Effect of magnetic pair breaking on Andreev bound states and resonant supercurrent in quantum dot Josephson junctions

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We propose a model for resonant Josephson tunneling through quantum dots that accounts for Cooper pair-breaking processes in the superconducting leads caused by a magnetic field or spin-flip scattering. The pair-breaking effect on the critical supercurrent I_c and the Josephson current-phase relation $I(\varphi)$ is largely due to the modification of the spectrum of Andreev bound states below the reduced (Abrikosov-Gorkov) quasiparticle gap. For a quantum dot formed in a quasi-one-dimensional channel, both I_c and $I(\varphi)$ can show a significant magnetic-field dependence induced by pair breaking despite the suppression of the orbital magnetic-field effect in the channel. This case is relevant to recent experiments on quantum dot Josephson junctions in carbon nanotubes. Pair-breaking processes are taken into account via the relation between the Andreev scattering matrix and the quasiclassical Green functions of the superconductors in the Usadel limit.

I. INTRODUCTION

Since its discovery, the Josephson effect[1] has been studied for a variety of superconducting weak links.[2–4] The research has recently entered another phase with the experimental realization of quantum dot weak links, exploiting electronic properties of finite-length carbon nanotubes coupled to superconducting leads.[5–7] In particular, since its theoretical prediction,[8–10] resonant Josephson tunneling through discrete electronic states has been observed in carbon nanotube quantum dots.[6] As demonstrated in Refs. 6 and 7, the quantum dot junctions exhibit transistorlike functionalities, e.g., a periodic modulation of the critical current with a gate voltage tuning successive energy levels in the dot on- and off-resonances with the Fermi energy in the leads. This property has already been implemented in a recently proposed carbon nanotube superconducting quantum interference device[11] with possible applications in the field of molecular magnetism.

Motivated by the experiments on resonant Josephson tunneling, in this paper, we investigate theoretically how robust it is with respect to pair-breaking perturbations in the superconducting leads. Cooper pair breaking can be induced by a number of factors, e.g., by paramagnetic impurities,[12] an external magnetic field,[13] or by structural inhomogeneities producing spatial fluctuations of the superconducting coupling constant.[14] It can cause a drastic distortion of the Bardeen-Cooper-Schrieffer (BCS) superconducting state, which manifests itself in the smearing of the BCS density of states leading to gapless superconductivity.[12,13]

While the pair-breaking effect on bulk superconductivity is now well understood, its implications for quantum superconducting transport have been studied to a much lesser extent (see, e.g., Refs. 4 and 15 and 16) which, to our knowledge, does not cover Josephson tunneling through quantum dots. On the other hand, in low-dimensional systems, pair-breaking effects may be observable in a common experimental situation when, for instance, a carbon nanotube weak link is subject to a magnetic field. Since the orbital field effect in the quasi-one-dimensional channel is strongly suppressed,

pair breaking in the superconducting leads can be the main source of the magnetic-field dependence of the Josephson current. This situation is addressed in our work.

The influence of pair breaking on the Josephson current cannot, in general, be accounted for by mere suppression of the order parameter in the superconducting leads. As was pointed out in Ref. 15, it is a more subtle effect involving the modification of the spectrum of current-carrying states in the junction, in particular, the subgap states usually referred to as Andreev bound states (ABSs).[10,17] We illustrate this idea for quantum dot junctions in the simple model of a short superconducting constriction with a scattering region containing a single Breit-Wigner resonance near the Fermi energy. The Josephson current is calculated using the normal-state scattering matrix of the system and the Andreev reflection matrix.[9,10] Unlike Refs. 9 and 10, we focus on dirty superconductors for which the Andreev matrix can be quite generally expressed in terms of the quasiclassical Green functions,[18] allowing us to treat pair breaking in the superconducting leads nonperturbatively. Although we account for all energies (below and above the Abrikosov-Gorkov gap Δ_g), it turns out that the behavior of the Josephson current can be well understood in terms of a pair-breaking-induced modification of the ABS, which depends sensitively on the relation between the Breit-Wigner resonance width Γ and the superconducting pairing energy Δ. Both the critical supercurrent and the Josephson current-phase relation are analyzed under experimentally realizable conditions.

