Current-Voltage Relations in $d$-wave Josephson Junctions: Effects of Midgap Interface States

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We investigate the dc current-voltage characteristics of $d$-wave Josephson junctions, where the barrier at the interface may have arbitrary strength. Dividing the current into $n$-particle currents $I_n$ ($n$ integer), we can explicitly show which physical processes are responsible for the subharmonic gap structure (SGS). For orientations where midgap states (MGS) exist, the resonances in the $n$-particle processes are drastically changed, giving rise to a strongly modified SGS. Introducing broadening in a phenomenological way, we show that MGS may produce a current peak near zero bias and we explain which physical processes are contributing to this peak. The agreement of our theory with recent experiments is discussed.

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1. INTRODUCTION

The formation of midgap states (MGS) at surfaces and interfaces of $d$-wave superconductors affects the current transport properties of junctions involving $d$-wave superconductors. It has been established that the zero-bias conductance peak (ZBCP) seen in normal metal/$d$-wave superconductor (N/$d$) junctions, are due to the MGS. For the ac Josephson effect it was shown that subharmonic gap structure (SGS) is in general different in $d$-wave junctions compared to $s$-wave junctions. In Ref. [1] it was shown that MGS produce current peaks at voltages of the order of the maximum gap, while in Ref. [2] also a singularity at zero bias was found. Later on, in Ref. [3] it was pointed out that this structure was not seen in Ref. [1], because the scattering theory did not include broadening effects. Numerical calculations including broadening confirmed the picture outlined in Ref. [3]. Despite all the
interest in the ac Josephson effect for \(d\)-wave junctions, the physics behind the current peaks has not been fully understood.

Recently, a scattering theory based approach has successfully explained SGS in conventional \((s\)-wave) junctions for arbitrary transparency of the barrier: it agrees for one-channel junctions with experiments without fitting parameters. In a recent reformulation of the theory it was shown that only currents from multi-particle processes creating real excitations need to be summed up, since non-physical currents, present in the original formulation of the theory, cancels. This proves that the Pauli exclusion principle is fulfilled.

In this paper we extend the reformulated scattering theory described above to junctions of \(d\)-wave superconductors and provide a deeper analysis of the SGS and the effects of MGS.

2. EXPRESSION FOR THE CURRENT

Considering transport in the \(ab\)-plane, we model the \(d_{\alpha L}/d_{\alpha R}\) junction \((\alpha_{L/R} \text{ is the orientation angle of the left/right superconductor})\) as described in Ref. [12]. This reference also provides a detailed description of the method we use to solve the time-dependent Bogoliubov-de Gennes (BdG) equation. A quasiparticle incident on the junction at energy \(E\) undergoes multiple Andreev reflections and builds up a scattering state with amplitudes at the sideband energies \(E_n = E + n\,eV\) \((V \text{ is the voltage; } n \text{ integer})\). It can be shown that the probability current \(I_{p n}\) leaking out at sideband \(E_n\) determines the \(n\)-particle current \(I_n\). At zero temperature we have [11,14]

\[
I_{dc}(V) = \sigma_0 \sum_n nI_n(V), \quad I_n(V) = \int_{-\pi/2}^{\pi/2} d\theta \cos \theta \int_{-eV}^{0} dE P_n^{\alpha}(\theta, E),
\]

\[
P_n^{\alpha}(\theta, E) = \sum_{\alpha_I = \{l,r\}} \left[ (1 - |a_0|^2) + (1 - |\bar{a}_0|^2)|a_0r_{0-}|^2 \right] |G_{n0}|^2 \times \left[ (1 - |a_n|^2) + (1 - |\bar{a}_n|^2)|a_n\bar{r}_{0+}|^2 \right],
\]

\[
G_{n0} = \frac{t_{n0}}{(1 - \bar{a}_0a_0r_{0-}\bar{r}_{n0})(1 - a_n\bar{a}_n\bar{r}_{0+}r_{n0}) - a_0\bar{a}_0a_n\bar{a}_n\bar{r}_{0+}r_{n0} + t_{n0}\tilde{t}_{n0}},
\]

where \(\sigma_0 = e k_F L_y / 2\pi h\). Above, \(a_0\) and \(a_n\) are the Andreev reflection amplitudes for the angle \(\theta\) at energies \(E_0\) and \(E_n\) respectively (the barred amplitudes are calculated at \(\bar{\theta} = \pi - \theta\); \(r_{0-}\) and \(r_{n+}\) describe reflections from minus and plus infinity in energy space; \(t_{n0}\), \(\tilde{t}_{n0}\), \(r_{n0}\), and \(\tilde{r}_{n0}\) are the elements of the scattering matrix describing the region between the injection point and the exit point. The weight \(n\) of \(I_n\) appears because the \(n\)-particle process involves an effective transfer of the charge \(ne\) over the junction.
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Fig. 1. Contributions from the first four $n$-particle currents to SGS for the $d_0/d_0$ junction in (a), and the $d_0/d_{45}$ junction in (b). The dashed lines are the total currents. In (b) broadening $\eta = 0.01$ has been introduced revealing a current peak near zero bias. The angle averaged junction transparency is $D = 0.026$ and we assume zero temperature. Note the inverse voltage scale in (a).

