Interface effects in superconductor-nanotubes hybrid structures

N. Stefanakis  
e-mail: stefan@iesl.forth.gr  
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The objective of the present paper is to investigate the proximity effect in junctions of superconductors with carbon nanotubes. The method is the lattice BdG equations within the Hubbard model. The proximity effect depends sensitively on the connection giving the possibility to control the proximity effect by performing simple geometrical changes in the hybrid system.

I. INTRODUCTION

In the proximity effect the superconducting pair amplitude appears in a region where the pair interaction is zero. During the last decades it has been investigated in several mesoscopic structures e.g. metallic wires made of normal metals between two macroscopic superconducting electrodes [1]. More recently it was probed in superconductor ferromagnet hybrid structures where the pair amplitude shows decaying oscillations with alternating sign inside the ferromagnetic layer [2].

In the past decade transport measurements were used to explore the properties of nanometer-scale structures. An example is the carbon nanotube [3]. A carbon nanotube is obtained from a slice of graphene sheet wrapped into a seamless cylinder. The conducting properties depend sensitively on the diameter and the helicity. They can be classified to 'armchair', 'zigzag', and 'chiral' depending on their wrapping vector. They come in two forms, the multiwall (MWNT) with diameter \(10 - 30\) nm and the single wall (SWNT) with diameter \(1 - 2\) nm. Due to their small diameter SWNT provide ideal systems to study transport properties of 1D conductors.

It is possible to create superconducting junctions with SWNT embedded between superconducting contacts. In superconductor - SWNT - superconductor junctions, proximity induced superconductivity has been observed [4]. The temperature and magnetic field dependence of the critical current shows unusual features due to their strong one dimensional character. More explicitly the critical current exceeds the predicted one for SNS junctions by a large factor. Also the temperature and magnetic field dependence of the critical current is almost linear. In contrast in superconductor - SWNT - superconductor junctions with high transparent interfaces a dip in a differential resistance was observed [5]. This was attributed to Andreev reflection processes. When the transparency was low a peak was observed due to normal tunneling processes. Recently observation of 1D superconductivity in single-walled 4A carbon nanotubes was reported [6].

In this paper we describe the proximity effect in superconductor - SWNT junctions by solving the numerically Bogoliubov de Gennes equations within the Hubbard model. We calculate the local density of states (LDOS) and the pair amplitude self consistently. We find that the LDOS is strongly modified in the interface of superconductor with the nanotube and depends sensitively on the pairing symmetry of the superconductor, the chirality of the nanotube, and the connection between the two structures giving the opportunity to control the electronic properties at nanometer scale by performing topological changes to the hybrid system. The junctions of superconductor with nanotubes differ from the conventional junctions in their cross section which is of nanometer scale.

In the following we describe the numerical method in Sec II. In Sec III we present the results for the proximity effect in superconductor-side(-end) connected nanotube junction, we examine the effect of the pairing symmetry and chirality and finish with the conclusions.

II. METHOD

In our paper we describe the proximity effect in superconductor - SWNT junctions by solving the Bogoliubov de Gennes equations within the Hubbard model [7–9]. The Hamiltonian for the extended Hubbard model on a two dimensional square lattice is

\[
H = -t \sum_{<i,j>,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \mu \sum_{i\sigma} n_{i\sigma}
\]
\[ + V_0 \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{V_1}{2} \sum_{<ij>\sigma\sigma'} n_{i\sigma} n_{j\sigma'}, \]  

(1)

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, and \(V_0, V_1\) are on site and nearest-neighbor interaction strength. Negative values of \(V_0\) and \(V_1\) mean attractive interaction and positive values mean repulsive interaction. Within the mean field approximation Eq. (1) is reduced to the Bogoliubov deGennes equations:

\[
\begin{pmatrix}
\hat{\xi} & \hat{\Delta} \\
\hat{\Delta}^* & -\hat{\xi}
\end{pmatrix}
\begin{pmatrix}
u_n(r_i) \\
v_n(r_i)
\end{pmatrix} = \epsilon_n \begin{pmatrix}
u_n(r_i) \\
v_n(r_i)
\end{pmatrix},
\]  

(2)

such that

\[
\hat{\xi} u_n(r_i) = -t \sum_{\delta} u_n(r_i + \hat{\delta}) + \mu u_n(r_i),
\]  

