Josephson Coupling through a Quantum Dot

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Abstract

We derive, via fourth order perturbation theory, an expression for the Josephson current through a gated interacting quantum dot. We analyze our expression for two different models of the superconductor-dot-superconductor (SDS) system. When the matrix elements connecting dot and leads are featureless constants, we compute the Josephson coupling \( J_c \) as a function of the gate voltage and Coulomb interaction. In the limit of a diffusive dot, we compute the probability distribution \( P(J_c) \) of Josephson couplings. In both cases, \( \pi \) junction behavior \( (J_c < 0) \) is possible, and is not simply dependent on the parity of the dot occupancy.

Magnetic impurities in Josephson junctions tend to degrade the critical current \([1,7]\). This result has been known since the work of Kulik \([1]\), who analyzed a simple model in which spin-preserving as well as spin-flip hopping processes (with amplitudes \( t \) and \( t' \), respectively) are present. The critical current in such a junction is given by the expression \( I_c = I_{cAB} \cdot (|t|^2 - |t'|^2)/(|t|^2 + |t'|^2) \), where \( I_{cAB} \) is the Ambegaokar-Baratoff critical current. Since spin-flip tunneling results in a sign change of the Cooper pair singlet \((\uparrow \downarrow \rightarrow \downarrow \uparrow)\), the spin-flip hopping contribution is negative, and reduces \( I_c \) \([5]\). When \( I_c < 0 \), one has a \( \pi \) junction, for which the ground state energy is minimized when the superconducting phase difference is \( \delta = \pi \). A ring containing a single \( \pi \) junction will enclose trapped flux \([3]\). A related effect occurs in Josephson tunneling through a ferromagnetic layer \([8,11]\), and recent experiments on Nb-Cu\(_x\)Ni\(_{1-x}\)-Nb junctions suggest that \( I_c < 0 \) states have been observed \([12]\).

In this paper, we investigate Josephson coupling mediated by a quantum dot \([13]\), generalizing the case of a single impurity to a system with many quantized energy levels. We derive first a general expression, within fourth-order perturbation theory, for the Josephson coupling \( J_c \) \((I_c = 2eJ_c/\hbar)\). We then consider two models for the tunneling amplitudes \( t_{\alpha j} \) from the leads to the dot. As we shall see, in contrast to the single impurity case, the parity of the number of electrons on the dot, \( N_0 \), does not uniquely determine the sign of the Josephson coupling.

It is well-known in the theory of elastic co-tunneling that if the Coulomb repulsion \( U \) is large then the conductance through a dot is independent of \( U \). Correspondingly, we find the critical current is insensitive to \( U \) in this regime, and furthermore when the system is close to a charge degeneracy point, the probability distribution \( P(J_c) \) for a disordered dot has universal properties.

Our Hamiltonian is a sum of three terms:
\[ H_{\text{sc}} = \sum_{k,\alpha} \left( \psi_{k\alpha}^\dagger \psi_{-k\alpha} \right) \left( \begin{array}{cc} \varepsilon_{k\alpha} - \mu + \Delta_{\alpha} & \Delta_{\alpha} \\ \Delta_{\alpha} & \mu - \varepsilon_{k\alpha} \end{array} \right) \left( \begin{array}{c} \psi_{k\alpha} \\ \psi_{-k\alpha}^\dagger \end{array} \right) \]

\[ H_{\text{tun}} = - \sum_{k,\alpha,j,\sigma} (S_{\alpha}S_d)^{-1/2} \left( t_{aj} \psi_{k\alpha\sigma}^\dagger c_{j,\sigma} + t_{aj}^* c_{j,\sigma}^\dagger \psi_{k\alpha\sigma} \right) \]

\[ H_{\text{dot}} = \sum_{j,\sigma} (\varepsilon_j - \mu + V) c_{j,\sigma}^\dagger c_{j,\sigma} + \frac{1}{2} N(N - 1) U. \]

Here, \( S_{\alpha,d} \) are the areas of the \( \alpha \) electrode and the dot, \( V \) is the gate voltage on the dot and \( U \) is the Hubbard interaction on the dot. Electron states on the dot are assumed to be disordered by a spin-independent random potential.

