Current-voltage relation for superconducting $d$-wave junctions

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We calculate the current-voltage ($I-V$) relation for planar superconducting $d$-wave junctions for both arbitrary transmission of the junction and arbitrary orientation of the $d$-wave superconductors. The midgap states (MGS) present at interfaces/surfaces of a $d$-wave superconductor influence the $I-V$ relation. In some arrangements we find considerable negative differential conductance and lower threshold voltage for non-zero current due to resonant conduction through MGS.

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Soon after the discovery of the high-$T_c$ cuprates it was realized that these materials did not in a straightforward way conform to the conventional BCS scheme. Therefore, a number of researchers started to speculate whether the symmetry of the order parameter in the high-$T_c$ cuprates might deviate from the spherical symmetric one ($s$-wave) found in the conventional superconductors. Recently, an already lively discussion on the subject has become even more intensified. Quite a few experiments probing the $d$-wave symmetry of the order parameter are claimed to exclude the possibility of an order parameter with symmetries different from $s$-wave. In fact, some experiments sensitive to the phase of the order parameter do at least not exclude the possibility of an order parameter with symmetry different from $s$-wave. In addition to the discussion above, Hu has pointed out a possible connection between the often observed zero-bias conductance peaks in high-$T_c$ junctions and the zero-energy bound states or midgap states (MGS) theoretically predicted to be present at interfaces/surfaces of $d$-wave superconductors. The origin of MGS is due to normal scattering at the interface/surface. A quasiparticle in the superconductor changes its momentum when scattered. Therefore, the quasiparticle in general experiences a different order parameter before and after the scattering event, since in the $d$-wave case the order parameter depends on the momentum. Due to Andreev reflection the quasiparticle will retrace its path and form a closed loop, leading to a bound state when the order parameter before and after scattering differs in sign.

We calculate the current-voltage ($I-V$) relation for planar superconducting $d$-wave junctions for both arbitrary transmission of the junction and arbitrary orientation of the $d$-wave superconductors. The midgap states (MGS) present at interfaces/surfaces of a $d$-wave superconductor influence the $I-V$ relation. In some arrangements we find considerable negative differential conductance and lower threshold voltage for non-zero current due to resonant conduction through MGS.

Calculations of $I-V$ curves for normal metal-superconductor (NS) junctions indeed confirmed the importance of MGS in the $d$-wave case. Due to conduction through MGS, a peak at zero voltage grows up in the conductance as the transmission of the junction is decreased, which is different from the $s$-wave case. Motivated by both the general discussion regarding the underlying symmetry of the order parameter of the cuprates and the new understanding of MGS in $d$-wave junctions we calculate in this paper the current-voltage ($I-V$) relation for junctions with anisotropic superconductors. To produce numerical results allowing us to compare our calculation to earlier calculations we specialize to the case of $d$-wave symmetry. Therefore we choose the order parameter to be $\Delta(\theta) = \Delta_0 \cos(2(\theta-\alpha))$, where $\theta$ is the angle of incidence for a quasiparticle approaching the junction and $\alpha$ is the angle of orientation of the $d$-wave superconductor with respect to the interface as explained in Fig. 1. The cases $\alpha = 0$ and $\alpha = \pi/4$ correspond to $d_{x^2-y^2}$ and $d_{xy}$ symmetry, respectively. For the $s$-wave case, $\Delta(\theta) = \Delta_s$.

There are some calculations of $I-V$ curves for $d$-wave junctions in the literature. Using the tunneling hamiltonian formalism one can calculate the conductance as a convolution of the density of states in the $d$-wave superconductors. Unmodified, such an approach cannot describe the action of MGS. Now, in some con-
figurations of d-wave superconductors there are no MGS, and we can therefore compare the curves with our calculations (in the tunneling limit) as we will do later in this paper. Refs. 12 and 14 are using methods somewhat similar to ours; however, the presence of MGS is not discussed. There is also work on asymmetric (different gaps of the electrodes) SNS junctions in point-contact geometry (one or few conducting modes in the normal region). 15, 16 This theory applies straight to the d-wave case since for point-contacts the modes making it through the contact correspond to $\theta \approx 0$. In this case the MGS are absent. However, for the planar junction quasiparticles with any angle $\theta$ of incidence come into play, making it necessary to consider the MGS.

