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Influence of electron-electron interactions on supercurrent in SNS structures

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We consider a superconductor-normal quantum dot-superconductor structure in which the number of electrons in the dot can be controlled by a gate voltage. We study the effect of electron-electron interactions on the supercurrent between the two superconductors. Using both an analytic model and numerical density functional calculations, we find that Coulomb interactions may serve to make the system quantum mechanically more «rigid», i.e., increasing its sensitivity to phase gradients, hence *enhancing* the supercurrent through the structure, especially at small phase differences. Accordingly, we find that in this structure the supercurrent can be controlled by the gate voltage.

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1. Introduction

The impact of quantum mechanical coherence on macroscopic quantities, such as electrical currents, is interesting both for basic research and for potential applications. In view of the latter, an ability to control the supercurrent in hybrid normal/superconducting systems — preferably by electrical means — is desirable. Examples of structures which exhibit a controlled supercurrent is the Josephson field effect transistor (JOFET) [1], the injected-current SNS transistor [2], and devices which effectuate Cooper-pair transport via tunable resonant states [3,4].

In the above works, novel effects were essentially of single-particle origin. The effects of Coulomb interactions on transport of Cooper pairs through confined regions have been investigated using different formulations of the tunneling-Hamiltonian formalism, in which interactions were modeled by a (repulsive) on-site Hubbard term. It was established that a single impurity level in general suppresses the supercurrent [5,6], except in the presence of spin-flip processes, when it may in fact be enhanced by means of the Kondo effect [5]. Strictly one-dimensional approaches, in which a Luttinger liquid description of the system was employed, likewise yielded significant suppression of the Josephson current with increasing interaction strength [7,8], except in the case of perfectly transmitting NS interfaces, when interactions were found to have virtually no impact on the supercurrent [8]. Recently, Rozhkov et al. [9] considered Josephson tunneling through an interacting gated quantum dot and showed that for strong enough interactions the system is a π-junction, i.e., the energy of the system is minimized at a phase difference π between the order parameters of the two superconducting leads, in certain ranges of the gate voltage.

In the work cited above, the interaction Hamiltonian describes a situation in which the interacting charge is allowed to fluctuate, so that the electrostatic potential is constant throughout the system. We shall here consider the opposite boundary condition of *fixed* interacting charge, and discuss its consequences, in terms of a simple qualitative model and a more rigorous density functional theory formulation.

In this article we study a superconductor-quantum dot-superconductor structure, and show that Coulomb interactions in the dot can be used to electrostatically control the supercurrent. The fundamental question we address is how electrostatic «rigidity» (reluctance towards changes in charge configuration) interplays with superconducting «rigidity», i.e., the macroscopic quantum coherence described by the phase of the superconducting order parameter. Usually, electrostatic interactions cause fluctuations of the phase by fixing the number of charges, in accordance with the well-known particle number-phase uncertainty relation, $\Delta N \Delta\varphi \gtrsim 1$, thereby destroying global phase coherence. In the present case, however, we have a unique situation when electrostatic rigidity *reinforces* phase rigidity. This possibility arises due to accumulation of non-quantized electronic charge, *controlled by the phase difference*, in the *non-superconducting* part of the device, where the charge-phase uncertainty relation is not applicable. This charge, associated with the formation of an Andreev state [10] which is confined to the vicinity of the junction, introduces additional electrostatic rigidity into the quantum mechanical coherent coupling across the junction. As a result, the supercurrent — which is related to coupling strength — increases. This is a consequence of the constraint that the charge confined in the normal region is fixed, in part by the superconducting pair potential (Andreev contribution) and in part by a gate potential (normal contribution). Due to the novel operating principle of the present device, the maximum supercurrent is thus greatly enhanced.

2. System

We consider a structure of the type depicted in the inset of Fig. 1. The electronic states in the normal region can be divided into confined states that reside in the potential well (quantum dot) created by the gate electrode, and states that couple the two superconductors. The latter consist of discrete Andreev states [10] whose energies, which lie within the superconducting gap, depend on the superconducting phase difference across the junction, and continuum states outside the gap.