We calculate the Josephson current via fourth order perturbation theory in \( H_{\text{tun}} \). For this to be applicable both the typical distance between consecutive energy levels \( \delta \varepsilon \) and the gap in the superconductors must be large compared to the broadening of the individual level due to tunneling: \( \Gamma_{\alpha} \ll \delta \varepsilon, \Delta_{\alpha} \), where \( \Gamma_{\alpha} = \pi \nu_{\alpha} \langle |t_{\alpha}|^2 \rangle / S_d \), where \( \nu_{\alpha} \) is the metallic density of states per unit area in the \( \alpha \) electrode.

We also have to be far enough from charge degeneracy points, where the gap for charge excitations on the dot vanishes. We measure \( V \) relative to the charge degeneracy point, which is equivalent to setting \( \mu \equiv \varepsilon_\frac{1}{2}N_0 + 1 + U N_0 \).

In computing the fourth order correction to the ground state energy, we only consider terms which depend on the phase difference \( \delta \) between the two superconductors.

\[ E_J(\delta) = -4\nu_1 \nu_2 \Delta_1 \Delta_2 \text{Re} \ e^{i\delta} \left\{ \sum_{\xi_j > 0} t_{1j} t_{1j'} t_{2j} t_{2j'}^* J_{ee}(\xi_j, \xi_j') + \sum_{\xi_k < 0} t_{1k} t_{1k'} t_{2k} t_{2k'}^* J_{hh}(\xi_k, \xi_k') - \sum_{\xi_j > 0} t_{1j} t_{1j'} t_{2j} t_{2j'}^* J_{eh}(\xi_j, \xi_k) \right\}, \]

where \( J_{ee}, J_{hh} \) and \( J_{eh} \) are given by

\[ J(\xi, \xi') = \int_0^\infty d\theta_1 \int_0^\infty d\theta_2 J(\xi, \xi', \theta_1, \theta_2) \]

\[ J_{ee} = [(\Delta_1 \cosh \theta_1 + \xi + V) (\xi + \xi' + 2V + U) (\Delta_2 \cosh \theta_2 + \xi' + V)]^{-1} + [(\Delta_1 \cosh \theta_1 + \xi + V) (\Delta_1 \cosh \theta_1 + \Delta_2 \cosh \theta_2) (\Delta_2 \cosh \theta_2 + \xi' + V)]^{-1} + [(\Delta_1 \cosh \theta_1 + \xi + V) (\xi + \xi' + 2V + U) (\Delta_2 \cosh \theta_2 + \xi + V)]^{-1} \]

\[ J_{hh} = [(\Delta_1 \cosh \theta_1 + \xi - V + U) (\xi - \xi' - 2V + 3U) (\Delta_2 \cosh \theta_2 - \xi - V + U)]^{-1} + [(\Delta_1 \cosh \theta_1 + \xi - V + U) (\Delta_1 \cosh \theta_1 + \Delta_2 \cosh \theta_2) (\Delta_2 \cosh \theta_2 - \xi' - V + U)]^{-1} + [(\Delta_1 \cosh \theta_1 + \xi - V + U) (\xi - \xi' - 2V + 3U) (\Delta_2 \cosh \theta_2 - \xi - V + U)]^{-1} \]

\[ J_{eh} = [(\Delta_1 \cosh \theta_1 + \xi' - V + U) (\Delta_1 \cosh \theta_1 + \Delta_2 \cosh \theta_2 + \xi - \xi') (\Delta_2 \cosh \theta_2 - \xi' - V + U)]^{-1} + [(\Delta_1 \cosh \theta_1 + \xi + V) (\Delta_1 \cosh \theta_1 + \Delta_2 \cosh \theta_2 + \xi - \xi') (\Delta_2 \cosh \theta_2 + \xi + V)]^{-1} + [(\Delta_1 \cosh \theta_1 + \xi + V) (\Delta_1 \cosh \theta_1 + \Delta_2 \cosh \theta_2) (\Delta_1 \cosh \theta_1 - \xi' - V + U)]^{-1} + [(\Delta_2 \cosh \theta_2 + \xi + V) (\Delta_2 \cosh \theta_2 + \Delta_2 \cosh \theta_2 + \xi - \xi') (\Delta_2 \cosh \theta_2 - \xi' - V + U)]^{-1} \]
where $\xi \equiv \varepsilon - \mu$.

To proceed further we have to make some assumptions about the tunneling amplitudes and energy spectrum of the dot. Initially, we ignore any structure to the hopping amplitudes and set $t_{o\alpha} \equiv t_{\alpha}$. This choice of the amplitudes is equivalent to a situation where both leads are connected to the same point on the surface of the dot.

