper, we will investigate the MQT in the d-wave junctions parallel to the ab-plane (see Fig. 1), e.g., the YBCO grain boundary junctions [12,13] and the ramp-edge junctions.[14] In such junctions, the zero-energy bound states (ZES)[15–18] are formed near the interface between the superconductor and the insulating barrier. (Note that in the d_0/d_0 junction [Fig. 1(a)] no ZES are formed as will be mentioned later.) The ZES are generated by the combined effect of multiple Andreev reflections and the sign change of the d-wave order parameter symmetry, and are bound states for the quasiparticle at the Fermi energy. Below, we will show that the ZES give rise to the ohmic type strong dissipation so the MQT is considerably suppressed compared with the c-axis and the d_0/d_0 junction cases.

Note that recently Amin and Smirnov have theoretically calculated the decoherence time of a d-wave qubit and discussed the effect of the ZES on the qubit operation.[19] They, however, phenomenologically assumed that the system coupled to an ohmic heat bath. Instead, we will calculate the effective action starting from microscopic Hamiltonian without any phenomenological assumptions. Moreover, by using this effective action we will derive the theoretical formula of the MQT rate and discuss the influence of the ZES on the MQT.

The grandcanonical Hamiltonian of the d-wave junctions [Figs. 1(a) and 1(b)] is given by

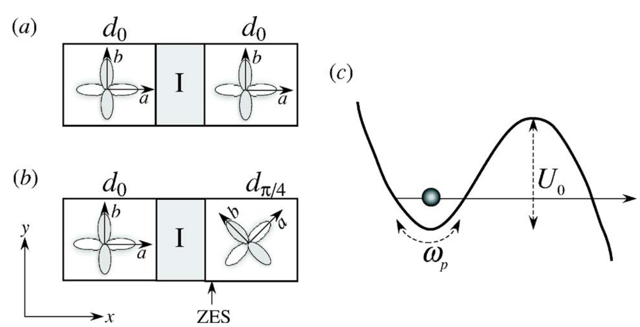

FIG. 1. (Color online) Schematic drawing of the d-wave Josephson junction. (a) d_0/d_0 junction and (b) $d_0/d_{\pi/4}$ junction. In the case of the $d_0/d_{\pi/4}$ junction, the ZES are formed near the boundary between superconductor $d_{\pi/4}$ and insulating barrier I (arrow). (c) Potential $U(\phi)$ vs the phase difference ϕ between two superconductors. U_0 is the barrier height and ω_p is the Josephson plasma frequency.

$$\mathcal{H} = \sum_{\sigma} \int d\boldsymbol{r}\psi^{\dagger}_{\sigma}(\boldsymbol{r})\left[-\frac{\hbar^2\nabla^2}{2m} - \mu + W(\boldsymbol{r})\right]\psi_{\sigma}(\boldsymbol{r}) - \frac{1}{2}\sum_{\sigma,\sigma'} \int d\boldsymbol{r}d\boldsymbol{r}'\,\psi^{\dagger}_{\sigma}(\boldsymbol{r})\psi^{\dagger}_{\sigma'}(\boldsymbol{r}')g(\boldsymbol{r}-\boldsymbol{r}')\psi_{\sigma'}(\boldsymbol{r}')\psi_{\sigma}(\boldsymbol{r}), \tag{1}$$

where μ is the chemical potential. This Hamiltonian describes conduction electrons in a potential $W(\boldsymbol{r})$ which includes a boundary. The second term in $\mathcal{H}$ describes the anisotropic attractive interaction of strength $g(\boldsymbol{r})$. This model also includes the insulating tunnel barrier I where $g(\boldsymbol{r})=0$ by a suitable choice of $W(\boldsymbol{r})$. Below, we will assume that the tunnel barrier is given by a delta function potential, i.e., $W(\boldsymbol{r})=w_0\delta(x)$ and consider the high barrier limit $z_0 \equiv mw_0/\hbar^2k_F \gg 1$ (m is the mass of the electron and k_F is the Fermi wave number) which corresponds to typical experimental situations.