In general, both types of states contribute to the phase-dependent supercurrent through the structure. In non-interacting short junctions the contribution from the continuum states has been shown to be negligible [11,12], especially for states far outside the gap; however, in more general situations the two contributions tend to have opposite signs [11–14]. The most dramatic manifestation of the charge accumulation effect occurs in a situation in which the continuous and discrete parts of the spectrum are discriminated with respect to their contribution to the supercurrent. Such discrimination might originate from an energy dependence of the transmission amplitude through the structure. If, for example, the interfaces between the dot and leads form adiabatic microconstrictions [15], such discrimination occurs when only one transverse mode contributes to the transmission. The contribution of the corresponding continuous spectrum of such a mode (with longitudinal energy $\mu + \epsilon < \mu - |\Delta|$) is suppressed with respect to the contribution of the Andreev states by a factor

$$D^{(1)}(E) \simeq \frac{1}{1 + e^{-\kappa(E - V_{\text{th}}^{(1)})}}, \quad \kappa \approx \pi^2 \sqrt{\frac{R}{d_0}}\frac{1}{\mu},$$

where E is the energy, $V_{\text{th}}^{(1)}$ is the threshold energy of the lowest transverse mode, d_0 is the minimum width of the neck, and R is the radius of curvature at the neck. The discrimination is then determined by the parameter $\kappa|\Delta|$, and is substantial already for constriction length $l = \sqrt{d_0 R/2} \sim \xi_0/5$, implying that significant discrimination can be realized for a wide range of structure lengths.

Our main concern shall be the contribution from discrete states. To minimize the contribution from continuum states we choose the lead-dot-lead geometry such that (i) only the lowest transverse mode contributes to the charge transport, and (ii) the transmission amplitude $D(\epsilon)$ for this mode is very small below the lower gap edge and increases sharply for $\epsilon \gtrsim |\Delta|$. Indeed, the scenario which most vividly illustrates the new effect is the extreme limit of $D \sim \Theta(\epsilon + |\Delta|)$, and in the following we shall take this to be the case. A more comprehensive investigation including other states will be pursued elsewhere. Moreover we shall, for simplicity, neglect possible transmission resonances associated with normal reflection.

We first present an analytic model that accounts for qualitative deviations from the noninteracting problem, and then proceed with a more general density functional theory (DFT) formulation of the problem.

3. Analytics

The equilibrium zero-temperature current I can be obtained from the total energy E of the system as $I = (2e/\hbar)\partial E/\partial\varphi$ [16], where φ is the phase difference across the junction. In the spirit of the constant-interaction (CI) model [17] we approximate the total energy of the system as*

$$E(V_g,\varphi) = \frac{[Q_c - \overline{Q}]^2}{2C_\Sigma} + \frac{1}{C_A} Q_c Q_A(\varphi) + \\ + \sum_j \epsilon_{c,j} + \epsilon_A(\varphi), \quad (1)$$

where $Q_c = N_c e$ is the confined normal charge, $\overline{Q}$ is a linear function of V_g, C_Σ is the total dot capacitance and C_A is an effective capacitance of the order of C_Σ. Here Q_A is the amount of charge inside the normal region that is associated with formation of an Andreev level. Importantly, we shall impose the boundary condition that Q_c is fixed (at a value determined by V_g). The last two terms represent the eigenenergies of confined and Andreev electronic states, respectively. Due to efficient screening we neglect the effects of Coulomb interactions inside the superconductors. Apart from the last term, which is responsible for the usual Josephson supercurrent, the second term gives an additional contribution which we now set out to investigate.

We confine our attention to ballistic, short weak links with adiabatic leads, so that only one Andreev level is relevant. For simplicity, we consider a quasi-1D system, although the essential features of the problem are independent of dimensionality. We shall, furthermore, assume ideal junctions, i.e., absence of Schottky barriers and entailing normal reflection, in order to emphasize the role of Andreev reflection as a significant scattering mechanism.

