Perturbation theory for a quantum dot with Andreev bound states: Saturation of spin symmetric solution

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(Dated: January 7, 2014)

A quantum dot with Coulomb repulsion attached to left and right superconducting leads is studied via the perturbation expansion in the interaction strength. We use the Nambu formalism and the standard many-body diagrammatic representation of the impurity Green functions. We formulate the perturbation expansion in the spectral representation so that to be able to distinguish contributions from the isolated Andreev bound states in the gap and continuous band states. We analyze the spin-symmetric solution in the weak-coupling regime and show that no crossing of Andreev states is possible. We find that a spin-symmetric state reaches saturation at which the gap states merge and freeze at the Fermi energy and no direct Josephson current flows through the impurity.

I. INTRODUCTION

Nanostructures attached to leads with specific properties display interesting and important quantum effects at low temperatures. Much attention, both from experimentalists and theorists, and has been paid in recent years to a quantum dot with well separated energy levels attached to BCS superconductors. In particular the behavior of the supercurrent (Josephson current) that can flow through the impurity without any external voltage bias between two superconducting leads in equilibrium was in the center of interest. The Josephson current is normally (non-interacting dot) proportional to the sine of the phase difference between the left and right superconductor. But when it goes through the impurity with tangible Coulomb repulsion it undergoes a transition signaled by a reversal of the sign of the current. Full and unambiguous understanding of this quantum phase transition has not yet been reached. There is a general consensus that the sign reversal of the Josephson current has origin in a transition from a spin-singlet state (0-phase), where the supercurrent is proportional to the sine of the phase difference, to a spin-doublet state ($\pi$-phase) where the supercurrent is proportional to the sine of the phase difference shifted by angle $\pi$. It remains, however, unclear whether this transition is accompanied by emergence of a stable magnetic order on the impurity. Weak-coupling mean-field static solutions obtain a $0 - \pi$ transition in the Josephson current as a consequence of a first-order transition from a spin-symmetric to a spin-polarized state. This Hartree-Fock solution does not contain dynamical fluctuations and its conclusion about the existence of a magnetic order in the $\pi$-phase is not reliable. More advanced, mostly numerical approaches such as numerical renormalization group Monte-Carlo simulations or a functional renormalization group produce a $0 - \pi$ transition without any equilibrium symmetry breaking.

The question whether the $0 - \pi$ transition is a consequence of a transition from a spin-symmetric to a spin-polarized state is subtle and essentially demands knowledge of spectral properties of the one-electron propagator on the impurity. Numerical methods and most of the analytic approaches are formulated in the Matsubara formalism within which spectral properties are not directly accessible. A few approaches have tried to address the impurity Green function for real frequencies and to understand the $0 - \pi$ transition from changes in spectral properties. The principal result of these analyses is that the $0 - \pi$ transition is a consequence of a crossing of gap states. Due to the proximity effect the gap of the superconducting leads is imposed on the impurity spectrum, while the original atomic levels for the electron and the hole of the dot transform to Andreev bound states (ABS). There are two Andreev (bound and anti-bound) states in the singlet 0-phase while it seems that other two emerge in the $\pi$-phase. The Andreev states are always symmetrically distributed around the Fermi energy. At the transition point the existing two ABS from the 0-phase reach the Fermi energy and interchange their positions in the $\pi$-phase. These conclusions were confirmed experimentally via scanning tunneling spectroscopy.

The Andreev bound states are important for the transfer of the Cooper pairs (supercurrent) through the impurity. They are generally dependent on the phase difference between the attached superconducting leads. They have the dominant contribution to the Josephson current in the 0-phase. When the bound and anti-bound Andreev states reach the Fermi energy and cross in the $\pi$-phase their contribution to the Josephson current reverse the sign and leads to the observed transition.

The existing spectral analysis has not yet resolved the
question whether the $\pi$-phase is a spin-polarized state. The weak-coupling Hartree-Fock approximation and an expansion beyond it lead to the spin-polarized $\pi$-phase, while the numerical solutions connect the $\pi$-phase with a degenerate state but still without equilibrium (static) spin polarization. The question whether we can obtain a degenerate state but still without equilibrium (static) spin polarization. The question whether we can obtain the $0 - \pi$ transition where Andreev bound states cross without breaking spin-reflexion symmetry remains to be answered.

The aim of this paper to analyze the spin-symmetric phase via the perturbation expansion in the interaction strength and to find out whether dynamical corrections beyond the Hartree-Fock solution can lead to crossing of Andreev bound states. We present rules for a systematic treatment of the perturbation expansion in the spectral representation with separate contributions from the isolated gap states and from continuously distributed band states. We resort to the weak-coupling regime and start with the static, spin-symmetric Hartree-Fock approximation that we later enrich with dynamical corrections due to multiple electron-hole scatterings. We stay in the spin-symmetric solution below the unphysical transition to the magnetic state caused by insufficient treatment of dynamical effects of the Coulomb repulsion connected with the Kondo effect.

The paper is organized as follows. In Sec. II we introduce the model and the Andreev states for the noninteracting impurity. In Sec. III we introduce a diagrammatic representation of the perturbation expansion with normal and anomalous contributions to the one- and two-particle Green functions. We introduce rules for analytic continuation from imaginary Matsubara frequencies to real ones with contributions from isolated poles in the energy gap and continuous cuts due to the band states in Sec. IV. The simplest dynamical approximation with multiple electron-hole scatterings equivalent to the random phase approximation (RPA) is presented. Explicit equations in the spectral representation for the Hartree-Fock approximation (HFA) are derived in Sec. V. We solved these equations numerically. To confirm the observed general trend of the spin-symmetric solution we added numerical results with dynamical fluctuations via RPA. Sec. VI contains discussion of the results and conclusions.

