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Correlations in Hexagonal Lattice Systems — Application to Carbon Nanotubes

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We present exact diagonalization studies of two-dimensional electron gas on hexagonal lattice. Using Lanczös method we analyze the influence of the Coulomb correlations on the density of states and spectral functions. Choosing appropriate boundary conditions we simulate the geometry of a single wall carbon nanotube. In particular, integration over the boundary condition in one direction and summation in the other one allows us to perform cluster calculations for a tube-like system with a finite diameter and infinite length.

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1. Introduction

Since the discovery of carbon nanotubes, their electronic properties attract much attention. However, most of the band structure calculations neglects the influence of the Coulomb interaction. Generally, the Coulomb interaction can be treated exactly for small systems (exact diagonalization techniques using the Lanczös algorithm [1]), or analytically for large (infinite) systems. Unfortunately, approximations which have to be used in analytical approaches to a strongly correlated system are often uncontrolled. The Lanczös algorithm is one of the most effective computational tools for searching the ground state and some low laying excited states for finite systems. From the ground state, one can compute all static and dynamic properties, and in this sense, one obtains a complete characterization of a model at zero temperature except for finite size effects. Unfortunately, this

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drawback is a very serious one, since the memory requirements strongly restrict the maximum size of the system. Some approaches are known to reduce the finite size corrections. In the present paper we make use of one of them in order to investigate the role the correlations play in carbon nanotubes.

2. Averaging over boundary conditions

To analyze influence of Coulomb interaction in hexagonal lattice we use the Hubbard Hamiltonian

$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}, \tag{1}$$

$c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) an electron at site i with spin $\sigma =\uparrow,\downarrow$, $n_{i,\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ represents a number of electrons at site i, t_{ij} is the hopping integral between nearest neighbors $\langle ij\rangle$, and U is the Coulomb interaction.

Since the analytical solution of two-dimensional (2D) Hubbard model is unknown, we make use of the exact diagonalization method. In this case we have to apply appropriate boundary conditions (BC). Unfortunately, commonly used open or (anti)periodic BC gives only a few points in the Brillouin zone (BZ) — the number of points in BZ is equal to the number of cluster sites. This feature makes difficult to analyze the momentum dependence of physical quantities. As a partial solution of this problem we propose *averaging over boundary conditions* (ABC) [2]. The idea is the following: each time the hopping term makes a particular electron jump out of the cluster, it is mapped back into the cluster with the wave function multiplied by $\exp(\mathrm{i}\varphi_x)$ or $\exp(\mathrm{i}\varphi_y)$, for jumps along the x or y axis, respectively. $\varphi_x = \varphi_y = 0$ corresponds to periodic BC, whereas $\varphi_x = \varphi_y = \pi$ to antiperiodic BC (Fig. 1).

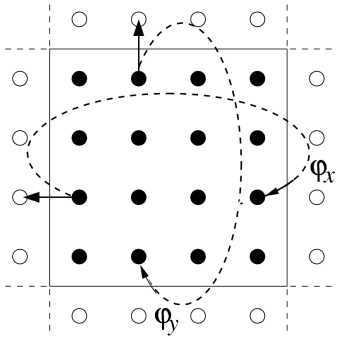

Fig. 1. Explanation of the meaning of the parameters φ_x and φ_y.

The *whole* reciprocal space can be swept, when φ_x and φ_y are allowed to vary *continuously*. The density of states or spectral functions, calculated as a sum

of delta functions for each φ_x and φ_y, integrated over φ_x and φ_y from continuous functions, e.g.:

$$\varrho(\omega) = \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \mathrm{d}\varphi_x \int_{-\pi}^{\pi} \mathrm{d}\varphi_y \varrho(\omega, \varphi_x, \varphi_y), \tag{2}$$

where $\varrho(\omega, \varphi_x, \varphi_y)$ is the density of states determined for a particular boundary conditions specified by φ_x and φ_y. In practice, the integrals are replaced by an average over a rectangular mesh.

3. Hexagonal lattice and nanotubes

Carbon nanotubes are rolled up graphite planes. There are three basic kinds of nanotubes: armchair, zig-zag, and chiral. The type of nanotube determines their electron properties and they can be semimetallic (like graphite), semiconducting or metallic.

