An exact solution to the extended Hubbard model in 2D for finite size system

S Harir\(^1\), M Bennai\(^1,3\) and Y Boughaleb\(^1,2,4\)

\(^1\) Laboratoire de Physique de la Matière Condensée, Faculté des Sciences Ben M’Sik, Université Hassan II-Mohammedia Casablanca, Morocco
\(^2\) LPMC, Faculté des Sciences d’El Jadida, Université Chouaib Doukkali, Morocco
\(^3\) Groupement National de Physique des Hautes Energies, LabUFR-PHE, Rabat, Morocco
\(^4\) Hassan II Academy of Sciences and Technology, Morocco

E-mail: harirsaid@gmail.com, bennai.jdriissi@yahoo.fr and yboughaleb@yahoo.fr

Received 10 December 2007
Accepted for publication 21 May 2008
Published 25 July 2008
Online at stacks.iop.org/PhysScr/78/025701

Abstract
An exact analytical diagonalization is used to solve the two-dimensional extended Hubbard model (EHM) for a system with finite size. We have considered an EHM including on-site and off-site interactions with interaction energies \(U\) and \(V\), respectively, for a square lattice containing 4 \(\times\) 4 sites at one-eighth filling with periodic boundary conditions, recently treated by Kovacs and Gulacsi (2006 Phil. Mag. 86 2073). Taking into account the symmetric properties of this square lattice and using a translation linear operator, we have constructed a \(r\)-space basis only with 85 state-vectors which describe all possible distributions for four electrons in the 4 \(\times\) 4 square lattice. The diagonalization of the 85 \(\times\) 85 matrix energy allows us to study the local properties of the above system as a function of the on-site and off-site interactions energies, where we have shown that the off-site interaction encourages the existence of the double occupancies at the first excited state and induces a supplementary conductivity of the system.

PACS numbers: 71.10.−W, 75.10.Jm, 72.15.Nj

1. Introduction
In the last few years, the extended Hubbard model (EHM) was introduced to explain some interesting phenomena including metal–insulator transitions [2–6], antiferromagnetism [7–10] and high-\(T_c\) superconductivity [11–13]. This EHM is a standard simple model of interacting itinerant electrons in a solid [14–19]. Although this model is too idealized to be regarded as a quantitatively reliable model of real solids, it contains physically essential features of interacting itinerant electron systems. Despite being one of the most studied models to describe strongly the correlated electrons system, many questions concerning the Hubbard model remain as open problems. In [20], we have applied the self-consistent random phase approximation (SCRPA) [21, 22] to solve the EHM in one-dimension (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 the supplementary conductivity, since the SCRPA energy gap vanishes when the closed chains of the EHM are governed by a strong repulsive on-site and an intermediate repulsive off-site interaction. But due to the restricted motion along one direction in space, the Hubbard model chain does not exhibit any ferromagnetic feature. Thus, the 1D Hubbard is a nice prototype to describe only the 1D classical conductors.

Stimulated by the discovery of high-\(T_c\) superconductivity in the cuprate plans, the 2D Hubbard model has attracted a great deal of attention in the last two decades [23, 24]. In spite of its simple description in square lattice, it is not easy to solve the 2D Hubbard model in the general case. The exact solution of the 2D Hubbard model is still not achieved, but a great variety of approximate treatments have been proposed [25, 26].

Very recently, Kovacs and Gulacsi [1] proposed an exact solution of the usual Hubbard model for 4 \(\times\) 4 sites cluster...
with low concentration, where each cluster presents four electrons. The dynamics of these electrons is described by the usual kinetic of electrons with hopping energy $t$ and the repulsive on-site interaction between the electrons in the same site with the interaction energy $U$.

In the present paper, we aim to apply this method to an EHM which takes into account the off-site interaction with an interaction energy $V$.

This paper is organized as follows. In section 2, we present the model and the calculation procedure which allows us to construct the Hamiltonian matrix of dimension 85 × 85. In section 3, we present our results for ground state and gap energies and discuss the effect of the off-site interaction on the dynamics of system. Finally, in section 4 we give our conclusions.