II. MODEL AND FORMALISM

We consider a junction between two superconductors S_1 and S_2 adiabatically narrowing into quasi-one-dimensional ballistic wires S_1' and S_2' coupled to a normal conductor N (Fig. 1). The transformation from the superconducting electron spectrum to the normal-metal one is assumed to take place at the boundaries $S_1 S_1'$ and $S_2' S_2$, implying the pairing potential of the form[2] $\Delta(x) = \Delta e^{i\varphi_1}$ for $x < -L/2$, $\Delta(x) = 0$ for $|x| \leqslant L/2$, and $\Delta(x) = \Delta e^{i\varphi_2}$ for $x > L/2$ with the order param-
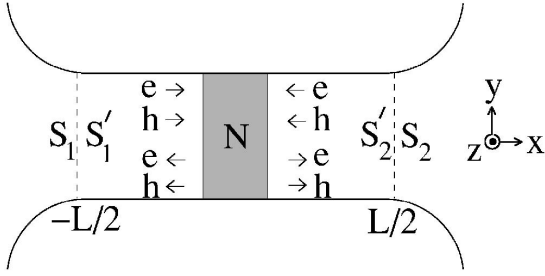
FIG. 1. Scheme of a superconducting constriction with a normal scattering region N. The arrows indicate the electrons (e) and holes (h) incident on and outgoing from N.

eter phase difference $\varphi \equiv \varphi_2 - \varphi_1$ and the junction length $L \ll \hbar v_F / \Delta$ (v_F is the Fermi velocity in $S_{1,2}$).

The Josephson coupling can be interpreted in terms of the Andreev process,[19] whereby an electron is retroreflected as a Fermi-sea hole from one of the superconductors with the subsequent hole-to-electron conversion in the other one. Such an Andreev reflection circle facilitates a Cooper pair transfer between S_1 and S_2. Normal backscattering from disordered superconducting bulk into a single-channel junction is suppressed due to the smallness of the junction width compared to the elastic mean free path ℓ. The N region in the middle of the junction is thus supposed to be the only source of normal scattering. In such type of weak links, the Josephson current is conveniently described by the scattering matrix expression of Refs. 10 and 20 that can be written at finite temperature T as the following sum over the Matsubara frequencies $\omega_n = (2n+1)\pi k_B T$ (Ref. 20):

$$I = -\frac{2e}{\hbar} 2k_B T \frac{\partial}{\partial \varphi} \sum_{n=0}^{\infty} \ln \mathrm{Det}[\hat{1} - \hat{s}_A(E)\hat{s}_N(E)]_{E=i\omega_n}. \quad (1)$$

Here, $\hat{s}_N(E)$ is a 4×4 unitary matrix relating the incident electron and hole waves on the N region to the outgoing ones (Fig. 1). It is diagonal in the electron-hole space,

$$\hat{s}_N = \begin{bmatrix} s_{ee}(E) & 0 \\ 0 & s_{hh}(E) \end{bmatrix}, \quad s_{ee}(E) = \begin{bmatrix} r_{11}(E) & t_{12}(E) \\ t_{21}(E) & r_{22}(E) \end{bmatrix}.$$

The matrix $s_{ee}(E)$ describes electron scattering in terms of the reflection and transmission amplitudes, $r_{jk}(E)$ and $t_{jk}(E)$, for a transition from S'_k to S'_j ($j,k=1,2$). The hole scattering matrix is related to the electron one by $s_{hh}(E)=s^*_{ee}(-E)$. The Andreev scattering matrix $\hat{s}_A(E)$ is off-diagonal in the electron-hole space,

$$\hat{s}_A = \begin{bmatrix} 0 & s_{eh}(E) \\ s_{he}(E) & 0 \end{bmatrix}, \quad (2)$$

where the 2×2 matrices $s_{he}(E)$ and $s_{eh}(E)$ govern the electron-to-hole and hole-to-electron scatterings of the superconductors. Equation (1) is valid for all energies as long as normal scattering from the superconductors is absent.[10,20]