3. RESULTS AND DISCUSSION

Analyzing the current in Eq. (1), we see that resonances may appear in the propagator $G_{n0}$, which describes the transmission process from energy $E$ to $E_n$. There are two types of resonances: bare transmission resonances (appearing in $t_{n0}$) and boundary resonances (due to the denominator). A bare transmission resonance may appear when the trajectory hits a bound state at the IS interface, so called de Gennes state. In a short $d_0/d_0$ junction (as in the short $s$-wave junction) the de Gennes states are located at the gap edges, giving rise to the usual SGS at the voltages $eV = 2\Delta/n$. In the $s$-wave case the SGS is due to the combination of onset of the $n$-particle current and resonances in the $n + 1$-particle current (due to an overlap of a bare transmission resonance and a boundary resonance) and the $n + 2$-particle current (two overlapping bare transmission resonances). For the $d_0/d_0$ case [see Fig. 1(a)] the physics behind the SGS is the same, but for two reasons the structure is smeared and suppressed. First, there are no real onsets (the $d$-wave gap has nodes), meaning that the 1-particle current background dominates at all voltages. In addition, the resonances in the higher order currents are not sharp because of angular averaging.

Rotating the right $d$-wave gap away from the $\alpha_R = 0$ orientation, the de Gennes states are moved from the gap edges to zero energy (MGS) for those angles where the gap changes sign after normal reflection at the junc-
Fig. 2. Introducing broadening reveals a current peak near zero bias in the $d_{45}/d_{45}$ junction. Decreasing $\eta$, sharpens the peak and moves it to lower voltage. In the limit $\eta \to 0$ (dashed line) the peak becomes a delta spike at $V = 0$. In (b) we show that particle currents of high order contribute to the peak. The angle averaged junction transparency is $D = 0.026$ and we assume zero temperature.

The bare transmission resonance is then moved and, in addition, the boundary resonances are lost for quasiparticles injected from the right superconductor. This result in a drastically changed SGS: for the $d_0/d_{45}$ junction [see Fig. 1(b)] the only surviving structure is at $eV = \Delta_0$ and it is mainly due to the 2-particle current: an overlap between the bare MGS resonance and boundary resonances (near the left gap edges) produces the peak. This happens also in the $s/d_{45}$ junction. We introduce, on a phenomenological level, inelastic scattering into the problem by adding a small imaginary part $i\eta$ to the quasiparticle energy, which results in broadening of all resonances. For the $d_0/d_{45}$ junction, a small current peak is then revealed near zero bias, as seen in Fig. 1(b). The peak is due to resonances in particle currents of order $n = 2$ and higher and was therefore not discussed in connection to the tunnel limit calculations in Ref. 5 and 6.

When MGS are present on both sides of the junction (the $d_{45}/d_{45}$ junction) boundary resonances can never appear. Consequently current peaks are not seen in the IV-characteristics, leaving only an onset of the current at $eV = \Delta_0$ (due to the bare MGS resonance). Again, introducing broadening reveals a peak near zero bias, see Fig. 2(a). In Fig. 2(b) we show that processes of many orders are in this case contributing to the peak.

In recent experiments on bicrystal grain boundary junctions of hole-doped cuprates a ZBCP was seen for all orientations of the superconductors. No real SGS was seen, only a gap-like structure at $eV = \Delta_0$. Our predictions
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agree with the experimental results, apart from that negative differential conductance was not found in the experiments. In another experiment weak SGS (although not perfectly at $eV = 2\Delta_0/n$) was observed for edge junctions with the $d_0/d_0$ orientation, as we also report here.

4. SUMMARY

Dividing the current into $n$-particle currents, we have shown which physical processes are giving rise to SGS and current peaks near zero bias. For orientations where no MGS are present in the junction the SGS is at $eV = 2\Delta_0/n$ as in the $s$-wave case. When MGS are present on at least one side of the junction SGS is lost and a current peak appears near zero bias (if we include broadening into the formalism). Currents of high orders are contributing to this peak.

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