Magnetotunneling spectroscopy as a probe for pairing symmetry determination in quasi-2D anisotropic superconductors

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As a probe to determine the pairing symmetry of quasi-two-dimensional anisotropic superconductors, we propose tunneling spectroscopy in the presence of magnetic field, where the magnetic field is parallel to the two-dimensional planes and rotated. As a case study, we apply this idea to the models of high-$T_c$ cuprates and organic superconductors $\kappa$-(ET)$_2$X. The surface density of states at the Fermi energy exhibits a characteristic oscillation upon rotating the direction of the magnetic field due to the Doppler shift of the energy of quasiparticles. The surface density of states has a minimum when the applied magnetic field is parallel to the node direction of the pair potential independent of the detailed shape of the Fermi surface. The amplitude of the oscillation is sensitively affected by the shape of Fermi surface.

Nowadays, there are various superconductors in which the pairing mechanism seems to be unconventional. In order to clarify the pairing mechanism of these superconductors, it is crucial to identify the pairing symmetry, which is characterized by the sign change and the presence of nodes in the pair potential. In order to determine the pairing symmetry, several phase-sensitive probes have been used, among which is the tunneling spectroscopy, which enables us to detect the sign change in the pair potential as well as its nodal structure. Namely, a reliable evidence of the sign change of the pair potential is an observation of a zero-bias conductance peak (ZBCP), which is originated from Andreev bound states (ABS) formed at the surfaces or interfaces\textsuperscript{1,2}. The existence of ZBCP has been actually observed for several unconventional superconductors\textsuperscript{3,4}.

In principle, it is possible to determine the pairing symmetry through the tunneling spectroscopy via ABS if one can make well oriented surfaces or interfaces for arbitrary orientations. However, in quasi-two-dimensional (2D) superconductors, it is by no means easy to make a well oriented surface/interface in the direction perpendicular to the 2D planes. For example, for the high-$T_c$ cuprates, it is predicted theoretically that ZBCP is observed most prominently for (110) surface/interface and is not observed for (100) oriented surface/interface\textsuperscript{5}. However, in the actual experiments, it is not easy to prepare well controlled surface/interface, and only few exceptional cases\textsuperscript{6-8} have succeeded in discriminating the difference between the tunneling conductance of (100) and (110) oriented junctions. Moreover, it has been clarified that atomic-scale roughness has influence on the tunneling spectroscopy via ABS\textsuperscript{9,10}. Thus, in order to clearly determine the positions of nodes in the pair potential, \textit{i.e.}, the symmetry of the pair potential, through tunneling spectroscopy via ABS, a preparation of well oriented junctions is necessary.

The situation can even be more severe for quasi-2D organic superconductors such as $\kappa$-(BEDT-TTF)$_2$X salts\textsuperscript{11} [abbreviated $\kappa$-(ET)$_2$X hereafter], $(X = \text{Cu(NCS)}_2, \text{Cu[N(NCN)}_2\text{]Br, or } \text{I}_3\text{]}$, which is another candidate for anisotropic pairing superconductors. It is even more difficult to make well oriented junctions compared to the high-$T_c$ cuprates.

For quasi-2D superconductors, it is much more promising to make films well oriented in the direction parallel to the planes, but the problem is that in that case, ZBCP is not obtained in the tunneling spectroscopy due to the absence of the interference of the sign change of the pair potential felt by the quasiparticle. Thus, even if there are nodes in the pair potential, only a V-shaped tunneling conductance is expected, and the direction of the nodes cannot be determined. In order to overcome this difficulty, we propose in the present study tunneling spectroscopy for surfaces parallel to the planes in the presence of a magnetic field applied parallel to the planes.

