

Subharmonic gap structure in d -wave superconductors

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We present a self-consistent theory of current-voltage characteristics of d -wave/ d -wave contacts at arbitrary transparency. In particular, we address the open problem of the observation of subharmonic gap structure (SGS) in cuprate junctions. Our analysis shows that (i) the SGS is possible in d -wave superconductors; (ii) the existence of bound states within the gap results in an even-odd effect in the SGS; (iii) elastic scattering mechanisms, like impurities or surface roughness, may suppress the SGS; and (iv) in the presence of a magnetic field the Doppler shift of the Andreev bound states leads to a splitting of the SGS, which is an unambiguous fingerprint of d -wave superconductivity.

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Although the d -wave scenario is emerging as the new paradigm in superconducting cuprates,¹⁻³ there is still lacking a consensus with regards to current transport in superconductor/superconductor (SIS) junctions.⁴ By now it is clear that tunneling in unconventional superconductors is a phase-sensitive technique. An important consequence of an order parameter showing a sign change in different momentum directions is the formation of Andreev bound states at zero energy confined to the surface.^{5,6} One of the consequences of the presence of these bound states is the appearance of a zero-bias conductance peak in the current-voltage characteristics. This peak has been observed in different experiments using superconductor/normal metal (SIN) junctions⁷ and SIS grain boundaries.⁸ However, there is still a controversy related to the observation of the subharmonic gap structure (SGS) in cuprate SIS junctions. Devereaux and Fulde suggested that the Andreev scattering in SNS contacts could be used to identify the symmetry of the order parameter.⁹ Based on their analysis the SGS revealed in different experiments in YBa₂Cu₃O_{7-x} (YBCO) contacts were interpreted as an evidence of the existence of a well-defined nonvanishing gap.^{10,11} After a more detailed but non-self-consistent analysis, different authors concluded that SGS's are weak in d -wave superconductors, since averaging over the anisotropic gap washes out any prominent features.^{12,13} However, there are also more recent experimental reports of SGS's in YBCO edge Josephson junctions,^{14,15} and even in the c -axis tunneling of different cuprate contacts.¹⁶ Auerbach and Altman proposed an alternative interpretation of the appearance of pronounced SGS's in Ref. 15, claiming that this structure is an indication of magnon tunneling that can be explained in the context of the SO(5) theory.¹⁷

In this Communication we present a self-consistent theoretical analysis of the ac Josephson effect in d -wave superconductors. Using quasiclassical methods we determine the local electronic properties of the superconductors in the interface region. This includes effects on the order-parameter (OP) profile and on the local density of states (DOS) by pair breaking caused both by quasiparticle scattering off the interface and off homogeneously distributed impurities in the crystals.¹⁸⁻²³ The I - V characteristics of the d -wave/ d -wave SIS junction are computed using the local surface Green's

functions containing all relevant information of superconducting electrodes and solving the appropriate boundary conditions for a point contact.²⁴ We shall show that, not only does the SGS survive after averaging for all crystal misorientations, but there are qualitatively new features in the I - V characteristics that can only be captured by a truly self-consistent calculation. For instance, there is an even-odd effect in the SGS which originates from processes connecting the zero-energy states with Andreev states formed close to the gap edges. Such an even-odd effect in the differential resistance was reported in YBCO edge junctions by Neshor and Koren.¹⁵ These states are missed in a non-self-consistent calculation where the suppression of the OP close to the interface is neglected. We also show that the SGS in d -wave contacts can be tuned with a magnetic field. The Doppler shift of the Andreev bound states^{20,25} leads to a very peculiar splitting of the SGS, which provides a clear signature of d -wave superconductivity.

