Interface effects in superconductor–carbon nanotube hybrid structures

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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 Bogoliubov de Gennes (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.

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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 nanotube (MWNT) with diameter 10–30 nm and the single-wall nanotube (SWNT) with diameter 1–2 nm. Due to their small diameter SWNTs provide ideal systems to study transport properties of 1D conductors.

It is possible to create superconducting junctions with a 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 1D 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 4*A* carbon nanotubes was reported.[6]

In this paper we describe the proximity effect in superconductor–SWNT junctions by solving numerically the Bogoliubov de Gennes (BdG) 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.

We describe the proximity effect in superconductor–SWNT junctions by solving numerically the BdG equations in a square lattice within the extended Hubbard model. The description of the numerical method can be found in our previous publications.[7–9] This model describes better the class of superconducting materials that have *d*-wave pairing symmetry, e.g., cuprate superconductors. In these materials the coherence length is small, the pairing symmetry is nonlocal, and the superconducting correlations occur in a 2D square lattice space. Within the same model, 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 there is a tunneling element t between neighboring atoms. SWNTs are formed by rolling the honeycomb sheet into a cylinder. We describe armchair or zigzag structures. The coupling between the two structures is through multiple bonds connecting the edge or side sites of the tube to the 2D superconductor. We calculate the LDOS and pair amplitude.

We would like to describe the LDOS for a SWNT that exhibits superconductivity. Within the lattice Hubbard model the presence of on-site attractive interaction gives rise to *s*-wave superconductivity. The main characteristic that is visible in the LDOS is the presence of gap. For the bulk LDOS the gap coexists with bands showing 1D Van Hove singularities at the band edges. However close to the interface the LDOS is modified due to boundary effects.

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. We investigate for example the effect of the rotation of the nanotube with respect to the superconductor. We study first the case of an end-connected armchair SWNT to a superconductor as seen in Fig. 1(a). We see in Fig. 2 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

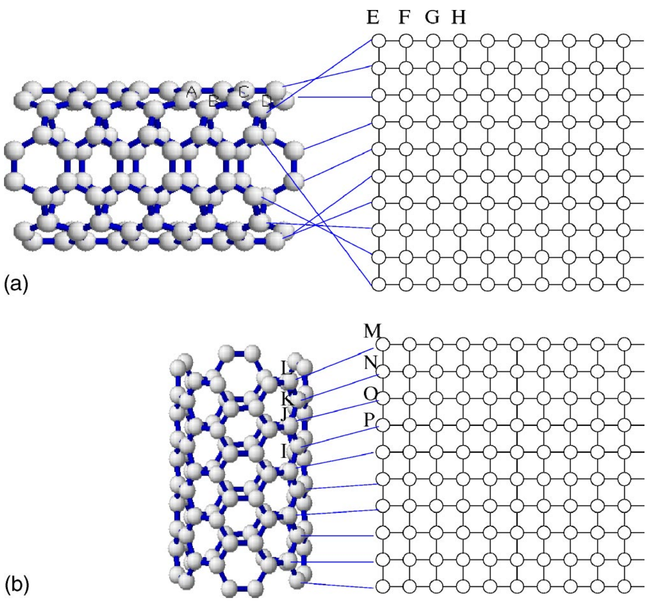

FIG. 1. The open armchair (5,5) nanotube composed of 10 layers (a) end-connected and (b) side-connected to a 2D superconductor of 10×10 sites.

present the side-connected SWNT to a superconductor as seen in Fig. 1(b). In the LDOS in Fig. 2 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. 3 we compare the pair amplitude for the side- and end-connection cases. In the end-connection case, the pair amplitude decays toward the bulk of the SWNT showing plateaus across the nanotube. In the side-connection case, the pair amplitude is almost homogeneous along the nanotube, but is varied across the nanotube.

