Analytical result on the supercurrent through a superconductor/quantum-dot/superconductor junction Postprint

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Full Text

Preamble

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Abstract

We present an analytical result for the supercurrent across a superconductor/quantum-dot/superconductor junction. By converting the current integration into a special contour integral, we can express the current as a sum of the residues of poles. These poles are real and provide a natural definition of the Andreev bound states. We also use the exact result to explain several features of the supercurrent transport behavior.

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Introduction

The mesoscopic superconductor/quantum-dot/superconductor (S-QD-S) junction is a canonical structure for studying phase-coherent current transport in mesoscopic hybrid systems [**?**]. When using the Keldysh Green' s function technique [**?**] to evaluate the current across the S-QD-S junction, conventional methods require numerical integration and encounter difficulties in explaining certain features of the current transport behavior [**?**]. In this paper, we employ a new method to analytically compute the current across the S-QD-S junction in the absence of voltage bias, and use these analytical results to explain several features of the current transport properties.

Model and Hamiltonian

In the system under consideration, a quantum dot defined in a two-dimensional electron gas (2DEG) is coupled to two BCS superconducting leads. We model this system with the Hamiltonian $\hat{H} = \hat{H}_L + \hat{H}_d + \hat{H}_R + \hat{H}_T$, where

$$\hat{H}_L = \sum_k a^\dagger_{k\sigma} a_{k\sigma} + [\Delta_L a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} + \text{h.c.}]$$

$$\hat{H}_d = \epsilon_0 (d^\dagger_\sigma d_\sigma)$$

$$\hat{H}_R = \sum_p b^\dagger_{p\sigma} b_{p\sigma} + [\Delta_R b^\dagger_{p\uparrow} b^\dagger_{-p\downarrow} + \text{h.c.}]$$

are the isolated (unperturbed) Hamiltonians of the left superconductor, the quantum dot, and the right superconductor, respectively.

We consider only a quantum dot with negligible intra-dot Coulomb interaction. The reason is that we wish to focus on the superconducting proximity effect on the QD, which arises from Andreev reflections, whereas a large charging effect caused by intra-dot Coulomb repulsion suppresses transport mediated by the Andreev process [**?**, **?**]. A study of the competition between intermediate intra-dot Coulomb interaction and Andreev reflections in S-QD-S junctions will be presented in future work. Furthermore, we consider only a single energy level inside the QD. Generalization to QDs with several energy levels is straightforward.

The tunneling term

$$\hat{H}_T = \sum_k [t_L a^\dagger_{k\sigma} d_\sigma + \text{h.c.}] + \sum_p [t_R b^\dagger_{p\sigma} d_\sigma + \text{h.c.}]$$

describes electron transfer between the QD and the leads.

Current Formula

The current flowing across the junction is [**?**]

$$I = \frac{e}{\hbar} \int \frac{d\omega}{2\pi} \text{Tr}[\hat{\tau}_z (\hat{G}^<_d(\omega) \hat{\Sigma}^>_L(\omega) + \hat{G}^>_d(\omega) \hat{\Sigma}^<_L(\omega) + \hat{G}^r_d(\omega) \hat{\Sigma}^<_L(\omega) + \hat{G}^<_d(\omega) \hat{\Sigma}^a_L(\omega))]$$

where $\hat{G}_d$ and $\hat{\Sigma}_L$ are the Keldysh Green' s functions of the QD and the left superconductor in Nambu space [**?**]. The retarded Green' s function of the superconductor is

$$\hat{g}_{L/R}(\omega) = -\frac{i\pi\rho_{L/R}}{\sqrt{\Delta^2-(\omega+i0^+)^2}} \begin{pmatrix} \omega & \Delta_{L/R} \\ \Delta^*_{L/R} & \omega \end{pmatrix}$$

where $\rho_{L/R}$ is the normal-state density of states and $\Delta_{L/R} = \Delta e^{i\phi_{L/R}}$.

After solving the matrix Dyson equation, we obtain the retarded Green' s function of the QD:

$$\hat{G}^r_d(\omega) = \frac{1}{D(\omega)} \begin{pmatrix} \omega - \epsilon_0 - \Sigma^r_{11}(\omega) & \Sigma^r_{12}(\omega) \\ \Sigma^r_{21}(\omega) & \omega + \epsilon_0 - \Sigma^r_{22}(\omega) \end{pmatrix}$$

where $\hat{g}^r_d(\omega) = \begin{pmatrix} \frac{1}{\omega-\epsilon_0+i0^+} & 0 \\ 0 & \frac{1}{\omega+\epsilon_0+i0^+} \end{pmatrix}$ is the unperturbed retarded Green' s function of the QD. The QD' s self-energy $\hat{\Sigma}(\omega) = \hat{\Sigma}_L(\omega) + \hat{\Sigma}_R(\omega)$ describes the proximity effect of the superconductors on the QD; here we have used the wide-bandwidth approximation [**?**]. $D(\omega)$ in Eq. [8] is the determinant of the matrix $(\hat{g}^r_d(\omega) - \hat{\Sigma}^r(\omega))$:

$$D(\omega) = [\hat{g}^r_d(\omega)_{11} - \Sigma^r_{11}(\omega)][\hat{g}^r_d(\omega)_{22} - \Sigma^r_{22}(\omega)] - \Sigma^r_{12}(\omega)\Sigma^r_{21}(\omega)$$

