PHYSICAL REVIEW B **67**, 100503(R) (2003)

Phase-breaking effects in superconducting heterostructures

Mikhail Belogolovskii
Donetsk Physical and Technical Institute, National Academy of Sciences of Ukraine, Donetsk 83114, Ukraine
(Received 3 December 2002; published 19 March 2003)

We present a theoretical analysis of a zero-temperature charge transport in a double-barrier structure formed by normal and superconducting electrodes with a partially dephasing mesoscopic region between two insulating layers. A scattering theory approach permits us to investigate a crossover from phase-coherent to sequential carrier transmission caused by inelastic phase-randomizing events. For a weakly transmitting junction, we derive a simple expression describing their effect on the superconducting tunneling density of states. For moderate-strength barriers, numerically simulated conductance-versus-voltage spectra exhibit a double-peaked structure in the case of *s*-wave superconductors and a dramatic reduction of a zero-bias maximum for *d*-wave pairing.

DOI: 10.1103/PhysRevB.67.100503 PACS number(s): 74.78.Fk, 73.23.−b, 72.10.−d, 03.65.Yz

Because of the gapped energy spectrum of a superconductor *S*, current *I* versus voltage *V* characteristics of mesoscopic devices formed by normal *N*, and *S* regions are strongly nonlinear and their measurement is one of the most high-resolution probes for analyzing quasiparticle spectra in *S* electrodes.[1] At the same time, the method is known to be an extremely interface-sensitive technique, with curves strongly governed by the nature of a transition region between *N* and *S* electrodes. Most of the theoretical results in this field have been obtained under the assumption of quantum-coherent transport.[2] What is less established is the effect of incoherent scattering events. After the work of Dynes *et al.*,[3] it is usually considered by introducing a damping parameter Γ into the normalized quasiparticle density of states $N_{\mathrm{T}}(\varepsilon)$. This paper is motivated by recent findings that cannot be described by the Dynes formula obtained from an entirely *ad hoc* procedure and valid only for an *s*-wave superconductor very close to its gap value Δ_s. The experiments were carried out for contacts with doped copper and manganese perovskites, where a weak Cu-O or Mn-O bond oxygen easily outdiffuses from the surface reducing the oxygen stoichiometry near the intrinsic metal oxide surface.[4] As it was argued in Ref. 5, it should result in an enhancement of antiferromagnetic spin fluctuations. Strong inelastic scatterings of transferring carriers from excitations located in and/or near the insulating layer in a tunnel device not only modify the background characteristic and smear $N_{\mathrm{T}}(\varepsilon)$, but also produce gradual changes of the gap features in conductance spectra. It follows, in particular, from our experiment for a cuprate $LaBa_2Cu_3O_{7-x}$ (Ref. 6) that was designed to directly address the issue of environment-induced decoherence. Another nonconventional finding is a double-peaked structure in the lead gap region in conductance spectra for contacts between a manganite and a superconducting Pb [the inset (a) in Fig. 5 of Ref. 7]. As it will be clarified below, such anomalies can arise as an effect of a near-interface decohering mechanism on the carrier transmission across a superconductng heterojunction. The aim of this work is to present a theoretical analysis of the impact of inelastic scatterings, stressing the way where and how they can reveal themselves.

What we want to study, in fact, is a continuous transition between limiting regimes of completely coherent charge transmission and pure macroscopic sequential transport in a heterogeneous double-barrier structure with a superconducting electrode. In order to bridge between the two extreme cases, we refer to the paper by Büttiker[8] where such a crossover was discussed for a normal N-I_1-n-I_2-N device with a thin *n* interlayer with inelastic phase-destroying processes and two barriers I_1 and I_2 (the effect of incoherent scattering on transport and noise in other normal structures was studied in Ref. 9 and papers cited in this work). In the following, we show how the results of Ref. 8 can be extended for a two-terminal device where one of *N* electrodes is replaced with a superconductor. The main new issues introduced in the scheme[8] are (i) Andreev reflection events when electrons incident from the normal side are rejected back by the pairing potential as time-reversed particles (holes) with phases related through the macroscopic phase of a superconductor,[10] and (ii) a three-dimensional generalization important for anisotropic *S* electrodes, in particular, those with a *d*-wave order parameter symmetry. It should be noted that an effect of phase-breaking events on the charge transport in a one-dimensional junction with an *s*-wave superconductor was studied in the paper of Mortensen *et al.*[11] but only for a zero-bias conductance whereas for our purposes just finite voltages are important. Concerning the three-dimensional generalization, up to our knowledge, it has not been done yet.