In the limit of not too low interface transparency, $D \geq 0.1$, the main feature of the I - V characteristics of conventional SIS contacts is the appearance of a SGS, which consists of a series of maxima in the conductance at voltages $eV = 2\Delta/n$, where Δ is the superconducting gap and n is an integer number. This peculiar structure is due to the occurrence of multiple Andreev reflections (MAR), and is by now well established both theoretically²⁶ and experimentally²⁷ in the case of s -wave superconductors. In this work, our goal is to extend the analysis of the SGS to the case of superconducting cuprates. For this purpose, we consider a voltage-biased contact, consisting of two $d_{x^2-y^2}$ superconductors separated by a single interface of arbitrary transparency. The order parameter on side i , $i=L,R$, is rotated by α_i with respect to the surface normal, and we denote the junction type by the relative crystal orientations as $d_{\alpha_L} - d_{\alpha_R}$. There are several experimental realizations of this system, among which the bicrystal grain-boundary junctions are ideal examples.⁸ We carry out the calculation of the current following the formulation introduced by two of the authors in Ref. 24, and refer the reader to this work for all the technical details. In the case of a constant bias voltage V , one can show that the current oscillates in time with all the harmonics of the Jo-

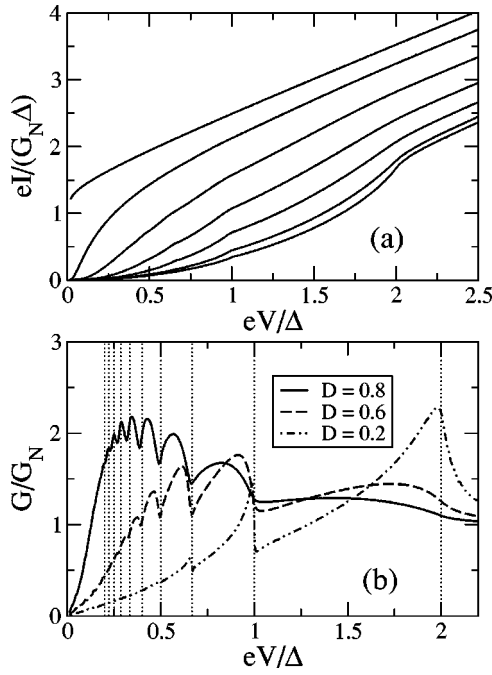


FIG. 1. d_0 - d_0 contact in the clean case: (a) I - V characteristics for different transmissions, from bottom to top $D=0.1, 0.2, 0.4, 0.6, 0.8, 0.95$, and 1.0 . (b) Differential conductance normalized by the normal state conductance G_N . The dotted vertical lines indicate $eV=2\Delta/n$.

sophon frequency, i.e., $I(t)=\sum_m I_m e^{im\phi(t)}$, where $\phi(t)=\phi_0+(2eV/\hbar)t$ is the time-dependent superconducting phase difference. We concentrate ourselves in the analysis of the dc current, denoted from now on as I . Furthermore, we assume that the interface conserves the momentum of the quasiclassical trajectories, which allows us to write the current as a sum over independent trajectory contributions: $I=\frac{1}{2}\int_{-\pi/2}^{\pi/2} d\hat{p}_F I(\hat{p}_F)\cos(\hat{p}_F)$, where \hat{p}_F defines the Fermi surface position. For the angular dependence of the transmission coefficient we use the expression $D(\hat{p}_F)=D\cos^2(\hat{p}_F)/[1-D\sin^2(\hat{p}_F)]$, resulting from a δ -like potential. Here D is the transmission for the trajectory perpendicular to the interface.

Let us start by analyzing the case of a symmetric d_0 - d_0 junction in the clean limit. In this case, the order parameter is constant up to the surface, and there are no bound states for any trajectory. The I - V characteristics of a single trajectory, $I(\hat{p}_F)$, coincide with those of isotropic s -wave superconductors, and exhibit a pronounced SGS at $eV=2\Delta(\hat{p}_F)/n$.²⁶ Since the different trajectories see different gaps, the relevant question is whether the SGS survives after averaging. The answer can be seen in Fig. 1, where both the current and differential conductance are shown for different transmissions. One can clearly see a SGS at $eV=2\Delta/n$, although it is more rounded than in the s -wave case. Also note that SGS's are better defined as minima in the conductance at the subharmonic voltages, i.e., as maxima in the differential resistance. At this point a natural question arises: why is the maximum gap the energy scale revealed in the SGS? The idea is that the jump of the current at the opening of a new MAR scales with the gap of the corresponding trajectory.