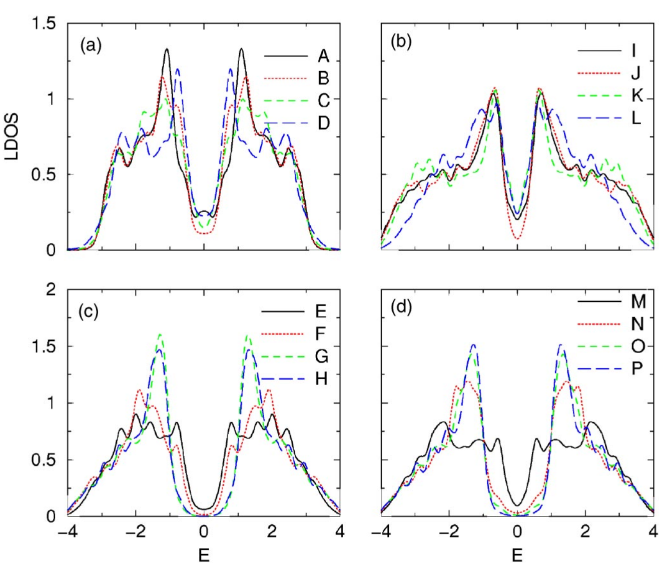

FIG. 2. (a) and (c) The LDOS for the hybrid structure shown in Fig. 1(a). The points A,B,C,D belong to the end-connected nanotube while the points E,F,G,H to the superconductor. (b) and (d) The LDOS for the hybrid structure shown in Fig. 1(b). The points I, J, K, and L belong to the side-connected nanotube, while the points M, N, O, and P to the superconductor.

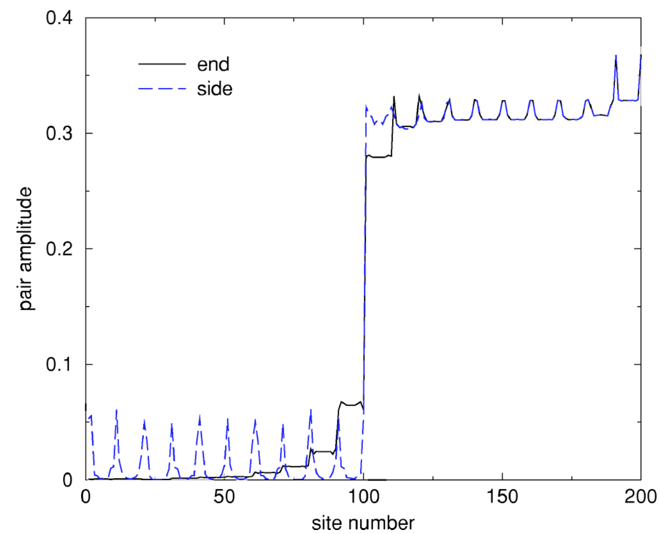

FIG. 3. The comparison of the pair amplitude for the superconductor side- and end-connected SWNT.

We see in Fig. 4 the LDOS for an end-connected nanotube to a *d*-wave superconductor. The geometry is the same as in Fig. 1. We see the evolution of the LDOS from the metallic state to the *d*-wave superconducting state. 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. In the LDOS in Fig. 4 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 end-connection case. In Fig. 5 we compare the pair amplitude for the side- and end-connection cases. In the end-connection case, the pair amplitude decays toward the bulk of the SWNT showing plateaus across the nanotube. In the side-

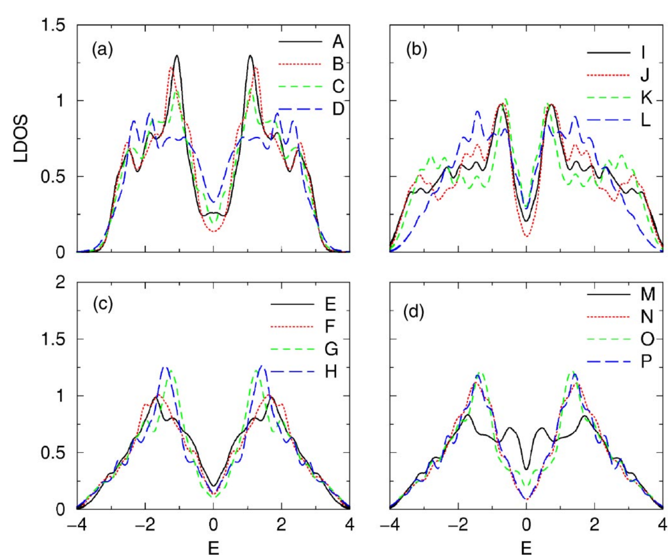

FIG. 4. The same as in Fig. 2 but for the *d*-wave superconductor.

