Tunneling conductance in normal metal - high $T_C$ cuprate junctions in the presence of magnetic field

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The magnetic field responses of the zero-bias conductance peak (ZBCP) in tunneling spectra of high $T_C$ cuprate junctions are studied theoretically. Our calculation is based on the lattice Green’s function method and takes the realistic electronic structure of the high $T_C$ cuprates into account. In marked contrast to previous works, it is shown that the critical magnetic field strength $H_C$ exists for the splittings of the ZBCP’s to be discernible. $H_C$ is almost proportional to the product of the magnitude of pair potential, transmissivity of the junction, and the inverse of the Fermi velocity parallel to the interface ($1/v_{Fy}$). The calculated $H_C$’s for the hole-doped superconductors are higher than those for electron-doped ones because of relatively large magnitude of pair potential and the small magnitude of $v_{Fy}$ originating from peculiar shape of the Fermi surface.

KEYWORDS: $d$-wave superconductor, Doppler shift, zero-bias conductance peak, Fermi velocity

1. Introduction

Nowadays, almost all of the high-$T_C$ cuprates are classified to be $d$-wave superconductors$^{1-3}$ and several experiments reported the existence of phase coherent phenomena peculiar to the $d$-wave symmetry. One of this is so called the zero bias conductance peak (ZBCP) observed in the tunneling spectroscopy in high $T_C$ cuprate junctions. It was clarified that ZBCP is a direct consequence of $d_{x^2-y^2}$ symmetry of the pair potential.$^{4,14-19}$ The presence of ZBCP is a manifestation of the formation of the Andreev bound state (ABS) at the Fermi energy (zero-energy) near a specularly reflecting surface$^5$ or interface$^{14}$ when the angle between the lobe direction of the $d_{x^2-y^2}$-wave pair potential and the normal to the interface is nonzero. This state originates from the interference effect between the injected and reflected quasiparticles at the surface or interface and the sign change of the $d_{x^2-y^2}$-wave pair potential. There is a large number of studies on ZBCP,$^{4,15-18}$ and its related problems.$^{19-28}$ However, the experimental results of the dependence of ZBCP on an external magnetic field are not converged yet. The splitting of the ZBCP in a magnetic field has been reported in some experiments$^{19,22-24}$ while others can not reproduce it.$^{15-18}$ We can consider whether splitting of ZBCP is observed or not is quite sensitive to the experimental situations and doping concentration of actual high $T_C$ cuprates.

The effect of screening currents which is so called Doppler shift of the energy levels of quasiparticles is considered to be the most promising idea to understand the origin of the peak splitting.$^{19,22,26}$ It was pointed out that in an applied magnetic field $H$, screening currents shift the ABS spectrum$^{29-31}$ and lead to a splitting of ZBCP that is linear in $H$ at low fields.$^{26}$ The previous theory$^{26}$ predicts the splitting of ZBCP in any case and is consistent with some experimental results.$^{19,21}$ However, the absence of ZBCP splitting has not been clarified yet. We must need further study which takes into account the electronic structures peculiar to actual junctions of high $T_C$ cuprates. Recently, four of the authors study about the effect of transmissivity of the junction on the splitting of ZBCP.$^{32}$ It was found there is a critical value of the magnetic field $H_C$ above which ZBCP splits by external magnetic field below which it does not.$^{32}$ The critical field is almost proportional to the width of ZBCP in the absence of magnetic field and equivalently to the transparency of the junctions. However, in this paper, the shape of Fermi surface is assumed to be cylindrical and the reduction of the magnitude of the Fermi velocity parallel to the interface in the actual Fermi surface is not taken into account. Since the degree of the Doppler shift is determined by the Fermi velocity parallel to the interface, it is natural to expect that the shape of Fermi surface influence significantly on the ZBCP splitting. In order to understand the actual line shape of the tunneling conductance, it is indispensable to calculate tunneling conductance taking into account the effect of the shape of Fermi surface.

The aim of this paper is to predict the tunneling conductance of normal metal - high $T_C$ superconductor junctions in the presence of magnetic field taking into account the shape of Fermi surface. In the present paper, based on the Kubo formula,$^{33-37}$ we will clarify that there is a critical value of the magnetic field $H_C$, which crucially determines the peak structure of the tunneling conductance. For $H > H_C$, ZBCP splits into two by the magnetic field.$^{26}$ On the other hand, for $H < H_C$, ZBCP does not split at least explicitly and only the height of ZBCP is reduced. It is revealed that $H_C$ is proportional

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to the product of the width $\Gamma$ of ZBCP for $H = 0$ and the inverse of the magnitude of Fermi velocity in $d$-wave superconductor parallel to the interface ($v_F y$). Since the magnitude of $\Gamma$ is roughly proportional to the product of the transmissivity of the junctions and the magnitude of the pair potential, $H_C$ is enhanced (suppressed) for high (low) transmissive junctions and large (small) magnitude of the pair potential of $d$-wave superconductors. We also clarify the asymmetric behavior of $H_C$ with respect to the carrier type of the high $T_C$ cuprates mainly due to the difference in the shapes of the Fermi surface.