II. MODEL HAMILTONIAN AND ANDREEV BOUND STATES

A single impurity is used to simulate a nanostructure with separated energy levels connecting superconducting leads in the experimental setup. The Hamiltonian of the system consisting of a single impurity attached to left-right BCS superconductors is

$$\mathcal{H} = \mathcal{H}_{\text{dot}} + \sum_{s=R,L} (\mathcal{H}_{\text{lead}}^s + \mathcal{H}_{\text{imp}}^s),$$

where the impurity Hamiltonian is a single-level atom with the level energy $\pm \epsilon$ for single electron (hole) and Coulomb repulsion $U$

$$\mathcal{H}_{\text{dot}} = \epsilon \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma} + U (d_{\uparrow}^\dagger d_{\uparrow} d_{\downarrow}^\dagger d_{\downarrow}) .$$

The Hamiltonian of the leads is

$$\mathcal{H}_{\text{lead}}^s = \sum_{\kappa \sigma} \epsilon(k) c_{\kappa \sigma}^\dagger c_{\kappa \sigma} - \Delta_s \sum_{k} (e^{i\Phi_k} c_{\kappa \uparrow}^\dagger c_{\kappa \downarrow} + \text{H.c.} )$$

with $s = L, R$ denoting left, right lead. Finally, the hybridization term for the contacts reads

$$\mathcal{H}_{\text{h}}^s = -t_s \sum_{\kappa \sigma} (c_{\kappa \sigma}^\dagger d_{\sigma} + \text{H.c.} ) .$$

The most direct way to handle Cooper pairs and anomalous functions breaking charge conservation is to introduce the Nambu spinor representation. We first introduce Nambu spinors in the superconducting leads

$$\hat{\varphi}_{\kappa \sigma} = \begin{pmatrix} c_{\kappa \sigma}^\dagger \\ c_{\kappa \sigma} \end{pmatrix} , \quad \hat{\varphi}_{\kappa \sigma}^\dagger = \begin{pmatrix} c_{\kappa \sigma}^\dagger & c_{\kappa \sigma} \end{pmatrix} .$$

Due to the hybridization the Cooper pairs can penetrate onto the impurity giving rise to an anomalous impurity Green function. Hence, we introduce Nambu spinors also for the impurity (local) operators

$$\hat{\varphi}_{\sigma} = \begin{pmatrix} d_{\sigma} \\ d_{\sigma}^\dagger \end{pmatrix} , \quad \hat{\varphi}_{\sigma}^\dagger = \begin{pmatrix} d_{\sigma}^\dagger & d_{\sigma} \end{pmatrix} .$$

The individual degrees of freedom of the leads are unimportant for the studied problem and are generally integrated out leaving us with only the active variables and functions on the impurity. The fundamental function is the one-electron impurity Green function measuring (imaginary) time fluctuations that in the Nambu formalism is a $2 \times 2$ matrix

$$\hat{G}_{\sigma}(\tau - \tau') = \frac{1}{\mathcal{T} \left[ G_{\sigma}(\tau) G_{\sigma}^\dagger(\tau') \right] - \mathcal{T} \left[ G_{\sigma}^\dagger(\tau) G_{\sigma}(\tau') \right]}$$

$$= \begin{pmatrix} G_{\sigma}(\tau - \tau') & G_{-\sigma}(\tau - \tau') \\ G_{\sigma}^\dagger(\tau - \tau') & G_{-\sigma}^\dagger(\tau - \tau') \end{pmatrix}$$

correlating appearance of the electron with spin $\sigma$ and the hole with spin $-\sigma$. We introduced particle $G_{\sigma}, G_{-\sigma}$ and hole $G_{\sigma}^\dagger, G_{-\sigma}^\dagger$ Green functions for individual spins. They are connected by symmetry relations $G_{\sigma}^\dagger(\tau) = -G_{-\sigma}(\tau)$ and $G_{-\sigma}^\dagger(\tau) = G_{\sigma}(\tau)$, since the normal Green function is odd while the anomalous is an even function of the imaginary time.
The problem can be exactly solved for an impurity without onsite interaction, \( U = 0 \). In this case the inverse unperturbed propagator for the spin-symmetric situation and for identical left and right superconductors can directly be found in the Nambu formalism. Due to energy conservation it is convenient to use Fourier transform from (imaginary) time to frequency (energy) where the Green function can analytically be continued to complex values. The matrix of the inverse Green function for a complex energy \( z \) reads

\[
\hat{G}_0^{-1}(z) = \begin{pmatrix} \Delta \cos(\Phi/2)\sigma(z) & z[1 + \sigma(z)] + \epsilon \\ \Delta \cos(\Phi/2)\sigma(z) & z[1 + \sigma(z)] - \epsilon \end{pmatrix},
\]

(8)

where

\[
\sigma(z) = i\frac{\Gamma_0}{\zeta} \text{sgn}(\Im z),
\]

(9)
is the “hybridization self-energy” \( \sigma(z) \), that is, a dynamical renormalization of the impurity energy level due to the hybridization to the superconducting leads. We approximated the Green function in the leads by its value at the Fermi energy and denote \( \Gamma_0 = 2\pi i^2\rho_0 \) being the effective hybridization strength. We further denoted \( \Phi = \Phi_L - \Phi_R \) the difference between the phases of the left and right superconducting leads and \( \rho_0 \) the density of states of the lead electrons at the Fermi energy. To represent explicitly the hybridization self-energy we introduced a new complex number \( \zeta = \xi + i\eta \) derived from the complex energy \( z = x + iy \) by a quadratic equation \( \zeta^2 = x^2 - \Delta^2 \). Thereby the following convention for the complex square root has been used

\[
\xi\eta = xy, \quad \text{sgn}(\xi) = \text{sgn}(x), \quad \text{sgn}(\eta) = \text{sgn}(y).
\]

(10)
The renormalized energy \( \zeta \) along the real axis \( z = x \pm i0 \) is real outside the energy gap (\( \Delta, -\Delta \)) and imaginary within it

\[
\zeta = \text{sgn}(x)\sqrt{x^2 - \Delta^2} \quad \text{for} \quad |x| > \Delta,
\]

\[
\zeta = \pm i\sqrt{\Delta^2 - x^2} \quad \text{for} \quad |x| < \Delta.
\]

(11)

Accordingly the hybridization energy is purely imaginary outside the gap and real within it

\[
\sigma(x \pm i0) = \pm \frac{i\Gamma_0 \text{sgn}(x)}{\sqrt{x^2 - \Delta^2}} \quad \text{for} \quad |x| > \Delta,
\]

\[
\sigma(x \pm i0) = \frac{\Gamma_0}{\sqrt{\Delta^2 - x^2}} \quad \text{for} \quad |x| < \Delta.
\]

(12)

