BdG equations within lattice Hubbard model for the description of $\pi$-states in nanoscale S-FF-S junctions

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(March 22, 2022)

We calculate the persistent currents in $S - F_{\uparrow}, F_{\downarrow} - S$ structures ($S$ denotes the superconductor in a closed ring geometry, $F$ the ferromagnet in a two dimensional geometry, and the arrows the alignment of exchange field) as a function of the applied magnetic flux, self consistently by solving the Bogoliubov-de Gennes equations within the two dimensional Hubbard model. The local current shows a sign change i.e. a 0 to $\pi$ transition in the parallel alignment of the magnetizations and it does not change sign in antiparallel alignment.

I. INTRODUCTION

Presently the study of $\pi$ states is a subject of intensive theoretical and experimental investigation. The $\pi$ states have been predicted theoretically long time ago in junctions containing magnetic impurities. They appear as a sign change of the Josephson critical current in SFS structures ($S$ denotes the superconductor and $F$ the ferromagnet). The crossover from the 0 to $\pi$ state has been observed recently in the critical current versus temperature in SFS junctions [1], and in the critical current versus ferromagnetic layer thickness in SIFS junctions [2]. More recently the concept of $\pi$ state was used to explain the observed shift in the critical versus magnetic field pattern by half the flux quantum in the ferromagnetic $0 - \pi$ SQUID [3], and the decaying density of states oscillations in $s$-wave superconductor ferromagnet hybrid structures [4]. Similar effects have been observed in $d$-wave [5,6] superconductor ferromagnet hybrid structures. Theoretical explanation has been given in the framework of the quasiclassical theory for $s$-wave [7] and $d$-wave case [8].

Alternatively $\pi$ states appear in Josephson junctions involving $d$-wave superconductor due to the sign change of the superconducting order parameter [9]. For example the 0 to $\pi$ transition occurs in the critical current versus temperature in Josephson junctions with $d$-wave symmetry and depends on the orientation of the lobes of the $d$-wave order parameter with respect to the interface. The Josephson effect has been studied in junctions between unconventional superconductors across different types of magnetic barriers [10].

In superconductor - ferromagnet multiterminal hybrid structures the proximity effect can be controlled by the alignment of magnetizations in ferromagnetic electrodes connected to superconductor [11–13] or by the magnetic flux in an Aharonov-Bohm loop connected to superconductor [14]. In two superconductor - ferromagnet bilayers separated by thin insulating film, the enhancement of the Josephson critical current when the orientations of the magnetic moments in the ferromagnetic layers are antiparallel has been predicted [15]. Since then several S-FF-S, SF-SF structures have been examined in the limit of thin F layer and in the diffusive limit by solving the Usadel equations [16,17]. They found that in the case of antiparallel alignment of magnetizations in the ferromagnetic electrodes the critical current enhances with the exchange field, while in the parallel alignment the junction exhibits a transition to the $\pi$ state [16]. Also non-sinusoidal current phase relation in S-F-S, SF-c-SF junctions has been predicted [17]. The same problem has been treated in the ballistic regime [18].

In this paper our goal is to explore several new aspects related to the control of the Josephson effect in nanosstructures. We study two dimensional $F_{\uparrow}, F_{\downarrow}$ embedded in a superconducting wire. The method is based on exact diagonalizations of the Bogoliubov-de Gennes equations associated to the mean field solution of an extended Hubbard model. The basic quantity which we calculate is the local current as a function of several relevant parameters: the distance from the surface, the magnetic field that penetrates the superconducting loop and exchange field.

We find that the local current is periodic function of the flux and is controlled by the orientation of magnetization in the ferromagnetic electrodes. The local current shows a sign change i.e. a 0 to $\pi$ transition in the parallel alignment of the magnetizations and it does not change sign in antiparallel alignment. Our predictions from the simulations of this model are of interest in view of future experiments on nanoscale Josephson junctions.

The article is organized as follows. In Sec. II we develop the model and discuss the formalism. In Sec. III we discuss metallic or ferromagnetic structures embedded inside a superconducting loop. Finally summary and discussions are presented in the last section.
II. BDG EQUATIONS WITHIN THE HUBBARD MODEL

The Hamiltonian for the Hubbard lattice model is

\[ H = -t \sum_{<i,j>,\sigma} c_i^\dagger c_j^\sigma + \mu \sum_i n_i^\sigma + \sum_i h_i n_i^\sigma + V_0 \sum_i n_i^\uparrow n_i^\downarrow, \]

where \( i, j \) are sites indices and the angle brackets indicate that the hopping is only to nearest neighbors, \( n_i^\sigma = c_i^\dagger c_i^\sigma \) is the electron number operator in site \( i \), \( \mu \) is the chemical potential which is set to zero. \( h_i = -h \sigma_z \) 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 [19]:

