Proximity effect in superconductor Aharonov Bohm loop hybrid structures

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Abstract

We study the proximity effect in superconductor - metallic or ferromagnetic Aharonov Bohm loop hybrid structures self consistently using the Bogoliubov-deGennes formalism within the two dimensional extended Hubbard model. We calculate the local density of states, the pair amplitude, and persistent currents as a function of several modulation parameters, the position around the loop, the exchange field, the magnetic flux through the loop, the loop size, and the chemical potential in the loop atoms. We find that the parameters above can modulate the proximity effect.
I. INTRODUCTION

Recently the proximity effect has been probed as decaying oscillations of the density of states in $s$-wave superconductor ferromagnet hybrid structures [1] and a phase shift of half flux quantum in the diffraction pattern of a ferromagnetic $0 - \pi$ SQUID [2]. Similar effects have been observed in $d$-wave [3,4] superconductor ferromagnet hybrid structures. Theoretical explanation has been given in the framework of the quasiclassical theory for $s$-wave [5] and $d$-wave case [6]. In these structures the exchange field modulates the period of the pair amplitude oscillations.

Moreover much interest has been focused recently on the manipulation of entangled states which are formed by extracting Cooper pairs from the superconductor. For example a beam splitter has been proposed [7] and also several experiments that involve ferromagnetic electrodes connected to superconductors [8–10]. These structures have acquired considerable interest the last years due to the possibility to use the $\pi$ states in solid state qubit implementation.

Moreover great experimental efforts have been devoted the last years to control the conductance in mesoscopic structures by phase sensitive methods. For example the differential conductance of a mesoscopic metallic loop in contact with two superconducting electrodes has been examined [11].

In this paper our goal is to explore several new aspects related to the control of the proximity effect in superconductor - Aharonov Bohm loop (AB) structures. The basic quantities which we calculate are the local density of states (LDOS), the pair amplitude, and persistent currents, as a function of the magnetic field, exchange field, loop size, position in the loop, and chemical potential in the loop atoms. We find that the quasiparticle properties of the hybrid structure are modulated by these parameters. The method that we use is based on exact diagonalizations of the Bogoliubov-de Gennes equations associated to the mean field solution of an extended Hubbard model. Our predictions from the simulations of this model are of interest in view of future STM spectroscopy experiments on nanostructures.
The article is organized as follows. In Sec. II we develop the model and discuss the formalism. In Sec. III we discuss the effect of the magnetic field on the LDOS. In Sec. IV we present the results for the calculation of the currents. Finally summary and discussions are presented in the last section.

II. BDGEQUTIONS WITHIN THE HUBBARD MODEL

The Hamiltonian for the Hubbard lattice model is

\[
H = -t \sum_{<i,j>\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \mu \sum_i n_{i\sigma} + \sum_i h_{i\sigma} n_{i\sigma} + V_0 \sum_i n_{i\uparrow} n_{i\downarrow},
\]

where \( i, j \) are sites indices and the angle brackets indicate that the hopping is only to nearest neighbors, \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) is the electron number operator in site \( i \), \( \mu \) is the chemical potential.

\[ h_{i\sigma} = -h \sigma_z, \]

is the exchange field in the ferromagnetic region and \( \sigma_z = \pm 1 \) is the eigenvalue of the \( z \) component of the Pauli matrix. \( V_0 \) is the on site interaction strength which gives rise to superconductivity. Within the mean field approximation Eq. (1) is reduced to the Bogoliubov deGennes equations [12]:

\[
\begin{pmatrix}
\hat{\xi} & \hat{\Delta} \\
\hat{\Delta}^* & -\hat{\xi}
\end{pmatrix}
\begin{pmatrix}
u_{n\uparrow}(r_i) \\
v_{n\downarrow}(r_i)
\end{pmatrix} = \varepsilon_{n\gamma_1}
\begin{pmatrix}
u_{n\uparrow}(r_i) \\
v_{n\downarrow}(r_i)
\end{pmatrix},
\]

\( \hat{\xi}u_{n\sigma}(r_i) = -t \sum_\delta u_{n\sigma}(r_i + \delta) + (\mu I(r_i) + \mu)u_{n\sigma}(r_i) + h_{i\sigma} \sigma_z u_{n\sigma}(r_i), \)

\[
\hat{\Delta}u_{n\sigma}(r_i) = \Delta_0(r_i)u_{n\sigma}(r_i),
\]

where the pair potential is defined by
\[ \Delta_0(r_i) \equiv V_0 < c_\uparrow(r_i)c_\downarrow(r_i) > . \] (6)

Equations (2,3) are subject to the self consistency requirement
\[ \Delta_0(r_i) = V_0(r_i) F(r_i) = V_0(r_i) \sum_n \left[ u_{n\uparrow}(r_i)v_{n\downarrow}^*(r_i)(1 - f(\beta\epsilon_{n\eta})) + u_{n\downarrow}(r_i)v_{n\uparrow}^*(r_i)f(\beta\epsilon_{n\eta}) \right], \] (7)

\( F(r_i) \) is the pair amplitude. We solve the above equations self consistently. The numerical procedure has been described elsewhere [10,13–15].