With the above definitions the unperturbed \( (U = 0) \) impurity Green function is

\[
\hat{G}^{(0)}(z) = \frac{1}{D_0(z)} \begin{pmatrix} z[1 + \sigma(z)] + \epsilon & -\Delta_0\sigma(z) \\ -\Delta_0\sigma(z) & z[1 + \sigma(z)] - \epsilon \end{pmatrix},
\]

(13)

where we denoted \( \Delta_0 = \Delta \cos(\Phi/2) \) and introduced

\[
D_0(z) = z^2 [1 + \sigma(z)]^2 - \epsilon^2 - \Delta_0^2 \sigma(z)^2
\]

the determinant of the matrix of the inverse unperturbed impurity Green function. It is decisive for the determination of the gap states. This determinant is real within the gap and can go through zero determining the gap (Andreev) states. It is easy to find the defining equation for the energy \( \omega_0 \) of the Andreev states that are symmetrically placed around the Fermi energy (center of the gap). From Eq. (13) we directly obtain

\[
\omega_0(1 + \sigma_0) = \pm \sqrt{\epsilon^2 + \Delta_0^2 \sigma_0^2}.
\]

(14)

We abbreviated \( \sigma_0 = \sigma(\omega_0) \).

The Andreev states are important for the transport of the Cooper pairs through the quantum dot. They allow the direct pass through the impurity and dominate over the tunneling contributions from one lead to the other through a potential barrier due to the Coulomb repulsion on the dot. The Josephson current flows through the impurity also in equilibrium and can be represented at zero temperature via the anomalous Green function

\[
J = \int_0^\infty \frac{dx}{\pi} \Im \left[ G^*(i\omega)S^{(0)}(i\omega) \right]
\]

\[
= -2\Delta\Gamma_0 \sin(\Phi/2)
\]

\[
\times \left[ \int_{-\infty}^{-\Delta} d\omega \frac{\Re[G^*(\omega)]}{\sqrt{\omega^2 - \Delta^2}} + \text{Res}[G^*, -\omega_0] \right].
\]

(15)

where we denoted \( S^{(0)}(i\omega_n) = \Delta \sigma(i\omega)e^{\Phi/2} \). We see that the contribution from the Andreev states to the Josephson current cannot be determined from the thermal representation via Matsubara frequencies. Only the spectral representation allows us to distinguish the direct current from the residues of the anomalous impurity Green function at the frequencies of the Andreev states from the tunneling current between the band states. One can check that the tunneling current is much smaller than that due to the Andreev states and has opposite sign. Introducing the Coulomb repulsion hinders creation of Andreev states on the impurity and hence diminish the direct contribution to the Josephson current. To control this effect one has to work in the spectral representation with real frequencies. Such a control is not accessible to numerically exact solutions but it is the main asset of our spectral representation of the perturbation expansion in the interaction strength.

III. PERTURBATION EXPANSION: DIAGRAMMATIC REPRESENTATION

The full inclusion of the Coulomb repulsion on the impurity cannot be exactly (analytically) performed and we hence must resort to approximations. A systematic way to assess the impact of the Coulomb repulsion on equilibrium properties is a renormalized perturbation expansion. The best way to control the individual contributions from the perturbation expansion is to represent them diagrammatically.
We start with the Nambu spinor of the impurity propagator to which we assign solid lines decorated with arrows
\[
\begin{pmatrix}
G_\sigma(\tau - \tau') , & G_{-\sigma}(\tau - \tau') \\
G^*_\sigma(\tau - \tau') , & G^*_{-\sigma}(\tau - \tau')
\end{pmatrix}
\]
\[= \begin{pmatrix}
\text{ } & \text{ } \\
\text{ } & \text{ }
\end{pmatrix}
\]
(16)

We keep the time (charge) propagation (from left to right) and spin of the propagators in the diagrammatic representation, whereby the upper/lower line corresponds to spin up/down. We can construct standard Feynman many-body diagrams for processes induced by the Coulomb interaction of the electrons on the impurity between two superconducting leads. The Coulomb interaction will be represented via a wavy line. Since the interaction is static, the interaction wavy line is always vertical. Before we start to analyze the diagrammatic contributions from the perturbation expansion we resume basic exact relations.

The impact of the Coulomb repulsion on the Green function is included in a matrix self-energy \(\hat{\Sigma}(z)\) so that the full inverse propagator in the spin-symmetric situation reads \(\hat{G}^{-1}(z) = \hat{G}^{-1}_0(z) - \hat{\Sigma}(z)\). Its explicit component representation is
\[
\hat{G}^{-1}(z) = \begin{pmatrix}
z[1 + \sigma(z)] - \epsilon - \Sigma(z) , & \Delta_\Phi [\sigma(z) - S(z)] \\
\Delta_\Phi [\sigma(z) - S^*(z)] , & z[1 + \sigma(z)] + \epsilon - \Sigma^*(z)
\end{pmatrix}.
\]
(17)

We denoted \(\Sigma\) and \(S\) the normal and anomalous parts of the interaction-induced self-energy. The symmetry relations for the unperturbed Green function are conserved and read in (complex) energy representation
\[
G^*_\sigma(z) = -G_\sigma(-z) \quad \text{and} \quad G^*_{-\sigma}(z) = G_{-\sigma}(-z).
\]
(18)

Consequently, the same relations hold for the self-energies
\[
\Sigma^*_\sigma(z) = -\Sigma_\sigma(-z) \quad \text{and} \quad S^*_\sigma(z) = S_\sigma(-z).
\]
(19)

If we denote \(D(z) = \det[\hat{G}^{-1}(z)]\), the determinant of the inverse Green function, then with the electron-hole symmetry we obtain
\[
D(z) = z^2 [1 + \sigma(z)]^2 - [\epsilon + \Sigma(z)][\epsilon + \Sigma(-z)]
- \Delta_\Phi [\sigma(z) - S(z)][\sigma(z) - S(-z)]
\]
(20)

and the full one-particle Green function can be represented with the above notation as
\[
\hat{G}(z) = \frac{1}{D(z)} \times \begin{pmatrix}
z[1 + \sigma(z)] + \epsilon + \Sigma(z) , & -\Delta_\Phi [\sigma(z) - S(z)] \\
-\Delta_\Phi [\sigma(z) - S(-z)] , & z[1 + \sigma(z)] - \epsilon - \Sigma(z)
\end{pmatrix}.
\]
(21)

The existence and positions of the Andreev states are again determined from zeros of determinant \(D(z)\). They depend on the behavior of the normal and anomalous self-energies for which we introduce a diagrammatic expansion. We resort throughout the paper to the spin-symmetric situation. We first formulate the perturbation expansion in the thermodynamic language using the Matsubara representation. Only after having constructed contributions to the perturbation expansion and approximations we perform analytic continuation to real frequencies so that to control the behavior of Andreev states.

