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GROUND STATE ENERGY OF 2D EXTENDED HUBBARD MODEL FOR FINITE SIZE SYSTEM WITH AN EXACT DIAGONALIZATION

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Using an exact analytical diagonalization for an extended Hubbard model, we study the first nearest-neighbour repulsion effect on the behaviour of a two-dimensional system of finite size at low density of electrons. The obtained results show that the introduction of the nearest-neighbour off-site interaction allows the correlation effects to become more remarkable and to play an essential role in the electron dynamics, and this off-site interaction encourages the formation of double occupancies.

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1. Introduction

The Hubbard model (HM) and its extensions play a key role in the analysis of correlated electron systems, where it is widely used for describing the high T_c temperature superconductivity [1, 2] and the Mott metal-insulator transition [3, 4]. In its extended version (EHM), the model exhibits the competition between the usual kinetic, the on-site and the off-site Coulomb interactions. In spite of its simple definition, the general exact solution of the EHM has still not been reached, but, a great variety of approximate treatments have been proposed in order to establish an appropriate theoretical framework. In Refs. [5, 6], we have generalized the self-consistent random-phase approximation (SCRPA) [7, 8] to solve the EHM in 1D, where we have shown that this approach treats the correlations of closed chains in a rigorous manner. The behaviour of our SCRPA ground state and gap energies shows that the repulsive off-site interaction between the electrons

of the neighbouring atoms induces a supplementary conductivity. But, due to the restricted motion along one direction in space, the Hubbard model chain doesn't exhibit any ferromagnetic feature, where the Pauli principle requires that even the neighbouring electrons must have the opposite spins, so that the hopping of these electrons between neighbour's sites will be possible. Thus, the 1D Hubbard is a nice prototype to describe, only, the 1D classical conductors.

Recently, the two-dimensional (2D) extended Hubbard model (EHM) has been intensively studied [9, 10]. This activity increased rapidly after the discovery of the high-T_c superconductors, since it is widely believed that this high-T_c superconductivity exists in the CuO_2 planes. Despite considerable efforts, there is still a need for simple methods that can contribute to the resolution and the understanding of the two-dimensional EHM.

In this paper, we perform a numerical diagonalization of the 2D EHM for finite size systems using an analytical diagonalization procedure developed in Ref. [11], and to study the local properties of this model.

2. *Model and formalism*

The two-dimensional extended Hubbard model on a square lattice is given by

$$H = -t \sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + V \sum_{\langle i,j\rangle,\sigma,\sigma'} n_{i,\sigma} n_{j,\sigma'} \,, \tag{1}$$

where $c^{\dagger}_{i,\sigma}$ ($c_{j,\sigma}$) are the creation (annihilation) operators for a fermion of spin σ at the site i (j) under the periodic boundary conditions and t is the hopping term from the site j to the site i. The $\langle i,j\rangle$ sums are over nearest neighbour sites. The second term describes the local repulsive interaction with parameter U. The last term takes into account the nearest-neighbour repulsion between electrons with energy V.

The solution of the model (1) in the case of a finite-size system, gives the exact solution of some physical quantities such as the ground state energy and the occupation numbers. We consider, thus, a two dimensional $L \times L = N = 16$ square lattice at one-eighth filling (four electrons per cluster), under the periodic boundary conditions in both directions. For the considered system, three types of particle configurations may occur. First, we can have two double occupancies at sites i and j ($i \neq j$). Second, we may have a double occupancy at site i and two electrons with opposite spins at sites j and k ($i \neq j$, $i \neq k$ and $j \neq k$). Finally, we may have four single occupancies placed at different sites of this 4×4 square lattice. These three possible configurations provide, respectively, the three states:

$$|a\rangle = \left(c^{\dagger}_{i,\sigma} c^{\dagger}_{i,-\sigma}\right) \left(c^{\dagger}_{j,\sigma} c^{\dagger}_{j,-\sigma}\right) |0\rangle \,,$$

$$|b\rangle = \left(c^{\dagger}_{i,\sigma} c^{\dagger}_{i,-\sigma}\right) \left(c^{\dagger}_{j,\sigma} c^{\dagger}_{k,-\sigma}\right) |0\rangle \,,$$

$$|c\rangle = \left(c^{\dagger}_{i,\sigma} c^{\dagger}_{j,\sigma}\right) \left(c^{\dagger}_{k,-\sigma} c^{\dagger}_{l,-\sigma}\right) |0\rangle \ ,$$

where $|0\rangle$ represents the state vacuum with no electron present.

The states $|a\rangle$, $|b\rangle$ and $|c\rangle$ generate 14400 states, which describe all possible distributions of our four electrons in the 4×4 cluster. In order to construct a r–space basis, it is convient to define a linear operator T [11], which satisfies the relation

$$T(A + B) = T(A) + T(B) \, ,$$

where A and B represent the particle configurations as described in Fig. 1. $T(A)$ is the linear combination of the 16 contributions obtained by the translation of the configuration A to each site of the 4×4 cluster.