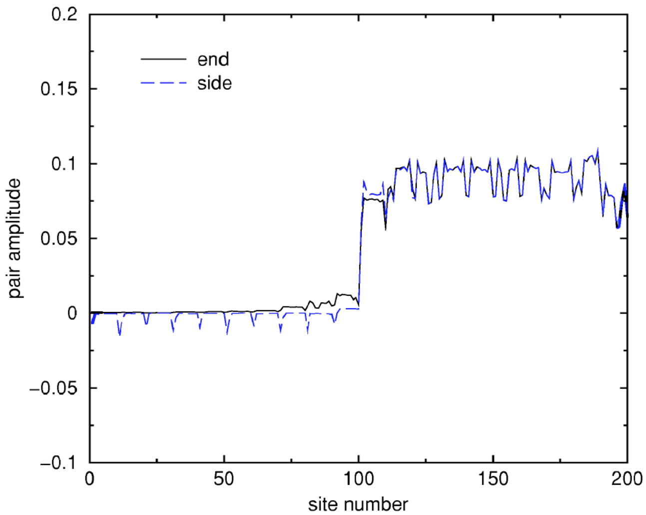

FIG. 5. The comparison of the pair amplitude for the *d*-wave superconductor: side- and end-connected SWNT.

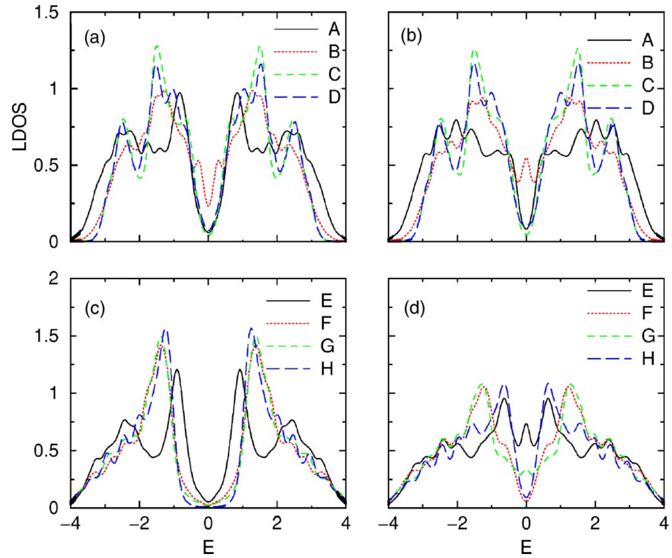

FIG. 7. (a) and (c) The LDOS for the hybrid structure shown in Fig. 6. The points A, B, C, and D belong to the end-connected nanotube, while the points E, F, G, and H to the *s*-wave superconductor. (b) and (d) The same but for the *d*-wave superconductor.

connection case, 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 nonlocal 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.

We study then the effect of the chirality of the nanotube. We present the proximity effect in the superconductor–zigzag nanotube junction seen in Fig. 6. We see that differently from the armchair case; inside the nanotube the LDOS practically does not change with position (see Fig. 7). Also the LDOS is reduced due to the semiconducting character of the material. Inside the 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 a longer distance.

We also tested the case of the different pairing symmetry, i.e., *d*-wave. As seen in Fig. 7 the main difference with the armchair case is the appearance of the zero bias conductance peak (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–zigzag 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–zigzag nanotube due to the absence of charge carriers in the SWNT. As a consequence for *d*-wave superconductor–zigzag 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.

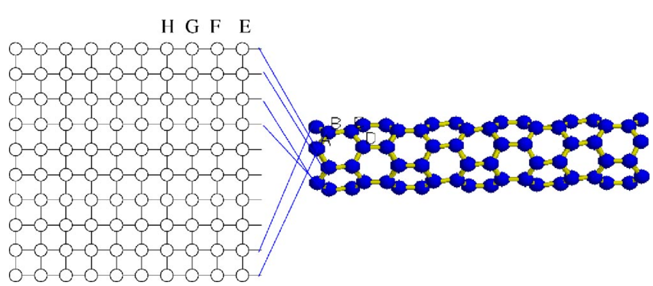

FIG. 6. The open zigzag (5,0) nanotube composed of 10 layers end-connected to a 2D 10×10 superconductor.

We have also considered the case of superconductor–SWNT–superconductor, and we state here the most important conclusions. The electronic properties for this structure depend on the length and the chirality of the nanotube. In particular the critical current is substantialy modified when the nanotube is zigzag. The transition temperature shows an almost linear variation as observed in experiment[4] due to the quasi-1D structure. Moreover a maximum length exists for the nanotube bellow at which the whole system becomes superconducting.

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 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, such as rotation of the SWNT, with respect to the superconductor. We found that the proximity-induced gap is reduced for side-connection cases. 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 metallic (armchair) or insulating (zigzag) interfaces. So one could say that the proximity effect can be viewed as a different way to classify the nanotubes in metallic or semiconducting nanotubes. 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.

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