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# Disorder and Superconductivity in Doped Semiconductor Nanotubes

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**Abstract.** Finite-size systems of the one-dimensional attractive Hubbard model with random potential are studied as an effective model for doped semiconductor nanotubes. We calculate the binding energy of Cooper pairs and pair correlation function by the density-matrix renormalization group method. We show that, when the scattering potential is strong, there appears the ground state where Cooper pairs are formed but are localized spatially, with a decay length of pair correlation smaller than the system size. Experimental relevance is discussed.

## 1. Introduction

Superconductivity has been found [1, 2] to occur in boron (B) doped diamond where carbon (C) ions in the diamond structure are substituted randomly by B ions. The effects of disorder in this system are reported to be so strong that the dimensionless characteristic parameter  $E_F\tau \sim 1$  where  $E_F$  is the Fermi energy and  $\tau$  is the lifetime of electrons [3]. In such a situation, Bloch-like coherent electron conduction does not occur and Fermi surface is no longer well defined in momentum space [4]. The effects of disorder on superconductivity in such systems have been examined based on the coherent potential approximation (CPA) [5] and the superconducting critical temperature  $T_c$  is found to be strongly suppressed by disorder. Regarding the nature of the ground state as a function of doping rate, the electrical resistivity at low temperatures [6] appears to indicate that there exists a superconductor-to-insulator transition, which cannot be treated by CPA. We therefore want to consider the issue “Anderson localization versus superconductivity” at  $T = 0$  K in the present paper.

In the case of boron-nitride (BN) nanotubes, the electric resistance is reduced strongly by doping of fluorine (F) ions, resulting in a highly metallic conduction comparable with that of heavily doped semiconductors [7]. It is well known that pure BN nanotubes are insulating with a band gap of  $\sim 5$  eV [8, 9], irrespective of their chirality. The first-principles local-density-approximation (LDA) band calculation suggests that, upon doping of F ions, the impurity state appears above the top of the valence band and hole carriers are introduced into the system, so that the system becomes a  $p$ -type semiconductor [10]. One may then expect that superconductivity with appreciable  $T_c$  should be realized because the hole carriers are introduced near the top of the valence band with high density of states due to the one-dimensionality. However, occurrence of superconductivity has not so far been reported. We suppose that the

absence of superconductivity in F-doped BN nanotubes may be due to the presence of strong impurity scattering of carriers in spite of the presence of strong attractive interaction.

In this paper, the competition of the formation of Cooper pairs and Anderson localization is studied by finite-size clusters of the one-dimensional attractive Hubbard model for simulating BN nanotubes, where we numerically calculate the binding energy of Cooper pairs and pair correlation function by the density-matrix renormalization group (DMRG) method.

## 2. Model and method

The one-dimensional negative- $U$  Hubbard model with random potential  $\Delta$  is defined by the Hamiltonian

$$H = t \sum_{i\sigma} \left( c_{i+1\sigma}^\dagger c_{i\sigma} + \text{H.c.} \right) - \Delta \sum_{i \in \text{imp.}} n_i + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

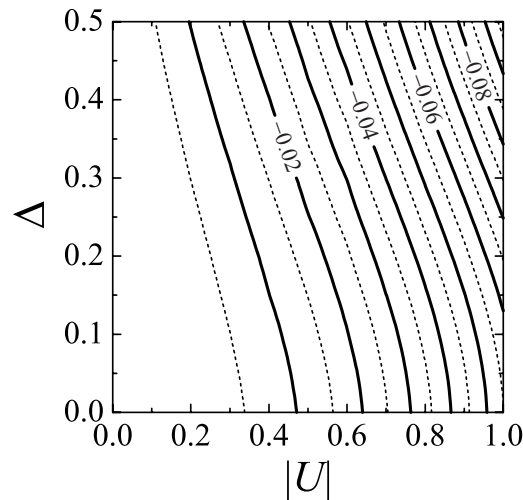
where  $c_{i\sigma}^\dagger$  ( $c_{i\sigma}$ ) is the creation (annihilation) operator of a hole with spin  $\sigma$  ( $=\uparrow, \downarrow$ ) at site  $i$ ,  $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$  is the density operator, and  $n_i = n_{i\uparrow} + n_{i\downarrow}$ .  $t$  is the hopping integral and  $\Delta$  is the strength of the scattering potential at the impurity sites distributed randomly in the system.  $U$  is the attractive interaction ( $U < 0$ ) between carriers, which may come from the electron-phonon coupling, though we do not specify its origin explicitly. We assume that the number of impurity sites is equal to the number of carriers and we take the impurity concentration to be 10%. From the tight-binding band structure calculation, we choose the value of  $t$  so as to reproduce the effective mass of the top of the valence band. Because the difference in energy between the impurity state and the top of the valence band is given in our model as  $\Delta E = \sqrt{4t^2 + \Delta^2} - 2t$  in the dilute limit, we can estimate the impurity potential  $\Delta$  from the results of the band calculation [10]. We thus have the values  $t = 0.25$  eV and  $\Delta/t \simeq 0.3$ . In the following, we take  $t = 1$  as the unit of energy.