By using the method developed by Ambegaokar *et al.*,[20–22] the partition function of the system can be described by a functional integral over the macroscopic variable (the phase difference ϕ), $\mathcal{Z}=\int\mathcal{D}\phi(\tau)\exp(-\mathcal{S}_{eff}[\phi]/\hbar)$, where the effective action $\mathcal{S}_{eff}$ in the *high barrier limit* is given by

$$\mathcal{S}_{eff}[\phi] = \int_0^{\hbar\beta} d\tau\left[\frac{M}{2}\left(\frac{\partial\phi(\tau)}{\partial\tau}\right)^2 + U(\phi)\right] - \int_0^{\hbar\beta} d\tau\int_0^{\hbar\beta} d\tau'\left[\alpha(\tau-\tau')\cos\frac{\phi(\tau)-\phi(\tau')}{2}\right]. \tag{2}$$

In this equation, $\beta=1/k_BT$, $M=C(\hbar/2e)^2$ is the mass (C is the junction capacitance), and the potential $U(\phi)$ is described by

$$U(\phi) = \frac{\hbar}{2e}\left[\int_0^1 d\lambda\,\phi I_J(\lambda\phi) - \phi I_{ext}\right], \tag{3}$$

where I_J is the Josephson current and I_{ext} is the external bias current, respectively. The dissipation kernel $\alpha(\tau)$ is related to the quasiparticle current I_{qp} under constant bias voltage V by

$$\alpha(\tau) = \frac{\hbar}{e}\int_0^{\infty}\frac{d\omega}{2\pi}D_{\omega}(\tau)I_{qp}\left(V=\frac{\hbar\omega}{e}\right). \tag{4}$$

In this equation, $D_{\omega}(\tau)$ is the Matsubara Green's function of a free boson

$$D_{\omega}(\tau) = \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}\frac{2\hbar\omega}{\nu_n^2+(\hbar\omega)^2}\exp(i\nu_n\tau), \tag{5}$$

where $\nu_n=2n\pi/\hbar\beta$ is the bosonic Matsubara frequency (n is an integer). At the zero temperature, $D_{\omega}(\tau)=e^{-\omega\tau}$.

Below, we will derive the effective action for the two types of the d-wave junction (d_0/d_0 and $d_0/d_{\pi/4}$) in order to investigate the effect of the ZES on the MQT (see Fig. 1). In the case of the d_0/d_0 junction, the node-to-node quasiparticle tunneling can contribute to the dissipative quasiparticle current. However, the ZES are completely absent. These behaviors are qualitatively identical with that for the c-axis Josephson junctions.[6] On the other hand, in the case of the $d_0/d_{\pi/4}$ junction, the ZES are formed around the surface of the right superconductor $d_{\pi/4}$. Therefore the node to the ZES quasiparticle tunneling becomes possible.

First, we will calculate the potential energy U in the effective action (2). As mentioned above, U can be described by the Josephson current through the junction in the high barrier limit ($z_0\gg 1$). In order to obtain the Josephson current, we solve the Bogoliubov-de Gennes equation together with the appropriate boundary conditions.[17] Then we can get the Andreev reflection coefficient for the electron (hole)-like quasiparticle $r_{he}(r_{eh})$. By substituting $r_{he}(r_{eh})$ into the formula of the Josephson current for unconventional superconductors (the Tanaka-Kashiwaya formula),[17,23–25] we can obtain ϕ dependence of the Josephson current. In the case of low temperatures ($\beta^{-1}\ll\Delta_0$) and the high barrier limit ($z_0\gg 1$), we get

$$I_J(\phi) \approx \begin{cases} I_1\sin\phi & \text{for } d_0/d_0 \\ -I_2\sin 2\phi & \text{for } d_0/d_{\pi/4}, \end{cases} \tag{6}$$