Fig. 1. Schematic illustration of the geometry of the normal metal (N)/ insulator (I)/ $d_{x^2-y^2}$-wave superconductor (D) junction. N and I are stacked along (100) axis of a square lattice while D is stacked along (110) axis. Lattice spacing is $a$ for N and I and $a'(=a/\sqrt{2})$ for D.

2. Formulation

We consider a $N/I/D$ junction on 2-dimensional lattice system, where $N$ and $I$ are stacked along (100) axis of square lattice with lattice spacing $a$ and $I$ is connected to the (110) surface of $D$ (see Fig. 1). In order to describe the $d$-wave superconductor, we use the $t$-$J$ model which is one of the promising models for high $T_C$ cuprates. By using a mean-field approximation based on the Gutzwiller approximation, the model can be mapped into a BCS like mean-field Hamiltonian $^38$ $H + \Delta$ with

$$ H = -t_1 \sum_{(i,j),\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - t_2 \sum_{(i,j)\prime,\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - \mu n, \quad (1) $$

$$ \Delta = \sum_{(i,j),\sigma} (\Delta_{i,j}^\dagger c_{j,-\sigma}^\dagger c_{i,\sigma} + H.c.), \quad (2) $$

where summations over $\cdots$ and $\cdots'$ run nearest-neighbor and next-nearest-neighbor pairs, respectively. The hopping parameters $t_1$ and $t_2$ include so-called Gutzwiller factor and the pair potential $\Delta_{i,j}$ has $d_{x^2-y^2}$ symmetry. In the middle of the superconductor, $\Delta_{i,j}$ is $\Delta_0(\delta)$ for $j = i \pm (1/2, 1/2)$, $-\Delta_0(\delta)$ for $j = i \pm (1/2, -1/2)$, and zero for others, where $\delta$ denotes the doping concentration of hole or electron. Due to the translational invariance along the $y$ direction, the creation and annihilation operator $c_{i,\sigma}^\dagger$ and $c_{i,\sigma}$ can be expressed as $c_{i,\sigma} = \sum_{k_y} c_{i,x,\sigma}(k_y) \exp(-ik_y j_y a)$. Since the coherence length of the high $T_C$ cuprates $\xi$ is much smaller than the penetration depth of the magnetic field $\lambda$, and the effect of the magnetic field on the normal metal is not important, we can choose the spatial dependence of vector potential as $A_y(x) = -H \lambda$, where $H$ is the applied magnetic field.$^26$ The quantity $k_y$ is replaced with $k_y - eH \lambda/h$. In the following, the applied magnetic field is normalized by $H_0 = \phi_0/(\pi^2 \xi_0 \lambda)$ with $\phi_0 = \hbar/(2e)$ and $\xi_0 = \hbar v_F)/(\Delta_0 \pi)$. The order of the magnitude of $H_0$ becomes about 1 Tesla when we choose $\xi_0$ and $\lambda$ as 10Å and 1500Å, respectively, for hole-doped cuprates with $\delta = 0.1$, where $\Delta_0 = 0.12t_0$ and $v_F = 0.16t_0 a'/h$ with the lattice constant $a'$ of cuprates and the unit $t_0$ of energy.

As for the normal region ($N$ and $I$), we use the single-orbital tight-binding model. The Hamiltonian is

$$ H = -t \sum_{l,m,\sigma} \left( c_{l+1,m,\sigma}^\dagger c_{l,m,\sigma} + c_{l,m+1,\sigma}^\dagger c_{l,m,\sigma} + H.c. \right) $$

$$ + \sum_{l,m,\sigma} v_{l,m} c_{l,m,\sigma}^\dagger c_{l,m,\sigma}, \quad (3) $$

where $t$ is the hopp ing integral between nearest neighbor sites and $v_{l,m}$ is the on-site potential at a site $(l,m)$. Since the system considered has the translational invariance in $y$-direction, the conductance $\Gamma_S(eV)$ of the junction is given by Kubo formula$^{33-35}$ using the Green’s function $G(E)$ as

$$ \Gamma_S(E) = \frac{2e^2 v_F^2}{\hbar} \sum_{k_y} \left[ \tilde{G}_{1,l+1}^{k_y} \tilde{G}_{1,l+1}^{k_y} + \tilde{G}_{1,l}^{k_y} \tilde{G}_{1,l+1}^{k_y} \right]_{11}, \quad (4) $$