In Ref. 10, the Andreev matrix [Eq. (2)] was obtained by matching the solutions of the Bogolubov–de Gennes equations in the wires $S'_{1,2}$ to the corresponding solutions in impurity-free leads. Gorkov's Green function formalism in

combination with the quasiclassical theory[21] allows one to generalize the results of Ref. 10 to dirty leads with a short mean free path $\ell \ll \hbar v_F / \Delta$. In the latter case, the matrices $s_{he}(E)$ and $s_{eh}(E)$ can be expressed in terms of the quasiclassical Green functions of the superconductors as follows:[18]

$$s_{eh} = \begin{bmatrix} \dfrac{f_1(E)}{g_1(E)+1} & 0 \\ 0 & \dfrac{f_2(E)}{g_2(E)+1} \end{bmatrix},$$

$$s_{he} = \begin{bmatrix} \dfrac{-f_1^\dagger(E)}{g_1(E)+1} & 0 \\ 0 & \dfrac{-f_2^\dagger(E)}{g_2(E)+1} \end{bmatrix}.$$

Here, $g_{1,2}$ and $f_{1,2}$ ($f_{1,2}^\dagger$) are, respectively, the normal and anomalous retarded Green functions in $S_{1,2}$. These matrices are diagonal in the electrode space due to a local character of Andreev reflection in our geometry.

Neglecting the influence of the narrow weak link on the bulk superconductivity, we can use the Green functions of the uncoupled superconductors $S_{1,2}$ described by the position-independent Usadel equation,[21]

$$\left[E\hat{\tau}_3 + \hat{\Delta}_j + \frac{i\hbar}{2\tau_{pb}} \hat{\tau}_3 \hat{g}_j \hat{\tau}_3, \hat{g}_j \right] = 0, \quad (3)$$

with the normalization condition $\hat{g}_j^2 = \hat{\tau}_0$ for the matrix Green function,

$$\hat{g}_j = \begin{bmatrix} g_j & f_j \\ f_j^\dagger & -g_j \end{bmatrix}, \quad \hat{\Delta}_j = \begin{bmatrix} 0 & \Delta e^{i\varphi_j} \\ -\Delta e^{-i\varphi_j} & 0 \end{bmatrix}, \quad j=1,2.$$

Here, $\hat{\tau}_0$ and $\hat{\tau}_3$ are the unity and Pauli matrices, respectively, and $[\cdots,\cdots]$ denotes a commutator. Equation (3) accounts for a finite pair-breaking rate τ_{pb}^{-1} whose microscopic expression depends on the nature of the pair-breaking mechanism. For instance, for thin superconducting films in a parallel magnetic field, $\tau_{pb}^{-1}=(v_F\ell/18)(\pi dB/\Phi_0)^2$ (Ref. 13), where d is the film thickness and Φ_0 is the flux quantum. For paramagnetic impurities, τ_{pb} coincides with the spin-flip time.[12] In the case of the spatial fluctuations of the superconducting coupling, τ_{pb}^{-1} is proportional to the variance of the fluctuations.[14]

From Eq. (3), one obtains the Green functions

$$g_j = \frac{u}{\sqrt{u^2-1}} = ue^{-i\varphi_j}f_j, \quad f_j^\dagger = -e^{-2i\varphi_j}f_j, \quad (4)$$

$$\frac{E}{\Delta} = u\left(1 - \frac{\zeta}{\sqrt{1-u^2}}\right), \quad \zeta = \frac{\hbar}{\tau_{pb}\Delta}, \quad (5)$$

where, following Refs. 12 and 13, we introduce a dimensionless pair-breaking parameter ζ. The matrices s_{eh} and s_{he} can be expressed using Eq. (4) as follows:

$$s_{eh} = \alpha \begin{bmatrix} e^{i\varphi_1} & 0 \\ 0 & e^{i\varphi_2} \end{bmatrix}, \quad s_{he} = \alpha \begin{bmatrix} e^{-i\varphi_1} & 0 \\ 0 & e^{-i\varphi_2} \end{bmatrix}, \quad (6)$$

$$\alpha = u - \sqrt{u^2 - 1}. \tag{7}$$

We note that pair breaking modifies the energy dependence of the Andreev reflection amplitude α according to the non-BCS Green functions [Eqs. (4) and (5)]. A few words concerning the applicability of this result are due here.