In the presence of a magnetic field, it is known that the energy spectrum of the quasiparticle is influenced by the Doppler shift\textsuperscript{12}. Due to this effect, specific heat and thermal conductivity show characteristic oscillation by rotating the direction of the magnetic field within the 2D plane reflecting the nodal structure of the pair potential\textsuperscript{13-15}. Recently, based on this idea, pairing symmetry of several unconventional superconductors have been discussed using thermal conductivity measurements\textsuperscript{16,17}. Although thermal conductivity and specific heat measurements are powerful ways to determine the pairing symmetry, these quantities are strongly influenced by phonons, so that the actual analysis of the experimental data, namely the subtraction of the phonon contributions, can be subtle. Thus, it is desirable to propose a complementary method to determine the positions of nodes. In this sense, tunneling spectroscopy in the presence of a magnetic field, \textit{magnetotunneling}, is a promising method\textsuperscript{18}. In the present paper, we apply our idea to models of the above mentioned quasi-2D superconductors, namely the high-$T_c$ cuprates and...
\( \kappa-(\text{ET})_2X \)

As regards \( \kappa-(\text{ET})_2X \), the existence of nodes of the pair potentials has been suggested from various experiments. However, the position of nodes is still a controversial issue. Although early theories support \( d_{xy} \)-wave pairing, recent experiments support \( d_{xy} \) pairing. Stimulated by these recent experiments, two of the present authors revisited this issue theoretically, and found that a \( d_{xy} \)-like pairing can slightly dominate over \( d_{xy} \)-wave pairing when the dimerization of the BEDT-TTF molecules is not so strong. Thus, it is intriguing to clarify what is expected in the magnetotunneling spectroscopy for each of the plausible pairing symmetries.

We calculate surface density of states (SDOS) at the Fermi energy, which corresponds to zero-bias tunneling conductance in the high barrier limit. We find that SDOS oscillates as a function of the direction of the magnetic field applied in the antinodal direction, and a minimum for the magnetic field along the node. Although this result is similar to those obtained in Ref. 22, where the bulk density of states is considered for free electrons (namely for a round Fermi surface), it is by no means evident from the beginning whether similar results can be obtained at surfaces and for realistic lattice structures and band fillings (namely for realistic shapes of the Fermi surface).

\[ \begin{align*}
\xi_k &= -2 \left(t_{\text{eff}} + J_{\text{eff}} \chi \right) \left( \cos \kappa_x a + \cos \kappa_y a \right) \\
&\quad -4t' \cos \kappa_x a \cos \kappa_y a - \mu, \\
\Delta_k &= 2\Delta_0 \left( \cos \kappa_x a - \cos \kappa_y a \right). 
\end{align*} \]

with \( t_{\text{eff}} = \frac{\kappa a}{1 + \delta} t \), and \( J_{\text{eff}} = \frac{\kappa a}{4 \left(1+\delta^2\right)} J \). Here, the quantities \( \chi \), \( \mu \), and \( \Delta_0 \) are determined self-consistently for each doping ratio \( \delta \). In the following calculation, we fix \( J/t = 0.3 \) and \( t'/t = -0.5 \) \( [t'/t = 0.5] \) as a typical values of hole-doped [electron-doped] cases.

(ii) \( \kappa-(\text{ET})_2X \): Although this material has four molecules per unit cell (four bands), we may reduce it to a single band model for the present purpose. The single band description is not sufficient for determining which pairing symmetry is more favorable but it suffices for the argument here, where we discuss the tunneling spectrum for a given pairing symmetry. In the single band description, the quantity \( \xi_k \) in Eq. (4) is given by

\[ \begin{align*}
\xi_k &= -2t \left( \cos \kappa_x a + \cos \kappa_y a \right) \\
&\quad -2t' \cos \kappa_x a a - \mu. 
\end{align*} \]
The values of $t$, $t'$, and $\mu$ are chosen as to reproduce the Fermi surface observed by Shubnikov-de Haas experiments. As for plausible pairing symmetries in $\kappa$-(ET)$_2$X, we consider the $d_{x^2-y^2}$-wave pairing given by Eq. (5), and a $d_{xy}$-like pairing given by

$$\Delta_k = 2\Delta_0 \left[ \cos k_xa + \cos k_ya - \alpha \cos(k_xa + k_ya) \right] , \quad (7)$$

with $\alpha \sim 0.8$. These pairing symmetries have been found to closely compete with each other in Ref. [4].