To begin with, we consider the limiting case of perfect normal transmission, $D(\epsilon) = 1$, in the interval $-|\Delta| < \epsilon < |\Delta|$ around the chemical potential, and stepwise constant gap parameter $\Delta(x)$ [12,18–20]. By matching bulk solutions $(u(x); v(x))$ of the Bogoliubov–de Gennes equation [22] at the NS interfaces and employing the Andreev approximation [10,19], we find the Andreev bound state to lowest order in L/ξ_0, where L is the dot size and ξ_0 is the superconducting coherence length. The single-particle energy $\epsilon_A(\varphi)$ may be obtained from an asymptotic analysis [11,21] and is given by $\epsilon_A^2 = |\Delta|^2(1 - D\sin^2(\varphi/2))$. The charge within the normal region, $-L/2 < x < L/2$, associated with the coupling between the superconductors, is obtained from [22,23]

$$Q_A = 2e \int_{-L/2}^{L/2} [|v|^2 + f(\epsilon_A)(|u|^2 - |v|^2)]\, dx,$$

where $f(\epsilon)$ is the Fermi–Dirac distribution. For $D(\epsilon > -|\Delta|) = 1$, we find $Q_A = eL/\xi_0 |\sin(\varphi/2)|$ to leading order in L/ξ_0 at zero temperature (Fig. 1). The current may now be calculated, and we find, for $\varphi \in [-\pi, \pi]$ and under the assumption that the superconductors are coupled**

$$I \approx I_{c,0} \sin\left(\frac{\varphi}{2}\right) + I_{c,0} N_c \frac{E_c}{|\Delta|} \frac{L}{\xi_0} \cos\left(\frac{\varphi}{2}\right) \mathrm{sgn}(\varphi). \quad (2)$$

Here $I_{c,0} \equiv e|\Delta|/\hbar$, N_c is the (quantized) number of confined electrons in the dot and $E_c = e^2/2C_A$. This suggests that the current is radically different from the ordinary Josephson effect: (i) The magnitude of the current depends on the gate voltage, and (ii) the phase-current relationship is not of the familiar sinusoidal form at zero temperature. The first term of Eq. (2) gives the usual current-phase relationship of

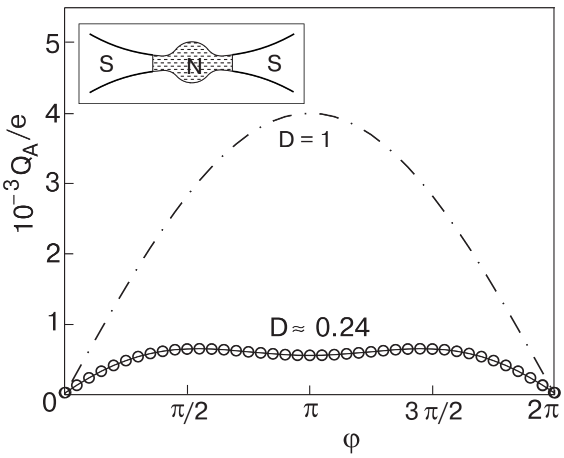


Fig. 1. Charge Q_A as a function of phase difference φ across the junction. Circles (O) correspond to numerical DFT results. Top curve corresponds to the case D ≈ 1, for which a simple analytic expression can be obtained (dash-dotted curve), whereas the lower curve is for the more realistic case of small *D*. Inset: Bird's-eye view of the SNS setup. «S» denotes the superconducting leads, «N» denotes the normal interacting «dot». A positively charged gate electrode is situated beneath the N region.

* The separation of the total energy into interacting and non-interacting parts as in Eq. (1) is valid provided that the interaction energy is small compared with $|\Delta|$. In this limit the wave functions of both Andreev and confined states are largely unperturbed.

** Corrections to the Andreev approximation are required only for φ very close to $n\pi$. At these phase values the corrections ensure that $\partial Q_A/\partial\varphi \to 0$.

the Andreev level by itself. The second term originates from the fact that the mid-gap Andreev states penetrate the leads by a distance that depends on the energy of the states and, hence, on the phase difference between the superconductors. Consequently, the charge in the normal region associated with these states is also phase-dependent, which results in a phase-dependent electrostatic interaction with the confined charge in the quantum dot. This situation is unique in the sense that the customary phase-dependent Josephson energy is accompanied by a phase-dependent electrostatic energy; usually, the uncertainty relation $\Delta N \Delta\varphi \lesssim 1$ precludes such an effect, but here the charge relevant to the electrostatics resides in the normal part of the device and is not subject to the uncertainty relation — charges in the superconducting banks are free to fluctuate as required to establish a well-defined phase difference φ.