First of all, there is no restriction on energy E; e.g., for $\zeta \leq 1$, Eqs. (6) and (7) are valid both below and above the reduced (Abrikosov-Gorkov) quasiparticle gap $\Delta_\mathbf{g} = \Delta(1 - \zeta^{2/3})^{3/2}$. In particular, for $|E| \leq \Delta_\mathbf{g}$ one can show that u is real and $|u| \leq (1 - \zeta^{2/3})^{1/2} < 1$ (Ref. 13), corresponding to perfect Andreev reflection with $\alpha = \exp[-i \arccos(u)]$. Since in the Usadel limit $\ell \ll v_F \tau_{pb}$, normal scattering from the superconductors is suppressed due to the smallness of the junction width also in the presence of pair breaking. The absence of normal transmission at $|E| \leq \Delta_\mathbf{g}$ is consistent with the Abrikosov-Gorkov approach assuming no impurity states inside the gap and the validity of the Born approximation.[12,13] For $|E| \geq \Delta_\mathbf{g}$, the relevant solution of Eq. (5) is complex and has positive $\mathrm{Im}\, u$ related to the density of states of the superconductor.[13] Equations (5) and (7) are thus the generalization of the known result $\alpha = (E/\Delta_0) - \sqrt{(E/\Delta_0)^2 - 1}$ (Ref. 22) for transparent point contact, where $\Delta_0 \equiv \Delta|_{\zeta=0}$ is the BCS gap. It is convenient to measure all energies in units of Δ_0 for which Eqs. (4)–(7) should be complemented with the self-consistency equation for Δ. At $T=0$, the case we are eventually interested in, this equation can be written as[12,13]

$$\ln(\zeta_0/\zeta) = -\pi\zeta/4, \quad \zeta \leq 1, \tag{8}$$

$$\ln(\zeta_0/\zeta) = \sqrt{\zeta^2 - 1}/(2\zeta) - \ln(\zeta + \sqrt{\zeta^2 - 1}) \\ - (\zeta/2)\arctan(1/\sqrt{\zeta^2 - 1}), \quad \zeta \geq 1, \tag{9}$$

with ζ being now a function of a new pair-breaking parameter $\zeta_0 = \hbar/(\tau_{pb}\Delta_0)$ ranging from zero to the critical value $\zeta_0 = 0.5$ at which $\zeta = \infty$ and $\Delta = 0$.[12,13]

Inserting Eqs. (2) and (6) for $\hat{s}_A(E)$ into Eq. (1) and taking the limit $T \to 0$, we obtain the Josephson current for an arbitrary $\hat{s}_N(E)$ as

$$I = -\frac{4e}{h} \int_0^\infty d\omega \frac{\partial}{\partial\varphi} \ln\{1 + \alpha^4 \, \mathrm{Det}\, s_{ee}(E) \, \mathrm{Det}\, s_{ee}^*(-E) \\ - \alpha^2 [r_{11}(E) r_{11}^*(-E) + r_{22}(E) r_{22}^*(-E) + e^{-i\varphi} t_{21}(E) t_{12}^*(-E) \\ + e^{i\varphi} t_{12}(E) t_{21}^*(-E)]\}_{E=i\omega}. \tag{10}$$

III. ANDREEV BOUND STATES IN A RESONANT JUNCTION

Let us assume that the N region is a small quantum dot and electrons can only tunnel via one of its levels characterized by its position E_r with respect to the Fermi level and broadening Γ. For the simplest Breit-Wigner scattering matrix with $r_{11} = r_{22} = (E - E_r)/(E - E_r + i\Gamma)$ and $t_{12} = t_{21} = \Gamma/i(E - E_r + i\Gamma)$, Eq. (10) reads
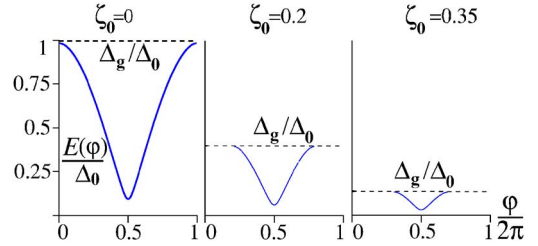