In order to compare our theory with scanning tunneling microscopy (STM) experiments, we assume that the STM tip is metallic with a constant density of states, and that the tunneling occurs only for the site nearest to the tip. This has been shown to be valid through the study of tunneling conductance of unconventional superconductors. The tunneling conductance spectrum at zero-energy is then given at low temperatures by the normalized SDOS.

$$\rho(\theta) = \frac{\int_{-\infty}^{\infty} d \omega \rho_S(\omega) \text{sech}^2 \left( \frac{\omega}{2k_B T} \right)}{\int_{-\infty}^{\infty} d \omega N(\omega) \text{sech}^2 \left( \frac{\omega - \delta}{2k_B T} \right)} , \quad (8)$$

$$\rho_S(\omega) = \left\{ \begin{array}{ll} \frac{1}{2} \sum_k \left[ |u_k|^2 \left[ \delta(\omega - E_k) + \delta(\omega - E_{-k}) \right] ight. & \left. \text{for } \rho(\theta) \right. \\
+ |v_k|^2 \left[ \delta(\omega + E_k) + \delta(\omega + E_{-k}) \right] & \left. \text{for } \rho_N(\omega) \right. \end{array} \right. \quad (9)$$

Here $\rho_S(\omega)$ denotes the SDOS for the superconducting state while $\rho_N(\omega)$ the bulk density of states in the normal state.

![FIG. 2: The angle variation of SDOS for the model of cuprates in $H = 0.5H_c$. (a) $t'/t = -0.5$ and (b) $0.5$.](image)

First, we look into the case of the cuprates. $\rho(\theta)$ is plotted in Fig. 2 for various $\delta$. In the overdoped regime, SDOS exhibits clear fourfold oscillations, which has a maximum for the magnetic field applied in the antinodal direction, and a minimum for the magnetic field along the nodes. Thus, through the analysis of the position of maxima and minima of $\rho(\theta)$, we can identify the nodal and antinodal directions. With the increase of $\delta$, the magnitude of the difference between the maximum and minimum is enhanced. In the underdoped region, the difference of the magnitude between maximum and minimum is reduced reflecting on the square shape of Fermi surface (see Fig. 2). We now move on to the case of $\kappa$-(ET)$_2$X. For both of $d_{x^2-y^2}$ and $d_{xy}$-like cases, $\rho(\theta)$ exhibits a characteristic oscillation reflecting the nodal structure and the twofold symmetry of the Fermi surface. For $d_{x^2-y^2}$-wave pairing, $\rho(\theta)$ has local minimum [maximum] around $(2n + 1)\pi/4$ [$n\pi/2$] with integer $n$, while for $d_{xy}$-wave pairing, $\rho(\theta)$ has local minimum [maximum] around $n\pi/2$ [$(2n + 1)\pi/4$]. As seen from this result, we can discriminate $d_{x^2-y^2}$-wave from $d_{xy}$.

![FIG. 3: The Fermi surface and $d$-wave pairings. Dots lines represent the nodal lines. (a) a model of cuprates with a $d_{x^2-y^2}$-wave: left and right panels are plotted for $t'/t = -0.5$ and 0.5, respectively. (b) a model of $\kappa$-(ET)$_2$X for $d_{x^2-y^2}$-wave (left) and $d_{xy}$-like (right).](image)

To summarize, we have proposed tunneling spectroscopy in the presence of a magnetic field, magnetotunneling, for quasi-2D anisotropic superconductors, where the magnetic field is rotated within the 2D plane. SDOS at the Fermi energy, $\rho(\theta)$, exhibits a characteristic oscillation upon rotating the direction of the magnetic field. As case studies, we have applied this idea to the high $T_C$ cuprates and $\kappa$-(ET)$_2$X salts. $\rho(\theta)$ is found to take its (local) minimum value when the applied magnetic field is parallel to the nodal direction of the pair potential independent of the detailed shape of the Fermi surface. The origin of the oscillation $\rho(\theta)$ is considered to be essentially the same as that given in Ref. [22], but we stress that it is not expected from the beginning that the phase of the oscillation is the same as that in Ref. [22] for arbitrary doping concentrations and/or for various lattice...
structures. In fact, we have seen that in the underdoped regime of the cuprates, the oscillation, although it still has the same phase as that in Ref. 22, becomes extremely weak reflecting the characteristic band structure near half-filling. Although only two kinds of quasi-2D superconductors are studied here, the proposed magnetotunneling spectroscopy should serve as a strong probe to identify the pairing symmetry for various unconventional superconductors.

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