EXACT GROUND STATES FOR QUASI 1D SYSTEMS WITH HUBBARD INTERACTION

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ABSTRACT

Using a positive semidefinite operator technique we deduced exact ground states for a modified diamond chain described by a non-integrable Hubbard model with on-site repulsion. Our results are valid for arbitrary length of the chain and strength of the Hubbard interaction. For the analyzed quasi 1D chain structure we found that two flat bands are present in the bare band structure of the system, both for zero and for a fixed value of magnetic field. We obtained ground states of nonmagnetic and ferromagnetic insulator type and studied their physical properties.

Keywords: Strongly interacting systems, Hubbard model, nanowires, ferromagnetism

INTRODUCTION

The investigations of nanostructure objects with itinerant electrons are one of the most quickly progressing fields in the modern material science.These systems present a drastic change of physical properties under given conditions, e.g. fixed external magnetic field or given site-selective gate potential[1, 2]. In this frame we investigate below electron systems where the interaction between the electrons is the well-known Hubbard on-site term. Our goal is to find exact ground-state wave functions for arbitrary strength of the interaction, thus we do not use perturbation theory or any other approximations. It is worth to mention that the full exact solution of the Hubbard model is still unknown for dimensions larger than 1. In the paper [1] a new method was developed and applied for the diamond Hubbard chain. In this paper we used the same method to a similar, but modified system.

THE STUDIED SYSTEM

Figure 1. shows the modified Hubbard diamond chain we analyzed. The sites of the chain for the cell defined at the site i are denoted by $i+r_s$, where s = 1, 2, 3 is the sublattice index. The Bravais vector of the lattice is a, horizontal in the figure. N_C is the number of unit cells, N is the number of electrons, N_S is the number of sites, and one has $N_S = 4N_C$.

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$$\hat{H} = \sum_{\sigma}\sum_{i=1}^{N_C}\Big[te^{i\delta/2}(c^{\dagger}_{i+r_1,\sigma}c_{i,\sigma} + c^{\dagger}_{i+a,\sigma}c_{i+r_1,\sigma} + c^{\dagger}_{i+r_2,\sigma}c_{i+a,\sigma} + c^{\dagger}_{i,\sigma}c_{i+r_2,\sigma})$$
$$+ t_3 c^{\dagger}_{i+r_3,\sigma}c_{i,\sigma} + t_{\perp}c^{\dagger}_{i+r_1,\sigma}c_{i+r_2,\sigma} + t_{\parallel}c^{\dagger}_{i+a,\sigma}c_{i,\sigma} + H.c.$$
$$+ \epsilon_0 n_{i,\sigma} + \epsilon_1 n_{i+r_1,\sigma} + \epsilon_2 n_{i+r_2,\sigma} + \epsilon_3 n_{i+r_3,\sigma}\Big] + U\hat{U}$$

The operator $c^{\dagger}_{i,\sigma}$ creates an electron with spin σ in at site i, $n_{i,\sigma} = c^{\dagger}_{i,\sigma}c_{i,\sigma}$ is the particle number operator, while $\hat{U} = \sum_{i=1}^{N_S} n_{i,\uparrow}n_{i,\downarrow}$ the operator of the on-site Coulomb repulsion, U>0. The movements of the electrons are described by the hopping matrix elements t, $t_{\parallel}$, $t_{\perp}$ and t_3.

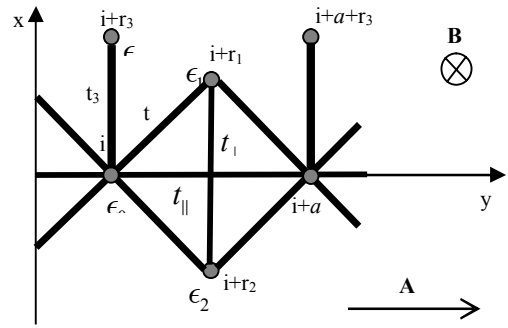

Fig. 1 – The Hubbard chain, Case I

The first one characterize the nearest-neighbor hoppings (except for sites i+r_3) while $t_{\parallel}$ and $t_{\perp}$ the second nearest neighbor terms parallel and perpendicular to a, respectively. The last hopping term t_3 refers to movements along the external leg, and the epsilons are one-site one particle potentials. The system is placed in an external magnetic field perpendicular to the plane of the chain and described by the Peierls phase factor delta. During the calculations arbitrary but fixed N and periodic boundary conditions are taken into account along the chain. One notes that the presence of the external legs into the system allows the use of external site selective gate potentials in order to modify and easily manipulate the potential T_3 and therefore the physical behavior of the system.

ABOUT THE METHOD

First we calculate the non-interacting band-structure of the system. For this we have to write the Hamiltonian without the $U\hat{U}$ term into the k-space

by Fourier transformation. Then, by diagonalizing the obtained expression we derive an algebraic equation with four unknowns – as we have four sites in the primitive cell – and the solutions of this equation as a function of k gives the four bands of the bare band structure. We obtained that the lowest two bands are always flat.