where $I_1\equiv 3\pi\Delta_0/10eR_N$, $I_2\equiv\pi^2\hbar\beta\Delta_0^2/35e^3N_cR_N^2$ ($R_N=3\pi\hbar z_0^2/2e^2N_c$ is the normal state resistance of the junction and N_c is the number of channel at the Fermi energy). In calculation, we have assumed that the amplitude of the pair potential is given by $\Delta_0\cos 2\theta\equiv\Delta_{d_0}(\theta)$ for d_0 and $\Delta_0\sin 2\theta\equiv\Delta_{d_{\pi/4}}(\theta)$ for $d_{\pi/4}$. By using Eq. (3), we obtain the analytical expression of the potential U, i.e.,

$$U(\phi) \approx \begin{cases} -\dfrac{\hbar I_1}{2e}\left(\cos\phi + \dfrac{I_{ext}}{I_1}\phi\right) & \text{for } d_0/d_0 \\ -\dfrac{\hbar I_2}{4e}\left(-\cos 2\phi + 2\dfrac{I_{ext}}{I_2}\phi\right) & \text{for } d_0/d_{\pi/4}. \end{cases} \tag{7}$$

As in the case of the s-wave[20,21] and the c-axis junctions,[6] U can be expressed as the tilted washboard potential [see Fig. 1(c)].

Next we will calculate the dissipation kernel $\alpha(\tau)$ in the effective action (2). In the high barrier limit ($z_0\gg 1$), the quasiparticle current is given by[17,18]

$$I_{qp}(V) = \frac{2e}{h}\sum_{p}|t_N|^2\int_{-\infty}^{\infty}dE N_L(E,\theta)N_R(E+eV,\theta) \times [f(E)-f(E+eV)], \tag{8}$$

where $t_N\approx\cos\theta/z_0$ is the transmission coefficient of the barrier I, $N_{L(R)}(E,\theta)$ is the quasiparticle surface density of states ($L=d_0$ and $R=d_0$ or $d_{\pi/4}$), and $f(E)$ is the Fermi-Dirac distribution function. The explicit expression of the surface density of states is obtained by Matsumoto and Shiba.[26] In the case of d_0, there are no ZES. Therefore the angle θ dependence of $N_{d_0}(E,\theta)$ is the same as the bulk and is given by

$$N_{d_0}(E,\theta) = \mathrm{Re}\,\frac{|E|}{\sqrt{E^2-\Delta_{d_0}(\theta)^2}}. \tag{9}$$

On the other hand, $N_{d_{\pi/4}}(E,\theta)$ is given by

$$N_{d_{\pi/4}}(E,\theta)=\mathrm{Re}\,\frac{\sqrt{E^2-\Delta_{d_{\pi/4}}(\theta)^2}}{|E|}+\pi|\Delta_{d_{\pi/4}}(\theta)|\delta(E). \tag{10}$$

The delta function peak at $E=0$ corresponds to the ZES. Because of the bound state at $E=0$, the quasiparticle current for the $d_0/d_{\pi/4}$ junctions is drastically different from that for the d_0/d_0 junctions in which no ZES are formed. By substituting Eqs. (9) and (10) into Eq. (8), we can obtain the analytical expression of the quasiparticle current $I_{qp}(V)$. In the limit of low bias voltages ($eV \ll \Delta_0$) and low temperatures ($\beta^{-1} \ll \Delta_0$), this can be approximated as

$$I_{qp}(V)\approx\begin{cases}\dfrac{3^2\pi^2}{2^8\sqrt{2}}\dfrac{eV^2}{\Delta_0 R_N} & \text{for } d_0/d_0\\[2ex] \dfrac{3\pi^2}{2^4\sqrt{2}}\dfrac{V}{R_N} & \text{for } d_0/d_{\pi/4}.\end{cases} \tag{11}$$

It is apparent from Eq. (11) that, in the case of d_0/d_0 junctions, the dissipation is the superohmic type[1] as in the case of the c-axis junctions.[6] This can be attributed to the effect of the node-to-node quasiparticle tunneling. Thus the quasiparticle dissipation is very weak. On the other hand, in the case of the $d_0/d_{\pi/4}$ junctions, the node-to-ZES quasiparticle tunneling gives the ohmic dissipation which is similar to that in normal junctions.[20,21] Therefore the dissipation for the $d_0/d_{\pi/4}$ junctions is enormously stronger than that for the d_0/d_0 junctions. This is the principal result of this paper.