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

(2)

\[
\begin{pmatrix}
\hat{\xi} & \hat{\Delta} \\
\hat{\Delta}^* & -\hat{\xi}
\end{pmatrix}
\begin{pmatrix}
u_{n\downarrow}(r_i)
\v_n \uparrow(r_i)
\end{pmatrix}
= \epsilon_{n\gamma_2}
\begin{pmatrix}
u_{n\downarrow}(r_i)
\v_n \uparrow(r_i)
\end{pmatrix},
\]

(3)

such that

\[
\hat{\theta} u_{n\sigma}(r_i) = -t \sum_{\delta} u_{n\sigma}(r_i + \delta) + \mu u_{n\sigma}(r_i) + h_i \sigma_z u_{n\sigma}(r_i),
\]

(4)

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

(5)

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

\[
\Delta_0(r_i) = V_0(r_i) F(r_i) = \frac{V_0(r_i)}{2} \sum_n [u_{n\uparrow}(r_i) v_{n\downarrow}(r_i) \tanh(\beta \epsilon_{n\gamma_1}/2) + u_{n\downarrow}(r_i) v_{n\uparrow}(r_i) \tanh(\beta \epsilon_{n\gamma_2}/2)],
\]

(7)

\( F(r_i) \) is the pair amplitude. We solve the above equations self consistently. The numerical procedure has been described elsewhere [12,13,20–22].

The local current between sites \( i, j \) is given by

\[
I_{ij} = \frac{ie}{\hbar} (t < c_i^\dagger c_j > -t^* < c_j^\dagger c_i >).
\]

III. RESULTS

We study the quasiparticle properties of a two dimensional plane to which a superconducting wire is attached at two points and a magnetic flux is applied through the wire. The magnetic flux creates a phase difference between sites \( \alpha \) and \( \beta \) (see Fig. 1), which is proportional to the applied flux. Alternatively a current through the wire can create this phase difference. We demonstrate in this section that the magnetic flux through the wire 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 \( \Phi = \frac{2\pi \Phi_0}{\hbar} = 2\pi \phi \) in the hopping integral. \( \Phi_0 = \frac{\Phi}{2\pi} \) is the normal flux quantum. In the calculation we used a small cluster of \( 8 \times 8 \) sites to model the 2DEG and also open boundary conditions, while a chain of 20 sites models the superconducting wire. The hybrid normal-superconducting ring has been discussed in Refs. [23,24].
They found that the persistent currents depend on the length of the N segment compared to the S. For large length of the superconducting region the quasiparticle wave function is localized in the normal metal region and quasiparticles are entering the superconductor via Andreev reflection. In this case the persistent currents have period half the flux quantum. In the opposite limit where the length of the superconducting region is small compared to the coherence length the quasiparticle wave function becomes extended and the persistent currents have period equal to the flux quantum. In our case the quasiparticle properties are more close to the former case. We checked the case where the wire and the reservoir are both normal metals. In that case we found that the persistent currents have period $\Phi_0$. Also the phase of the persistent currents is zero in a loop with even number of carriers and equal to $\pi$ in a loop with odd number of carriers. However in our case we fix the loop size and study the response of the system to the magnetic field and exchange field. We distinguish the following cases depending on the quality of the barrier

A. S-N-S

We discuss first the case where a superconducting wire is connected to a 2DEG as seen in Fig. 1. We demonstrate that the flux through the loop modulates in a periodic way the quasiparticle properties of the film, so that the proximity effect is controlled by the applied flux. The local current-magnetic flux relation is seen in Fig. 2 between sites $\alpha a$, $\alpha \beta$ and $\beta b$. It shows the characteristic sinusoidal form, with period almost $\Phi_0/2$.

B. S-F-S

We discuss now the case where a superconducting wire is connected to a ferromagnetic film as seen in Fig. 3. The objective is to investigate the effect of the exchange field in the current. The ferromagnetic atoms at sites $\alpha$ and $\beta$ where the superconducting wire is connected to the film have the same orientation of magnetizations. Due to proximity effect the pair amplitude shows decaying oscillations with alternating positive and negative signs inside the ferromagnet away from the connection points $\alpha, \beta$. The local current oscillates with $\phi$ as seen in Fig. 4. The Josephson effect occurs due to transfer of Cooper pairs across the interface via Andreev reflection. In the ferromagnetic site with spin up orientation of magnetization $\alpha$ and in the ballistic limit the phase difference between the electron and Andreev reflected hole depends on the exchange field i.e. $\delta \phi = 2 h x / h \nu_F$. In the other ferromagnetic site with the same orientation of magnetization $\beta$ the phase shift has the same sign. So in total in the parallel alignment of magnetizations there is a phase shift which can be equal to $\pi$, and the critical current is expected to change sign compared to the SNS case. Indeed $I_{\alpha \beta}$ has opposite sign in relation to the normal metal case as seen in Fig. 4.