In a two-terminal three-dimensional N-I_1-n-I_2-S structure with a partially dephasing interlayer *n*, the current *I* is a sum of two noninterfering contributions arisen from phase-coherent and incoherent transferring channels (Fig. 1). We suppose that a carrier entering the interlayer has a certain probability ζ to undergo phase-destroying scatterings determining a finite value l_{in} of the carrier inelastic mean free path in an *n* electrode of a thickness *l*. whereas with a probability $1-\zeta$ a charge transfers it without any interaction with a phase-randomizing agent. The first effect is modeled by considering the interlayer as consisting of two parts with an inelastic phase-randomizing source between them. Then the charge sequential transmission consists of three stages: it transfers the barrier I_1 crossing the N-I_1-n junction,

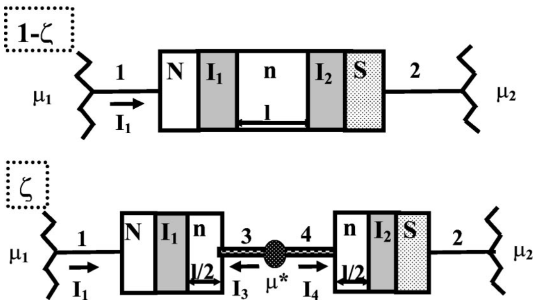

FIG. 1. A sketch of a two-probe heterostructure considered illustrating the Büttiker approach (Ref. 8) to dephasing effects in a double-barrier device. The upper scheme corresponds to the case of charge coherent transmission across the n interlayer (with the probability $1-\zeta$). The bottom one illustrates sequential transmission of a charge losing its phase in the interlayer center shown by a darkened circle.

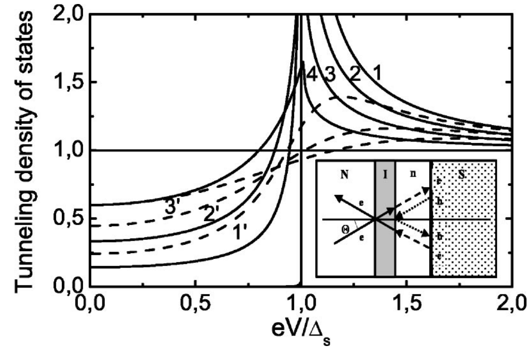

FIG. 2. Tunneling density of states of a one-dimensional s-wave superconductor for a dephasing parameter ζ equal to 0, 0.25, 0.5, 0.75 (curves 1, 2, 3, and 4, respectively) compared with the Dynes formula (Ref. 3) $N_T(\varepsilon)=\mathrm{Re}[(\varepsilon-i\Gamma)/\sqrt{(\varepsilon-i\Gamma)^2-\Delta_s^2}]$ with a damping parameter $\Gamma=0.25$, 0.5, 0.75 (curves $1'$, $2'$, and $3'$, respectively). The inset: scattering processes in a tunneling junction consisting of a normal injector, low-transparent barrier, a normal-metal interlayer of a vanishing thickness, and a superconductor.

''forgets'' its phase in a conductor connecting two intermediate regions (it is shown in Fig. 1 with a darkened circle) and transmits the n-I_2-S interface. The three-step process allows the leakage of current carriers into the energy region $eV<\Delta_s$ even if it is forbidden for a charge in a purely phase-coherent channel. To proceed with a scatteringlike technique, we introduce two auxiliary leads 3 and 4 shown in Fig. 1 and a steplike nonequilibrium distribution function with a chemical potential $\mu^\star$ in the interface region (see the bottom curve in Fig. 4 in Ref. 9). In the general case, $\mu^\star$ is a function of the applied bias $V=(\mu_1-\mu_2)/e$ and should be found from a natural condition of coincidence of currents incoming and outcoming from the interlayer $I_3=I_4$.[8] In the following, we limit ourselves to a zero-temperature case because thermal dephasing cannot be accounted for by this model (see the discussion in Ref. 11) and to a planar structure in a quasi-one-dimensional geometry with the x axis as the interface normal.