(3)

\[
\hat{\Delta} u_n(r_i) = \Delta_0(r_i) u_n(r_i) + \sum_{\delta} \Delta_\delta(r_i) u_n(r_i + \hat{\delta}),
\]  

(4)

where the gap functions are defined by

\[
\Delta_0(r_i) \equiv V_0 < c_{\uparrow}(r_i) c_{\downarrow}(r_i) >,
\]  

(5)

\[
\Delta_\delta(r_i) \equiv V_1 < c_{\uparrow}(r_i + \hat{\delta}) c_{\downarrow}(r_i) >,
\]  

(6)

where \(\hat{\delta} = \hat{x}, -\hat{x}, \hat{y}, -\hat{y}\). Equations (2) are subject to the self consistency requirements

\[
\Delta_0(r_i) = V_0 \sum_n u_n(r_i) v_n^*(r_i) \tanh \left( \frac{\beta \epsilon_n}{2} \right),
\]  

(7)

\[
\Delta_\delta(r_i) = \frac{V_1}{2} \sum_n (u_n(r_i + \hat{\delta}) v_n^*(r_i)
\]

\[
+ u_n(r_i) v_n^*(r_i + \hat{\delta}) \tanh \left( \frac{\beta \epsilon_n}{2} \right).
\]  

(8)

We start with the approximate initial conditions for the gap functions (7,8). After exact diagonalization of Eq. (2) we obtain the \(u(r_i)\) and \(v(r_i)\) and the eigenenergies \(\epsilon_n\). The quasiparticle amplitudes are then inserted into Eq. (7,8) and new gap functions \(\Delta_0(r_i)\) and \(\Delta_\delta(r_i)\) are evaluated. We reinsert these quantities into Eqs. (3,4), and we proceed in the same way until we achieve self-consistency: i.e. when the norm of the difference of \(\Delta_0(r_i)\) and \(\Delta_\delta(r_i)\) from their previous values is less than the desired accuracy. We then compute the \(d\)-wave gap function given by the expression:

\[
\Delta_d(r_i) = \frac{1}{4} |\Delta_x(r_i) + \Delta_{-x}(r_i) - \Delta_y(r_i) - \Delta_{-y}(r_i)|,
\]  

(9)

and the LDOS at the \(i\)th site which is given by

\[
\rho_i(E) = -2 \sum_n \left[ |u_n(r_i)|^2 f'(E - \epsilon_n) + |v_n(r_i)|^2 f'(E + \epsilon_n) \right],
\]  

(10)

where the factor 2 comes from the twofold spin degeneracy, \(f'\) is the derivative of the Fermi function,

\[
f(\epsilon) = \frac{1}{\exp(\epsilon/k_B T) + 1}
\]  

(11)

The SWNT is described as a single sheet of graphite composed of carbon atoms arranged on the sites of a honeycomb lattice. Within the tight binding method one orbital is associated per carbon atom, and a tunneling element \(t\) between neighboring atoms. SWNT are formed by rolling the honeycomb sheet into a cylinder. We describe armchair or zigzag structures. The coupling between the two structures is through single bond or multiple bonds connecting the edge or side sites of the tube to the 2d superconductor. We calculate the LDOS, and pair amplitude.
III. RESULTS

A. 1d-superconductivity in SWNT

We would like to describe the LDOS for a SWNT which exhibits superconductivity. Within lattice Hubbard model the presence of on site attractive interaction give rise to s-wave superconductivity. The main characteristic which is visible in the LDOS is the presence of gap (see Fig. 2). For the bulk LDOS the gap coexists with bands showing one-dimensional Van-Hove singularities at the band edges. However close to the interface the LDOS is modified due to boundary effects.