The reason for the appearance of the ohmic type dissipation for the $d_0/d_{\pi/4}$ junctions can be explained as follows. In the $d_0/d_{\pi/4}$ junctions, the ZES delta function term in $N_{d_{\pi/4}}$ [Eq. (10)] results in $I_{qp}(V) \sim N_{d_0}(V)$, where $N_{d_0}(V)$ is the angle θ integral of $N_{d_0}(V,\theta)$. This can be physically attributed to the effect of the node-to-ZES quasiparticle tunneling. The density of states $N_{d_0}(E)$ is proportional to E for $E \ll \Delta_0$.[17,18] Thus $I_{qp}(V) \sim V$ for $eV \ll \Delta_0$ [Eq. (11)]. Therefore the existence of ZES results in the ohmic dissipation.

From Eq. (4), the explicit and asymptotic form of the dissipation kernel at the zero temperature is given by

$$\alpha(\tau)=\frac{3}{2^4\sqrt{2}\pi}\frac{\Delta_0^2}{e^2R_N}\int_{-1}^{1}dy\frac{1+y}{\sqrt{1-y}}y^2K_1\left(\frac{\Delta_0|\tau y|}{\hbar}\right)^2 \tag{12}$$

$$\approx\frac{3^2}{2^7\sqrt{2}}\frac{\hbar^2R_Q}{\Delta_0R_N}\frac{1}{|\tau|^3}\quad \text{for } \tau\gg\frac{\hbar}{\Delta_0} \tag{13}$$

for the d_0/d_0 junctions and

$$\alpha(\tau)=\frac{3}{2^3\sqrt{2}\pi}\frac{\Delta_0^2R_Q}{\hbar R_N}\int_{-1}^{1}dy(1-y)^{3/2}K_1\left(\frac{\Delta_0|\tau y|}{\hbar}\right) \tag{14}$$

$$\approx\frac{3}{2^4\sqrt{2}}\frac{\hbar R_Q}{R_N}\frac{1}{\tau^2}\quad \text{for } \tau\gg\frac{\hbar}{\Delta_0} \tag{15}$$

for the $d_0/d_{\pi/4}$ junctions, where $R_Q=h/4e^2$ is the resistance quantum. In Eqs. (12) and (14), K_1 is the modified Bessel function.

Let us move to the calculation of the MQT rate Γ for the d-wave Josephson junctions based on the standard Caldeira and Leggett theory.[27,28] At the zero temperature Γ is given by $\Gamma=\lim_{\beta\to\infty}(2/\beta)\ln\mathcal{Z}$.[1] Within the WKB approximation the partition function $\mathcal{Z}$ is evaluated by the saddle-point approximation. Then Γ in the low viscosity limit is obtained by a perturbative treatment as $\Gamma\approx A\exp(-S_B/\hbar)$, where $S_B\equiv\mathcal{S}_{eff}[\phi_B]$ and ϕ_B is the bounce solution. Following the procedures as mentioned above, we finally obtain the central results of this paper, i.e., the analytical formulas of the MQT rate for the d-wave junctions, as[29,30]

$$\frac{\Gamma}{\Gamma_0}\approx\begin{cases}\exp\left[-\left(c_0\dfrac{3^5\pi}{2^7\sqrt{2}}\dfrac{\hbar\eta}{\Delta_0}+\dfrac{18}{5}\dfrac{\delta M}{\hbar}\right)\dfrac{U_0}{M\omega_p}\right] & \text{for } d_0/d_0\\[2ex] \exp\left[-\dfrac{3^4\zeta(3)}{2^5\sqrt{2}\pi^2}\eta(1-x^2)\right] & \text{for } d_0/d_{\pi/4},\end{cases} \tag{16}$$