The LDOS at the \( i \)th site is given by
\[ \rho_i(E) = -\sum_{n\sigma} \left[ |u_{n\sigma}(r_i)|^2 f'(E - \epsilon_n) + |v_{n\sigma}(r_i)|^2 f'(E + \epsilon_n) \right], \] (8)
where \( f' \) is the derivative of the Fermi function,
\[ f(\epsilon) = \frac{1}{\exp(\epsilon/k_B T) + 1}. \] (9)

III. LDOS AS A FUNCTION OF THE MAGNETIC FIELD

We demonstrate in this section that the magnetic flux through a metallic or ferromagnetic AB loop which is connected to a superconductor as seen in Fig. 1 can be used to control the proximity effect in this hybrid structure. The magnetic flux through the loop is modeled as a factor \( e^{i\phi} \) where \( \phi = 2\pi\Phi/\Phi_0 = 2\pi f \), in the hopping element, where \( \Phi_0 \) is the unit of the flux quantum. In the calculation we used a small cluster of 7 \( \times \) 7 sites to model the superconductor and 6 sites to model the metallic or ferromagnetic loop. The AB effect appears as periodic oscillations of the conductance of a ring as a function of the enclosed magnetic flux \( f \).

A. isolated AB loop

We first study the case of an isolated AB loop. Magnetoresistance oscillations with period \( h/e \) have been observed in Au ring along with weaker \( h/2e \) oscillations [16]. Also magne-
toresistance oscillations of period $h/2e$ (corresponding to a superconducting flux quantum) were observed on a two dimensional honeycomb Mg network of loops and were attributed to weak localization effects [17]. We present in Fig. 2 the LDOS versus energy for site 0, for different values of the flux. The pair interaction in the superconductor is zero, and the ring is disconnected from the normal metal reservoir namely the corresponding hopping element of the tight binding Hamiltonian is zero. We see that the LDOS shows oscillations as a function of the applied magnetic flux $f$. Also the LDOS for finite exchange field can be obtained by adding the LDOS for spin up and spin down Hamiltonian, so the number of peaks is double.

B. AB loop in contact with normal metal reservoir

Secondly we would like to make a comparison of the results derived above with the case where AB loop is connected to a normal metal reservoir. We present in Fig. 3 the LDOS versus energy for site 0, for different values of the flux. The basic results are summarized as follows. The LDOS shows again modulation with the applied flux. However the form of the LDOS is changed due to the exchange of electrons between the ring and the reservoir. For all values of the enclosed flux it presents a $U$-like form which is characteristic for chain of atoms.

C. superconductor-metallic AB loop

We discuss in the subsection the case where a metallic AB loop is connected to a superconductor. The quasiparticle properties in the ring are modified by the proximity effect. In the usual proximity effect in the superconductor normal metal bilayer the pair amplitude decays away from the interface inside the normal metal. However in the case of a normal metal loop in contact with a superconductor, the pair amplitude decays inside the loop, symmetrically around the site where the superconductor is connected to the loop (see the symmetry between sites 1 and 5 Fig. 4(a) for a 6 sites loop and between sites 1, 2 in Fig.
4(b), for a 3 sites loop). The pair amplitude changes with the magnetic flux. This may be related to size effects. The evolution of the LDOS around the loop is not periodic. The LDOS shows the $U$-like form which is characteristic of a line of atoms which changes as we move around the loop as seen in Fig. 5(a). Especially for $\phi = 4/8$ it shows a peak at zero energy (see Fig. 5(b)). This means that the proximity effect becomes long ranged one for this particular value of the magnetic flux. However the evolution with respect to the enclosed magnetic flux is periodic. This is seen in Fig. 6 where the LDOS is presented for fixed site on the loop but for different values of the magnetic flux. We present only $f < 4/8$ due to symmetry. So the proximity effect can be modulated by the AB magnetic flux.