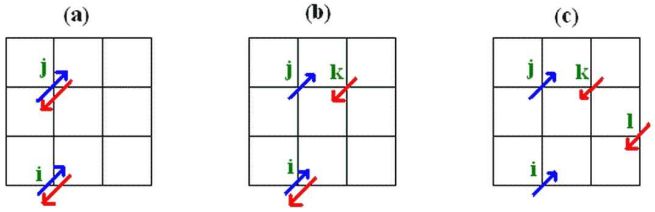
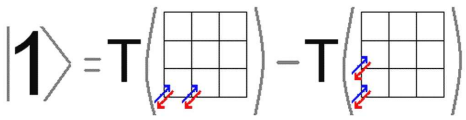


Fig. 1. The three possible types of particle configurations (a: two double occupancies, b: double occupancy and two single occupancies, c: four single occupancies).

Using this linear operator, the Hilbert space of our considered system has the dimension 176. As found in Ref. [11], one can check that, even in the case of the extended Hubbard model, this space of the 176 cluster states can be decoupled in two independent parts. The first and second parts are, respectively, the difference and the sum of horizontally and vertically generated vectors. The application of the Hamiltonian (1) on the different vectors of the first parts allows the conclusion that this first subspace generates the ground state of our considered system described by the parameters t, U and the additional term V. In this manner, we can regroup all states of the four electrons on 85 cluster states denoted $|n\rangle$, where $n = 1, 2, \ldots, 85$, which are all orthogonal vectors. For example, $|1\rangle$ describes all states $|a\rangle$ with $|R_i - R_j| = a$



(For the definition of the other 84 vectors, see Ref. [11]).

In order to analyze the properties of the ground and excited states of this regular cluster, we have written the energy matrix in the subspace of the 85 cluster states, then, we have performed a numerical diagonalization of the finite-size clusters using an analytical diagonalization procedure developed in Ref. [11].

3. Results and discussion

3.1. Local properties of the 4×4 cluster for $V = 0$

First, we started our study with the analysis of the pure Hubbard case, where the interaction was taken into consideration only between the electrons at the same site, that is $V = 0$.

The study of the eigenstates of the matrix energy $E_{85\times85}$ leads to an interesting observation, since 34 states (40% of the eigenstates) are U independent. This independence means that the single-particle physics is dominating in these 34 excited states. This is a logical result, knowing that our electron system is placed in the limit of the low concentration, where the correlation effects are very weak.

In the following, we turn our interest to the ground state and the lowest excited state of the U-independent eigenstates in the subspace of the 85 cluster states.

In Fig. 2, we have plotted the ground state and the lowest excited state energies as a function of the on-site interaction energy U. The curves show that the ground state energy E_{GS} has smooth (less than linear) U dependence, whereas the lowest excited state energy E^* is U independent; it is equal to $-8t$ for any value of U.

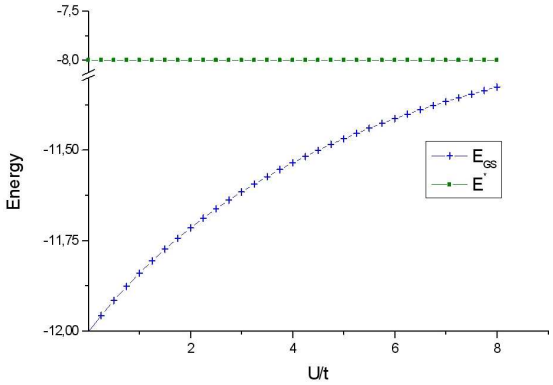


Fig. 2. Ground state energy E_{GS} and lowest excited state energy E^* as functions of U for $V = 0$.

Thus, it is clear that this lowest excited state is an eigenvector of the kinetic energy $\left(-\sum_{\langle i,j\rangle,\sigma} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma}\right)$, since this excited state avoids completely any formation of the double occupancy. But the ground state is not an eigenstate of the kinetic energy or of the on-site interacting part of H only, but is an eigenvector of the sum of both. With this scenario, in the ground state, electrons can jump between the neighbouring sites due to the term t, without, necessarily, avoiding the double occupancy.

In order to analyze the on-site interaction effect on the repartition of our four electrons in the above system, we define the double-occupancy coefficients D and D^* as the probabilities to have a couple of electrons ($\uparrow\downarrow$) on the same site in the

ground state and the lowest excited state, respectively:

$$D = \frac{1}{N} \sum_i \langle GS \, | n_{i\uparrow} n_{i\downarrow} | \, GS \rangle \ ,$$

$$D^* = \frac{1}{N} \sum_i \langle excited \, | n_{i\uparrow} n_{i\downarrow} | \, excited \rangle \ ,$$

where the sums are over all 4×4 cluster sites. $|GS\rangle$ and $|excited\rangle$ are, respectively, the corresponding eigenvectors to E_{GS} and E^*.