### A. One-particle diagrams

We start with summing diagrams directly for the self-energy, that is, summing one-particle irreducible diagrams. The simplest diagrams are the Hartree-Fock contributions represented for the normal and anomalous parts in the following two relations
\[
\Sigma_{HF} = \frac{U}{\beta} \sum_n G(i\omega_n), \quad \Delta_\Phi S_{HF} = \frac{U}{\beta} \sum_n G(i\omega_n).
\]
(24)

The Hartree-Fock approximation leads to a static self-energy that does not cover dynamical effects induced by strong particle interaction. The simplest dynamical self-energy comes from the second order of the perturbation expansion. At this order we have to include different types of intermediate propagation consisting either of the normal or the anomalous Green functions. The full contribution from the second order for the normal and
The anomalous self-energy is

\[
\Sigma = - \left( \begin{array}{c}
\text{normal} \\
\text{anomalous}
\end{array} \right),
\]

(25)

which is mathematically expressed as

\[
\Sigma^{(2)}(i\omega_n) = - \frac{U^2}{\beta} \sum_n G(i\omega_n + iv_m)[\chi(iv_m) + \psi(iv_m)],
\]

(26)

\[
\Delta_{\Phi}S^{(2)}(i\omega_n) = - \frac{U^2}{\beta} \sum_n G(i\omega_n + iv_m)[\chi(iv_m) + \psi(iv_m)].
\]

(27)

We introduced normal and anomalous two-particle bubbles

\[
\chi(iv_m) = \frac{1}{\beta} \sum_n G(i\omega_n)G(i\omega_n + iv_m),
\]

\[
\psi(iv_m) = \frac{1}{\beta} \sum_n G(i\omega_n)G^*(-i\omega_n - iv_m).
\]

(28)

Notice that the two-particle bubbles appear in diagrams in pairs, the normal and the anomalous together.

The first two orders of the perturbation expansion are well controllable on the one-particle level. The higher-order contributions to the self-energy become more complex and their classification more intricate. It is convenient to introduce and classify diagrams with two and more particles involved in the diagrammatic contributions via vertex functions. Most of the approximations rely on and do not go beyond classification of two-particle contributions.

### B. Two-particle diagrams

To classify the two-particle diagrams in the perturbation expansion we introduce a notation for the two-particle vertex. We use the electron-hole notation, which means that the fundamental (normal) vertex contains one electron and one hole. We must assign three independent dynamical variables, Matsubara frequencies in this case, to four end points of the two-particle vertex. We do it for the normal vertex in the following way

\[
X(i\omega_n, i\omega_n'; iv_m) = X^{i\omega_n + iv_m \downarrow \uparrow}.
\]

(29)

The upper lines carry spin up, while the lower ones spin down. We have to add to the normal vertex also anomalous vertex functions that can have different end points (orientations of the fermionic lines attached to the corners of the vertex). All possible two-particle vertex functions are plotted in Fig. 1. They differ in orientations of upper and/or lower lines. The anomalous vertices do not conserve either spin or/and charge.

In analogy with the one-particle irreducible diagrams summed in the self-energy, we introduce two-particle irreducible vertices and use Bethe-Salpeter equations to build the full two-particle vertex of the given type. The most common diagrams contributing to the vertex are summed via a geometric series of two-particle bubbles. There are three different types of such series corresponding to three different two-particle scattering channels. An example of such a series is plotted in Fig. 2. Again the normal and anomalous two-particle propagators appear simultaneously and thereby double the contribution from the vertex. The corresponding Bethe-Salpeter equation in the electron-hole channel for the normal vertex is

\[
\Gamma = \Lambda - \Lambda \Gamma - \Lambda \Gamma,
\]

(30)

where we denoted \( \Lambda \) the irreducible electron-hole vertex.

This irreducible vertex in the simplest approximation is
FIG. 1: Normal ($X$) and anomalous ($X'$) vertices and their symmetries. We used the electron-hole representation. Asterisk denotes inversion of the lower line while bar the inversion of the upper line. Notice that anomalous vertices (a) and (b) conserve charge but do not conserve spin, while vertices (c) and (d) conserve neither spin nor charge.

The full two-particle vertex $\Gamma$ is then used to determine the self-energy. A relation connecting the two-particle vertex with the one-particle self-energy is the Schwinger-Dyson equation and has a diagrammatic representation for the normal component of the self-energy

$$ \Sigma = - \left( \begin{array}{c} \Gamma + \Gamma \end{array} \right) + \left( \begin{array}{c} \Gamma + \Gamma \end{array} \right) \quad \text{(31)} $$

and for the anomalous one

$$ \Sigma = - \left( \begin{array}{c} \Gamma + \Gamma \end{array} \right) + \left( \begin{array}{c} \Gamma + \Gamma \end{array} \right) \quad \text{(32)} $$

Notice that it is only the normal part of the two-particle vertex that contributes to the self-energy, either normal or anomalous. Equations (31) and (32) are used to assess dynamical corrections to the static Hartree-Fock mean-field approximation.

IV. SPECTRAL REPRESENTATION OF THE PERTURBATION EXPANSION

General diagrammatic representation with its rules directly gives expressions in Matsubara frequencies. The Matsubara representation on the temperature axis carries no direct information about the gap and the Andreev states. To control the Andreev states and their dependence on the interaction strength we must analyt-
ically continue the sums over Matsubara frequencies to spectral integrals over real frequencies. The sums over fermionic and bosonic Matsubara frequencies to be analytically continued generally are

\[ X(i\nu_m) = \frac{1}{\beta} \sum_n A(i\omega_n + i\nu_m)B(i\omega_n) , \]  

\[ C(i\omega_n) = \frac{1}{\beta} \sum_m Z(i\nu_m)B(i\omega_n + i\nu_m) . \]  

(33)  

(34)

Their spectral representations, assuming vanishing of the functions at infinity, are

\[ X(z) = -\int_{-\infty}^{\infty} \frac{dx}{\pi} f(x) \left[ 3A(x^+)B(x + z) + 3B(x^+)A(x - z) \right] \]  

(35)

and

\[ C(z) = \frac{1}{\beta} \int_{-\infty}^{\infty} \frac{dx}{\pi} \left[ b(x)3Z(x^+)B(x + z) - f(x)3B(x^+)Z(x - z) \right] \]  

(36)

where \( f(x) \) and \( b(x) \) are Fermi-Dirac and Bose-Einstein distributions. We abbreviated \( x^+ = x + i0^+ \).