**D. superconductor-ferromagnetic AB loop**

We now study a ferromagnetic AB loop in contact with a superconductor. When the magnetic flux is zero the proximity effect appears in the loop sites as oscillations of the pairing amplitude inside the ferromagnetic material. In the usual proximity effect in the superconductor ferromagnet bilayer the proximity effect appears as decaying oscillations of the pair amplitude with alternating sign away from the interface inside the ferromagnetic material. However due to the annular geometry of our structure the proximity effect appears symmetrically around the loop (note the symmetry between sites 1 and 5 in Fig. 7(a) for the 6 site loop and between sites 1 and 2 for the 3 site loop structure in Fig. 7(b)). A second difference is that the proximity effect oscillations for very small loop sizes are not decaying but are rather symmetric. As indicated in these figures the oscillations of pair amplitude inside the ferromagnetic material change as we change magnetic flux that is applied through the loop. The pair amplitude function returns to itself after one period in $\Phi_0$ is completed. The flux can change the amplitude of the oscillations but not the period.

The modulation of the oscillations of the pair amplitude with $f$ induces additional effects in the LDOS seen in Fig. 8. When $\phi = 0$ the ZEP in the LDOS practically does not change around the loop as seen in Fig. 8(a). This means that the proximity effect becomes long
ranged as in the metallic loop case. The presence of the pic at \( f = 0 \) which is absent in the case where \( h = 0 \) is attributed to the exchange field. Namely the effect of the ferromagnetism is to shift the LDOS that corresponds to \( h = 0 \) by an energy \( E = h \), so that a peak appears at zero energy when the van Hove singularity crosses the Fermi energy. Also when \( f = 2/8 \) (see Fig. 8(b)) a peak develops at zero energy. Moreover the LDOS is a periodic function of the applied magnetic flux as seen in Fig. 9 and it shows a different form for \( h = 0 \) and \( h = 2 \) (see Fig. 10).

Comparing with Figs. 2 and 3 we see that the main effect of the superconductor is to enhance the LDOS and also to induce long range proximity effects for certain values of \( f \), e.g. \( f = 4/8 \). The long range proximity effect appears in the LDOS as a peak at zero energy for some values of \( f \).

IV. PERSISTENT CURRENTS

We would like in this section to describe the effect of the proximity effect on the persistent currents of a small loop that encloses magnetic flux and is coupled to a superconductor. For small isolated one dimensional metallic rings enclosing magnetic flux, the existence of persistent currents has been predicted in theory [18] and verified in magnetization response of isolated Cooper rings to a slowly varying magnetic flux [19]. In isolated loops the relation of the persistent current as a function of the flux \( I(f) \) is modulated by the loop circumference and the chemical potential. The relation \( I(f) \) is periodic with period \( \Phi_0 \) and in some cases \( \Phi_0/2 \).

We study first the case of an isolated AB loop. In this case one can give simple physical argument for the persistent currents as follows. The phase coherence of the wave function enters the calculation through the flux modulated boundary conditions

\[
\Psi_n(x + L) = \exp[2i\pi f]\Psi_n(x),
\]

where \( L \) is the loop circumference. Then the current is \( I_n = \frac{e\nu_n}{L} \) where \( \nu_n = \frac{1}{h}\frac{\partial E_n}{\partial k_n} \). Then by identifying \( 2\pi f \) and \( kL \) we have \( I_n = \frac{e}{h}\frac{\partial E_n}{\partial f} \).
In our case the energy spectrum is obtained from the eigenvalues of the BdG Hamiltonian. Then the current for the $n$ state is $I_n = \frac{e}{h} \frac{\partial E_n}{\partial f}$. To calculate the total current we perform a summation over the eigenvalues of the system. We present in Fig. 11 the $I(f)$ relation for $V_0 = 0$ and hopping elements connecting the AB loop and the normal metal reservoir equal to zero, for different loop sizes and exchange fields. We see that the $I(f)$ relation changes with the loop size and exchange field depending on the number of electrons in the loop and presents linear variation with the applied flux.

We study then the case where $V_0$ equals zero, and the AB loop is connected to a normal metal reservoir. We present in Fig. 12 the $I(f)$ relation for different loop sizes and exchange fields. We see that the $I(f)$ relation changes with the loop size. Also for fixed loop size the $I(f)$ relation changes sign as we increase the exchange field and the critical current is reduced for large values of the exchange field. Moreover due to the presence of the electron exchange with the reservoir the $I(f)$ relation is not linear but is rounded.

We now turn to the case where the proximity effect is present. The pairing interaction in the superconductor is set equal to $V_0 = -3.5$. We present in Fig. 13 the $I(f)$ relation for different loop sizes and exchange fields. We see that the $I(f)$ relation is enhanced comparable to the case where $V_0 = 0$. Also the period of the $I(f)$ relation changes with the exchange field.

