Generalized method of image and the tunneling spectroscopy in high-$T_c$ superconductors

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A generalized method of image is developed to investigate the tunneling spectrum from the metal into a class of states, with the tight-binding dispersion fully included. The broken reflection symmetry is shown to be the necessary condition for the appearance of the zero-bias conductance peak (ZBCP). Applying this method to the $d$-wave superconductor yields results in agreement with experiments regarding the splitting of ZBCP’s in magnetic fields. Furthermore, a ZBCP is predicted for tunneling into the (110) direction of the $d$-density-wave state, providing a signature to look for in experiments.

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The current transport through a heterojunction consisting of a normal metal and another different material ($X$) has been a subject of interest for many years. In this setup, the normal metal with known spectral properties is used as a probe to analyze the electronic states of the material $X$. Although such measurements have provided useful insights into the bulk spectral properties of $X$, it has been also realized that the presence of the interface matters. The zero-bias conductance peak (ZBCP) observed in the tunneling spectra when $X$ is a $d$-wave superconductor (ND junction) in the (110) direction is a well-known example of interface effects. However, the issue of exactly how the tunneling measurements are related to the bulk properties has never been answered satisfactorily.

Conventionally, the ND junction is analyzed in the mean-field level, using the Bogoliubov–de Gennes (BdG) equations in which continuum and quasiclassical approximations are often invoked. While these approximations are valid for conventional superconductors, they are certainly not justified for high-$T_c$ cuprates where proximity to the Mott insulators entails fully consideration of the tight-binding nature. Previously, this was done by numerically solving the discrete BdG equation for each interface orientation individually without elucidating their relations to the bulk properties. This technical inconvenience makes it difficult to include fluctuations systematically in this approach.

In this work, we shall adopt a different approach based on the nonequilibrium Keldysh-Green’s function formalism which enables one to construct systematically higher-order corrections from the mean-field lattice Green’s functions. In this approach, because $X$ extends over a semi-infinite space, one shall need the half-space Green’s functions. For simple configurations such as the (100) orientation of a $d$-wave superconductor, it turns out that these half-space Green’s functions only differ from the bulk ones by sinusoidal factors. This relation certainly does not hold for other orientations as it predicts no ZBCP in the (110) direction. We shall develop a generalized method of image which enables us to construct half-space Green’s functions from the bulk ones. We emphasize the generality of this method and its ability to account for the low-energy features in the tunneling spectrum for a whole class of states. As a demonstration, in this paper we will focus mostly on the study of ND junctions and only briefly mention the applications to other systems. The effects of interactions and fluctuations will be addressed elsewhere.

Our results indicate broken reflection symmetry is necessary for the emergence of ZBCP’s. For ND junctions our method can reproduce earlier results on the ZBCP in the continuous-wave approximation. In a full tight-binding calculation for (110) and (210) directions, we obtain the doping dependence of ZBCP’s which exhibits its sensitivity to the Fermi surface topology. In particular, the splitting of the ZBCP in the current-carrying state is also calculated and is shown to be in agreement with experiments.

We start by considering a junction consisting of a two-dimensional (2D) normal metal on the left ($L$) hand side ($-\infty<x<-d$, where $d$ is the lattice constant of the metal side) and a $d$-wave superconductor ($0\leq x<\infty$) on the right ($R$) hand side (see Fig. 1), governed by the Hamiltonians $H_L$ and $H_R$, respectively. At the mean-field level, we have

$$H_R = -\sum_{\langle ij \rangle, \sigma} t_R c_{i\sigma}^\dagger c_{j\sigma} - \sum_{\langle ij \rangle} t'_R c_{i\sigma}^\dagger c_{j\sigma}$$

$$+ \sum_{\langle ij \rangle} \Delta_{ij} (c_{i\uparrow}^\dagger c_{j\downarrow} - c_{i\downarrow}^\dagger c_{j\uparrow}) + \text{H.c.,}$$