To calculate a current I_m in an m lead in the normal side ($m=1$, 3, and 4), we use the Landauer-Büttiker formalism applied to superconducting structures[12]

$$I_m(V)=\mathrm{const}\int d\Omega\,\cos\Theta\left[\int_0^{\mu_1}G_{m,1}(\varepsilon,\Theta)d\varepsilon+\int_0^{\mu^\star(V)}\{G_{m,3}(\varepsilon,\Theta)+G_{m,4}(\varepsilon,\Theta)\}d\varepsilon\right],\quad(1)$$

where the injection angle Θ between an electron wave vector $\mathbf{k}_e$ and the x axis is shown in Fig. 2, the reference potential of a superconductng side is put to zero, $\mu^\star(V)$ is a Θ-independent quantity, and

$$G_{m,n}(\varepsilon,\Theta)=\delta_{mn}-|R_{mn}^{ee}(\varepsilon,\Theta)|^2+|R_{mn}^{he}(\varepsilon,\Theta)|^2.\quad(2)$$

$R_{mn}^{ee}(\varepsilon,\Theta)$ and $R_{mn}^{he}(\varepsilon,\Theta)$ are angle-dependent probability amplitudes for an electron entering the lead m to be scattered into the nth lead as an electron and as a hole, respectively. In Eq. (1), we do not write an explicit expression for the coefficient const as it will be canceled in the normalized conductance spectra equal to the ratio of $dI_1(V)/dV$ in S and N states.

Let us now take into the account possible incoherent scattering events that are happened with a probability $\zeta(\Theta)=1-\exp[-l/(l_{\mathrm{in}}\cos\Theta)]$ supposed to be energy independent. For a superconducting order parameter the usual step-function approximation will be assumed and the self-consistency of its spatial variation will be ignored that is valid for an s-wave pairing and for biases near $V=0$ in the d-wave case. Probability amplitudes for $m,n=1$, 3, and 4 can be found by summarizing all possible charge paths including Andreev transformations (as it was done for a phase-coherent contribution in Ref. 13):

$$R_{mn}^{ee}(\Theta)=s_{mn}^{e}(\Theta)+\frac{s_{m2}^{e}(\Theta)r^{he}(\Theta)s_{22}^{h}(\pi+\Theta)r^{eh}(-\Theta)s_{2n}^{e}(\pi-\Theta)}{1-s_{22}^{e}(\pi-\Theta)r^{he}(\Theta)s_{22}^{h}(\pi+\Theta)r^{eh}(-\Theta)},$$

$$R_{mn}^{he}=\frac{s_{m2}^{e}(\Theta)r^{he}(\Theta)s_{2n}^{h}(\pi+\Theta)}{1-s_{22}^{e}(\pi-\Theta)r^{he}(\Theta)s_{22}^{h}(\pi+\Theta)r^{eh}(-\Theta)}.\quad(3)$$

Here the energy dependencies of all quantities are omitted, r^{he} and r^{eh} are scattering characteristics for an electron retroreflected into a hole and vice versa[10]

$$r^{he(eh)}(\Theta)=\frac{\varepsilon-\mathrm{sgn}(\varepsilon)\sqrt{\varepsilon^2-|\Delta(\Theta)|^2}}{|\Delta(\Theta)|}e^{\mp i\phi(\Theta)}, \qquad (4)$$

where $\phi(\Theta)$ is the order parameter phase, $\Delta(\Theta)$ is a constant Δ_s for an s-wave superconductor and for a d-wave pairing $\Delta(\Theta)=\Delta_d\cos[2(\Theta-\Theta_0)]$ with the misorientation angle Θ_0 between the surface normal and the crystalline axis along which the order parameter reaches maximum. Probability amplitudes for scatterings between m and n leads in the junction driven into a normal state s_{mn} can be found by the same scattering procedure as in Ref. 8. To show how they can be derived in an informal way, we present an example for s_{11}^e

$$\begin{aligned} s_{11}^e &= r_1^e+t_1^e a r_2^e a t_1^e + t_1^e a r_2^e a r_1^e a r_2^e a t_1^e+\cdots \\ &= r_1^e+\frac{a^2 t_1^e r_2^e t_1^e}{1-a^2 r_1^e r_2^e}, \end{aligned} \qquad (5)$$

where each transfer across the n interlayer without loss of phase memory contributes with an amplitude $a=\sqrt{1-\zeta}\exp(i\chi^e)$, $\chi^e=k_e l\cos\Theta$ is the phase shift acquired by an electron traveling between two interlayer boundaries, $t_{1,2}^e$ and $r_{1,2}^e$ are transmission and reflection amplitudes for insulating layers I_1 and I_2, respectively. In numerical simulations the barriers are modeled by repulsive potentials $U_{1,2}(x)$ that are characterized by their dimensionless strengths[14] $Z_{1,2}=k_F\int U_{1,2}(x)dx/\varepsilon_F$, with Fermi energy ε_F and wave number k_F.