FIG. 2. (Color online) Phase dependence of the Andreev bound state for a broad resonant level with $\Gamma = 15\Delta_0$ close to the Fermi energy ($E_r = 0.1\Gamma$); dashed line shows the normalized gap for a given value of the pair-breaking parameter ζ_0.

$$I = -(2e/h)\mathcal{T}\sin\varphi \int_0^\infty d\omega \left\{ u^2\left[\mathcal{R} + \mathcal{T}\left(1 + \frac{\sqrt{1 - u^2} - \zeta}{\Gamma/\Delta} \right)^2 \right] \right. \\ \left. - 1 + \mathcal{T}\sin^2\left(\frac{\varphi}{2}\right) \right\}^{-1}_{E=i\omega}, \tag{11}$$

where $\mathcal{T} = 1 - \mathcal{R} = \Gamma^2/(E_r^2 + \Gamma^2)$ is the Breit-Wigner transmission probability at the Fermi level. The parameter Γ/Δ accounts for the energy dependence of the resonant superconducting tunneling. In Eq. (11), the integrand has, in general, poles given by the equation

$$u^2\left[\mathcal{R} + \mathcal{T}\left(1 + \frac{\sqrt{1 - u^2} - \zeta}{\Gamma/\Delta} \right)^2 \right] = 1 - \mathcal{T}\sin^2\left(\frac{\varphi}{2}\right). \tag{12}$$

Along with Eq. (5), they determine the energies of the ABSs localized below the Abrikosov-Gorkov gap $\Delta_\mathbf{g} = \Delta(1 - \zeta^{2/3})^{3/2}$. It is instructive to understand how the pair breaking modifies the ABS spectrum since this is reflected on both the current-phase relation $I(\varphi)$ and the critical current $I_c \equiv \max I(\varphi)$.

We start our analysis with an analytically accessible case of an infinitely broad resonant level, $\Gamma/\Delta \to \infty$, where Eq. (12) reduces to $u^2 = 1 - \mathcal{T}\sin^2(\varphi/2)$, yielding the ABS energies $\pm E(\varphi)$ (see Eq. (5)),

$$E(\varphi) = \Delta\sqrt{1 - \mathcal{T}\sin^2(\varphi/2)}\left[1 - \frac{\zeta}{\sqrt{\mathcal{T}}|\sin(\varphi/2)|} \right]. \tag{13}$$

Requiring $E(\varphi) \leq \Delta_\mathbf{g}$, we find that the ABSs exist in the phase interval where $\sin^2(\varphi/2) \geq \zeta^{2/3}/\mathcal{T}$ and only if $\zeta^{2/3} \leq \mathcal{T}$. The numerical solution of Eqs. (5), (8), and (12) confirms that the interval of the existence of ABSs gradually shrinks from $0 \leq \varphi \leq 2\pi$ to a narrower one with increasing pair breaking (see Fig. 2). Outside this interval the Josephson current is carried by the continuum states ($E \geq \Delta_\mathbf{g}$) alone, which is automatically accounted for by Eq. (11). An equation of the same form as Eq. (13) was derived earlier for a nonresonant system and by a different method.[15]

By contrast, the ABS spectrum for a narrow resonant level turns out to be much less sensitive to pair breaking. Indeed, under condition $\Gamma/\Delta \ll 1 - \zeta$, Eqs. (5) and (12) reproduce the known result, $E(\varphi) = \sqrt{E_r^2 + \Gamma^2}\sqrt{1 - \mathcal{T}\sin^2(\varphi/2)}$ (Refs. 4 and 9). In particular, for $E_r \to 0$, the ABSs exist within the resonance width $E(\varphi) < \Gamma$ and are separated from the continuum
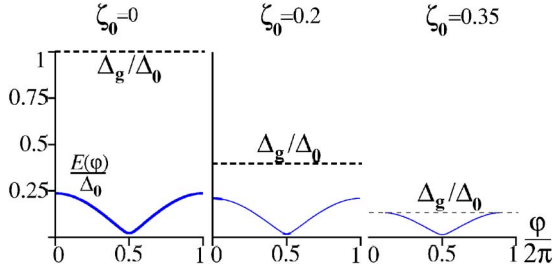
FIG. 3. (Color online) Phase dependence of the Andreev bound state for a narrow resonant level with $\Gamma = 0.3\Delta_0$ and $E_r = 0.1\Gamma$.