In Fig. 3, we have plotted the coefficients D and D^* as functions of U. In the lowest excited state, we have $D^* = 0$. Thus, effectively, this excited state avoids completely any formation of the double occupancy. Figure 3 shows, also, that $D \neq 0$, where the probability to find a double occupancy in the ground state is important for a weak on-site interaction. But, this ground state has the tendency to avoid the double occupancy for strong on-site interaction.

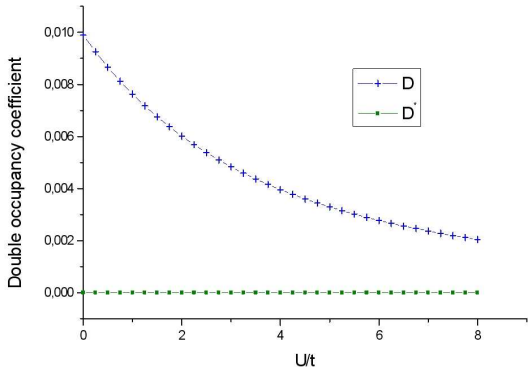


Fig. 3. Double occupancy coefficients D and D^* in the ground state and in the lowest excited state, respectively, as functions of U for $V = 0$.

3.2. Local properties of the 4×4 cluster for $V \neq 0$

As described in Sec. 3.1, Kovacs et al. show that the 4×4 cluster avoids completely the double occupancy in a great number of excited states. In order to investigate how far is this result near to the real description of this cluster, it is necessary to take into account all possible interactions which govern the dynamics of this 4×4 cluster of electrons, as the off-site interaction. Thus, in the following, we present the V effect on the local properties of the cluster.

In Fig. 4, the ground state energy E_{GS} is shown as a function of U/t for different values of V/t. The curves show that the energy E_{GS} has a smooth U dependence, whereas it has a quasi-linear V dependence. This behaviour is similar to the one obtained for the ground state energy of the chains extended Hubbard model with the self consistent random phase approximation (SCRPA) [5, 6]. These curves show,

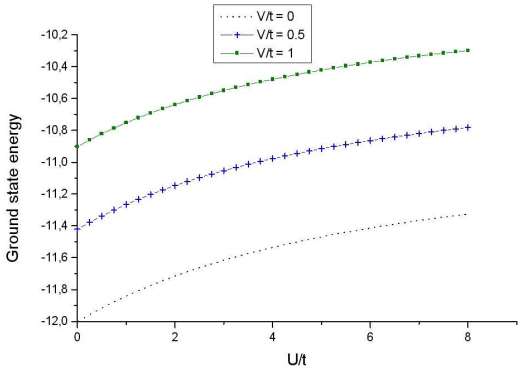


Fig. 4. Ground state energy as the function of U/t for different values of V/t.

also, that E_{GS} decreases with V for a fixed value of U. Thus, we can conclude that this off-site interaction imposes to the electron system to avoid, partially, the double occupancy of the ground state.

In Fig. 5, the lowest excited state energy E^* is shown as a function of U/t for different values of V/t. The curves show that the lowest excited state energy becomes U dependent for $V \neq 0$. Thus, the off-site interaction encourages the existence of double occupancies in this excited state. For a weak off-site interaction ($V/t = 0.5$), the corresponding curve shows that E^* becomes U independent for the high values of U. But for an intermediate off-site interaction ($V/t = 1$), E^* still remains dependent on U, since we have the opportunity to have double occupancies even for the high values of U.

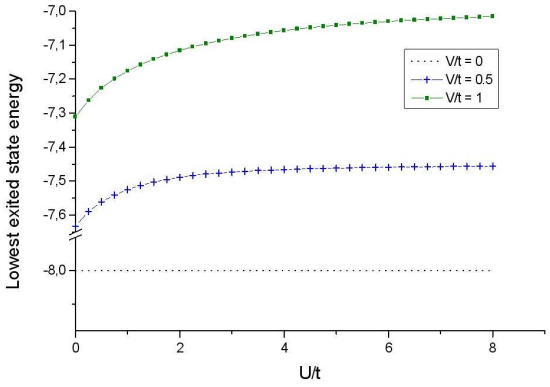


Fig. 5. Lowest excited state energy as the function of U/t for different values of V/t.