Before to go to a common case of a double-barrier structure, let us discuss a more simple tunnelinglike problem. It is widely accepted now that zero-bias conductance peaks in high-T_c superconductors arise from the formation of midgap surface states[15] as a result of a sign change of the d-wave pair potential. We will show that tunneling characteristics of an s-wave superconductor can be also interpreted as a surface effect. We introduce (see the inset in Fig. 2) a normal auxiliary interlayer n with a vanishing thickness into a two-terminal N-I-s-wave S junction with a potential barrier of a very low transparency T, i.e., with a very great strength Z. For a zero-temperature phase-coherent contribution, we have a region of vanishing conductivity up to $V=\Delta_s/e$ with a huge peak at the gap edge. But it is not so if a significant amount of incoherent scatterings is present in the n layer. Then the three-step process described above allows the leakage of carriers into the energy region $V<\Delta_s/e$. A charge sequentially transfers the N-I-n junction without any restrictions and after that the n/S interface (the latter process contains no barrier and the transmission is always able by converting a normal current into the superconducting one). In the weak-transmitting (tunneling) limit, the ratio of the n/S interface resistance to that of the all-normal N-I-n device is vanishing and only terms of the order of T should be retained in all quantities. We put $\mu^\star$ to zero and $r_1=-1$ in Eq. (5) to consider only one-particle transmissions across the barrier I.

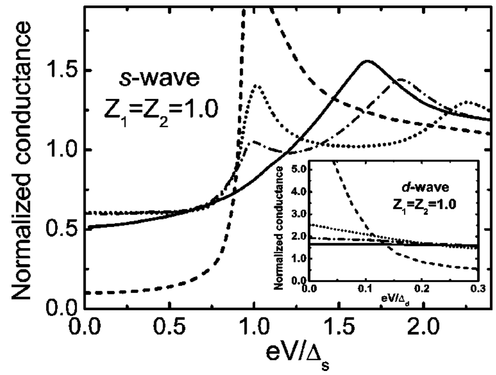

FIG. 3. Decoherence effect on the normalized differential conductance versus voltage of a double-barrier junction with an s-wave superconductor and two identical barriers of a strength $Z=1.0$ for completely coherent charge transmission (dashed curve), incoherent transport (solid line), and intermediate cases with $l/l_{\rm in}$ equal to 0.5 and 1.0 (dotted and dash-dotted curves, respectively). Inset: the same characteristics for a (110) oriented d-wave superconductor ($\Theta_0=\pi/4$).

After some algebra, we obtain the normalized tunneling conductance spectrum that for one-dimensional geometry looks as

$$N_{\rm T}(\varepsilon)=\mathrm{Re}\left[\frac{1+(1-\zeta)r^{he}r^{eh}}{1-(1-\zeta)r^{he}r^{eh}}\right]. \qquad (6)$$

Refer now to the work of Schopohl[16] who showed that the local density of states of a superconductor is simply a rational function of solutions of modified quasiclassical Eilenberger equations. Combining Eqs. (12) and (68) from Ref. 16, we get the same result (6) but for $\zeta=0$. Our simulation data for $\zeta\neq 0$ are presented in Fig. 2, where they are compared with the behavior predicted by the Dynes equation.[3] We emphasize again that the latter formula was obtained from an *ad hoc* procedure and was proposed to describe the impact of inelastic scatterings inside a superconductor. It results in a gradual smearing of $N_{\rm T}(\varepsilon)$ with a shift of a maximum to higher biases, whereas in the case of phase-randomizing effects inside a normal transferring region the main effect is the spectrum suppression without any shift of the conductance peak. This difference can serve as an indication of where the dephasing agent is located.

Let us return to a three-dimensional case of arbitrary moderate-strength barriers and present results of numerical simulations. In this communication we assume that the interlayer thickness l is vanishing but the ratio $l/l_{\rm in}$, that serves us as a parameter characterizing an impact of dephasing effects is finite. Figure 3 shows the data for two identical barriers of a strength $Z=1.0$. Without any decoherence, for an s-wave superconductor we obtain a well known, from the Blonder-Tinkham-Klapwijk paper,[14] curve with a peak at $V=\Delta_s/e$ (a dashed curve in the main panel). When the impact of incoherent-scattering events increases, a second peak appears at high biases and for a completely sequential tunneling only a shifted maximum remains in the spectrum. It is interesting that the position of a high-voltage peak depends

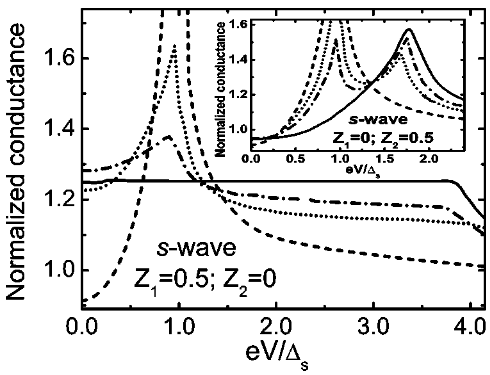

FIG. 4. Decoherence effect on the normalized differential conductance versus voltage of a double-barrier heterostructure with an *s*-wave superconductor and two barriers of strengths $Z_1=0.5$ and $Z_2=0$ for completely coherent charge transmission (dashed curve), incoherent transport (solid line), and intermediate cases with l/l_{in} equal to 0.5 and 1.0 (dotted and dash-dotted curves, respectively). Inset: the same characteristics for $Z_1=0$ and $Z_2=0.5$.