Since N_c and E_c can be varied considerably by varying the depth and width of the confining potential, the current contribution from the last term may dominate the Andreev term.

While the case of perfect normal transmission is instructive as a limiting behavior, it is not very realistic. Whereas ϵ_A is independent of the details of the scattering potential in the short-junction limit, this is not true for the charge Q_A. However, since the quantity $\sqrt{|\Delta|^2 - \epsilon_A^2}$, which determines the inverse decay length of the wavefunction inside the leads, is reduced by a factor $\sqrt{D}$ in the presence of normal reflection, the charge Q_A is typically reduced by very roughly the same factor. Hence, normal reflection has a less severe effect on the interaction term than on the ordinary Josephson term ($\sim D$), especially for small D. A quantitative determination of the charge Q_A in the presence of normal reflection will be obtained from numerical DFT calculations.

In the absence of electron-electron interactions, the coupling between two superconductors through the formation of an Andreev level always reduces the total energy. In the present configuration, in contrast, Coulomb interactions in the dot result in a destruction of the Josephson coupling for large phase differences. However, there still exists a phase difference interval $[-\varphi_A, \varphi_A]$ — henceforth termed an «Andreev window» (AW) — where formation of an Andreev state is energetically favorable. Remarkably, the supercurrent in these regions is greatly enhanced, and is to a good approximation (especially for $D \approx 1$) constant throughout the interval.

The criterion for formation of an Andreev level at zero temperature (i.e., stability with respect to fluctuations of the superconducting phase, corresponding to a negative Josephson coupling energy) demands, for $D = 1$, that $|\varphi| \lesssim \varphi_A$, where $\varphi_A = \frac{1}{N_c}\frac{\xi_0}{L}\frac{|\Delta|}{E_c} \propto (I^{\max})^{-1}$, the latter quantity being the maximum supercurrent through the link. By tuning the gate voltage we may change the number N_c by discrete amounts, which in turn changes φ_A and $I^{\max}$ in a stepwise manner. In the $D < 1$ case, the width of the Andreev window increases as a consequence of the diminished charge Q_A. Since the phase difference φ_A corresponds to an interaction energy that is equal to $|\Delta|$, it also represents the limit of validity of Eq. (1). Consequently, the transition from finite to zero supercurrent will be continuous rather than abrupt as implied by Eq. (2).

4. Numerics

Here we present a numerical analysis which supports the above qualitative analysis. Density functional theory [24] has proven very successful in the study of small quantum mechanical systems, and is particularly well suited to equilibrium situations such as the one at hand. Oliveira et al. [25] have shown that DFT can be extended to describe systems with general mixed normal and superconducting elements. The Bogoliubov—de Gennes—Kohn—Sham (BdGKS) equations [25,26] take the form

$$\begin{pmatrix} \mathcal{H}(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -\mathcal{H}(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_\kappa(\mathbf{r}) \\ v_\kappa(\mathbf{r}) \end{pmatrix} = \epsilon_\kappa \begin{pmatrix} u_\kappa(\mathbf{r}) \\ v_\kappa(\mathbf{r}) \end{pmatrix}, \quad (3)$$

where u_κ and v_κ are the two components of the κth solution, ϵ_κ is the energy measured from the chemical potential, $\mathcal{H}$ is the appropriate effective Hamiltonian, and Δ is the self-consistent pair potential. In long weak links ($L \geq \xi_0$) a self-consistent determination of the pair potential is crucial [27]. For short and narrow junctions ($\xi_0 << L$), however, the exact shape of Δ inside the link is unimportant [11], and we use the approximation that it is piecewise constant, $\Delta(x) = |\Delta| e^{i\frac{\varphi}{2}\mathrm{sgn}(x)} \Theta(|x| - L/2)$. In this approximation, the BdGKS equations simplify significantly in the normal region, coupling the u and v components only through a boundary condition at the interfaces.