$$ \tilde{G} = G(E - i0) - G(E + i0), \quad (5) $$

$$ G(z) = \left( \begin{array}{cc} z1 - H & \Delta \\ \Delta^\dagger & z1 + H^* \end{array} \right)^{-1}, \quad (6) $$

where the relation $c_{l,\sigma}(k_y) = \sum_{m} c_{l,m,\sigma} \exp(ik_y m a)$ was used and $\tilde{G}_{1,l}^{k_y}$ is a $2 \times 2$ matrix. First, we calculate the isolated Green’s function of the $d$-wave superconductor and normal metal. Then we obtain the combined Green’s function by solving Dyson’s equation iteratively and finally we obtain the tunneling conductance $\Gamma_S(eV)$. We also calculate the corresponding quantity $\Gamma_N(eV)$, where the $d$-wave superconductor is in the normal state and the pair potential is, then, zero. Hereafter, we will look at the normalized value $\sigma\Gamma_S(eV)/\Gamma_N(eV)$.

In the actual calculation, we choose material parameters in the $d$-wave superconductor determined by applying the Gutzwiller approximations to $t$-$J$ model. For both the normal metal and insulator, we use $t = 10t_0$ and $\mu = 0$. As regards $v_{l,m}$, we choose $v_{l,m} = 20t_0$ for normal metal, while for insulator we choose $v_{l,m} = 35t_0$ for the junction with high transmissivity, and $v_{l,m} = 65t_0$ for junctions with low transmissivity. The corresponding transmissivities $\gamma$ are given by 0.4 and 0.1, respectively. The thickness of the insulator is chosen as one atomic layer.

3. Numerical calculation and results

First, we study the electron over-doped case, i.e., $\delta = 0.2$, (Fig. 2), where $t_1 = 0.415t_0$, $t_2 = 0.133t_0$, $\lambda = 1/2t_0$, $\Delta_0 = 0.12t_0$, and $\phi_0 = 0.16t_0 a'/h$.
where $\mu = 0.0214 t_0$ for the $d$-wave superconductor.\textsuperscript{38}) The ZBCP splits into two as the magnetic field increases (see Fig. 2). The degree of the splitting is crucially influenced by the transmissivity of the junctions. With an increase in transmissivity of the junctions, the critical value of magnetic field $H_C$ above which ZBCP splits into two decreases.

In Fig. 3, corresponding plot for hole over-doped case ($\delta = 0.2$) is shown, where material parameters are chosen as $t_1 = 0.4117 t_0$, $t_2 = -0.1335 t_0$, and $\mu = -0.4601 t_0$.$\textsuperscript{38}$ For hole-doped materials, the degree of ZBCP splitting is weakened, and ZBCP does not split into two by magnetic field except for low transmissivity and high magnetic field junctions. As compared to Fig. 2, the magnitude of $H_C$ is drastically enhanced.

To clarify this point, $\delta$ dependence of $H_C = H_C(\delta)$ is plotted in Fig. 4 both for electron and hole-doped cases with low and high transmissivity of the junctions. The magnitude of $H_C(\delta)$ is a decreasing function with $\delta$ both for electron and hole-doped cases. In the following, we will consider a microscopic origin of $H_C(\delta)$.

In the presence of magnetic field, the energy of the quasiparticle $E$ is substituted with

$$E - e v_{Fy} A_y(x) = E + \frac{H\Delta_0 v_{Fy}}{H_0 v_{F0}}. \quad (7)$$

Since positive $H$ is chosen, quasiparticles energy $E$ increases (decreases) by $H$ for $v_{Fy} > 0$ ($v_{Fy} < 0$). The amplitude of this energy shift is $H\Delta_0 < v_{Fy} >/(H_0 v_{F0})$, where $< | v_{Fy} | >$ denotes the average of the $y$ component of the Fermi velocity on the Fermi surface. By comparing the energy shift and the width $\Gamma$ of ZBCP with $\sigma_T(\gamma) = \frac{1}{2} \sigma_T(0)$ for $H = 0$, we can analytically estimate critical value $H_C$ which we call $H_{th}(\delta)$ to distinguish from $H_C(\delta)$ in Fig. 4. The resulting $H_{th}(\delta)$ is given by

$$H_{th}(\delta) = \frac{C T H_0 v_{F0}}{2\Delta_0 < | v_{Fy} | >}. \quad (8)$$

where $C$ is a constant. To confirm the correspondence between $H_C(\delta)$ and $H_{th}(\delta)$, we plot $H_C(\delta)/H_C$ (0.10; electron-dope) and $H_{th}(\delta)/H_{th}$ (0.10; electron-dope) in Fig. 5 for low and high transmissivity of the junctions with both electron and hole-doped cases.