B. rotation of nanotube with respect to the superconductor

The next step is to describe the proximity effect in superconductor SWNT. Here the SWNT shows superconductivity which is due to the proximity with a metal that exhibits superconductivity. We show that the LDOS due to proximity between the two structures can be modulated by simple geometrical transformations like rotation of the SWNT with respect to the superconductor. We study first the case of an end-connected SWNT to a superconductor as seen in Fig. 3. We see in Fig. 4 the crossover from the metallic behavior which appears as finite LDOS at zero energy to the superconducting state where a gap appears. The deviation from the metallic behavior which appears as finite LDOS at Fermi energy becomes weaker as we go to the bulk. Next we present the side-connected SWNT to a superconductor as seen in Fig. 5. In the LDOS in Fig. 6 we see that it deviates from the metallic behavior and is modulated by the distance from the surface. The proximity induced gap in the superconductor is of smaller magnitude compared to the end-connection case. In Fig. 7 we compare the pair amplitude for the side- and end- connection cases. In the end connection the pair amplitude decays toward the bulk of the SWNT showing plateaus across the nanotube. In the side connection the pair amplitude is almost homogeneous along the nanotube, but is varied across the nanotube.

We see in Fig. 8 an end connected nanotube to a d-wave superconductor. We see in Fig. 9 that the LDOS changes from metallic A to superconducting D like where a gap appears as we approach the interface. The form of the gap in the LDOS is V like due to the presence of nodes in the pair amplitude along certain directions in k-space. Next we present the side-connected SWNT to a d-wave superconductor as seen in Fig. 10. In the LDOS in Fig. 11 we see that it deviates from the metallic behavior and is modulated by the distance from the surface. Moreover the proximity induced gap in the superconductor is of smaller magnitude compared to the armchair case. In Fig. 7 we compare the pair amplitude for the side- and end- connection cases. In the end connection the pair amplitude decays toward the bulk of the SWNT showing plateaus across the nanotube. In the side connection the pair amplitude is almost homogeneous along the nanotube, but is varied across the nanotube. Negative pair amplitude appears in the proximity induced superconductivity due to the absence of hopping elements in the x direction. Therefore due to the fact that the pair interaction in d-wave is strongly non local and depends on the number of nearest neighbors that are available, the induced proximity pair amplitude inside the honeycomb lattice is modified for d-wave compared to s-wave. Concluding this section we could say that independently on the pairing symmetry the proximity induced gap is smaller for the side connection than the end connection. The induced pair amplitude is also different for the side than the end connection and shows additional features due to the pairing symmetry.

C. effect of chirality of nanotube

We present now the proximity effect in superconductor - zig zag nanotube junction seen in Fig. 13. We see that differently to the armchair case, inside nanotube the LDOS practically does not change with position (see 14). Also the LDOS is reduced due to the semiconducting character of the material. Inside superconductor we see that the LDOS recovers the bulk value in few lattice layers from the surface while in the armchair case the bulk value appears for larger distance.

We also tested the case of the different pairing symmetry i.e. d-wave. As seen in Fig. 15 the main difference with the armchair case is the appearance of the ZBCP [10,11]. This is attributed to the insulating character of nanotube which causes reflection of quasiparticles from the surface and appearance of peak due to the sign change of the pair amplitude. We note that the interface is along the [100] direction where for usual junctions the ZBCP is not expected. However in the present case the appearance of ZBCP is due to the distortion of the interface from the [100] direction by the honeycomb lattice. The conclusion from this section is that the proximity effect is reduced
for superconductor zig-zag nanotube due to the insulating character of the nanotube. We can provide an additional explanation in terms of Andreev reflection which is responsible for the proximity effect. The Andreev reflection is modified for superconductor zig-zag nanotube due to the absence of charge carriers in the SWNT. As a consequence for d-wave superconductor zig-zag nanotube hybrid structure, ZBCP appears similarly to the appearance of ZBCP in d-wave superconductors having the appropriate orientation, close to rigid insulating surfaces, where the reflected quasiparticles experience different sign of the pair amplitude.

D. more realistic geometries

Finally we would like to present the more realistic geometry where the nanotube is connected on top of the two dimensional superconducting film as shown in Fig. 16. We restrict here to s-wave superconductors since as is well known d-wave superconductivity actually occurs in the 2-D plane and important effects due to sign change of the pair amplitude can not be observed when tunneling in the z-direction is considered. The LDOS presented for open armchair nanotube in Fig. 17 shows that no important conclusions can be drawn compared to the previous connection geometries. Also here the gap coexists with the one dimensional bands. However the present structure has the advantage that novel phenomena may appear due to the confinement of the superconducting sites inside the restricted region which is defined by the periphery of the tube. This may become more obvious when the transparency of the interface is low and the superconducting atoms are encapsulated inside the tube. In the latter case we may speak about few atom nano grain superconductivity. In order to test the latter case more precisely we present the case where the superconductor is connected to a zigzag nanotube as shown in Fig. 18. Here the interface is of reduced transparency due to the insulating features of the zig-zag nanotube. The LDOS ( see Fig. 19) shows residual states inside the gap due to the semiconducting (6,0) nanotube which acts a pair breaking mechanism.