### 2. Model and formalism

The 2D EHM on a square lattice is given by:

$$H = - \sum_{\langle i,j \rangle} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_{\langle i,j \rangle,\sigma,\sigma'} n_{i,\sigma} n_{j,\sigma'},$$

where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) are the creation (annihilation) operators for a fermion of spin $\sigma$ at site $i$ ($j$) with periodic boundary conditions. $t$ is the hopping term from the site $i$ to the site $j$, where $(i, j)$ sums over the 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 the electrons with energy $V$.

The resolution of the model (1) in the case of the finite size system gives the exact solution of some physical quantities such as the ground state energy, the energy gap and the occupation numbers. We consider thus a 2D $L \times L = N = 16$ square lattice at one-eighth filling (four electrons per cluster), with periodic boundary conditions in both directions. For this considered system, three types of particle configuration may occur. Firstly, we can have two double occupancies at sites $i$ and $j$ ($i \neq j$). Secondly, 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 on different sites of this 4 × 4 square lattice. These three possible configurations provide, respectively, the three states:

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

$$|b\rangle = \left( c_{i,\sigma}^\dagger c_{i,\sigma}^\dagger \right) \left( c_{k,\sigma}^\dagger c_{k,\sigma}^\dagger \right) |0\rangle,$$

$$|c\rangle = \left( c_{i,\sigma}^\dagger c_{i,\sigma}^\dagger \right) \left( c_{k,\sigma}^\dagger c_{k,\sigma}^\dagger \right) |0\rangle,$$

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

The states $|a\rangle$, $|b\rangle$ and $|c\rangle$ generate $N_d = 16 \times 16 \times 15 \times 15 = 28\ 800$ 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 convenient to define a linear operator $T$ [1], which verifies the relation:

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

where $A$ and $B$ represent the particle configurations as mentioned in figure 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. Using this linear operator and taking into account the symmetric proprieties of the 4 × 4 cluster in $r$-space representation, we can regroup these $N_d$ states in 85 cluster states denoted by $|n\rangle$, where $n = 1, 2, \ldots, 85$, and are all orthogonal vectors. For example, $|1\rangle$ is the linear combination of all states $|a\rangle$ with $|R_i - R_j| = a$, where $R_i$ ($R_j$) is the lattice position of the site $i$ ($j$) and $a$ is the square lattice parameter. (2) is the linear combination of all states $|b\rangle$ with $|R_i - R_j| = |R_j - R_k| = a$ and $|R_i - R_k| = 2a$, whereas (3) is also the linear combination of all states $|b\rangle$ with $|R_i - R_j| = |R_j - R_k| = a$, but $|R_i - R_k| = \sqrt{2}a$ (for the definition of the other 82 vectors, see [1]).

The application of the Hamiltonian (1) on the basis vector $|1\rangle$ gives:

$$H|1\rangle = (2U + 4V) |1\rangle + t(|2\rangle - |3\rangle).$$

It is clear that the Hamiltonian would not be diagonal in our $r$-space basis, since the application of the kinetic term $H_0 = - \sum_{\langle i,j \rangle} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma}$ on a vector $|n\rangle$ gives, always, the new states $|n'\rangle$ after the creation and the annihilation of electrons in the different lattice sites. Thus, it is necessary to define the matrix energy $E_{85 \times 85}$ as:

$$E_{nm} = \langle n | H | m \rangle,$$

where $|n\rangle$ and $|m\rangle$ are two vectors of the $r$-space basis. In order to study the local properties of the 4 × 4 square lattice, it is appropriate to determine, numerically, the eigenvalues and the eigenvectors of the matrix energy $E_{85 \times 85}$. We consider the obtained first and second minima of the eigenvalues as, respectively, the ground state and the first excited energies.