In carbon nanotubes hopping between nearest neighbors is in three directions and within the framework of the ABC approach we have three different hopping integrals (see Fig. 2):

$$t_1 = -t \exp\left[\frac{\mathrm{i}}{2}(\varphi_x + \sqrt{3}\varphi_y)\right], \quad t_2 = -t \exp\left[\frac{\mathrm{i}}{2}(\varphi_x - \sqrt{3}\varphi_y)\right],$$
$$t_3 = -t \exp(-\mathrm{i}\varphi_x). \tag{3}$$

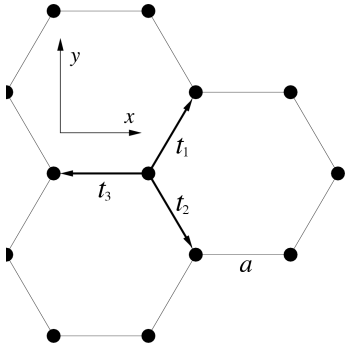

Fig. 2. Hopping integrals in hexagonal lattice.

Since carbon nanotubes are seamless objects, the wave functions have to obey periodic boundary conditions around the circumference, and the component of the wavevector perpendicular to the nanotube axis is quantized. This feature makes carbon nanotubes well suited for the ABC approach. In this case the averaging over BC along the nanotube circumference reduces itself to a summation over only a few distinct values, to reproduce the quantized values of the component of the wavevector (k_y). On the other hand, a particular BC along the nanotube

corresponds to a specific one (or several, depending on the cluster size and shape) value(s) of the component of the wavevector along the nanotube axis (k_x).

4. Results and conclusions

In order to demonstrate the proposed approach we have performed numerical calculations for 8–site clusters cut out of zig–zag and armchair nanotubes. Both these clusters, presented in Fig. 3, have the same shape, but different orientations.

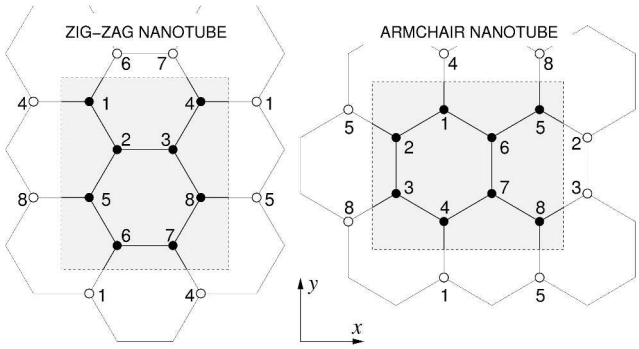

Fig. 3. Clusters used in numerical calculations. The nanotube is along the x-axis.

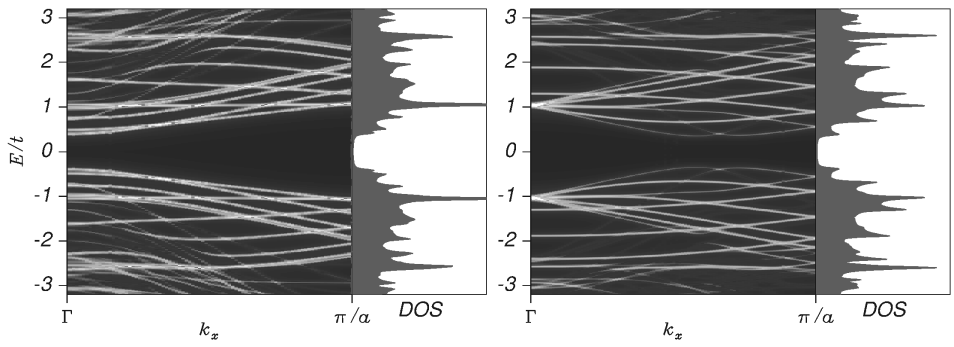

Fig. 4. Band structures and densities of states for zig-zag (left panel) and armchair (right panel) nanotubes in the presence of the Coulomb interactions with $U = t$.

The summation over a finite set of φ_y's mimics the quantized values of k_y. On the other hand, continuous values of φ_x correspond to a dense set of k_x. This allows us to determine, using the Lanczös method, the spectral functions for a given k_x. Summation over k_x gives the density of states. In the case of $U = 0$, the proposed approach exactly reproduces the tight-binding band structure of nanotubes. Examples of the band structure and the density of states for zig-zag and armchair nanotubes determined in the presence of the Coulomb interaction

are presented in Fig. 4. Note that the gap at the Fermi level in the armchair nanotube (semimetallic in the noninteracting case), opens due to the Coulomb interactions.

References

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