by a gap $\Delta_g - \Gamma$. Solving Eqs. (5), (8), and (12) numerically, we find that until this gap closes at a certain value of ζ_0, the ABS spectrum remains virtually intact (see Fig. 3). For bigger ζ_0, the spectrum gets modified in a way similar to the previous case (cf., third panels in Figs. 2 and 3). In the case of a very narrow resonance, the characteristic value of ζ_0 is ≈ 0.45, corresponding to $\zeta \approx 1$, i.e., to the onset of gapless superconductivity.[12,13]

IV. CRITICAL CURRENT AND CURRENT-PHASE RELATION: RESULTS AND DISCUSSION

For numerical evaluation of the Josephson current [Eq. (11)], we first set $E = i\omega$ in Eq. (5) and then make the transformation $u \to i\nu$, yielding $\omega/\Delta = \nu(1 - \zeta/\sqrt{1 + \nu^2})$. Using this relation, in Eq. (11) we change the integration over ν with the Jacobian $d\omega/d\nu = \Delta[1 - \zeta/(1 + \nu^2)^{3/2}]$,

$$I = (2e\Delta/h)\mathcal{T}\sin\varphi \int_{\nu_0}^{\infty} d\nu \left(1 - \frac{\zeta}{(1 + \nu^2)^{3/2}}\right)$$
$$\times \left\{\nu^2\left[\mathcal{R} + \mathcal{T}\left(1 + \frac{\sqrt{1 + \nu^2} - \zeta}{\Gamma/\Delta}\right)^2\right] + 1 - \mathcal{T}\sin^2\left(\frac{\varphi}{2}\right)\right\}^{-1}.$$
(14)

Positiveness of ω in Eq. (11) enforces the choice of the lower integration limit: $\nu_0 = 0$ for $\zeta \leq 1$ and $\nu_0 = \sqrt{\zeta^2 - 1}$ for $\zeta \geq 1$.

Using Eqs. (8), (9), and (14), we are able to analyze the critical current $I_c \equiv \max I(\varphi)$ in the whole range of the pair-
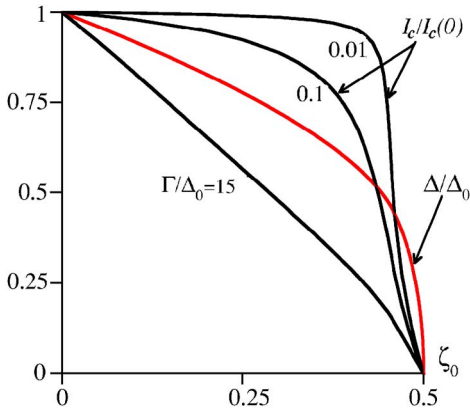

FIG. 4. (Color online) On-resonance critical current vs pair-breaking parameter $\zeta_0 = \hbar/(\tau_{pb}\Delta_0)$ for different Γ/Δ_0. The behavior of the normalized order parameter (Refs. 12 and 13) is shown, for comparison, in red.
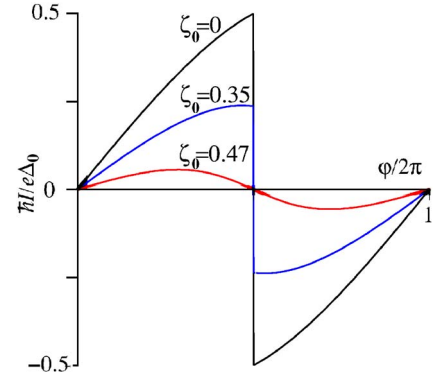

FIG. 5. (Color online) On-resonance current-phase relation for different values of the pair-breaking parameter ζ_0 and $\Gamma = \Delta_0$.