where $c_0=\int_0^\infty dy\, y^4\ln(1+1/y^2)/\sinh^2(\pi y)\approx 0.0135$, $\zeta(3)\approx 1.20$ is the Riemann zeta function, $\eta=R_Q/R_N$ is the dissipation parameter, $U_0=(\hbar I_{1(2)}/3e)(1-x^2)^{3/2}$ is the barrier height of the potential U, $\omega_p=\sqrt{\hbar I_{1(2)}/2eM}(1-x^2)^{1/4}$ is the Josephson plasma frequency, $x=I_{ext}/I_{1(2)}$, and $\Gamma_0=12\omega_p\sqrt{3U_0/2\pi\hbar\omega_p}\exp(-36U_0/5\hbar\omega_p)$ is the MQT rate without the dissipation. In Eq. (16) δM is the renormalized mass due to the high-frequency components ($\omega \gg \omega_p$) of the quasiparticle dissipation and is given by

$$\delta M=\frac{3}{2^4\sqrt{2}}\frac{\hbar^2\eta}{\Delta_0}\int_{-1}^{1}dy y^2\frac{1+y}{\sqrt{1-y}}\int_0^{\Delta_0/\hbar\omega_p}dz z^2K_1(z|y|)^2. \tag{17}$$

In order to compare the influence of the ZES and the nodal-quasiparticle on the MQT more clearly, we will estimate the MQT rate (16) numerically. For a mesoscopic bicrystal YBCO Josephson junction[31] ($\Delta_0=17.8$ meV, $C=20\times10^{-15}$ F, $R_N=100\ \Omega$, $x=0.95$), the MQT rate is estimated as

$$\frac{\Gamma}{\Gamma_0}\approx\begin{cases}83\% & \text{for } d_0/d_0\\ 25\% & \text{for } d_0/d_{\pi/4}.\end{cases} \tag{18}$$

As expected, the node-to-ZES quasiparticle tunneling in the $d_0/d_{\pi/4}$ junctions gives strong suppression of the MQT rate compared with the d_0/d_0 junction cases.

In conclusion, the MQT in the high-T_c superconductors has been theoretically investigated. The node-to-node quasiparticle tunneling in the d_0/d_0 junctions gives rise to the weak superohmic dissipation as in the case of the c-axis junctions.[6] For the $d_0/d_{\pi/4}$ junctions, on the other hand, we have found that the node-to-ZES quasiparticle tunneling leads to the strong ohmic dissipation. We have also analytically obtained the formulas of the MQT rate which can be used to analyze experiments.

In the context of an application to the d-wave phase qubit,[19,32–34] it is desirable to use the d_0/d_0 or the c-axis Josephson junctions in order to avoid the strong ohmic dissipation. However, the effect of the ZES can be abated by several mechanisms (e.g., by applying a magnetic field or by a disorder in the interface).[17,18] Therefore it is interesting to investigate the MQT of the $d_0/d_{\pi/4}$ junction in such situations.

Finally, we would like to comment about recent experimental research. Bauch *et al.* have succeeded in observing the MQT in a YBCO grain boundary biepitaxial Josephson junction ($T_{co} \sim 40$ mK).[35] In their pioneering experiment, however, the dominant dissipation comes from some *extrinsic* impedances rather than the *intrinsic* nodal quasiparticles or ZES. For example, the *I-V* curve of their junction shows small deviations from the typical SIS junction behavior. The existence of finite residual Josephson current would have a fatal influence on the MQT rate. Therefore the development of the junction fabrication techniques will enable us to directly compare our theory with experimental results.

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[29] In calculation we have approximated the potential $U(\phi)$ as the quadratic plus cubic type potential (Refs. 27 and 28). Therefore the expression (16) is only valid in the case where x is close to unity.

[30] In the case of the $d_0/d_{\pi/4}$ junctions (the ohmic type), the dissipation mainly comes from the low-frequency components of the dissipation kernel. Therefore we have used the low-frequency expression (15) in order to calculate the MQT rate. On the other hand, in the case of the d_0/d_0 junctions (the superohmic type), the dissipation from the high-frequency components can also give a large contribution to the MQT. Therefore we have used the exact expression (12) in order to obtain the MQT rate.

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