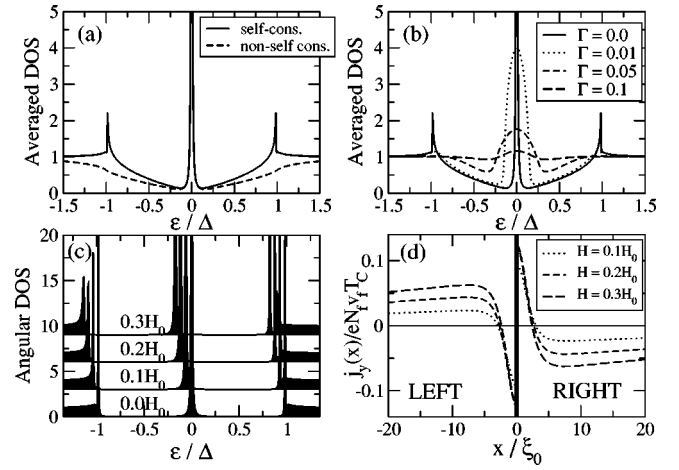


FIG. 2. (a) Angle-averaged local DOS at the interface for a 45° misorientation (clean case): self-consistent and non-self-consistent. (b) Local DOS for a 45° misorientation for different values of the bulk-impurity scattering rate Γ (Born scatterers), measured in units of $2\pi T_C$, where T_C is the critical temperature in the clean case. Δ is the maximum bulk gap for the clean superconductor. (c) Angular resolved DOS for a trajectory $\hat{p}_F=45^\circ$ for different magnetic fields. All the DOS's are normalized to the normal state DOS, N_f . (d) The current density parallel to the interface, j_y , at different applied fields for a $d_{\pi/4}$ - $d_{-\pi/4}$ contact. The distance to the interface, x , is normalized with the clean coherence length ξ_0 .

Therefore, the trajectories with the largest gaps dominate the contribution to the SGS.

Let us now consider the case of a $d_{\pi/4}$ - $d_{-\pi/4}$ junction. In this case, assuming specular quasiparticle scattering at the interface, an Andreev bound state forms at zero energy for every trajectory.⁶ This implies that the surface acts as a pair breaker,¹⁹ and the gap is depressed in the vicinity of the interface, vanishing exactly at the barrier. This order-parameter profile induces the appearance of new bound states at the gap edges for some trajectories,²¹ which are also visible in angle-averaged DOS; see Fig. 2(a). As we show in Fig. 2(a) these gap singularities are not present in the non-self-consistent calculation. This fact has important consequences in the I - V 's characteristics. As shown in Ref. 24, assuming a constant order parameter the most prominent feature of the I - V 's is the appearance of a SGS at $eV=\Delta/n$, instead of in $eV=2\Delta/n$ as in conventional superconductors. Its origin can be understood as follows. Inside the gap the current is dominated by MAR's. In this case there are two types of MAR processes: (a) those which connect the bound states with the gap edges, and (b) the usual ones connecting the gap edges. The first ones give rise to the SGS at $eV=\Delta/n$, while the second could give rise to the series $eV=2\Delta/n$. However, for the non-self-consistent calculation the DOS at the gap edges is rather small [see Fig. 2(a)], and thus, at the opening of this second type of process, their probability is small. In the self-consistent case the main consequence of the presence of the gap singularities is the recovery of the odd terms in the SGS series $eV=2\Delta/n$. The odd terms now appear due to the enhancement of the probability of the MAR's connecting the gap edges. However, the bound states