IV. CONCLUSIONS

We studied the electronic properties of SWNT - superconductor hybrid structures with in the Hubbard model self consistently. The results indicate that the LDOS is strongly modified close to the boundary layers of the nanotube as well as close to the interface of junctions with superconducting materials. We showed that the proximity LDOS between the superconductor and the nanotube can be modulated by simple geometrical transformations like rotation of the SWNT with respect to the superconductor. We found that the proximity induced gap is reduced for side connection. We demonstrated that the proximity effect depends on the chirality of the nanotube. We provided the explanation in terms of modified Andreev reflection in front of a metallic (armchair) or insulating (zigzag) interfaces. So one could say that the proximity effect can be viewed as a novel way to classify the nanotubes in metallic or semiconducting ones. Finally we found that the LDOS is sensitive to the pairing symmetry of the superconductor and shows features due to the geometric structure of the nanotube. In the last section we showed that the results that we presented here can be extended to more realistic geometries, and nanotubes with larger diameters where hybridization effects are absent and the approach what we used here is valid.

V. ACKNOWLEDGMENTS

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FIG. 1. The open armchair (5,5) nanotube composed of 21 layers.

FIG. 2. The LDOS for points A, B, C, D of an armchair (5,5) SWNT shown in Fig. 1 exhibiting superconductivity.
FIG. 3. The open armchair (5,5) nanotube composed of 10 layers end-connected to a two dimensional s-wave superconductor of $10 \times 10$ sites.

FIG. 4. a) The LDOS for the hybrid structure shown in Fig. 3. The points A,B,C,D belong to the end-connected nanotube while the points E,F,G,H to the superconductor.

FIG. 5. The open armchair (5,5) nanotube composed of 10 layers side-connected to a two dimensional $10 \times 10$ s-wave superconductor.
FIG. 6. The LDOS for the hybrid structure shown in Fig. 5. The points A, B, C, D belong to the side-connected nanotube while the points E, F, G, H to the superconductor.

FIG. 7. a) The comparison of the pair amplitude for the superconductor side- (end-) connected SWNT.

FIG. 8. The open armchair (5,5) nanotube composed of 10 layers end-connected to a two dimensional $10 \times 10$ d-wave superconductor.
FIG. 9. The LDOS for the hybrid structure shown in Fig. 8. The points A, B, C, D belong to the end-connected nanotube while the points E, F, G, H to the d-wave superconductor.

FIG. 10. The open armchair (5,5) nanotube composed of 10 layers side-connected to a two dimensional 10 × 10 d-wave superconductor.
FIG. 11. The LDOS for the hybrid structure shown in Fig. 10. The points A,B,C,D belong to the side-connected nanotube while the points E,F,G,H to the d-wave superconductor.

FIG. 12. a) The comparison of the pair amplitude for the d-wave superconductor - side- (end-) connected SWNT.

FIG. 13. The open zig-zag (5,0) nanotube composed of 10 layers end-connected to a two dimensional $10 \times 10$ superconductor.
FIG. 14. The LDOS for the hybrid structure shown in Fig. 13. The points A, B, C, D belong to the end-connected nanotube while the points E, F, G, H to the s-wave superconductor.

FIG. 15. The LDOS for the hybrid structure shown in Fig. 13. The points A, B, C, D belong to the end-connected nanotube while the points E, F, G, H to the d-wave superconductor.
FIG. 16. The open zig-zag (6,6) nanotube composed of 12 layers top-connected to a two dimensional 12 × 12 superconductor.

FIG. 17. The LDOS for the hybrid structure shown in Fig. 16. The points A,B,C belong to the superconductor while the points D,E,F to the top-connected nanotube.
FIG. 18. The open zig-zag (6,0) nanotube composed of 12 layers top-connected to a two dimensional $12 \times 12$ superconductor.

FIG. 19. The LDOS for the hybrid structure shown in Fig. 18. The points A,B,C belong to the superconductor while the points D,E,F to the top-connected nanotube.