We employ the DMRG method to calculate the energies and physical quantities in the ground state, where we use the finite-size clusters with both open-end (OBC) and periodic (PBC) boundary conditions. We keep up to  $m \sim 1200$  density-matrix eigenstates in the DMRG procedure; thus, the discarded weights are typically of the order  $10^{-8}$  and the ground-state energy is obtained in the accuracy of  $\sim (10^{-6} - 10^{-4})t$ . All the calculated energies are extrapolated to the limit  $m \rightarrow \infty$ . We use 100 samples for the distribution of the random potential and take the average for obtaining the physical quantities; no significant changes occur even if we use more samples.

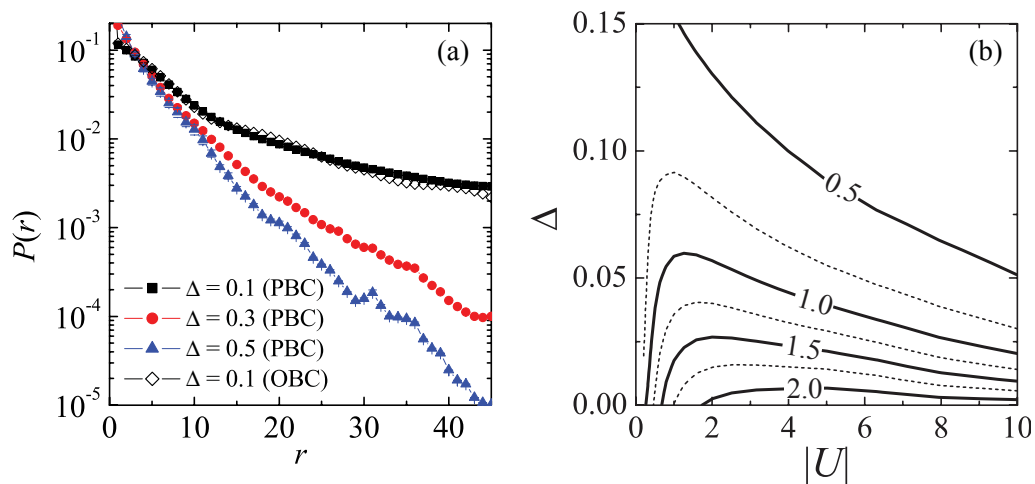
## 3. Results of calculation

We first estimate the localization length  $\xi_{\text{loc}}$  defined from the scaling relation  $\ln D(L) = A - L/\xi_{\text{loc}}$ , where  $A$  is a constant and  $D(L)$  is the Drude weight calculated for the system of size  $L$ . At  $U = 0$ , we find the power-law dependence  $\xi_{\text{loc}} \sim \Delta^{-2}$ . We may say that, if the localization length is larger (smaller) than the system size, the system should be metallic (insulating). In actual BN nanotubes, the system size is from 200 nm to 1  $\mu\text{m}$ , which corresponds to the system of size  $L = 500 - 2500$  in our model. In the following, we assume the system of  $L = 100$  for simplicity. In this case, we find that the system should be metallic if  $\Delta$  is less than  $\Delta_c \simeq 0.24$  at which  $\xi_{\text{loc}} \sim L$ .