on the dephasing strength and for intermediate ratios l/l_{in} a local maximum appears even at higher voltages than for the incoherent transmission. Switching on incoherent scatterings destroys interference effects forming a *d*-wave superconductor zero-bias conductance peak that is especially pronounced for $\Theta_0=\pi/4$.[15] The inset in Fig. 3 demonstrates how this feature is suppressed with increasing decoherence impact.

Figure 4 shows spectra of an *s*-wave superconductor for two nonidentical barriers. The initial characteristic for a phase-coherent transmission is the same (compare dashed curves in the main panel and in the inset) but for finite l/l_{in} two sets of data differ in a principal way. If the right barrier is absent (the main panel of Fig. 4), we have a tunnellike maximum at the superconducting gap superposed on a conductance step, a feature of a direct normal-superconducting contact. But in contrast to ideal Andreev measurements where it occurs at Δ_s/e and the suppression factor is 2, the step is shifted to higher voltages and the ratio of conductances at zero and high biases is significantly less than 2. The inset in Fig. 4 shows the effect of an inverse sequence of barriers when the principal behavior of conductance spectra is similar to that depicted in the main panel of Fig. 3.

The phenomenological approach developed here can be extended to treat decoherence phenomena in all-superconducting junctions (without delving into details of carrier interactions). Besides of a pure scientific interest, it can be useful for designing quantum circuits relied on principles of quantum superpositions.[17].

The author acknowledges M. Grajcar, V. Gokhfeld, and P. Seidel for helpful suggestions and useful discussions.

[1] E.L. Wolf, *Principles of Electron Tunneling Spectroscopy* (Oxford University Press, New York, 1985).

[2] C.W.J. Beenakker, Rev. Mod. Phys. **69**, 731 (1997).

[3] R.C. Dynes, V. Narayanamurti, and J.P. Garno, Phys. Rev. Lett. **41**, 1509 (1978).

[4] M. Naito, H. Yamamoto, and H. Sato, Physica C **335**, 201 (2000).

[5] A. Plecenik, M. Grajcar, P. Seidel, S. Takács, A. Matthes, M. Zuzcak, and Š. Beňačka, Physica C **301**, 234 (1998).

[6] M. Belogolovskii, Yu. Revenko, V. Svistunov, M. Grajcar, and P. Seidel, Physica C **367**, 218 (2002).

[7] V.Yu. Tarenkov, A.I. D'yachenko, and V.N. Krivoruchko, Zh. Éksp. Teor. Fiz. **120**, 205 (2001) [JETP **93**, 180 (2001)].

[8] M. Büttiker, IBM J. Res. Dev. **32**, 63 (1988).

[9] C. Texier and M. Büttiker, Phys. Rev. B **62**, 7454 (2000).

[10] A.F. Andreev, Zh. Éksp. Teor. Fiz. **46**, 1823 (1964) [Sov. Phys. JETP **19**, 1228 (1964)].

[11] N.A. Mortensen, A.-P. Jauho, and K. Flensberg, Superlattices Microstruct. **28**, 67 (2000).

[12] C.J. Lambert, V.C. Hui, and S.J. Robinson, J. Phys.: Condens. Matter **5**, 4187 (1993); M.P. Anantram and S. Datta, Phys. Rev. B **53**, 16 390 (1996).

[13] M. Belogolovskii, M. Grajcar, P. Kúš, A. Plecenik, Š. Beňačka, and P. Seidel, Phys. Rev. B **59**, 9617 (1999).

[14] G.E. Blonder, M. Tinkham, and T.M. Klapwijk, Phys. Rev. B **25**, 4515 (1982).

[15] C.-R. Hu, Phys. Rev. Lett. **72**, 1526 (1994).

[16] N. Schopohl, in *Quasiclassical Methods in the Theory of Superconductivity and Superfluidity*, edited by D. Rainer and J.A. Sauls, Bayreuth, Germany, 1998, cond-mat/9804064 (unpublished).

[17] C.H. van der Wal, F.K. Wilhelm, C.J.P.M. Harmans, and J.E. Mooij, cond-mat/0211664 (unpublished).