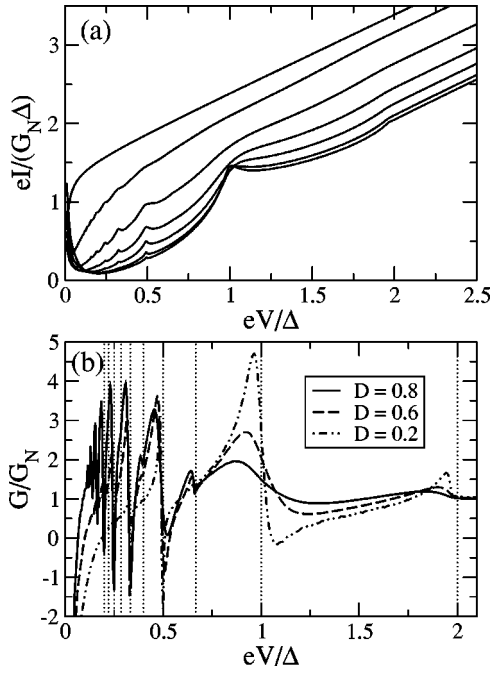


FIG. 3. $d_{\pi/4}$ - $d_{-\pi/4}$ contact in the clean case. (a) I - V characteristics for the same transmissions as in Fig. 2(a). (b) Differential conductance.

at the gap edges do not appear for every trajectory, which weakens the SGS due to these processes. In this sense, in Fig. 3 one can clearly see a difference between the even and odd maxima of the conductance. This even-odd effect was reported in Ref. 15. This result clearly shows the relevance of the self-consistency, even in the ideal clean case.

In d -wave superconductors the order parameter is very sensitive to scattering from nonmagnetic impurities and surface roughness. In particular, it is known that these elastic scattering mechanisms provide an intrinsic broadening for the zero-energy bound states (ZEBS).^{22,23} For the case of Born scatterers this broadening is $\propto \sqrt{\Gamma}\Delta$, where $\Gamma = 1/2\tau$ is the effective pair-breaking parameter locally at the surface. This is illustrated in Fig. 2(b) for the case of bulk impurities. The natural question now is: what is the influence of the broadening of the ZEBS in the SGS? In Fig. 4 we show the differential conductance of a $d_{\pi/4}$ - $d_{-\pi/4}$ junction for different values of the bulk-impurity scattering rate. Note that as the elastic scattering rate increases the SGS disappears, which can be understood as follows: the increase of density of states in the gap region enhances the probability of single-quasiparticle processes, producing the subsequent reduction of the probability of the Andreev processes, which in turn leads to the suppression of the SGS.

Probably the clearest signature of d -wave superconductivity in the SGS is its evolution with magnetic field. It is known that a magnetic field perpendicular to the ab plane, $\mathbf{H} = H\hat{z}$, leads to a Doppler shift in the continuum excitations given by $\mathbf{v}_F \cdot \mathbf{p}_s$, where the condensate momentum is $\mathbf{p}_s = -(e/c)A(x)\hat{y}$, with A the self-consistently determined vector potential.²⁰ As shown in Fig. 2(c), this means that the Andreev bound states are shifted to an energy which, in the

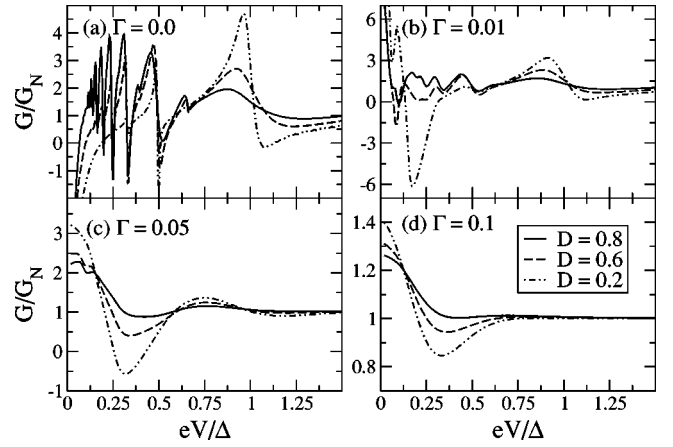


FIG. 4. Differential conductance for a $d_{\pi/4}$ - $d_{-\pi/4}$ contact for different values of the bulk-impurity scattering rate Γ . Transmission rates are as in Fig. 2(a).