We further assume the energy spacings on the dot satisfy $\delta\varepsilon \ll \Delta \alpha$. The summation over states on the dot can then be recast as an integral. We obtain $E_J = J_c(1 - \cos \delta)$, with

$$J_c = \frac{4}{\pi^2} \nu_d^2 \Gamma_1 \Gamma_2 \Delta_1 \Delta_2 \int_0^1 dx \int_0^1 dy \left[ B_e^2 J_{ee}(B_e x; B_e y) + B_h^2 J_{hh}(-B_h x, -B_h y) - B_e B_h J_{eh}(B_e x, -B_h y) \right],$$

where $B_e, h$ are the distance to the top/bottom of the dot spectrum from the Fermi level on the dot.

By numerical integration we obtain $J_c(V)$, shown in fig. 1a for different values of $U$. For small values of $U$ the Josephson coupling always is positive. However, above some critical value $U_c$ there is a finite interval of voltages in which $J_c < 0$. The phase diagram of the junction is presented in fig. 1b-c. Note that our approach does not apply close to the $V = 0$ or $V = U$ lines where the Coulomb blockade is lifted and the dot ground state is degenerate.

Disordered dot – When the leads are connected to the dot at two different points, it is necessary to account for the effects of disorder. In this case, we have $t_{o\alpha} = t_{\alpha} \psi_j(R_{\alpha})$, where $\psi_j(r)$ is the wave function corresponding to energy level $\varepsilon_j$ on the dot. These wave functions are functionals of the disorder potential. The Josephson coupling is now a random quantity and we must find its distribution, which is possible since the statistical properties of the $\psi_j$ are well-studied.

Let us define the dimensionless local density of states,

$$\rho_\omega(R_1, R_2) = \frac{G_R^\alpha(R_1, R_2) - G_A^\alpha(R_1, R_2)}{2\pi i \nu_d} = \nu_d^{-1} \sum_j \psi_j(R_1) \psi_j^*(R_2) \delta(\omega - \varepsilon_j),$$

where $\nu$ is the dot density of states $\nu_d = 1/(S_d \delta \varepsilon)$, and $G^{R,A}$ are the usual retarded/advanced single particle Green’s functions.

As it was discussed in [14] for $\omega$ less then Thouless energy $E_{Th}$ these objects have very simple disorder-averaged statistical properties:

$$\langle \rho_\omega(R) \rho_{\omega'}(R') \rangle = \delta \varepsilon \delta(\omega - \omega'),$$

$$\langle \rho_{\omega_1} \cdots \rho_{\omega_{2n}} \rangle = \sum_{\text{all pairwise contractions}} \langle \rho_{\omega_1} \rho_{\omega_2} \rangle \cdots \langle \rho_{\omega_{2n-1}} \rho_{\omega_{2n}} \rangle,$$

implying that the function $\rho_\omega$ is distributed according to the functional

$$P[\rho_\omega] \propto \exp \left\{ - \int_{-\infty}^{\infty} d\omega \frac{\rho_\omega^2}{2\delta \varepsilon} \right\}.$$

The Josephson energy is then a bilinear functional of $\rho_\omega$:
Formally, our task is straightforward. We have to obtain critical current distribution function $P(J_c) = \langle \delta (J_c - 4\Delta^2 g_1 g_2 \rho \cdot \tilde{J} \cdot \rho) \rangle$. We do that as follows. First, we find the eigenvalues of the matrix $\tilde{J}(\omega,\omega')$, where

$$2\tilde{J}(\omega,\omega') = \begin{cases} J_{ee}(\omega,\omega') + J_{ee}(\omega',\omega) & \text{if } \omega > 0, \omega' > 0 \\ -J_{eh}(\omega,\omega') & \text{if } \omega > 0, \omega' < 0 \\ -J_{eh}(\omega',\omega) & \text{if } \omega < 0, \omega' > 0 \\ J_{hh}(\omega,\omega') + J_{hh}(\omega',\omega) & \text{if } \omega < 0, \omega' < 0. \end{cases}$$

(9) The distribution $P(J_c)$ now has the form

$$P(J_c) = \langle \delta (J_c - 4\Delta^2 g_1 g_2 [\rho \cdot \tilde{J} \cdot \rho]) \rangle = \int_{-\infty}^{\infty} du \frac{e^{-iuJ_c}}{2\pi} \prod_{s}(1 - 4iu(\delta \varepsilon)\Delta^2 g_1 g_2 \lambda)^{-1/2},$$

(10) where the product is over all eigenvalues $\lambda$ of the matrix $\tilde{J}$. Normalization determines the appropriate branch cut.