The unperturbed one-electron Green functions have a gap around the Fermi energy \( -\Delta, \Delta \) and two poles at \( \pm \omega_0, |\omega_0| < \Delta \). Since the hybridization self-energy \( \sigma(z) \) has a square-root singularity at the gap/band edges, the gap is fixed and does not depend on the interaction strength. This does not hold for higher-order Green functions and the poles within the gap. They do depend on the interaction strength. We hence must be careful when treating the two-particle functions in the spectral representation.

The sum over the fermionic Matsubara frequencies for the one-particle function can then be rewritten in the spectral representation

\[ \frac{1}{\beta} \sum_n F(i\omega_n) \rightarrow \left[ \int_{-\infty}^{-\Delta} + \int_{\Delta}^{\infty} \right] \frac{dx}{\pi} f(x)3F(x + i0) + \sum_i f(x_i) \text{Res}[F, x_i] \]  

(37)

containing an integral over the band states and sum over isolated poles within the gap. Using formula (35), we analogously represent the two-particle bubbles. We resort in further reasoning to zero temperature. First the normal bubble

\[ \psi(z) = -\int_{-\infty}^{-\Delta} \frac{dx}{\pi} \left[ 3G(x^+)G(x - z) + 3G(x^+)G(x + z) \right] + \text{Res}[G, -\omega_0]G(-\omega_0 - z) + \text{Res}[G, -\omega_0]G(-\omega_0 + z) \]  

and then the anomalous one is

\[ \chi(z) = -\int_{-\infty}^{\infty} \frac{dx}{\pi} \left[ 3\tilde{G}(x^+)\tilde{G}(x - z) + \text{Res}[\tilde{G}, -\omega_0]\tilde{G}(-\omega_0 - z) + \text{Res}[\tilde{G}, -\omega_0]\tilde{G}(-\omega_0 + z) \right] \]  

(39)

The gap of the two-particle bubbles changed, but it is important that it was increased to \( -\Delta - \omega_0, \Delta + \omega_0 \). The bubbles contain as well gap states, poles at frequencies \( \pm 2\omega_0 \). The residues are multiples of the residues of the one-electron Green functions

\[ \text{Res}[\chi, 2\omega_0] = -\text{Res}[\tilde{G}, \omega_0]\text{Res}[\tilde{G}, -\omega_0], \]  

\[ \text{Res}[\chi, -2\omega_0] = \text{Res}[\tilde{G}, \omega_0]\text{Res}[\tilde{G}, -\omega_0], \]  

\[ \text{Res}[\psi, 2\omega_0] = -\text{Res}[\tilde{G}, \omega_0]\text{Res}[\tilde{G}, -\omega_0], \]  

\[ \text{Res}[\psi, -2\omega_0] = \text{Res}[\tilde{G}, \omega_0]\text{Res}[\tilde{G}, -\omega_0] . \]  

(40)

The gap extends to higher values by each convolution of the two-particle propagators. Notice that multiple scatterings in the electron-hole channel contain always a sum of the normal and anomalous bubble. It follows from the electron-hole symmetry, Eqs. (38) and (39) that the poles from the normal bubble are exactly compensated by the poles in the anomalous bubble. Consequently, the total two-particle bubble \( \chi(z) + \psi(z) \) in the electron-hole channel is free of gap singularities.

The infinite series of multiple electron-hole scatterings from Eq. 2 defines the normal vertex. It is the only one that is relevant for the one-electron self-energy. We can write

\[ \Gamma(z) = \frac{U}{1 + U[\chi(z) + \psi(z)]}. \]  

(41)

This vertex has no gap states in the weak-coupling regime. Generally, vertex \( \Gamma(z) \) can contain poles at the real axis for strong electron repulsion when the denominator on the right-hand side of Eq. (41) goes through zero. Such a pole is, however, unphysical and is suppressed by the Kondo effect. Its correct description demands inclusion of a dynamical renormalization of the interaction strength.

We now use vertex \( \Gamma \) in the Schwinger-Dyson equation (31) and (32) to determine the normal and anomalous self-energy \( \Sigma, S \)

\[ \Sigma(i\omega_n) = \frac{1}{\beta} \sum_m G(i\omega_n + i\nu_m)\Gamma(i\nu_m) \]  

\[ \Delta_\Phi S(i\omega_n) = \frac{1}{\beta} \sum_m \tilde{G}(i\omega_n + i\nu_m)\Gamma(i\nu_m) . \]  

(42)

We now analytically continue the equations for the self-energy to the spectral representation with real frequencies. Since each convolution increases the gap of the one-electron propagators, we know that the gap of vertex \( \Gamma \) is not smaller than that of this two-particle bubbles.
Using Eq. (35) we obtain
\[
\Sigma(z) = -\frac{1}{\pi} \int_{-\infty}^{-\omega_0} dx \Im \Gamma(x^+)^G(x+z) \\
- \frac{1}{\pi} \int_{-\infty}^{-\Delta} dx \Im G(x^+)^G(x-z) + \text{Res}[G,-\omega_0] \Gamma(-\omega_0-z) \tag{43}
\]
and
\[
\Delta_\Phi S(z) = -\frac{1}{\pi} \int_{-\infty}^{-\omega_0} dx \Im \Gamma(x^+)^G(x+z) \\
- \frac{1}{\pi} \int_{-\infty}^{-\Delta} dx \Im G(x^+)^G(x-z) + \text{Res}[G,-\omega_0] \Gamma(-\omega_0-z). \tag{44}
\]

We outlined the scheme how individual contributions to the perturbation theory expressed in the Matsubara formalism can be transformed to spectral representations with functions along the axis of real frequencies. The convolutions generally split into residues of isolated poles from the energy gap of the one-electron propagator and from cuts along the continuum of band states. Such decomposition is stable in the perturbation expansion, since the gap edges are independent of the interaction strength and the convolutions can only increase the gap of the unperturbed Green function.