where $\langle ij \rangle$ denotes the nearest-neighbor (NN) bond, the next-NN bond, and $\Delta_{ij}$ possesses $d$-wave symmetry. The tunneling Hamiltonian connects the interface points at $x=-d$ and $x=0$, and is given by $H_T = \sum_i t(y_L-y_R)(c_i^\dagger c_R + c_{iR}^\dagger c_L)$, where the summation is over lattice points along the interface, chosen to be in the $y$ direction. We shall assume that both sides are square lattices and characterize the orientation of right-hand side (RHS) by the Miller indices $(h0)$. The total grand Hamiltonian is then given by $K = (H_L - \mu_L N_L) + (H_R - \mu_R N_R) + H_T = K_0 + H_T$. Here $\mu_L$ and $\mu_R$ are the chemical potentials and their difference $\mu_L - \mu_R$ is fixed to be the voltage drop $eV$ across the junction.
dangling bonds, one needs to introduce two hard walls at consistent 52
\[ t_R, \]
where \( R \) is effectively a hard wall located at say, for the nearest-neighboring bonds to the interface sites are cut, there Bravais lattice and the lattice points in the half-plane usually do not form a simple the application of the method of image. However, because sider the case of Fourier transform in the direction is performed first. Con-
ty appearing problematic. To overcome these difficulties, a Fourier transform in the y direction is performed first. Con-
ider the case of (110) orientations; the Hamiltonian with only NN hopping becomes

\[ H_R = \sum_{i, \sigma, k_y} -2t_R \cos \left( \frac{k_y d}{2} \right) c_{i\sigma}^\dagger(k_y) c_{i+1\sigma}^\dagger(k_y) + \sum_{i, k_y} 2i\Delta_0 \sin \left( \frac{k_y d}{2} \right) \left( c_{i\sigma}^\dagger(k_y) c_{i+1\dagger}(-k_y) + c_{i\dagger}(-k_y) c_{i+1\sigma}(k_y) \right) + \text{H.c.}, \]

where \(-\pi/d < k_y < \pi/d\) and \(2\Delta_0\) is the gap value. The whole problem is now one dimensional, and the hard wall becomes a point. Note that the suppression of the gap near the interface can be taken into account by adding self-consistent \( \delta\Delta_0(i) \) to Eq.(2) and can be treated perturbatively later. In the presence of \( t_R' \), additional terms \( \Sigma_{i, \sigma, k_y} -2t_R' \cos(k_y d) c_{i\sigma}^\dagger(k_y) c_{i\dagger}(k_y) + \text{H.c.} \) appear. Since at the boundary, both \( t_R \) and \( t'_R \) are cut and become dangling bonds, one needs to introduce two hard walls at \( x = -d/2 \) and \( x = -d \). For clear presentation, we shall first set \( t_R' = 0 \). In this case, we are looking for the Green’s function \( \tilde{G}_0(\omega, k_y, x, x') \) (which is a 2x2 matrix in Nambu’s notation), which satisfies the boundary condition \( \tilde{G}_0 = 0 \) at \( x = -d/2 \). We shall suppress the dependence on \( \omega \) and \( k_y \). Here, since \( x' \) is the location of the point source and its image point is at \(-d-x'^{'}\), the method of image can be employed by constructing

\[ \tilde{G}_0(x, x') = \tilde{G}_0(x - x') - \tilde{G}_0(x + d + x') \alpha(x'), \]

where \( \tilde{G}_0 \) is the bulk bare Green’s function and \( \alpha \) is a matrix to be determined. The first term is the direct propagation from \( x' \) to \( x \), while the second term will reduce to the propagation from the image point to \( x \) in special situations (see below). In fact, since \( \tilde{G}_0 \) has to vanish at \( x = -d/2 \), we obtain \( \alpha(x') = \tilde{G}_0^{-1}(d/2 + x') \tilde{G}_0(-d/2 - x') \). Therefore, the second term describes the propagation from \( x' \) to \( x \) via the reflection of the hard wall. The matrix \( \alpha \), apart from fitting the boundary condition, carries important information about the gap structure along the reflected path from \( x' \) to \( x \). Note that in calculating the tunneling current, since \( H_T \) only connects points along the interface, only the surface Green’s function \( g_0(\omega, k_y) = \tilde{G}_0(x = 0, x' = 0) \) is needed.4,10 Writing \( G_0 \) in the Fourier \( k_y \) space, we find

\[ g_0(\omega, k_y) = \int_{-\pi/d}^{\pi/d} \frac{dk_y}{2\pi} G_0(\omega, k_y, k_x)[1 - \exp(ik_yd)\alpha_0], \]

where the factor \( \alpha_0 = G_0^{-1}(d/2)G_0(-d/2) \) is independent of \( k_x \). If the reflection symmetry holds for the state \( X \), such as \( d \)-wave superconductors in \( (100) \) direction (in this case, \( d/2 \) is replaced by \( d \)), one has \( \alpha_0 = 1 \) and hence it reduces to the familiar form

\[ g_0(\omega, k_y) = \int_{-\pi/d}^{\pi/d} \frac{dk_y}{\pi} \sin(k_yd) G_0(\omega, k_y, k_x). \]