C. S-F-F\textsuperscript{-}S

We discuss now the case where a superconducting wire is connected to a two dimensional ferromagnetic domain wall as seen in Fig. 5. We demonstrate that the alignment of the magnetization provides additional control parameter for the proximity effect. The ferromagnetic atoms at sites $\alpha$ and $\beta$ where the superconducting wire is attached have the opposite orientation of magnetizations. The local current oscillates with $\phi$ as seen in Fig. 6. However differently to the parallel alignment case, the local current $I_{\alpha \beta}$ does not change sign with the increase of the exchange field. These results indicate that the junction in the antiparallel alignment of magnetizations strongly resembles the SNS junction. We emphasize here that the ferromagnetic layers are small (one atomic layer) so there is no spatial variation of the pairing amplitude inside the ferromagnet. Therefore the $0$ to $\pi$ transition is explained in terms of phase discontinuities at the interface. For the antiparallel alignment the phase shift across the junctions is zero. The Josephson effect can be viewed as a transfer of Cooper pairs across the interface via Andreev reflection. In the ferromagnetic site with spin up orientation of magnetization $\alpha$ and in the ballistic limit the phase difference between the electron and Andreev reflected hole depends on the exchange field i.e. $\delta \phi = 2 h x / h \nu_F$. In the other ferromagnetic site with spin down orientation of magnetization $\beta$ the phase shift is the opposite. So in total in the antiparallel alignment of magnetizations there is not a phase shift, and the local current is expected to be similar to the SNS case. For the parallel alignment the phase shifts are added and this provides the possibility for a $\pi$ state. This $\pi$ phase shift in the phase of the order parameter is responsible for the sign change of the current. Similar analytical results have been obtained using the Usadel equations [16,17]. However in that case several approximations were used like constant order parameter in the superconducting electrodes and strongly coupled SF interfaces.
IV. CONCLUSIONS

We calculated the local current for normal and ferromagnetic planes with superconducting mirrors, in the presence of an external magnetic field within the extended Hubbard model, self consistently. The local current, is periodic function of the magnetic flux that is applied through the superconducting wire. The local current versus exchange field is further controlled by the alignment of the magnetizations in the ferromagnetic electrodes. Specifically it shows a sign change in the parallel alignment of the magnetizations but it does not change sign in the antiparallel alignment.

Our results are influenced from the details of the lattice structure and quantitative differences are found compared to the results of quasiclassical theory. The results can be generalized to extended contacts. We expect only quantitative differences. In the present paper we used superconducting rings where the applied flux creates a phase difference in the interruption points. However the results can be generalized to junctions instead of rings, where the current creates a phase difference between the two superconductors.

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FIG. 1. The SNS junction of the superconducting wire with the 2DEG. The loop contains 20 sites while the 2DEG is of 8 x 8 sites. The labeling of several sites close to the interface is shown.
FIG. 2. The local current $I_{ij}$ between sites $i, j$ of the SNS junction, where $ij = \alpha a, \alpha \beta, \beta b$ as a function of the magnetic flux. The exchange field is equal to $h = 0$ and the value of the superconducting gap is $V_0 = -3.5$.

FIG. 3. The S-F↑F↑-S junction of the superconducting wire with the ferromagnetic 2DEG. At the connections sites $\alpha, \beta$ the ferromagnetic atoms have the same orientation of magnetizations. The loop contains 20 sites while the 2DEG is of $8 \times 8$ sites.

FIG. 4. The local current $I_{ij}$ between sites $i, j$ of the S-F↑F↑-S junction, where $ij = \alpha a, \alpha \beta, \beta b$ as a function of the magnetic flux. The exchange field is equal to $h = 3$ and the value of the superconducting gap is $V_0 = -3.5$.

FIG. 5. The S-F↑F↓-S junction of the superconducting wire with the ferromagnet with antiparallel orientations of the magnetizations. The loop contains 20 sites while the 2DEG is of $8 \times 8$ sites.
FIG. 6. The local current $I_{ij}$ between sites $i, j$ of the S-F$_{\uparrow}$F$_{\downarrow}$-S junction, where $ij = \alpha\alpha, \alpha\beta, \beta\beta$ as a function of the magnetic flux. The exchange field is equal to $h = 3$ and the value of the superconducting gap is $V_0 = -3.5$. 