limit of a large ratio λ/ξ_0 , can be estimated to be $\epsilon_b(\hat{\mathbf{p}}_F) = (e/c)v_F H \lambda \sin \hat{\mathbf{p}}_F$, λ being the ab -plane penetration depth. We shall use a natural field scale set by a screening current of order the bulk critical current, $H_0 = c\Delta/ev_F\lambda$, which is of the order of a Tesla.²⁰ As can be seen in Fig. 2(d), the screening currents flow parallel to the interface and in opposite directions in both electrodes, which means that the trajectory resolved DOS's of the left and right superconductors are shifted by $2\epsilon_b(\hat{\mathbf{p}}_F)$ relative to each other. This shift modifies the threshold voltages of MAR's starting and ending in different electrodes, leading to the splitting of the peaks with an odd order n in the SGS. Conversely, since the magnetic field produces a rigid shift of the spectrum, the threshold voltages of those MAR's starting and ending in the same electrode are not modified. This means that the positions of the peaks with an even order n in the SGS remain unchanged. This fact gives rise to a rich SGS in the trajectory-resolved current, which consists of conductance peaks at the following voltage positions: (a) $[2\Delta(\hat{\mathbf{p}}_F) \pm 2\epsilon_b(\hat{\mathbf{p}}_F)]/n$, with n odd, due to MAR's connecting the gap edges of the left and right electrodes (the signs \pm correspond to electron and hole processes); (b) $[\Delta(\hat{\mathbf{p}}_F) \pm 2\epsilon_b(\hat{\mathbf{p}}_F)]/n$, with n odd, due to MAR's connecting the bound states and the gap edges of different

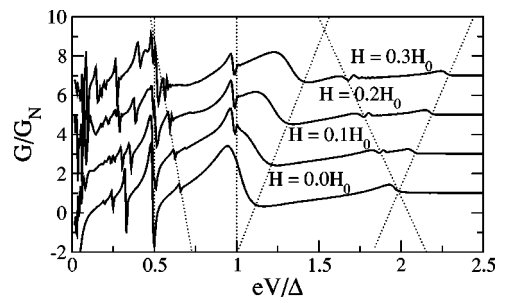


FIG. 5. Differential conductance of a clean $d_{\pi/4}$ - $d_{-\pi/4}$ junction with $D=0.4$ and different values of the magnetic field. The curves have been vertically displaced for clarity, and dotted lines have been added to guide the eye.

electrodes; (c) $2\Delta(\hat{p}_F)/n$, with n even, due to MAR's connecting the gap edges of the same electrode; (d) $\Delta(\hat{p}_F)/n$, with n even, due to MAR's connecting the bound states and the gap edges of the same electrode. Finally, there is also structure at $eV=2\epsilon_b(\hat{p}_F)/n$, with n odd, due to MAR's connecting the bound states.

After doing the angle average most of these features are still clearly visible. This is illustrated in Fig. 5, where we show the differential conductance of a $d_{\pi/4}-d_{-\pi/4}$ junction with transmission $D=0.4$ for different values of the magnetic field. Starting at large voltages, the weak structure seen at 2Δ splits with applied field. Around $eV=\Delta$ there are both type (b) and type (c) processes, leading to a maximum at $eV=\Delta$, unaffected by the applied field, as well as a field shift of the dip just above Δ . The field dependence of the differential conductance is most clearly resolved at larger biases, $eV\geq\Delta/2$, as the marks of the various processes begin to overlap at small bias. What is important to note is that it is still the bulk maximum gap that gives the characteristic en-

ergy scale for the SGS. The effect of the Doppler shift on the SGS or the differential conductance is only prominent in junctions with a sizable misorientation. For junctions close to the d_0-d_0 case, the main contribution to the SGS comes from trajectories close to perpendicular incidence, i.e., with $\sin\hat{p}_F\sim 0$ and thus having a vanishing Doppler shift.

In summary, we have presented a self-consistent analysis of the I - V characteristics of d -wave/ d -wave contacts at high transparencies. We have shown that it is possible to observe SGS for all crystal misorientations. We predict that the presence of bound states inside the gap gives rise to two new qualitative effects in the SGS: (a) an even-odd effect, and (b) a very peculiar splitting in an external magnetic field. These features are unique hallmarks of the d -wave scenario, and we hope that our analysis will trigger off a more detailed experimental study of the SGS in cuprate Josephson junctions.

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