### 3. Results and discussion

First, we disregard the off-site interaction, and we have plotted in figures 2 and 3 the ground state and the first excited state energies, respectively, as a function of the on-site interaction energy $U$. The corresponding curves of this case ($V = 0$) show that the ground state energy has smooth (less than linear) $U$ dependence, whereas the first excited state energy is $U$-independent and fixed at $−8t$ for any value of $U$. Thus, it is clear that the first excited state is an eigenvector of the kinetic energy ($−\sum_{\langle i,j \rangle,\sigma} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma}$), since this excited energy
state avoid totally the double occupancy. Whereas, the ground state is not an eigenstate of the kinetic energy or the on-site interacting part of $H$ only, but is an eigenvector for the sum of both. Thus, at the ground state, the dynamics of the electron system is governed by a competition between the habitual kinetic and the on-site interaction.

Then, we have taken into account the off-site interaction ($V \neq 0$) and we have plotted in the same previous figures (figures 2 and 3) the ground state and the first excited state energies, respectively, as a function of the on-site interaction $U$ for two values of $V/t$.

Figure 2 shows that the energy $E$ has a smooth $U$ dependence and a linear $V$ dependence. This behaviour is similar to the one obtained for the ground state energy of the chains EHM with the SCRPA [27], where we have also defined the matrix energy but in the basis of vectors impulsion-space ($k$-space) and not in $r$-space representation. The curves of figure 2 show also that $E$ decreases with $V$ for a fixed value of $U$. Thus, we can conclude that this off-site interaction imposes the electron system to avoid partially the double occupancy in this ground state.

Figure 3 shows that the first excited state energy becomes $U$-dependent for $V \neq 0$. Thus, the off-site interaction encourages the existence of the 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 $U$-dependent; since, we have the opportunity to have the double occupancies even for high values of $U$.

In order to analyse the on-site and off-site interaction effects on the repartition of our four electrons in the above system, we define the double occupancy coefficient in the first excited state $D^*$ as the probability to have a couple of electrons ($\uparrow \downarrow$) on the same site in this excited state,

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

where the sum over all $4 \times 4$ cluster sites and the mean values $\langle \ldots \rangle$ are taken in the corresponding eigenvector to $E^*$.

The double occupancy coefficient $D^*$ in the first excited state is shown in figure 4 as a 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 state. But after taking into account the off-site interaction, we have $D^* \neq 0$. For $V/t = 1$, we have $D^* \neq 0$ even for the strong values of $U/t$. But for $V/t = 0.5$, the coefficient $D^*$ vanishes for the strong 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 [1]. Where the authors have shown that 40% of the excited states of the $4 \times 4$ cluster are $U$-independent. But it is clear that the number of this $U$-independent excited states decreases if we take into account the off-site interaction, since this interaction encourages the formation of the double occupancies in the excited states.

Finally, in order to analyse the effect of the off-site interaction on the dynamics of electrons, we define the energy gap $\Delta \varepsilon$ as the difference between the first excited state energy $E^*$ and the ground state energy $E$

$$\Delta \varepsilon = E^* - E.$$

In figure 5, we plot the variation of this energy gap $\Delta \varepsilon$ as a function of the repulsive on-site interaction energy $U$ for different values of the off-site interaction energy $V$.

For a fixed value of $V/t$, the energy gap decreases with $U$. We deduce that the repulsive on-site interaction ($U > 0$) increases the conductivity of the system, since the repulsion between the two electrons of the same site...
encourages every electron to jump to the neighbouring site. Moreover, these curves show that the off-site interaction also increases the conductivity of this $4 \times 4$ cluster. For a weak off-site interaction ($V/t \leq 0.5$), the effect of $V$ is remarkable only for the weak on-site interaction, whereas it becomes practically non-existent for strong on-site interaction. But for an intermediate off-site interaction ($V/t = 1$), the effect remains remarkable even for the strong values of $U/t$. Thus, we can conclude that with a strong on-site and an intermediate off-site interaction, our $4 \times 4$ cluster has an important conductivity.