The modulation of the $I(f)$ relation with the exchange field is explained by the change of the number of electrons in the ring with the exchange field. Similar effects we observe when the chemical potential for the ring atoms is considered as modulation parameter. We present in Fig. 14 the $I(f)$ relation for $V_0 = -3.5$ and no exchange field for different loop sizes for different values of the chemical potential in the loop atoms. We see again that the $I(f)$ relation changes with the chemical potential in the loop atoms.
V. CONCLUSIONS

We calculated the LDOS, the pair amplitude, and the persistent currents for superconductor - AB loop hybrid structures, within the extended lattice Hubbard model. The quasiparticle properties depend on the loop size the magnetic flux, the exchange field and the chemical potential in the loop atoms. The proximity effect modifies the LDOS and for particular values of the magnetic flux it shows long range character. Also it enhances the persistent currents in the loop and modifies in some cases the $I(f)$ relation.
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FIG. 1. The junction of the normal metal or ferromagnetic AB loop with the superconductor.

The numbering of the sites along the loop is illustrated.

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FIG. 2. (a) The LDOS at $E = 0$ as a function of the energy, for different values of the magnetic flux $f = 0, 2/8, 4/8$, for site 0 of the AB loop, for $h = 0$. The pair interaction is $V_0 = 0$ and the hopping between the AB ring and the two dimensional reservoir is zero. (b) The same as in (a) but for $h = 2$. 


FIG. 3. (a) The LDOS at $E = 0$ as a function of the energy, for different values of the magnetic flux $f = 0, 2/8, 4/8$, for site 0 of the AB loop, for $h = 0$. The pair interaction is $V_0 = 0$, but the coupling between the ring and the normal metal reservoir is finite. (b) The same as in (a) but for $h = 2$. 
FIG. 4. (a) The pairing amplitude along the AB loop of 6 sites, which is in contact with a superconducting reservoir, for different values of the magnetic flux in the loop $f = 0, 2/8, 4/8$, and exchange field equal to $h = 0$. (b) The same as in (a) but for a 3 site AB loop.
FIG. 5. (a) The LDOS as a function of energy, for different sites along the AB loop $x = 0, 3, 5$ for magnetic flux equal to $f = 2/8$, and exchange field equal to $h = 0$. (b) The same as in (a) but for $f = 4/8$. 

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FIG. 6. (a) The LDOS as a function of energy, for site 0 of the AB loop, for different values of the magnetic flux $f = 0, 2/8, 4/8$, and exchange field equal to $h = 0$. (b) The same as in (a) but for the site 3.
FIG. 7. (a) The pairing amplitude along the AB loop of 6 sites, for different values of the magnetic flux in the loop \( f = 0, 2/8, 4/8, 6/8, 8/8 \), and exchange field equal to \( h = 2 \). (b) The same as in (a) but for a 3 site AB loop.
FIG. 8. (a) The LDOS as a function of energy, for a two dimensional electron gas, for different sites along the AB loop $x = 0, 3, 5$ for magnetic flux equal to $f = 0$, and exchange field equal to $h = 2$. (b) The same as in (a) but for $f = 2/8$. 
FIG. 9. (a) The LDOS as a function of energy, for site 0 of the AB loop, for different values of the magnetic flux $f = 0, 2/8, 4/8$, and exchange field equal to $h = 2$. (b) The same as in (a) but for the site 3.
FIG. 10. (a) The LDOS at $E = 0$ as a function of the magnetic field, for sites 0, 3, 5 of the AB loop, for $h = 0$. (b) The same as in (a) but for $h = 2$. 
FIG. 11. The current - flux relation for different values of the exchange field $h = 0, 1, 2$ and different number of sites in the ring (a) 6, (b) 7, (c) 8. The pair interaction is $V_0 = 0$ and the hopping between the AB ring and the two dimensional reservoir is zero.
FIG. 12. The current-flux relation for different values of the exchange field $h = 0, 1, 2$ and different number of sites in the ring (a) 6, (b) 7, (c) 8. The pair interaction is $V_0 = 0$ and the ring is coupled to a normal metal reservoir.
FIG. 13. The current - flux relation for different values of the exchange field $h = 0, 1, 2$ and different number of sites in the ring (a) 6, (b) 7, (c) 8. The pair interaction in the reservoir is $V_0 = -3.5$.
FIG. 14. The current-flux relation for different values of the chemical potential $\mu = 0, 1, 2$ in the loop atoms and different number of sites in the ring (a) 6, (b) 7, (c) 8. The exchange field is $h = 0$, and the pair interaction in the reservoir is $V_0 = -3.5$. 