Therefore, apart from modifications due to the sinusoidal factors, the density of state almost has the same feature as the bulk one. However, for other orientations such as the \( (110) \) direction, reflection symmetry with respect to the interface is broken. As a result, \( \alpha_0 \) is not the identity matrix and as we shall see, this will give rise to the ZBCP.

The advantage of Eq. (4) is that it is purely based on the bulk Green’s functions. The interface orientation is encoded in \( k_x \) and \( k_y \). In other words, \( g_0(\omega, k_y, k_x) \), which appears in Eq. (4) and \( \alpha_0 \) is simply the usual bulk BCS Green’s function but with \( k \) being rotated by 45°. This technical merit is retained for other interface orientations but with \( k \) being rotated by an angle in accordance with the interface orientation. More importantly, this also offers a scheme for studying fluctuations and interactions. Essentially one can take into account these effects through the bulk Green’s function \( G_0 \). This will be explained in more detail in a separate publication.

When evaluating \( G_0(x - x') \), the dominant contributions come from the poles determined by \( (\omega + i\eta)^2 - E_k^2 = 0 \), where \( E_k = \sqrt{\varepsilon_k^2 + \Delta_k^2} \). In the continuum limit, the dispersion becomes \( \varepsilon_k = \hbar^2(k^2_x + k^2_y)/2m \) and \( \Delta_k = \Delta_0 \cos(2\theta - \theta_h) \), where \( k^2_x = k^2_F - k^2_y \), \( \theta = \sin^{-1}(k_y/k_F) \), and \( \theta_h \) is the angle between the crystal axis \( a \) and \( x \) direction. At the same
time, the integration range of $k_z$ is extended to $\pm \infty$. There are four poles located at $\pm k_\perp \pm i k_z$ with $k_\perp = \sqrt{k_F^2 \pm 2 m \sqrt{(\omega + i \eta)^2 - \Delta_\perp^2}/\hbar^2}$, representing particles and holes along different directions. Here $\Delta_\perp$ are gaps in directions $\pm \theta$. By contour integration, one obtains $G_0(x-x')$ and thus $\alpha(x')$. After some algebra and assuming that $k_F$ is large,\textsuperscript{11} indeed Eq. (3) reproduces results obtained in Ref. 7 by directly solving the equations of motion. In our approach, the continuum approximation is not necessary. To investigate any effect that is due to the tight-binding nature, the full tight-binding dispersion has to be retained. In this case, the integration over $k_z$ cannot be extended to $\pm \infty$, and thus poles are in different structure and a substantial difference from the continuum approximation could result.

We now include the hopping $t'_R$ for the (110) direction. The main complication is to add a second hard wall at $x = -d$. This is a simple generalization of the single hard-wall problem. One simply requires $\tilde{G}_0$ to vanish on all these hard walls simultaneously. Therefore, we write

$$\tilde{G}_0(x,x') = G_0(x-x') - G_0(x-x')\alpha_1(x') - G_0(x-x')\alpha_2(x'),$$

where $x'_1 = x' - d$ and $x'_2 = x' - 2d$ are images of $x'$. The boundary conditions at $x = -d$ and $x = -2d$ determine $\alpha_1$ and $\alpha_2$. The surface Green’s function thus obtained is the bare one and will get renormalized by $H_{TR}$, giving rise to four different components in the differential conductance.\textsuperscript{4,11} The strength of $H_{TR}$, characterized by $t$, determines the relative weight among each component. In Fig. 2, we show our results for the spectrum of the total differential conductance for various dopings based on Eq. (4). The parameters adopted are determined self-consistently from the mean-field slave-boson theory for the $t$-$t'$-$J$ model.\textsuperscript{4} It is clear that the ZBCP's are the most important features at low energies.\textsuperscript{5} Since the