The coincidence between these two values are fairly well, and we can expect $H_C(\delta) \sim H_{th}(\delta)$. As discussed above, there are two crucial factors which determine the magnitude of $H_C$. First one is the magnitude of $\Gamma$ which is almost proportional to the product of the transmissivity of the junctions and the magnitude of the pair poten-

Fig. 2. Tunnel conductance $\sigma_T(eV)$ of N/ I / D(electron dope, $\delta = 0.2$) junctions with (a) high ($\gamma = 0.4$) and (b) low ($\gamma = 0.1$) transmissivities. Results obtained for $H = 0.0, 0.3, 0.5,$ and $1.0$ in a unit of $H_0$ are plotted by dashed, dotted, chained, and solid lines, respectively.

Fig. 3. Tunnel conductance $\sigma_T(eV)$ of N/ I / D(hole dope, $\delta = 0.2$) junctions with (a) high ($\gamma = 0.4$) and (b) low ($\gamma = 0.1$) transmissivities. Results obtained for $H = 0.0, 0.3, 0.5,$ and $1.0$ in a unit of $H_0$ are plotted by dashed, dotted, chained, and solid lines, respectively.

Fig. 4. $H_C(\delta)/H_0$ calculated for junctions with high ($\gamma = 0.4$) and low ($\gamma = 0.1$) transmissivities as a function of the doping rates $\delta$ of hole (triangles) and electron (circles). Solid and dashed curves are guides for eyes. $H_0$ is about 1T.
in detail where the realistic Fermi surfaces of high $T_C$ cuprates are taken into account. We concentrated on the splitting of the ZBCP due to the magnetic field for (110)-oriented junctions. We can define a critical magnetic field $H_C$, where only for $H > H_C$, ZBCP splitting occurs by magnetic field.$^{26}$ It is revealed that $H_C$ is proportional to the product of the transmissivity of the junction,$^{32}$ the magnitude of pair potential, and the inverse of the averaged Fermi velocity parallel to the interface. In the light of our theory, the absence of the splitting of ZBCP reported in several experiments$^{15-18}$ is due to the larger magnitude of $H_C$ originating from the low doping concentration or high transmissivity of the junctions. Systematic studies of tunneling experiments changing doping concentration in the presence of magnetic field are desired.

In the present paper, the effect of the impurity scattering or surface roughness is not taken into account.$^{11}$ These effects broaden the ZBCP$^{29,42,43}$ and the magnitude of $H_C(\delta)$ is expected to be enhanced. It is actually an interesting problem to clarify the influence of the impurity scattering on $H_C(\delta)$.

In the present paper, spatial dependence of the pair potential is not taken into account. It is revealed that if the symmetry of the pair potential is pure $d$-wave, the low bias property of the tunneling conductance is not influenced by the spatial modulation of the pair potential.$^{4}$ However, in the presence of the broken time reversal symmetry state (BTRSS) near the interface, where the mixing of subdominant $s$- or $d_{xy}$-wave component as the imaginary part of the pair potential to the predominant $d_{2-xy}$-wave component$^{25,39-41,44,45}$ occurs, the ZBCP splits into two even without magnetic field. It is also one of interesting problems to clarify the magnetic field dependence of the conductance in the presence of the BTRSS.$^{46}$

Finally, we must comment about recent experiments by Dagan and Deutscher.$^{23,24}$ They have found that the width of the splitting of ZBCP is thickness independent for films thinner than the penetration depth. This implies that the magnetic field splitting is not primarily a Doppler shift effect due to the Meissner screening currents. We must seek for other possibilities including field induced modification of the pair potential.$^{23,24,47}$

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Fig. 5. Normalized $H_C$ and $H_{th}$ calculated for junctions with high ($\gamma = 0.4$) and low ($\gamma = 0.1$) transmissivities as a function of the doping rates $\delta$ of (a) hole and (b) electron. $H_C(\delta)/H_C(0.1;\text{electron-dope})$ and $H_{th}(\delta)/H_{th}(0.1;\text{electron-dope})$ are plotted by solid and open symbols, respectively. Solid and dashed curves are guides for eyes.

Fig. 6. The magnitude of $v_{Fy}$ and $\Delta_0(\delta)$ as a function of $\delta$.

4. Conclusion

In this paper, influence of the magnetic field on the tunneling conductance in $N/I/D$ junctions is studied
Tunneling conductance in normal metal - high $T_C$ cuprate junctions in the presence of magnetic field

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