When there are superconductors on both sides of the junction multiple Andreev reflection (MAR) will take place. 15, 16 In this paper we use methods recently developed to calculate $I-V$ curves of SNS junctions for arbitrary transmission in the s-wave case. 17, 18 These methods will automatically take into account any effects from the MGS, if appropriately modified. The implementation of these modifications is our new contribution, as presented in this paper.

Our calculation is two-dimensional, using a cylindrical Fermi surface. Furthermore, the normal scattering will change the angle (or momentum) of a quasiparticle from $\theta$ to $\theta = \pi - \theta$. This simply means that the quasiparticle experiences a different pair potential before and after the scattering event, since in general $\Delta(\theta) \neq \Delta(\theta)$. (The exception is the case $\alpha = 0$.) Therefore, one has to book-keep the two different gaps in the calculation.

The system we study is shown in Fig. 1. The regions "Left" and "Right", separated by a barrier with transmission amplitude $t(\theta)$ and reflection amplitude $r(\theta)$, are only conceptual since we will only study the case when the normal region is short (zero-length limit). We model the barrier using a $\delta$-function potential to derive the angular dependence of $r$ and $t$. 17, 18

The time-dependent Bogoliubov-de Gennes equation for anisotropic superconductors is

$$\int \frac{dy}{\hbar} \begin{pmatrix} h_0(x, y) & \Delta(x, y, t) \\ \Delta^*(x, y, t) & -h_0(x, y) \end{pmatrix} \begin{pmatrix} u(x, t) \\ v(x, t) \end{pmatrix} = i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u(x, t) \\ v(x, t) \end{pmatrix}, \quad h_0(x, y) = \delta(x-y)(\frac{p_y^2}{2m} - \mu). \quad (1)$$

In the equation above, $\mu$ is the chemical potential, which is $\mu_1 - \mu_2$ in superconductor 1 (2). Since there is a voltage $eV$ between the two superconductors, the chemical potentials are different, $eV = \mu_2 - \mu_1$. Due to this difference, the phase $\phi$ of the order parameter $|\Delta|e^{i\phi}$ depends on time according to the Josephson relation $\partial_t \phi = 2eV/\hbar$, leading to inelastic scattering. (For details, see Ref. 13.)

Solving Eq. (1) piecewise in each region, we follow the standard treatment previously used in a number of papers. 15, 16 To this end, the center of mass coordinate $R = (x+y)/2$ and the relative coordinate $r = x-y$ are introduced, expressing the order parameter as $\Delta(r, R, t)$.

We will in the following assume approximate solutions to Eq. (1) of the form (in each region)

$$\begin{pmatrix} u(x, t) \\ v(x, t) \end{pmatrix} = \sum_k e^{i\delta_k \cdot \mathbf{r}} \begin{pmatrix} u_k \\ v_k \end{pmatrix} e^{-iE_k t}. \quad (2)$$

We approximate the integral operator of Eq. (1) by neglecting terms $u(\theta)$ of the order $(k_F \xi_0)^{-1}$ (the quasiclassical approximation). 19

$$\int dy \Delta(x, y) v(y, t) \approx \sum_k \Delta(k, x) v_k e^{ik \cdot \mathbf{r}} e^{-iE_k t}, \quad (3)$$

where we have introduced the Fourier transform $\Delta(k, R)$ of the order parameter $\Delta(r, R)$. Since in the weak-coupling limit the pair potential is expected to be non-zero only close to $k_F$, one can replace the momentum by an angle $\theta$. Neglecting self-consistency, we therefore model the order parameter as

$$\Delta(k, x, t) = \begin{cases} \Delta_1(\theta), & x < -L/2 \\ 0, & |x| < L/2 \\ \Delta_2(\theta)e^{i(\phi_0 + 2evt)/\hbar}, & x > L/2. \end{cases} \quad (4)$$

Since the overall phase is arbitrary, $\Delta_1$ is chosen real.