To find the GS of the interacting system, we use the method of positive semidefinite operators. A Hermitian operator is called positive semidefinite if its spectrum is nonnegative, i.e. its lowest eigenvalue is zero or positive. Therefore if H_+ is a positive semidefinite Hamiltonian and we have an eigenvector of H_+ with zero eigenvalue, then this vector belongs to the ground-state (GS) subspace of H_+. Suppose that we manage to write the H Hamiltonian of the interacting system in the form

$$H = H_+ + C \tag{1}$$

where H_+ is positive semidefinite and C is a constant which depends on the parameters of the Hamiltonian. Now if $|\psi_g\rangle$ is the most general element of the kernel of H_+, then $|\psi_g\rangle$ is the GS vector of H and the corresponding GS energy is C. Thus in our method we transform the Hamiltonian into the form (1) and calculate the kernel of H_+.

On this line we managed to transform the Hamiltonian into the form

$$\hat{\mathrm{H}} = \sum_{\sigma}\sum_{i=1}^{N}\left(A_{i,\sigma}^{\dagger}A_{i,\sigma} + B_{i,\sigma}^{\dagger}B_{i,\sigma}\right) + U\hat{U} - K\hat{N} \tag{2}$$

where the terms A and B are block operators which represent a linear combination of fermionic operators defined on a finite domain of the system. One can easily see that the terms in the bracket are positive semidefinite. On the other hand, the Hubbard-term is positive semidefinite, and presents its smallest possible zero eigenvalue if there are no doubly occupied sites in the system. Furthermore, $C = -K\hat{N}$, where $\hat{N}$ is the operator of total particle number of the system.

THE OBTAINED GROUND STATE

We obtained the GS wave vector in the form

$$|\Psi_{gs}\rangle = \prod_{i}\hat{G}_{i,\sigma_i}^{\dagger}|0\rangle \tag{3}$$

where $|0\rangle$ is the vacuum state. We consider the $\hat{G}_{i,\sigma}^{\dagger}$ operators as the most general linear combination of creation operators with acting on each lat-

tice site of the system. Furthermore, one takes into consideration that the lowest energy value must be provided by a state without doubly occupied sites. We found the following two families of $\hat{G}^{\dagger}_{i,\sigma}$ operators at $\delta = 0$:

$$D^{\dagger}_{i+a,\sigma} = \frac{t}{t_{\perp}} c^{\dagger}_{i+r_1,\sigma} - c^{\dagger}_{i+a,\sigma} + \frac{t_3}{\epsilon_3} c^{\dagger}_{i+a+r_3,\sigma} + \frac{t}{t_{\perp}} c^{\dagger}_{i+a+r_2,\sigma}$$

$$E^{\dagger}_{i,\sigma} = c^{\dagger}_{i+r_1,\sigma} - c^{\dagger}_{i+r_2,\sigma} \tag{4}$$

A similar expression is obtained for $\delta = \pi / 2$. So we have two sets of operators, namely $D^{\dagger}_{i,\sigma_i}$ and $E^{\dagger}_{i,\sigma_i}$ which can appear in the GS vectors, each with N_C terms for both up and down spins. Every vector from the kernel of the transformed Hamiltonian can be written as a product of these operators. The number of the operators in the product specifies the number of electrons in the system. The most general GS vector is obtained as a linear combination of these vectors. As $D^{\dagger}_{i,\sigma_i}$ and $E^{\dagger}_{i,\sigma_i}$ have no common lattice-points for different *i* (except for $D^{\dagger}_{i,\sigma_i}$ and $E^{\dagger}_{i+1,\sigma_i}$), the spin indices σ_i of them for different cells are usually independent. For the same cell, the $D^{\dagger}_{i,\sigma_i}$ and $E^{\dagger}_{i,\sigma_i}$ operators must have the same spin index in order to avoid the double occupancy. Physically this means that the solution is globally a non-magnetic phase up to the electron number $N<2N_C-1$. For the case when in the same cell both operators D and E are present, the cell itself is ferromagnetic and behaves as a ferromagnetic cluster. However, different cells are magnetically not correlated. This is the reason why the system globally is non-magnetic if $N<2N_C-1$. At $N=2N_C-1$ or $N=2N_C$ the D and E operators touch each other, the connectivity condition is satisfied and the system becomes ferromagnetic.

We also calculated the mean value of the long range hopping function

$$\frac{\langle \Psi_{gs} | \hat{c}^{\dagger}_{1+r_1+ra,\sigma} \hat{c}_{1+r_1,\sigma} + H.c. | \Psi_{gs} \rangle}{\langle \Psi_{gs} | \Psi_{gs} \rangle} \tag{5}$$

as a function of *r*, more precisely the logarithm of the absolute value of this function. We obtained that this is close to a straight curve, which means that the long range hopping function is exponentially decreasing. Thus we can conclude that the ground state electrons are localized, although not exactly to one lattice point. Therefore the GS is an insulator, albeit not a band insulator.

SUMMARY

An itinerant diamond chain with external link is analyzed in the presence of a perpendicular external magnetic field in the frame of a non-integrable Hubbard model. For this chain exact ground states are deduced by a method using positive semidefinite operator properties. The ground states turn out to be nonmagnetic and ferromagnetic in character being localized in the thermodynamic limit.

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