If both leads are connected to the same point on the surface of the dot, then $J_c \propto \int d\omega d\omega' \tilde{J}(\omega,\omega')$, which we have previously shown to be negative for certain $V,U$. Hence $\tilde{J}$ is not in general positive-definite, and we anticipate some finite probability for $\pi$ junction behavior.

Our numerical procedure consists of several steps. We introduce a cut-off $W$ and confine $\omega$ to the interval $-W/2 < \omega,\omega' < W/2$. Further, $\tilde{J}(\omega,\omega')$ is put on a uniform frequency grid. The Josephson coupling now is $J_c = 4\Delta^2 g_1 g_2 \sum_{s,s'} \tilde{J}_{ss'} \rho_s \rho_{s'}$ where the $2N \times 2N$ matrix $\tilde{J}_{ss'} = (W/2N) \tilde{J}(\omega_s,\omega_{s'})$ and $\rho_s = (W/2N)^{1/2} \rho_{s'}; \langle \rho_s \rho_{s'} \rangle = \delta \varepsilon \delta_{s,s'}$. $\tilde{J}_{ss'}$ is diagonalized and its eigenvalues $\lambda_s$ are substituted into (10). To make this integral more suitable for numerical evaluation a contour transformation is performed:

$$P(J_c) = \int_{0}^{+\infty} du \frac{1}{\pi} e^{\mp uJ_c} \prod_{s} \left(1 + 4u(\delta \varepsilon)\Delta^2 g_1 g_2 \lambda_s^2 \right)^{-1/2} \sin \left(\frac{\pi}{2} \sum_{s} \Theta(\mp u\lambda_s - 1) \right).$$

(11) One should pick upper sign for $J_c > 0$ and lower sign for $J_c < 0$.

The results of numerical calculation are quite insensitive to $W$ and $N$. The distribution function $P(J_c)$ is presented on fig. 2. It has a shape of asymmetric bell and it is non-zero for $J_c < 0$ per previous discussion. The total probability of having $\pi$-junction: $P_{\pi} = \int_{-\infty}^{0} P(J_c) \, dJ_c$, is shown in fig. 3.

Universal Limit – Generally the distribution $P(J_c)$ of Josephson couplings is dependent on nonuniversal parameters such as $V$ and $U$. In the limit $U \gg \Delta_1 = \Delta_2 \equiv \Delta$, though, there are universal aspects to the distribution. If the dot is close to the charge degeneracy point, i.e. $\Gamma \ll V \ll \Delta$ or $\Gamma \ll U - V \ll \Delta$ then the matrix $\tilde{J}$ is independent of both $U$
and $V$. Restricting our attention to the first case, we find the matrix $\tilde{J}$ is still given by (9) with $J_{hh} = 0$ and

$$ J_{ee} \approx \int_0^{\infty} d\theta_1 \int_0^{\infty} d\theta_2 \left[ (\Delta \cosh \theta_1 + \omega) (\Delta \cosh \theta_1 + \Delta \cosh \theta_2) (\Delta \cosh \theta_2 + \omega') \right]^{-1}, $$

$$ J_{eh} \approx \int_0^{\infty} d\theta_1 \int_0^{\infty} d\theta_2 \left[ (\Delta \cosh \theta_1 + \omega) (\Delta \cosh \theta_1 + \Delta \cosh \theta_2 + \omega - \omega') (\Delta \cosh \theta_2 + \omega) \right]^{-1}. $$

Thus, $\tilde{J}(\omega, \omega') = F(\omega/\Delta, \omega'/\Delta)/\Delta^3$ where $F(x, x')$ is a universal function of its arguments. We then find $P(J_c) = J_{AB}^{-1} f(J_c/J_{AB})$, where $f(x)$ is universal and $J_{AB} = \pi \langle G \rangle \Delta/\hbar$. The average conductance through the dot at $V = \Delta$ was calculated in [15] to be $\langle G \rangle = (2\pi e^2/\hbar) g_1 g_2 (\delta \varepsilon/\Delta)$.

There are several consequences of this universality. First, it means that all moments of this distribution are proportional to powers of $J_{AB}$, with universal coefficients. In particular, the ratio of the RMS and mean critical currents is $\sqrt{\langle (\Delta J_c)^2 \rangle / \langle J_c \rangle} \approx 1.59$. Second, the probability of having a $\pi$-junction is a universal number: $P_\pi = \int_0^{\infty} dx f(x) \approx 0.19$.