V. SPIN-SYMMETRIC STATE AT WEAK COUPLING

A. Hartree-Fock approximation

Although the experimental realization of the superconductor-dot-superconductor with carbon nanotubes represents a strongly correlated situation with the Coulomb repulsion being the dominant energy scale, we resort to weak coupling to analyze the impact of the repulsion on the positions of the Andreev states within the gap. In this regime already the Hartree-Fock approximation should give good qualitative estimates of the behavior of the Andreev states. We furthermore stay in the spin-symmetric state and keep control over the pole that can emerge in strong coupling in the two-particle vertex with Hartree-Fock propagators. The critical interaction strength for the impurity imbedded in a nonmagnetic metal is \( U_c = \pi w/2 \), where \( w \) is the effective bandwidth. This critical interaction is generally smaller on the dot attached to superconducting leads due to the gap around the Fermi energy. The value \( \pi w/2 \) is then the upper value for the interaction strength above which the Hartree-Fock approximation loses validity.

From the Hartree-Fock equations (22) and (23) we obtain
\[
\Sigma = Un, \quad S = Un \tag{45}
\]
where \( n \) and \( \nu \) are particle and Cooper-pair densities, respectively. Explicit equations for the two independent parameters of the spin-symmetric Hartree-Fock approximation are
\[
\begin{align*}
n & = \frac{1}{\beta} \sum_n \frac{e^{i\omega_n \beta}}{D(i\omega_n)} \left[ i\omega_n [1 + \sigma(i\omega_n)] + \epsilon + Un \right], \\
\nu & = -\frac{1}{\beta} \sum_n \frac{1}{D(i\omega_n)} \left[ \sigma(i\omega_n) - Un \right]. \tag{46}
\end{align*}
\]

We represent the HF Green function for complex energies as a matrix in the Nambu picture. It reads
\[
\hat{G}(z) = \frac{1}{D(z)} \left( z [1 + \sigma(z)] + \epsilon + Un - \Delta_\Phi [\sigma(z) - Un] \right) \tag{47}
\]
with the determinant
\[
D(z) = z^2 [1 + \sigma(z)]^2 - (\epsilon + Un)^2 - \Delta_\Phi^2 [\sigma(z) - Un]^2. \tag{48}
\]
We split the spectral representation for the HF parameters into the band and polar contributions. The determinant for the band states \(|x| \geq \Delta\) is
\[
D(x \pm i0) = x^2 \left[ 1 \pm \frac{i\Gamma_0 \text{sgn}(x)}{\sqrt{x^2 - \Delta^2}} \right]^2 - (\epsilon + Un)^2 \\
- \Delta_\Phi^2 \left[ Un \mp \frac{i\Gamma_0 \text{sgn}(x)}{\sqrt{x^2 - \Delta^2}} \right]^2. \tag{49}
\]
with real and imaginary parts
\[
\Re D(x \pm i0) = x^2 - (\epsilon + Un)^2 - \Delta_\Phi^2 U^2 \nu^2 - \Gamma_0 x^2 - \frac{\Delta_\Phi^2}{\Delta^2} \tag{50}
\]
\[
\Im D(x \pm i0) = \pm 2\Gamma_0 \text{sgn}(x) x^2 + \Delta_\Phi^2 U \nu. \frac{\sqrt{x^2 - \Delta^2}}{\sqrt{x^2 - \Delta^2}}.
\]
The determinant in the gap is real (except \( \delta \)-peaks at \( \pm \omega_0 \)) and it reads
\[
D(x) = x^2 \left[ 1 + \frac{\Gamma_0}{\sqrt{\Delta^2 - x^2}} \right]^2 - (\epsilon + Un)^2 \\
- \Delta_\Phi^2 \left[ Un - \frac{\Gamma_0}{\sqrt{\Delta^2 - x^2}} \right]^2. \tag{51}
\]
Zeros of \( D(x) \) determine the frequencies \( \pm \omega_0 \) of the Andreev bound states within the gap (\( 0 \leq \omega_0 \leq \Delta \)) symmetrically positioned around the Fermi energy. Let frequency \( \omega_0 \) be the positive root of the following equation
\[
\left[ 1 + \frac{\Gamma_0}{\sqrt{\Delta^2 - \omega_0^2}} \right] \omega_0^2 \\
= (\epsilon + Un)^2 + \Delta_\Phi^2 \left[ Un - \frac{\Gamma_0}{\sqrt{\Delta^2 - \omega_0^2}} \right]^2. \tag{52}
\]
The fundamental sum over Matsubara frequencies over the determinant of the Green function at zero temperature is

\[ D = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{1}{D(i\omega)} = \int_{-\infty}^{-\Delta} \frac{d\omega}{\pi} \Im D(x) + \text{Res} \left[ \frac{1}{\Delta^2 - \omega^2} \right] \]

\[ = -2\Gamma_0 \int_{-\infty}^{-\Delta} \frac{dx}{\pi} \frac{x^2 + \Delta^2 U\nu}{|D(x)|^2 \sqrt{x^2 - \Delta^2}} + \frac{1}{\Gamma(-\omega_0)}, \quad \text{(53)} \]

where \( K(x) = \partial D(x)/\partial x \) in the gap is

\[ K(x) = 2x \times \left[ 1 + \Gamma_0 \frac{2\Delta^2 + U\Delta^2 \nu - x^2}{(\Delta^2 - x^2)^{3/2}} + \Gamma_0 \frac{\Delta^2 - \Delta^2}{(\Delta^2 - x^2)^{3/2}} \right]. \quad \text{(54)} \]

To simplify the formulas for the solution of the HF equations we introduce the following notations for the contributions from the integrals over the band states

\[ I_0 = -\int_{-\infty}^{-\Delta} \frac{dx}{\pi} \Im D(x) , \]

\[ I_1 = \int_{-\infty}^{-\Delta} \frac{dx}{\pi} \frac{\Gamma_0 R D(x)}{|D(x)|^2 \sqrt{x^2 - \Delta^2}} , \]

\[ J_0 = \int_{-\infty}^{-\Delta} \frac{dx}{\pi} x \Im D(x) , \]

\[ J_1 = -\int_{-\infty}^{-\Delta} \frac{dx}{\pi} \frac{\Gamma_0 x R D(x)}{|D(x)|^2 \sqrt{x^2 - \Delta^2}} . \quad \text{(55)} \]