The problem separates naturally into a two-component formulation [28,29] in which the total energy functional is written as

$$E[\rho_c, \rho_A] = E_{\text{kin}}[\rho_c] + E_{\text{kin}}[\rho_A] + E_{\text{ext}}[\rho_{\text{tot}}] + \\ + E_H[\rho_{\text{tot}}] + E_{xc}[\rho_{\text{tot}}] - E_H[\rho_A] - E_{xc}[\rho_A]. \quad (4)$$

Here ρ_c and ρ_A denote the charge density of the confined and Andreev levels, respectively, and $\rho_{\text{tot}} = \rho_c + \rho_A$. The terms E_{kin}, E_{ext}, E_H and E_{xc} are, in this order, the kinetic energy, interaction with external potential, Hartree energy and the many-body exchange-correlation energy. The two last terms subtract the self-interaction of the Andreev state charge with itself (note that continuum states are not included in the DFT treatment). Provided that the potential well is deep enough, the confined states have decayed to a negligible value close to the interfaces and do not experience the presence of the superconducting leads. We assume that the screening is perfect everywhere in the leads so that their (infinite) energies are not included in the energy functional of Eq. (4). For the exchange-correlation energy E_{xc} a local density approximation for a 2D electron gas [30] was used. Since the Hartree term typically exceeds the XC term by several orders of magnitude, the choice of E_{xc} does not significantly affect our results. The minimization of the total energy of Eq. (4) with respect to ρ_c and ρ_A leads to generalized Kohn–Sham equations which must be solved self-consistently.

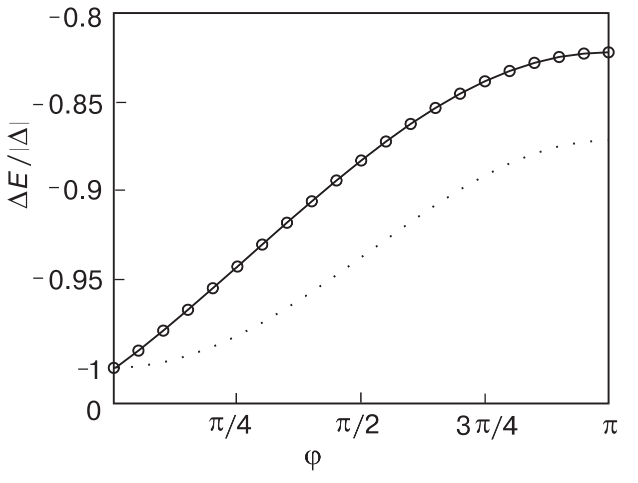
We perform the numerical calculation on a 1D grid containing the entire normal region (in the case of BdGKS equations the grid extends slightly into the leads in order to manage the boundary conditions). In practice, a narrow Gaussian charge distribution of width $W \lesssim k_F^{-1}$ is assumed in the transverse direction, facilitating the calculation of the Coulomb interactions and justifying the use of 2D XC-functionals.

We discretize the BdGKS equations, by which the problem of finding the Andreev state reduces to solving a generalized eigenvalue problem $\hat{K}(\epsilon_A)\Psi = \epsilon_A \Psi$, where $\hat{K}$ is the matrix corresponding to the BdGKS Hamiltonian and Ψ is the vector (u,v). The ϵ_A-dependence of the $\hat{K}$-matrix originates from the boundary conditions. In order to extract eigenvalues near the middle of the spectrum with required accuracy, we have used an iterative Arnoldi method [31], the performance of which was very satisfactory. The localized normal states in the quantum dot are solved on the 1D grid using an efficient Rayleigh quotient multigrid method [32].

We have chosen a channel length $L \simeq 50$ nm, and material parameters such that $|\Delta| = 0.2$ meV $<< \mu = 1$ eV and an effective mass $m^* = 0.024$ typical for InAs, so that $\xi_0 \approx 13$ μm. The gate potential was represented by a smooth well which was chosen to accommodate around 10 electrons. The charging energy corresponding to our choice of confining potential is $e^2/2C_A \approx 0.9$ meV.