To find consequences of the pairing interaction, we calculate the binding energy between two holes defined by  $E_B = (1/2)[E_0(N+2) + E_0(N) - 2E_0(N+1)]$ , where  $E_0(N)$  is the ground-state energy of the system with  $N = 10$  holes. The contour plot of the calculated binding energy is shown in Fig. 1. We find that, if we increase the strength of  $U$ ,  $|E_B|$  is increased, and if  $\Delta$  becomes larger,  $|E_B|$  also becomes larger for fixed  $U$ . We thus understand that, if the Cooper pairs are more localized, the holes feel the attractive interaction more strongly.



**Figure 1.** Contour map of the binding energy  $E_B$  in the  $|U|$ - $\Delta$  plane at  $L = 100$  with the impurity concentration of 10%.



**Figure 2.** (a) Pair correlation function calculated for different values of  $\Delta$  at  $U = -1$  and  $L = 100$  with the impurity concentration of 10%. The results obtained with PBC and OBC are shown. (b) Contour map of the exponent  $K$  in  $|U|$ - $\Delta$  plane at  $L = 100$  with the impurity concentration of 10%.

In order to see the degree of coherence of superconductivity, we calculate the pair correlation function  $P(r)$  defined by  $P(r) = (1/N) \sum_i \langle \psi_0 | \Delta(r+i)^\dagger \Delta(i) | \psi_0 \rangle$  with  $\Delta(i) = c_{i\uparrow} c_{i\downarrow}$ . The calculated results are shown in Fig. 2 (a). We find the power-like decay of  $P(r)$ , i.e.,  $P(r) \sim r^{-1/K}$ , if the impurity potential is sufficiently small  $\Delta < \Delta_c \sim 0.2$  (a boundary effect is little because the results with OBC are close to the results with PBC as shown in Fig. 2 (a)), where  $K$  corresponds to the Tomonaga-Luttinger-liquid parameter  $K_\rho$  in the weak-coupling theory. The estimated values of  $K$  are shown in Fig. 2 (b). We find the enhancement of  $K$  in the weak-coupling regime and suppression of  $K$  in the strong-coupling regime (see the values of  $K$  along the  $U$ -axis). The suppression of  $K$  in the strong-coupling regime would indicate that the effects of disorder have much influence on the pairs with shorter coherence length. If

the impurity potential is strong ( $\Delta > 0.3$ ), we find the exponential decay of  $P(r)$  as shown in Fig. 2 (a). Then, the system can not be superconducting. In this situation, however, there are Cooper pairs in the system because  $E_B < 0$ . We may conclude that the Cooper pairs are formed but they are localized by the effects of disorder and the superconductivity is not observed macroscopically in this parameter region.

#### 4. Summary and discussion

Our results may be summarised as follows. If  $\Delta$  is sufficiently small, the pair correlation extends over the system size and the superconductivity may occur if a bundle of such finite-size nanotubes is made in experiment. As for the issue "Anderson localization versus superconductivity" at  $T = 0$  K, we may say the following: If  $\Delta$  becomes larger, the binding energy becomes larger. The pair correlation is however suppressed and for sufficiently large values of  $\Delta$ , the pair correlation decays exponentially, so that the superconductivity does not occur. This is the case for both weak-coupling and strong-coupling regimes. In the strong-coupling regime, we note that, if  $|U|$  becomes larger for fixed  $\Delta$ , the pair correlation is suppressed more strongly because the coherence length becomes shorter.

The finite-temperature behavior of our system may be inferred from our results; i.e., if we assume that the binding energy corresponds to the temperature  $T_p$  at which the pairs begin to form and that the pair correlation corresponds to the temperature  $T_c$  at which the system begins to be superconducting, our results suggest that there appears the difference between  $T_c$  and  $T_p$  for  $\Delta > 0$ , indicating the existence of the preformed pairs at  $T_c < T < T_p$ . Note that, if  $\Delta$  becomes larger,  $T_p$  increases and  $T_c$  decreases.

We may therefore suggest that the absence of superconductivity in F-doped BN nanotubes should be due to the presence of strong impurity scattering of carriers. We may also suggest that, in B-doped diamond, the Cooper pairs are formed even in the temperature  $T > T_c$  but they are localized by the effects of disorder as in the case of Anderson localization.

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