The residues of the Green functions in the gap are

\[ \text{Res}[G, x] = \frac{1}{K(x)} \left[ x \left( 1 + \frac{\Gamma_0}{\sqrt{\Delta^2 - x^2}} \right) + \epsilon + U\nu \right] , \]

\[ \text{Res}[G, x] = -\frac{\Delta^2}{K(x)} \left( \frac{\Gamma_0}{\sqrt{\Delta^2 - x^2}} - U\nu \right) . \quad \text{(56)} \]

\[ \{ U\omega_0(1 + \sigma_0) + K_0 [\epsilon + U(J_1 + J_0)] \}^2 + \Delta^2 \left( \frac{\sigma_0(1 + U\nu_0) - U\nu_1 - \omega_0^2(1 + \sigma_0)^2 [U + K_0(1 + U\nu_0)]^2 = 0 \right. \quad \text{(62)} \]

Taking into account that \( K_0 \propto \omega \) we immediately see that \( \omega_0 = 0 \) is always a solution to Eq. (62). In the search for a positive solution \( \omega_0 > 0 \) we expand both sides of Eq. (62) in \( \omega_0 \). The leading term, proportional to \( \omega_0^2 \), goes through zero when increasing the interaction strength (for the fixed phase \( \Phi \)). When this term becomes negative, Eq. (62) has no positive root. It happens for a critical value \( U_c \) determined from equation

\[ U_c^2 = -2 \left( 1 + \frac{\Gamma_0}{\Delta} \right) [\epsilon + U_c(J_1 + J_0)] \left( 1 + \frac{\Gamma_0}{\Delta} \right) \left( \frac{\Gamma_0}{\Delta} (1 + U\nu_0) - U\nu_1 \right) \]

\[ \left. -4\Delta^2 \left( 1 + \frac{\Gamma_0}{\Delta} \right) \left[ \frac{\Gamma_0}{\Delta} (1 + U\nu_0) - U\nu_1 \right] \right] . \quad \text{(63)} \]

For interactions \( U > U_c \), Eq. (62) has only one solution \( \omega_0 = 0 \). A non-zero solution to Eq. (62) exists only in the weak-coupling regime \( U < U_c \). Notice that the critical field of the Hartree-Fock (unphysical) transition to a magnetic state is \( U_m = 1/I_0 \).
tributions, \( \omega_0^2 = \omega_c^2 + \omega_\Delta^2 \) that are from Eq. (62)

\[
\omega_c = \frac{(\epsilon + Un)^2}{(1 + \sigma_0)^2}, \quad \omega_\Delta = \Delta_0^2 \frac{(\sigma_0 - U\nu)^2}{(1 + \sigma_0)^2}.
\]

Frequency \( \mp \omega_c \) determines a renormalized impurity level for a single electron/hole, that is, with no Cooper pairs. The other frequency, \( \mp \omega_\Delta \), determines energy needed to form a Cooper/anti-Cooper pair (two electrons/two holes bound) on the impurity. Modulus of both frequencies decreases with the increasing interaction. It vanishes at the Fermi energy, when \( U = U_c \), at which electrons and holes are indistinguishable and the solution gets saturated. Beyond the critical point, \( U > U_c \), both frequencies stay zero and do not depend on the interaction strength. In this saturated state \( \omega_0 = 0 \) and \( n = -\epsilon/U, \nu = \Gamma_0/U\Delta \). It means that there is no crossing of Andreev states in the spin symmetric solution. This holds generally, not only for the Hartree-Fock solution but also beyond the static approximation.

\section*{B. Dynamical corrections}

The most important dynamical corrections to the Hartree-Fock approximation in the weak-coupling regime are contained in the self-energy from Eqs. (43) and (44) with the vertex from Eq. (41). This approximation includes both the second-order correction and all multiple electron-hole scatterings. The corrections do not move the gap edges of the one-electron Green function and hence the self-energy for \( \omega \in [-\Delta, \Delta] \) is real. The full solution with dynamical contributions changes the determinant \( D(z) \) as in Eq. (20) and reads

\[
D(z) = z^2 [1 + \sigma(z)]^2 - [\epsilon + Un + \Sigma(z)] [\epsilon + Un + \Sigma(-z)] - \Delta_0^2 [\sigma(z) - U\nu - S(z)] [\sigma(z) - U\nu - S(-z)].
\]

Dynamical corrections to the self-energy change the values of the integrals over the band states, but do not change the character and the number of the gap states. Due to the band-edge singularities the Andreev states cannot move outside of the gap. The equation for the energies of the gap states changes with respect to Eq. (62) only in that \( \epsilon \rightarrow \epsilon + \Sigma_0 \) and \( \sigma_0 \rightarrow \sigma_0 - S_0 \), where \( \Sigma_0 = \Sigma(\omega_0) \) and \( S_0 = S(\omega_0) \) are the values of the normal and anomalous self-energy at the positive frequency of the gap state. The electron-hole symmetry for the gap states at \( \pm \omega_0 \) is maintained. The integrals over the band are accordingly modified as well, but it is not important for the behavior of the gap states. The structure of Eq. (62) does not change by dynamical self-energy corrections and the frequencies of the poles appear in this equation only in even powers. It means that dynamical fluctuations beyond the static mean-field do not affect the transition to a saturated state and cannot lead to crossing of Andreev bound states.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3}
\caption{(Color online) Spectral density of the normal Green function for \( \epsilon = -U/2 \) and \( \Phi = \pi/2 \) calculated within the Hartree-Fock approximation (HFA) and for self-energy with dynamical corrections due to multiple electron-hole scattering (RPA).}
\end{figure}

\section*{C. Numerical results}

To obtain quantitative results in the Hartree-Fock approximation and in a solution with dynamical corrections we must use numerical methods. We solve numerically not only the static Hartree-Fock self-consistently but also add dynamical corrections to the self-energy due to multiple electron-hole scatterings contained in vertex \( \Gamma \) from Eq. (11). We use the Hartree-Fock one-electron propagators in the bubbles determining vertex \( \Gamma \). The dynamical self-energy is then determined from the Schwinger-Dyson equation, Eqs. (43) and (44). We use a small interaction strength \( U = 2\Delta \) and intermediate hybridization \( \Gamma_0 = \Delta \). All calculations were performed at zero temperature for which we derived explicit equations.