The double-occupancy coefficient D^* in the lowest excited state is shown in Fig. 6 as function of U/t for different values of V/t. For $V/t = 0$, we have $D^* = 0$. Thus, effectively, our system avoids completely the double occupancy at this excited

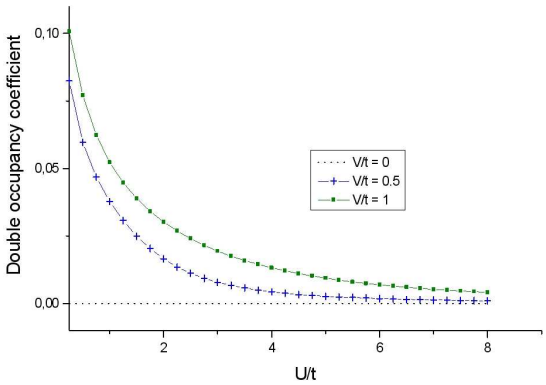


Fig. 6. Double occupancy coefficient D^* in the first excited state as the function of U/t for different values of V/t.

state. However, if we take into account the off-site interaction, we have $D^* \neq 0$. For $V/t = 1$, we have $D^* \neq 0$ even for the large values of U/t. But, for $V/t = 0.5$, the coefficient D^* vanishes for the large value of U/t, where the off-site interaction becomes very weak before the on-site interaction. Thus, the behaviour of our system in this regime ($U \ll V$) is similar to the one found in Ref. [11], where the authors have shown that 40% of the excited states of the 4×4 cluster are U independent. But, it is clear that the number of these U-independent excited states decreases if we take the off-site interaction, since this interaction encourages the double occupancy in the different excited states.

4. Conclusion

The present work represents an attempt for the generalization of the exact description of the 2D Hubbard model on finite-size systems in the low-density limit, to the extended case containing nearest-neighbour Coulomb repulsion. Thus, we have considered a two-dimensional square lattice containing 16 sites at one-eighth filling, recently treated in Ref. [11] with the pure Hubbard model and we have, then, studied the effect of the nearest-neighbour off-site interaction on the local properties of this square lattice.

In the first steep, we have shown that even in the case of the extended Hubbard model, the obtained Hilbert space for our electron system described by the parameters t, U and the additional term V has the dimension 85. Then, we have written the energy matrix in this subspace of the 85 cluster states and we have performed a numerical diagonalization of finite-size clusters using an analytical diagonalization. Finally, we have analyzed the behaviour of the obtained local properties of the ground state and excited state energies as functions of U and V.

The obtained results show that the behaviour of our system is similar to the one obtained in Ref. [11], but only in the ($V \ll U$) case, where we have found that the single-particle physics is dominating in 40% of the U independent excited

states. But for an intermediate and a strong off-site interaction, the correlations effects become more remarkable, where we have found an important reduction of the number of the U-independent excited states. The obtained results show, also, that the off-site interaction encourages the formation of double occupancies in the ground state.

References

[1] I. Martin, G. Ortiz, A. V. Balatsky and A. R. Bishop, Europhys. Lett. **56** (2001) 849.

[2] C. Halboth and W. Metzner, Phys. Rev. B **61** (2000) 7364.

[3] N. F. Mott, *Metal-Insulator Transitions*, 2nd ed., Taylor and Francis, London (1990).

[4] F. Gebhard, *The Mott Metal–Insulator Transition*, Springer, Berlin (1997).

[5] S. Harir, M. Bennai and Y. Boughaleb, Appl. Math. Sci. **1** (2007) 1651.

[6] S. Harir, M. Bennai and Y. Boughaleb, Phys. Scr. **76** (2007) 370.

[7] M. Jemai, P. Schuck, J. Dukelsky and R. Bennaceur, Phys. Rev. B **71** (2005) 85115.

[8] D. Davesne, M. Oertel and H. Hansen, Eur. Phys. J. A **16** (2003) 35.

[9] J. Beenen and D. M. Edwards, Phys. Rev. B **52** (1995) 13636.

[10] N. Stefanakis, Phys. Rev. B **66** (2002) 24514.

[11] E. Kovacs and Z. Gulacsi, Phil. Mag. **86** (2006) 2073.

ENERGIJA OSNOVNOG STANJA U PROŠIRENOM 2D HUBBARDOVOM MODELU ZA KONAČAN SUSTAV S EGZAKTNOM DIJAGONALIZACIJOM

Primjenom egzaktne analitičke dijagonalizacije za proširen Hubbardov model proučavamo učinak odbojne sile među prvim susjedima na svojstva konačnog dvodimenzijskog sustava pri niskim gustoćama elektrona. Postignuti ishodi pokazuju da uvođenje prvo-susjedskog međudjelovanja izvan sustava omogućuje pojačanje korelacijskih učinaka, igra bitnu ulogu u dinamici elektrona, te to međudjelovanje izvan sustava podstiče stvaranje dvostrukih popunjenja.