Choice of Integration Contour

The supercurrent formula can be expressed as

$$I_{sc} = \frac{e}{\hbar}\int \frac{d\omega}{2\pi}\mathrm{Tr}[\hat{\tau}_z(\hat{G}^<_d(\omega)\hat{g}^>_L(\omega) + \hat{G}^>_d(\omega)\hat{g}^<_L(\omega) + \hat{G}^r_d(\omega)\hat{g}^<_L(\omega) + \hat{G}^<_d(\omega)\hat{g}^a_L(\omega))]$$

To avoid calculating this integration numerically, we transform it into a contour integral. First, using the fluctuation-dissipation theorem $\hat{G}^<(\omega) = -\hat{G}^r(\omega)\hat{\Sigma}^<(\omega)\hat{G}^a(\omega)$ and $\hat{G}^>(\omega) = \hat{G}^r(\omega)\hat{\Sigma}^>(\omega)\hat{G}^a(\omega)$ for equilibrium systems, where $\hat{G}$ stands for any Green' s function and $f(\omega)$ is the Fermi distribution function, we have

$$I_{sc} = \frac{e}{\hbar}\int \frac{d\omega}{2\pi} f(\omega)\mathrm{Tr}[\hat{\tau}_z(\hat{G}^r_d(\omega)\hat{g}^r_L(\omega) - \hat{G}^a_d(\omega)\hat{g}^a_L(\omega))]$$

Then we make a change of integration variable $\omega \to \omega + i0^+$ for the retarded functions and $\omega \to \omega - i0^+$ for the advanced functions to divide I_{sc} into two integrals along different paths:

$$I_{sc} = \frac{e}{\hbar}\int \frac{d\omega}{2\pi} f(\omega + i0^+)\mathrm{Tr}[\hat{\tau}_z\hat{G}^r_d(\omega + i0^+)\hat{g}^r_L(\omega + i0^+)] - \frac{e}{\hbar}\int \frac{d\omega}{2\pi} f(\omega - i0^+)\mathrm{Tr}[\hat{\tau}_z\hat{G}^a_d(\omega - i0^+)\hat{g}^a_L(\omega - i0^+)]$$

Since the above two integrands are analytic continuations of the same function, we define a new integrand $J(\omega)$ equal to them:

$$J(\omega) = \frac{e}{\hbar} f(\omega)\mathrm{Tr}[\hat{\tau}_z\hat{G}^r_d(\omega)\hat{g}^r_L(\omega)]$$

Thus the current integration can be rewritten as a contour integral in the complex-ω plane:

$$I_{sc} = \oint_C \frac{d\omega}{2\pi i} J(\omega)$$

where the integration path $C = C_+ + C_-$ is a closed contour lying infinitely close to the real ω axis. The integral can then be evaluated analytically using Cauchy’ s theorem.

This choice of integration contour has the advantage of leaving all (infinitely many) poles at $\omega = i(2n+1)\pi/\beta$ of the Fermi function $f(\omega)$ outside the contour, thus avoiding the calculation of Matsubara frequency summations.

Poles and Definition of Andreev Bound States

Since the current is proportional to the sum of residues of the integrand $J(\omega)$ inside the contour C, only real poles of $J(\omega)$ contribute. For $J(\omega) = \mathrm{Tr}[\hat{\tau}_z \hat{G}_d^r(\omega)\hat{g}_L^r(\omega)]f(\omega)$, there are only two pairs of real poles originating from the singularities of the superconducting density of states and the QD’ s Green’ s function.

The poles at $\omega = \pm\Delta$ come from the DOS of the BCS superconductors. The poles at $\omega = \pm\epsilon^*$ come from the QD’ s Green’ s function and are the two real roots of the equation $D(\omega) = 0$ inside the gap ($|\omega| < \Delta$). These two poles give the positions of the quasi-particle states of the QD inside the gap. The fact that they are real indicates that these quasi-particle states are true bound states, commonly called Andreev bound states (ABS).

Before coupling to the superconductors, the unperturbed QD has a bound state at ϵ_0 for the electron spectrum and one at $-\epsilon_0$ for the hole spectrum. After coupling to the superconductors, through electron transfer with the two superconductors via Andreev processes, the electron and hole parts of the QD’ s Green’ s function become coupled, leading to significant modifications of the QD’ s energy spectrum: the original bound state at ϵ_0 for electrons (or $-\epsilon_0$ for holes) renormalizes into two symmetric bound states at $\pm\epsilon^*$ for both electron and hole spectra.