breaking parameter, $0 \leq \zeta_0 \leq 0.5$ (see Fig. 4). In line with the discussed behavior of the Andreev bound states, for a narrow resonance, $\Gamma/\Delta_0 \ll 1$, the critical current starts to drop significantly only upon entering the gapless superconductivity regime, $0.45 \leq \zeta_0 \leq 0.5$. On the other hand, for a broad resonance, $\Gamma/\Delta_0 \gg 1$, the suppression of I_c is almost linear in the whole range. We note that in both cases the behavior of I_c strongly deviates from that of the bulk order parameter (red curve) (Refs. 12 and 13) largely due to the pair-breaking effect on the ABS. In practice, the $I_c(\zeta_0)$ dependence can be measured by applying a magnetic field [the case where $\zeta_0 = (B/B_*)^2$ and $B_* = (\Phi_0/\pi d)\sqrt{18\Delta_0/\hbar v_F \ell}$] in an experiment similar to Ref. 6 where a quantum dot, defined in a single-wall carbon nanotube, was strongly coupled to the leads with the ratio $\Gamma/\Delta_0 \approx 10$. Carbon nanotube quantum dots with lower Γ/Δ_0 values are accessible experimentally, too.[5,11]

We also found that the crossover between the gapped and gapless regimes is accompanied by a qualitative change in the shape of the Josephson current-phase relation $I(\varphi)$, as demonstrated in Fig. 5 for the on-resonance case $E_r = 0$ and $\Gamma = \Delta_0$. The $I(\varphi)$ relation is anharmonic as long as the junction with $\Delta_g \neq 0$ supports the ABSs (black and blue curves). The vanishing of the ABSs upon entering the gapless regime leads to a nearly sinusoidal current-phase relation (red curve). A closely related effect is demonstrated in Fig. 6, showing the modification of the critical current resonance line shape with the increasing pair-breaking strength. In the absence of pair breaking, it is nonanalytic near $E_r = 0$ (black curves), reflecting the anharmonic $I(\varphi)$ due to the ABSs in a transparent channel.[9,10] On approaching the gapless regime,
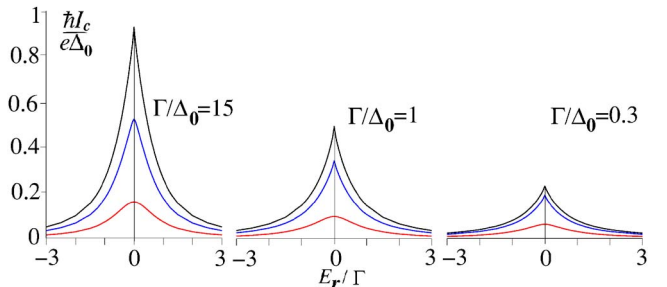

FIG. 6. (Color online) Critical current vs resonant level position: $\zeta_0 = 0$ (black), $\zeta_0 = 0.25$ (blue), and $\zeta_0 = 0.45$ (red).

this singularity is smeared out (red curves), which is accompanied by the suppression of the I_c amplitude. At finite temperatures $T \ll \Delta/k_B$, the pair-breaking-induced smearing of the resonance peak will enhance the usual temperature effect.

In conclusion, we have proposed a model describing resonant Josephson tunneling through a quantum dot beyond the conventional BCS picture of the superconducting state in the leads. It allows for nonperturbative treatment of pair-breaking processes induced by a magnetic field or paramagnetic impurities in diffusive superconductors. We considered no Coulomb blockade effects, assuming small charging energy in the dot $E_C \ll \Delta_0$, Γ, which was, for instance, the case in the experiment of Ref. 6. Our predictions, however, should be qualitatively correct also for weakly coupled dots with $\Gamma \lesssim E_C \ll \Delta_0$ at least as far as the dependence of the critical supercurrent on the pair-breaking parameter is concerned. Indeed, for a narrow resonance the Andreev bound states begin to respond to pair breaking only when the gap $\Delta_\mathbf{g}$ becomes sufficiently small (see Fig. 3) so that for a finite $E_C \ll \Delta_0$, one can expect a sharp transition to the resistive state, too, similar to that shown in Fig. 4 for $\Gamma/\Delta_0 \ll 1$.

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