Before solving Eq. (1), it is convenient to introduce some notational simplifications. First we define the BCS coherence factors

$$\frac{v_i(E, \theta)}{u_i(E, \theta)} = \frac{E - \text{sgn}(E)\sqrt{E^2 - \Delta_i(\theta)^2}}{\Delta_i(\theta)}, \quad |E| > |\Delta_i(\theta)|$$

$$\frac{v_i(E, \theta)}{u_i(E, \theta)} = \frac{E - i\sqrt{\Delta_i(\theta)^2 - E^2}}{\Delta_i(\theta)}, \quad |E| < |\Delta_i(\theta)| \quad (5)$$

where $|u_i|^2 + |v_i|^2 = 1$ and $i = 1, 2$ refers to superconductor 1 and 2. Using this definition, one can express the Andreev reflection amplitude at superconductor $i$ as $A_i(E_n, \theta) = A_{i,n} = v_i(E_n, \theta)/u_i(E_n, \theta)$ and $A_i(E_n, \theta) = A_{\bar{i},n}$, where $E_n = E + neV$. The transmission amplitude for an electron-like quasiparticle at energy $E$ and angle $\theta$ from superconductor $i$ to enter the electron branch in the normal region is $J_i(E, \theta) = J_i = (u_i^2(E, \theta) - v_i^2(E, \theta))/u_i(E, \theta)$.

Solving the scattering problem, we follow the approach by Averin and Bardas. 19 First, we assume that an electron-like quasiparticle is approaching the barrier from the left superconductor (labeled by $\rightarrow$) at energy $E$ and angle $\theta$. Since we will calculate the current in the normal region to the left of the barrier, see Fig. 1, we need the wave function $\Psi_L(E, \theta) \equiv \Psi_L$ that solves Eq. (1) in region "Left" (L), see Fig. 1.

$$\Psi_L^L = \sum_n \begin{pmatrix} a_n^* e^{ik \cdot x} + d_n^* e^{i\mathbf{k} \cdot x} \\ b_n e^{ik \cdot x} + c_n^* e^{i\mathbf{k} \cdot x} \end{pmatrix} e^{-i\frac{E_n^L t + a_n^* b_n + c_n^* d_n}{\hbar}}, \quad (6)$$

where $\mathbf{k} = (k_x, k_y) = k(\cos \theta, \sin \theta)$, $\mathbf{k} = (-k_x, k_y) = k(\cos \theta, \sin \theta)$ and $E_n = E + neV$ ($n$ is an even integer).
Matching the wave functions of the various regions at the two NS interfaces and the barrier, the following (recursive) relations can be derived that determine the coefficients \( a \), \( b \), \( c \) and \( d \). For \( d \) we have

\[
\alpha_n d_{n+2} + \beta_n d_n + \gamma_n d_{n-2} = r J_1 \delta_{n,0}, \tag{7}
\]

where \( \alpha_n \), \( \beta_n \) and \( \gamma_n \) are defined as

\[
\alpha_n = -|t|^2 \frac{\bar{A}_{2,n+1} \bar{A}_{1,n+2}}{1 - \bar{A}_{2,n+1} \bar{A}_{2,n+1}}
\]

\[
\beta_n = 1 - A_{1,n} \bar{A}_{1,n} + |t|^2 \left( \frac{A_{1,n} \bar{A}_{1,n}}{1 - A_{2,n-1} \bar{A}_{2,n-1}} + \frac{A_{2,n+1} \bar{A}_{2,n+1}}{1 - A_{2,n+1} \bar{A}_{2,n+1}} \right), \tag{8}
\]

\[
\gamma_n = -|t|^2 \frac{A_{2,n-1} A_{1,n}}{1 - A_{2,n-1} A_{2,n-1}}.
\]

The coefficient \( b \) is determined from

\[
b_{n+2} = \frac{|t|^2 A_{2,n+1} d_n + \bar{A}_{1,n+2} (|t|^2 - A_{2,n+1} \bar{A}_{2,n+1}) d_{n+2}}{r (1 - A_{2,n+1} A_{2,n+1})}.
\]