ZBCP arises from the existence of zero-energy states, it must appear as poles at zero energy in the Green’s function. For the (110) direction without $t'_R$, this is entirely determined by zeros of the denominator in $\alpha$:

$$\beta(\omega, k_z) = \det[G_0(d/2)].$$

In the continuum limit ($d \to 0$), $\beta$ can be evaluated analytically:

$$\beta = -[\omega^2/\Delta + (\Delta_+ \Delta_- + \Delta_- \Delta_+)]^{1/2},$$

where $\Delta = (\Delta_+ \Delta_-)/(\Delta_+ + \Delta_-)$. Therefore, poles of $\tilde{g}_0$ at $\omega = 0$ depend crucially on whether there is a sign change of the gap on the Fermi surface. This criterion, however, does not hold as one goes to the tight-binding limit because pairing no longer only occurs on the Fermi surface. As a result, a numerical computation of $\beta$ is necessary. Our results indicate that ZBCP’s are sensitive to the Fermi surface topology. In fact, for the (110) surface, the height of the peak depends on the volume of the Fermi surface. It reaches a maximum when $\mu_R = 0$ and decreases when $\mu_R \neq 0$. For other orientations, the ZBCP could even disappear.

For general orientations, there could be more than one hard wall. As a demonstration, we consider the (210) interface. In this case, when $t'_R = 0$, two hard walls are located at $x = -d/\sqrt{2}$ and $-2d/\sqrt{2}$, in analogy to the (110) surface with $t'_R$. A typical result for the small scale of $t$ is shown in the inset of Fig. 2. As $t$ increases, the zero-energy states are able to leak out, and thus the ZBCP’s get broadened. Note that lattice points with dangling bonds form a pair-breaking region near the interface, resulting in the peaks around $2\Delta_0$. They are due to quasiparticle bound states with nonzero energy.\textsuperscript{12}

The ZBCP’s split in the presence of magnetic fields $H$, essentially due to the Doppler shift caused by the supercurrent near the interface.\textsuperscript{13} In the tight-binding model, $\Delta_{ij}$ is shifted to $\Delta_{ij} \exp[iq \cdot (\mathbf{r}_i - \mathbf{r}_j)]$, where $q = eHx/2hc$ with $\lambda$ being the penetration depth. By redening $c_{i\sigma} = c_{i\sigma} \exp(iq \cdot \mathbf{r}_i)$, the dependence on $q$ can be absorbed into $\epsilon_k$. Figure 3 shows the field dependence of the splitting for the (110) in-

![FIG. 2. The total differential conductance of several dopings for the (110) interface with $\eta = 0.01$ and $t_2 = 1.0$. The weak link is modeled by the interface hopping $t(\omega) = \exp[-\sqrt{\omega \eta - |\omega|}/\Gamma]$ with $\omega_0 = 11\Delta_0$ and $\Gamma = \Delta_0$. Inset: $dI/dV$ curve for the (210) interface with $\delta = 0.08$.](image)

![FIG. 3. The field dependence of the splitting for an underdoped case ($\delta = 0.12$). Inset: doping dependence of the splitting for a fixed magnetic field.](image)
that for large $H$ the splitting deviates from linear dependence on $H$ due to the lattice effect in our approach. In fact, in the special case of the armchair interface, in agreement to recent experimental data.\textsuperscript{14} It is seen that how easily our formulation can tell whether there should be ZBCP’s or not. Further applications to other systems will be reported elsewhere.

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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4}
\caption{A typical $dI/dV$ curve for tunneling into the (110) direction of a $d$-density-wave state. Here $\mu_R=0$ and $\Delta_0=0.1$. Inset: a similar plot for tunneling from a wideband metal into the graphene sheet with zigzag interface. Here the hopping amplitude $\gamma_0=0.1$.}
\end{figure}


\textsuperscript{6} The Green’s function approach has also been attempted at the quasiclassical level. See, for example, T. Luck et al., Phys. Rev. B \textbf{63}, 064510 (2001).


\textsuperscript{9} In fact, for 1D, the image point can be chosen arbitrarily without affecting the result.


\textsuperscript{11} S.T. Wu and C.-Y. Mou (unpublished).


\textsuperscript{15} C. Honerkamp and M. Sigrist, cond-mat/0107550 (unpublished).