4. Conclusion

In this paper, an exact diagonalization in the $r$-space was proposed to solve the 2D EHM for a finite size system. In particular, we have considered a 2D $L \times L = N = 16$ square lattice at one-eighth filling with respect to the periodic boundary conditions in both directions. First, the numeric diagonalization of our Hamiltonian matrix allows us to determine some interesting local properties of our $4 \times 4$ square lattice: the ground state energy $E_{GS}$, the first excited state energy $E^*$, the gap energy $\Delta$ and the double occupation number per site $D^*$. Then, the analysis of the behaviours of these obtained local properties as a function of $U$ and $V$ allows us to study the distribution and the dynamics of the electrons system in two interesting states: ground and first excited states. Thus, we have found that our system always has the double occupancies in the ground state for any value of $U$ and $V$. In the first excited state, we have shown that the off-site interaction encourages the electron system to form the double occupancies, where the coefficient $D^*$ vanishes for $V = 0$. Whereas for an intermediate off-site interaction, we found that there is always the probability to have these double occupancies. But, this probability vanishes for strong on-site and weak off-site interactions, where the electrons system completely avoids the double occupancy. Thus, the behaviour of our system in this regime ($V \ll U$) is similar to the one found in [1]. Finally, the analysis of the off-site interaction effect on the energy gap shows that the repulsive off-site interaction induces supplementary conductivity of the system, where this effect of $V$ is more remarkable for an intermediate off-site interaction, since we have a reduction of the order of 20% in this regime.

References

[1] Kovacs E and Gulacsi Z 2006 Phil. Mag. 86 2073
[2] Mott N F 1990 Metal–Insulator Transitions 2nd edn (London: Taylor and Francis)
[3] Gebhard F 1997 The Mott Metal–Insulator Transition (Berlin: Springer)
[4] Imada M, Fujimori A and Tokura Y 1998 Rev. Mod. Phys. 70 1039
[5] Ono Y et al 2001 Eur. Phys. J. B 19 375
[6] Mancini F 2000 Europhys. Lett. 50 229
[7] Sanna S, Allodi G, Concas G, Hillier A D and De Renzi R 2004 Phys. Rev. Lett. 93 207001
[8] Niedermayer Ch, Bernhard C, Blasius T, Golnik A, Moodenbaugh A and Budiwick J 1998 Phys. Rev. Lett. 80 3843
[9] Yuan Q, Yuan F and Ting C S 2005 Phys. Rev. B 72 054504
[10] Korbel P et al 2003 Eur. Phys. J. B 32 315
[11] McElroy K, Lee D-H, Homan J E, Lang K M, Hudson E W, Eisaki H, Uchida S, Lee J and Davis J C 2004 Preprint cond-mat/0404005
[12] Martin I, Ortiz G, Balatsky A V and Bishop A R 2001 Europhys. Lett. 56 849
[13] Halboth C and Metzner W 2000 Phys. Rev. B 61 7364
[14] Lieb E H and Wu F Y 2003 Physica A 321 1
[15] Anderson P W 1987 Science 235 1196
[16] Zhang F C and Rice T M 1988 Phys. Rev. B 37 3759
[17] Takahashi A 1996 Phys. Rev. B 54 7965
[18] Zimanyi G T, Kivelson S A and Luther A 1988 Phys. Rev. Lett. 60 2089
[19] Hirsch J E 1985 Phys. Rev. B 31 6022
[20] Harir S, Bennai M and Boughaleb Y 2007 Appl. Math. Sci. 1 1651
[21] Jemai M, Schuck P, Dukelsky J and Bonnaud B 2005 Phys. Rev. B 71 85115
[22] Davidsne D, Oertel M and Hansen H 2005 Euro. Phys. J. A 16 35
[23] Beenen J and Edwards D M 1995 Phys. Rev. B 52 13636
[24] Stefanakis N 2002 Phys. Rev. B 66 24514
[25] Kotliar G, Savrasov S Y, Parson G and Birol G 2001 Phys. Rev. Lett. 87 186401
[26] Hettler M H, Tahvildar-Zadeh A N, Jarrell M, Pruschke T and Krishnamurthy H R 1998 Phys. Rev. B 58 7475
[27] Harir S, Bennai M and Boughaleb Y 2007 Phys. Scr. 76 370

Figure 5. Energy gap as a function of $U/t$ for different values of $V/t$. The Mott Metal–Insulator Transition

Phys. Scr. 78 (2008) 025701 S Harir et al