Spectral densities from the normal and anomalous Green functions are plotted in Figs. 3 and 4, respectively. The results are for a charge-symmetric case \( \epsilon = -U/2 \) and for the phase difference \( \Phi = \pi/2 \). We can see that the electron repulsion on the impurity site presses the poles of the gap states towards the Fermi energy. Dynamical corrections are visible only within the band. The non analyticity in the dynamical spectral function is caused by the convolution of an isolated pole (delta function) and continuous band states. The plots reveal also that dynamical corrections do not lead to qualitative changes of the Hartree-Fock spectral properties, in particular, the gap states.

The saturation of the spin-symmetric solution is demonstrated in Fig. 5. We remained in the charge-symmetric situation and traced dependence of the frequencies of the Andreev states on phase difference \( \Phi \). We again compared the static approximation with a solution with dynamical corrections to the self energy from Eqs. (11) and Eqs. (43), (44). We cannot observe any qualitative difference in the dependence of the gap states and their tendency to reach saturation with increasing the phase difference, which is equivalent to increasing...
We plot in Fig. 6 the Josephson current of the Hartree-Fock approximation \( J \) for the charge-symmetric situation and \( U = 2\Delta \) decomposed into its two different contributions. One from the direct current \( J_{ABS} \) mediated by the Andreev bound states and the tunneling one between the band states of the left and right leads, \( J_{band} \). At saturation, due to opposite signs of the residues of the anomalous Green function at \( \pm \omega_0 \), the direct current vanishes, abruptly falls to zero, since there is no energy difference between forming the bound pairs of two electrons and two holes. It costs no energy to build a Cooper and anti-Cooper pairs and the supercurrent vanishes. In saturation only the tunneling current through the potential barrier of the impurity survives.

It is interesting to find out whether and how the saturated solution is reached apart from the charge-symmetric situation. In Fig. 7 we plotted dependence of Andreev states on the impurity energy level \( \epsilon \) for \( U = 2\Delta \) and two phase differences. For small difference in the phases of the left and right superconductors and small Coulomb repulsion the saturated solution is not reached. The frequencies of the Andreev states do not reach the Fermi energy, only a minimal positive distance. Increasing either the interaction or the phase difference the Andreev states reach the Fermi energy and remain frozen there. The saturated phase is marked by nonexistence of the direct supercurrent via the Andreev states. When the upper and lower frequency of the Andreev state reach zero, their residues cancel each other leading to vanishing of the direct current. The direct current has a discontinuity at the point where saturation is reached. In the saturated phase the only supercurrent is the tunneling one, first term in the spectral representation on the right-hand side of Eq. (15). It is much smaller in its value than the direct one and has opposite sign, Fig. 8. We plotted in Fig. 9 behavior of the Hartree-Fock parameters \( n \) and \( \nu \), the particle and pair densities. The saturated phase is marked by linear dependence of the particle density and independence of the pair density on the impurity energy level as follows from Eqs. (57) and (58).
VI. CONCLUSIONS

We studied in this paper behavior of the Andreev bound states in a weakly interacting quantum dot attached to superconducting leads. We developed a systematic perturbation expansion in the interaction strength with normal and anomalous Green functions on the impurity. We presented a scheme how to assign spectral representation to individual contributions of the perturbation expansion in the Matsubara formalism. In this way we were able to separate contributions from the band and from the gap states of this model. It appears that separation of the two contributions is very important for the explanation of the observed $0 - \pi$ transition in the Josephson current.

We addressed the question whether the spin-reflection symmetry is broken in the $\pi$-phase. We resorted to weak coupling with the interaction strength below the unphysical mean-field transition to a magnetically ordered phase that is suppressed by the Kondo effect. We tried to answer the question whether crossing of Andreev states is possible within a spin-symmetric state, as indicated by exact numerical methods. We solved the Hartree-Fock equations and added dynamical corrections via multiple electron-hole scatterings. We found that frequencies of the gap states appear only in even powers in the equation defining the polar singularities within the gap. We also found that the energies of the gap states approach the Fermi energy with increasing interaction strength (or the phase difference between the superconducting leads). The energies are spin-independent and are symmetrically distributed around the Fermi energy. At a critical value of the interaction strength (phase difference) they meet at the Fermi energy and freeze there. It means that the spin symmetric solution does not allow for crossing of Andreev states. The gap states on the Fermi energy do not contribute to the Josephson current, since creation and annihilation of the Cooper pairs are equally probable. The only contribution to the supercurrent in the saturated state comes from tunneling through the potential barrier of the Coulomb potential on the impurity. These conclusions, although derived in the weak-coupling limit, seem to be generic and are not qualitatively affected by dynamical fluctuations. It hence means that the observed crossing must contain kind of symmetry breaking in the spin state.
Our results for the weak-coupling spin-symmetric state agree with the exact numerical results before saturation is reached. The Andreev states approach the Fermi energy and when they reach it, the solution becomes degenerate. This degeneracy can no longer be correctly described by a single, spin-independent equilibrium state. To treat a degenerate solution properly we must admit possibility of breaking of spin symmetry and define a perturbation expansion for spin-dependent solutions individually. One must be, however, careful so that emergence of the local magnetic moment is not unphysical, caused by a spurious divergence of the magnetic susceptibility of simple weak-coupling approximations. The spectral representation presented in this paper offers the appropriate tool to control spin fluctuations, since it separates the contributions from the gap and band states. The spurious magnetic state is caused by improper treatment of the band contributions to the perturbation theory, that is by neglecting the Kondo behavior. This can be, however, corrected by introducing a proper two-particle self-consistency via, e. g., simplified parquet equations correctly reproducing the Kondo asymptotics in the spin-symmetric state.\textsuperscript{21}

The encouraging result of our present analysis is that the $0 - \pi$ transition, or at least its qualitative features can be investigated already in the weak-coupling regime, since already the static mean-field approximation possesses substantial qualitative features of the exact solution.

Acknowledgment

We thank T. Novotný for valuable discussions on the physics of the quantum dot attached to two superconducting leads and careful reading of the manuscript. VJ and VP thank D. Shapiro for many fruitful discussions during his stay at the Institute of Physics, AS CR. Research on this problem was supported in part by Grant P204-11-J042 of the Czech Science Foundation.

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