The coefficients \( a \) and \( c \) are related to \( b \) and \( d \) through

\[
a_n = A_{1,n} b_n + J_1 \delta_{n,0}, \quad c_n = \bar{A}_{1,n} d_n. \tag{10}
\]

Using the wave function in Eq. (4) we can now calculate the current \( I \) per \( ab \)-plane (repeating the calculation above for the left-movers):

\[
\frac{I}{\sigma_0} = \frac{1}{2T} \int_{-\pi/2}^{\pi/2} d\theta \cos \theta \int_{-\infty}^{\infty} \frac{dE}{\Delta_0} \left[ T^\tau (E, \theta) - T^- (E, \theta) \right] + \frac{eV}{\Delta_0} \sigma_0 = L_y \frac{2^{3/2} e m^{1/2} \Delta_0^{1/2} \Delta_0 T}{\hbar^2}, \tag{11}
\]

where \( T = \int d\theta |t|^2 \cos \theta/2 \) and \( L_y \) is the junction length in the \( b \)-direction. The quantities \( T^\tau \) are defined as \( \tau \rightarrow \theta \), \( \tau \leftarrow \theta \)

\[
T^\tau (E, \theta) = N_r (E, \theta) \left| f(E) T^\tau_x (E, \theta) - f(-E) T^\tau_h (E, \theta) \right|, \tag{12}
\]

where \( N_r (E, \theta) \) is the bulk density of states evaluated in superconductor 1 (2) for \( \tau \rightarrow \theta \), \( \tau \leftarrow \theta \)

\[
T^\tau_x (E, \theta) = \sum_n \left| \alpha_n^\tau \right|^2 - \left| \beta_n^\tau \right|^2, \tag{13}
\]

\[
T^\tau_h (E, \theta) = \sum_n \left| \beta_n^\tau \right|^2 - \left| \gamma_n^\tau \right|^2.
\]

The Eqs. (6)-(11) are the main technical results of this paper. Together with Eq. (11) we will in the following use these equations to numerically calculate the \( I-V \) relation for some \( d \)-wave junctions. Putting \( A = \bar{A} \) (valid for \( s \)-wave) and assuming \( \Delta_1 = \Delta_2 \), Eqs. (6)-(11) will exactly transform to Eq. (5) of Ref. [14].

![FIG. 2](image-url)

**FIG. 2.** Varying the transmission \( T \), we show \( I-V \) curves for some arrangements of \( s \)-wave and \( d \)-wave superconductors. In (a) we show the results for the \( N/d_{xy} \) junction. In (b)-(f), the \( I-V \) curves for junctions with superconducting electrodes on both sides are shown: in (b) \( s/d_{xy} \) with \( \Delta_s = 0.1 \Delta_0 \); in (c) \( s/d_{xy} \) with \( \Delta_s = \Delta_0 \); in (d) \( d_{2s} - d_{2s} / d_{2s} - d_{2s} \); in (e) \( d_{xy} / d_{xy} \); in (f) \( d_{2s} / d_{xy} \). Zero-temperature is assumed.

In Fig. 2 we present some calculations of \( I-V \) curves involving \( d \)-wave superconductors. The MGS shows up in Eq. (8). The quantity \( 1 - A_n \bar{A}_n \) found in the denominators of Eq. (8) is zero when \( E_n = 0 \) for the case \( \Delta(\theta) = -\Delta(\bar{\theta}) \). This leads to transmission resonances which we explore in the following.

For the ballistic curves (transmission \( T = 1 \), no MGS in this case) involving two superconductors there is a non-vanishing zero-voltage current that disappears when the transmission is not unity. In Fig. 2(a) we confirm that using the Eqs. (3)-(11) reproduces previous results for the NS case. For low transmission, there is a huge increase of the current at small voltage leading to zero-bias conductance peaks.

