Numerical renormalization study on magnetic properties of edge states in carbon nanotubes

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Abstract

A π-electron network in carbon nanotubes with zigzag open edges exhibits strongly localized edge states, which are expected to show peculiar magnetic properties. We study the effect of the electron-electron interaction on the magnetic properties of the systems using the density-matrix renormalization-group method. We show that effective spins which can move almost freely appear around the zigzag open edges. A schematic picture representing the low-energy physics of nanographite systems with zigzag edges is proposed.

Key words: nanographite systems ; edge states ; electron-electron interaction ; density-matrix renormalization-group method

Recently, it has been realized that electronic and magnetic properties of graphite-based materials with nano-meter size are affected crucially by their edge shape: nanographites (NGs) with *zigzag* edges exhibit strongly localized edge states which form partly flat bands at the Fermi energy while such a edge state does not appear in NGs with *armchair* edges[1,2]. Since the partly flat bands, followed by a sharp peak of the local density of states, are expected to involve magnetic instability, it is important to study the effect of the electron-electron couplings on the magnetic properties of the NGs with zigzag edges. The effect of electron-electron couplings has been investigated within a mean-field approximation[1,3] and the density-functional theory[4]. It was suggested that a ferrimagnetic spontaneous spin polarization appears at the zigzag edges. However, it is also known that the approximations used in the studies are not appropriate for low-dimensional systems such as NGs. Thus, more detailed analysis with a controlled approximation is desired.

In this paper, we study magnetic properties of the zigzag carbon nanotubes (NTs) with open edges. We consider the Hubbard model on the (2,0) zigzag NTs[5] at half-filling given by

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} \left(c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c. \right) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}, \quad (1)$$

where $n_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$ and the sum $\sum_{\langle i,j \rangle}$ is taken only for the nearest-neighbor sites. We set $t = 1$ throughout this paper. Although the width of the NTs is quite narrow, magnetic properties expected to be common to general zigzag NTs already appear even for such a narrow NTs. We have employed the density-matrix renormalization-group (DMRG) method[6], which allows us to perform a highly accurate calculation even in the presence of electron-electron couplings. We have calculated the energy gap of spin excitations

$$\Delta_{01} = E_0(L/2+1, L/2-1) - E_0(L/2, L/2), \quad (2)$$

where $E_0(N_\uparrow, N_\downarrow)$ is the lowest energy of the system with $N_\uparrow$ up- and $N_\downarrow$ down-spin electrons and L is the total number of sites. We have also calculated the local spin polarization at each carbon site,

$$\langle S^z_i \rangle_M = \frac{1}{2} \langle n_{i,\uparrow} - n_{i,\downarrow} \rangle_M, \quad (3)$$

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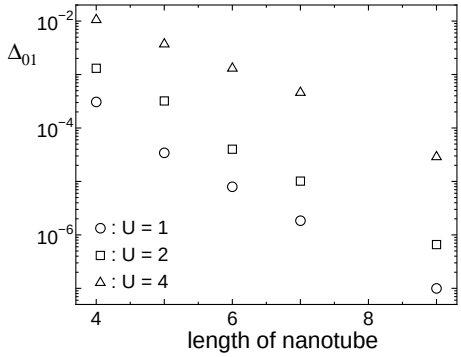

Fig. 1. The spin gap Δ_{01} of the (2,0) NTs for $U = 1$ (circles), $U = 2$ (squares), and $U = 4$ (triangles) as functions of the length of NTs. The numerical errors of the DMRG calculation are smaller than the symbols.

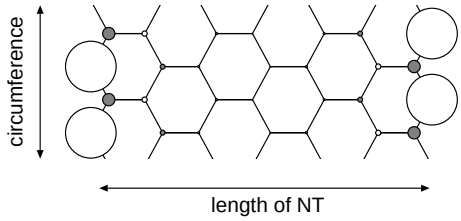

Fig. 2. The distribution of local spin polarization $\langle S_i^z \rangle_1$ on each carbon site in a (2,0) nanotube for $U = 1$. Open and gray circles represent the positive and negative values of the spin polarization, respectively. The area of each circle is proportional to the absolute value of the polarization.

where $\langle \cdots \rangle_M$ represents the expectation value in the lowest energy state in the subspace $(L/2+M, L/2-M)$. The number of kept states in the DMRG calculation is up to $m = 700$ per block. The numerical errors due to the truncation are estimated from the difference between the data with different m's.

Figure 1 shows the spin gap for several typical values of U as a function of the length of NTs. The spin gap takes non-zero values for all calculated U. This indicates that the ground state is a total spin-singlet for $U > 0$ and a finite magnetic field corresponding to the spin-gap energy is required to magnetize the system. However, we also find that the spin gap decreases exponentially as the length of NTs becomes larger. Thus, if the NT is long enough, one can magnetize the system by applying an extremely small (almost infinitesimal) field. In Fig. 2, we show the distribution of the spin polarization $\langle S_i^z \rangle_1$ in the magnetic excited state. It is clear that the magnetization appears almost only on the sites around the zigzag open edges. We thus conclude that only the spins of the electrons in the edge states are polarized easily by the small field while the spins in bulk sites are not.

The results obtained above can be understood in a schematic picture in the following. In the picture, the system is composed of two parts: one is the bulk electrons forming a spin-singlet state rigidly and the other is effective spins consisting of electrons around the zigzag-edge sites correlating loosely with each other. The effective spins interact via an antiferromagnetic effective coupling beyond the bulk sites, resulting in the ground state of total spin-singlet. The effective coupling, which corresponds to the spin-gap energy, becomes smaller as the length of the NT increases, and finally, the effective spins can move almost freely when the length becomes large enough.

To summarize, we have studied the magnetic properties of the zigzag NTs with open edges in the presence of the electron-electron couplings. We have found that the ground state of the system is a spin-singlet and a finite spin gap opens for $U > 0$. The system exhibits effective spins at zigzag edges which are easily magnetized by a small magnetic field. We note that we have also observed the similar magnetic behaviors in another typical NG system, called nanographite ribbons[7]. We thus expect that the picture proposed in this paper is valid not only for zigzag NTs but for general NG systems with zigzag edges.

Acknowledgements

We are grateful to K. Wakabayashi, S. Okada and A. Tanaka for fruitful discussion.

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[5] Carbon nanotubes are characterized by the two integers (N_+, N_-) specifying the wrapping vector $\mathbf{v} = N_+\mathbf{a}_+ + N_-\mathbf{a}_-$, where $\mathbf{a}_\pm$ are primitive lattice vectors of a graphene sheet. NTs with $N_- = 0$ are called as "zigzag" NTs.

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