5. Results

To excellent precision we find the expected short-junction result [11] $\epsilon_A^2 = |\Delta|^2(1 - D\sin^2(\varphi/2))$, with an effective normal transmission coefficient $D \approx 0.24$. Figure 2 describes our main results. For the parameters we have used, the total energy is clearly dominated by the interaction term. Due to the small effective mass of InAs, the Andreev window is very wide, $\varphi_A > \pi$, and supercurrent is non-zero for all values of the phase difference. The magnitude of the



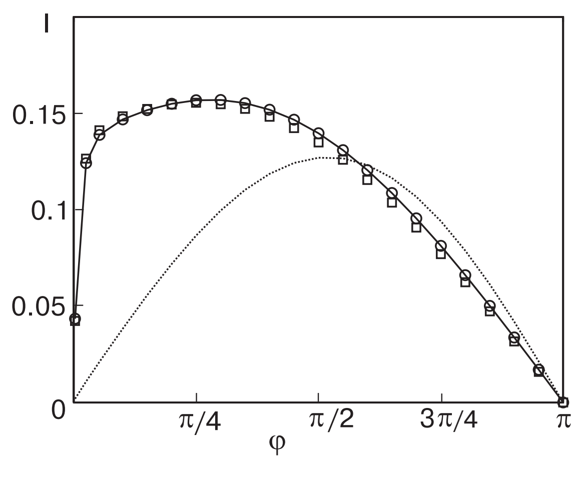


Fig. 2. Left: Circles: Total energy change due to formation of the Andreev level (solid line is a guide to the eye). Dotted line: Single-particle energy ϵ_A of the Andreev level. For the parameter values at hand, formation of the Andreev level is energetically advantageous throughout the entire phase interval $[0,2\pi]$. *Right*: Circles: Supercurrent in the presence of an Andreev level. Dotted line: Supercurrent in the absence of interactions (first term in Eq. (2)). Squares: Current as predicted by the CI-model (Eq. (1)) with numerically obtained values of Q_A and ϵ_A. Currents are given in units of $e|\Delta|/\hbar$. E and I are, respectively, even and odd with respect to $\varphi = 0$.

supercurrent at small phase differences is greatly enhanced, and exceeds the non-interacting contribution by as much as an order of magnitude. Normal reflection is responsible for the suppression of the supercurrent for small phase values.

6. Discussion

The main effect of electron-electron interactions is thus twofold: (i) Coupling of the superconductors through formation of an Andreev level is energetically favorable only for sufficiently small phase differences $\varphi < \varphi_A$. (ii) The supercurrent for small φ is greatly enhanced, and its magnitude is roughly quantized. This suggests two ways to accomplish a switching of the supercurrent: 1) By tuning φ, at fixed gate voltage, into or out of the AW; 2) Increasing the depth of the potential well by increasing V_g increases the number N_c of confined charges, which in turn reduces φ_A in a roughly stepwise fashion. For a fixed value of φ inside the initial AW, the supercurrent therefore increases in steps (for $D \approx 1$) of height $I_{c,0}(E_c/|\Delta|)(L/\xi_0)$ until $\varphi_A < \varphi$, at which point the supercurrent vanishes. The «phase-biasing» may be realized by integrating the SNS junction into a SQUID geometry and applying a small magnetic field.

The interaction effects also change the voltage response of the system. In the presence of a small bias voltage [33], the phase difference changes in time according to the Josephson relation $d\varphi/dt = 2eV/\hbar$. This brings the system periodically into the AW, $|\varphi - 2n\pi| < \varphi_A$, and results in a sequence of current pulses of alternating sign.

In conclusion, we have considered an SNS device in the short-junction limit, and investigated the consequences of Coulomb interaction between charges confined in the normal region and charge associated with coupling of the superconductors. We present a model which accurately describes the total energy of the system, and derive analytic results for a limiting case, which lets us qualitatively understand the phase dependence of the energy and the stability of the system, specifically the existence of an Andreev window and the essentially step-like magnitude of the maximum supercurrent inside this region. Numerical DFT results support analytical results. We find a dominant contribution to the total energy due to Coulomb interactions, leading to a supercurrent contribution that can greatly exceed the current of the non-interacting sistem. We discuss practical consequences and suggest the operation of a switchable weak link.

The quantitative results in this work were obtained at a relatively high value of the dielectric constant. The effects of interactions in real structures may therefore be even more pronounced than discussed.

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