Next, we study \( s/d_{xy} \) junctions, see Figs. 2(b)-(c). As the \( s \)-wave gap \( \Delta_s \) increases, the \( s \)-wave gap more and more "shadows" the zero-energy MGS on the \( d \)-wave
side. Since the width of the MGS decreases with decreasing transmission \( T \) this effect is more pronounced for low transmission. Subharmonic gap structure (SGS) appears at voltages \( \Delta_0/n \), \( n > 0 \) integer, see Fig. 6(a) in Ref. [3]. All other SGS predicted to occur in asymmetric junction\(^4\) is partly washed out after angular averaging since it involves also the gap of the \( d \)-wave superconductor (which depends on \( \theta \)). The SGS at voltages \( \Delta_0/n \) depends on \( n \) being even or odd. For odd \( n \) the scattering states originating from the left (\( s \)-wave) superconductor will hit the resonant MGS at the \( d \)-wave side, leading to negative differential resistance. For even \( n \) the scattering states responsible for SGS do not hit the MGS, and therefore this case resembles more what one finds in junctions with \( s \)-wave superconductors on both sides. When the transmission decreases, all SGS besides \( n = 1 \) vanishes, in which case the negative differential conductance is large.

We also study the case when there are \( d \)-wave superconductors on both sides of the junction. First, the case \( d_{x^2-y^2}/d_{x^2-y^2} \) is shown in Fig. 2(d). In this case the MGS are absent since \( \Delta(\theta) = \Delta(\bar{\theta}) \). We can therefore compare our low-transmission curve [the case \( T = 0.026 \) in Fig. 2(d)] with the tunneling calculation shown in Fig. 2 of Ref. [3] and we find that the curves are the same. At small voltage \( V \) there is a \( V^2 \) dependence of the current, and one finds a threshold voltage at \( eV = 2\Delta_0 \). For intermediate transmission [the case \( T = 0.38 \) in Fig. 2(d)] SGS appears at voltages \( 2\Delta_0/n \). The SGS is not as sharp as in the \( s \)-wave case because of angular averaging.

For the \( d_{xy}/d_{xy} \) configuration, see Fig. 2(e), there are MGS’s on either side of the junction. The difference compared to the \( d_{x^2-y^2}/d_{x^2-y^2} \) case is that the presence of MGS lower the threshold voltage to \( eV \approx \Delta_0 \). This behavior is similar to the case when a Breit-Wigner resonance is embedded in the normal region\(^1\). The reason for the lower threshold voltage is that the MGS transmission resonances at the right (left) hand side are most pronounced for \( \theta \approx \pi/4 \). At this angle a quasiparticle coming from the left (right) experiences the gap \( \Delta(\pi/4) = \Delta_0 \), resulting in a threshold voltage \( eV \approx \Delta_0 \) to make it possible for the quasiparticle from the left (right) side to hit the MGS on the right (left) side. Angular averaging smears out the threshold. For small voltage \( V \) there is a \( V^2 \) dependence of the current in the low-transmission limit. For intermediate transmission SGS again shows up at \( 2\Delta_0/n \), somewhat washed out because of angular averaging. In the \( s/d_{xy} \) case the negative differential conductance comes from resonant conduction of the right-moving scattering states through the MGS of the right-hand side. In the \( d_{xy}/d_{xy} \) case both left-movers and right-movers will pass through MGS (since there are MGS on both sides), and the resonant contribution from both left-movers and right-movers cancels. Therefore, there is in the \( d_{xy}/d_{xy} \) case no negative differential conductance.

In Fig. 2(f) we show the \( I-V \) curves for the \( d_{x^2-y^2}/d_{xy} \) case. This case is similar to the \( s/d_{xy} \) case shown in Figs. 2(b)-(c) since \( \Delta_1(\theta) = \Delta_1(\bar{\theta}) \). One important difference is that the angular averaging now results in non-zero current for small voltages. Still there is negative differential conductance close to the voltage \( eV \approx \Delta_0 \) in the low-transmission limit. One could understand the \( I-V \) curve in Fig. 2(f) as an averaging of the curves in Figs. 2(a)-(c). For small transmission the current is proportional to the voltage \( V \) in the small-voltage limit.

In summary, we have calculated \( I-V \) curves for planar \( d \)-wave junctions. In some arrangements we find considerable negative differential conductance and lower threshold voltage for non-zero current due to resonant conduction through MGS. These features have not been discussed before in the literature and they should be experimentally observable if superconducting gaps with \( d \)-wave symmetry exist in nature.

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