Odd $N_0$ – When the parameters of the dot are chosen in such a way that there is a single level ‘0’ occupied by only one electron, equation (4) must be modified. Consider a Cooper pair tunneling from the left to right superconductor. If none of two electrons passes through ‘0’ then their contribution to $E_J$ is already included in (4). Only those events where one or both electrons tunnel through ‘0’ will modify the expression for $E_J$. We find the corrections are given by

$$ \Delta J_{ee}(\omega, \omega') = \delta \varepsilon \delta(\omega') \left( J_{ee}(\omega, 0) - \frac{1}{2} J_{eh}(\omega, 0) \right) \Theta(\omega), $$

$$ \Delta J_{hh}(\omega, \omega') = \delta \varepsilon \delta(\omega') \left( J_{hh}(\omega, 0) - \frac{1}{2} J_{eh}(0, \omega) \right) \Theta(-\omega), $$

$$ \Delta J_{eh}(\omega, \omega') = (\delta \varepsilon)^2 \delta(\omega) \delta(\omega') J_{hh}(0, 0). \quad (12) $$

In the case of a single impurity level, we recover previous results [4]. Overall, this electron increases our chances to get $\pi$ junction. It is clear, however, that the influence of that electron is small for metallic dot where $\delta \varepsilon \ll \Delta$.

Discussion – Two superconductor-dot-superconductor models have been considered here. Assuming that both leads are attached to the same point on the dot surface and thus, ignoring any structure to the hopping matrix elements $t_{\alpha j}$, we find a critical $U$ above which $J_c$ can be driven negative by an appropriate dot gate voltage, $V$. As one can see from (3) and (4) there are six terms giving positive contribution to $J_c$ and six terms giving a negative contribution. They each depend in different ways on the gate voltage $V$, and one can suppress positive terms by varying $V$.

Another feature of our result is that it is derived for an even number of electrons on the dot. In the case of an Anderson impurity, the sign of $J_c$ depends on the parity of the impurity level occupancy $N_0$ [4]. Rather than being a parity effect, we offer the following interpretation: If two electrons of the Cooper pair both tunnel through empty states or both tunnel through filled states this gives positive contribution to $J_c$ (first and second term of (4)). To obtain a negative contribution (last term of (4)) one electron has to pass through filled states and the other through empty states. Thus, for a completely filled (empty) Anderson impurity both electrons must pass through filled (empty) states, yielding
a positive $J_c$. For a singly occupied orbital, one electron always tunnels through empty state while the other tunnels through filled state, and $J_c$ is negative. Therefore, the sign and magnitude of $J_c$ is determined in part by phase space considerations.

In the second model we allow leads to be ‘connected’ at different points on the surface of the dot. As a consequence the disorder has to be treated properly. We calculated the distribution function of critical current for the ensemble of junctions for different parameter values. The probability of $\pi$ junction as calculated from this distribution has very reasonable values to expect that such $\pi$ junction can be found experimentally. It is also predicted that the distribution function should possesses a remarkable universal property in the limit $U \gg \Delta$.

There are questions that remain unanswered. Within the framework of our first model, in order to have $\pi$ junction the value of $U$ must exceed some critical value $U_c$. From Fig. 3 one might infer that $U_c > 0$ for the second model as well. It has to noted, however, that our numerical procedure does not rule out the possibility of exponentially small tail for $U \to 0$. If this is true then $U_c$ corresponds to a crossover rather then a phase transition.
FIGURES

FIG. 1. (a) $J_c(V)$ versus $V/U$ for $U = 5, B_e = 80, B_h = 20$ (solid); $U = 2, B_e = 33.3, B_h = 66.7$ (dashed); $U = 3, B_e = 33.3, B_h = 66.7$ (dot-dashed). (b) phase diagram for $B_e = 50$ (solid), $B_e = 33.3$ (dashed), and $B_e = 10$ (dot-dashed) with $B_h = 100 - B_e$ The $\pi$ phase lies above the curve in each case.

FIG. 2. Probability distribution $P(J_c)$ for $U = 3, V = 0, W = 40$ (solid) and $U = 3, V = 1.5$, and $W = 40$ (dashed). $N = 100$ in both cases. The area under the total curve (i.e. out to $|J_c| = \infty$ is unity in both cases.
FIG. 3. $P_\pi$ versus $U/\Delta$ for $V = 0.1\Delta$. For very large values of $U/\Delta$, $P_\pi \to 0.19$. 
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