To express ϵ^* as an algebraic function of ϵ_0, ϕ and Γ, we transform the equation $D(\omega) = 0$ into a quartic equation for $x = \epsilon^{*2}$:

$$A_4 x^4 + (2A_2A_4 - 4\Gamma^2)x^3 + (A_4^2 + 2\Delta^2 B^2 - 4\Gamma^2\Delta^2)x^2 + (2A_2\Delta^2 B^2)x + (\Delta^2 B^2)^2 = 0$$

where $A_2 = \epsilon_0^2 + \Gamma^2 \cos^2\phi$, $A_4 = \epsilon_0^2 + \Gamma^2$, and $B^2 = \epsilon_0^2 - \Delta^2$ with $|\epsilon_0| < \Delta$.

This quartic equation in x has only one positive real solution $x_0 < \Delta^2$, giving $\epsilon^* = \sqrt{x_0}$. The quartic equation is solvable algebraically, but we omit the lengthy explicit solution. The dependence of ϵ^* on ϵ_0, ϕ and Γ is shown graphically in [**?**].

Residues and Analytical Result of the Current

The current is obtained by summing the residues at the four poles:

$I_{sc} = \frac{2e}{\hbar}\mathrm{Im}\left[\sum_i \mathrm{Res}\, J(\omega_i)\right]$, where $\omega_i = \pm\epsilon^*, \pm\Delta$.

The residues of J at $\pm\epsilon^*$ are:

$\mathrm{Res}_{\omega=\epsilon^*} J(\omega) = \lim_{\omega\to\epsilon^*}(\omega - \epsilon^*)J(\omega) = \frac{e\Gamma_L\Gamma_R \sin\phi}{2\hbar}\frac{\tanh(\beta\epsilon^*/2)}{\epsilon^*[(\Delta^2-\epsilon^{*2})+\Gamma^2(\Delta^2-\epsilon^{*2}\cos^2\phi)/(\Delta^2-\epsilon^{*2})]}$

The residues at $\pm\Delta$ vanish because the numerator of $J(\omega)$ also vanishes at these points. Thus the supercurrent is simply:

$I_{sc} = \frac{e\Gamma_L\Gamma_R \sin\phi}{\hbar}\frac{\tanh(\beta\epsilon^*/2)}{\epsilon^*[(\Delta^2-\epsilon^{*2})+\Gamma^2(\Delta^2-\epsilon^{*2}\cos^2\phi)/(\Delta^2-\epsilon^{*2})]}$

where $\phi = \phi_R - \phi_L$ is the phase difference between the two superconductors.

Discussion

In addition to the splitting of the original energy level ϵ_0 into the two ABS, another modification to the QD' s energy spectrum is that the QD develops a continuum energy spectrum outside the gap. In fact, one alternative method to calculate the current integral is to divide the QD' s spectrum into a continuum part ($|\omega| > \Delta$) and a discrete part ($|\omega| < \Delta$), then evaluate their contributions separately. However, this method involves numerical integration and cannot naturally explain why the peaks at $\omega = \pm\Delta$ in the $I_{\mathrm{continuum}}$ vs. ϵ_0 curve and in the I_{discrete} vs. ϵ_0 curve exactly cancel when the two parts are added to give the total current (see Fig. 1).

In contrast, our approach naturally demonstrates this exact cancellation. The current is obtained by summing the residues of the four poles. Since the residues at $\pm\Delta$ vanish, the total current curve has no peaks arising from the DOS singularities of the superconductors. Only the residues at $\pm\epsilon^*$ contribute to the total current, giving rise to a sharp peak in the I vs. ϵ_0 curve at $\epsilon_0 = 0$. The reason for this peak is that when $\epsilon_0 = 0$, the upper and lower ABS have the same phase. As ϵ_0 moves away from the Fermi level, the phases of the upper and lower ABS begin to differ, and this difference severely reduces the supercurrent across the junction. Fig. 2 shows the central peaks for different Γ values; the peaks broaden as Γ increases.

A direct application of this result is a method to align the energy level of the QD with the Fermi level of the superconductor in actual experiments: when changing the gate voltage, the state with maximum supercurrent occurs at $\epsilon_0 = 0$.

Conclusion

In summary, we have analytically calculated the supercurrent across an S-QD-S junction. The central results are Eq. [18] and Eq. [21], which give the analytical expressions for both the positions of the ABS and the supercurrent. We demonstrate two additional advantages of our method: (1) It provides a natural definition of the Andreev bound states inside the QD. (2) It explains the disappearance of peaks at the gap edge in the I vs. ϵ_0 curve. The method developed in this paper can also be applied to compute other equilibrium properties of superconductor-normal hybrid systems.

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FIGURE CAPTIONS

Fig. 1 [Figure 1: see original paper] Supercurrent vs. ϵ_0 when $\Gamma = 0.1$ and $\phi = \pi/2$. The dashed line shows the contribution from the discrete spectrum, and the dotted line from the continuum spectrum. The solid line is the total current. Note that the continuum spectrum contributes negative current.

Fig. 2 [Figure 2: see original paper] Supercurrent vs. ϵ_0 with $\phi = \pi/2$ for different Γ values. The curves correspond to $\Gamma = 0.1, 0.3, 1.0$, respectively. Note the broadening effect as Γ increases.

Note: Figure translations are in progress. See original paper for figures.

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