Two-particle correlations in the one-dimensional Hubbard model: a ground-state analytical solution

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Recibido el 29 de abril de 2002; aceptado el 27 de noviembre de 2002

A solution to the extended Hubbard Hamiltonian for the case of two-particles in an infinite one-dimensional lattice is presented, using a real-space mapping method and the Green function technique. This Hamiltonian considers the on-site (U) and the nearest-neighbor (V) interactions. The method is based on mapping the correlated many-body problem onto an equivalent site-impurity tight-binding one in a higher dimensional space. In this new space we obtained the analytical solution for the ground state binding energy. Results are in agreement with the numerical solution obtained previously [1], and with those obtained in the reciprocal space [2].

Keywords: Hubbard model, fermions in reduced dimensions,strongly correlated electron systems.

Se resolvió el hamiltoniano de Hubbard extendido para dos partículas en una red unidimensional, usando el método del mapeo en el espacio real y la técnica de la función de Green. Este hamiltoniano considera las interacciones intra-atómicas U e inter-atómicas V. El método mapea el problema de muchos cuerpos correlación de un problema equivalente de amarre fuerte en un espacio de mayor dimensión. Haciendo un análisis del problema en este espacio se obtuvo la solución analítica para la energía de enlace del estado base. Los resultados están en completo acuerdo con la soluciones obtenidas tanto numéricamente [1] como en el espacio recíproco [2].

Descriptores: Modelo de Hubbard, fermiones en dimensiones reducidas, sistemas electrónicos fuertemente correlacionados.

PACS: 71.10.fd; 71.10Pm; 71.10Li; 71.27.+a

1. Introduction

The one-dimensional Hubbard model is a good prototype for an exactly solvable model of correlated electrons in narrow-band systems [3, 4], where at half-filling the ground state is found to be antiferromagnetic and insulating for a repulsive potential. The other exact solution for the Hubbard Hamiltonian is the case an infinite dimensional lattice [5]. The exact solutions, particularly those obtained using the Bethe ansatz, have brought a very important progress in the understanding of strongly correlated systems. However, the conditions for integrability using the Bethe ansatz are very restrictive, and only a very limited class of realistic models can be solved with this technique [6]. For instance, it is difficult to include additional interactions in the Hubbard model so that the resulting Hamiltonian is still integrable.

The Hubbard model [7] is the simplest one used to describe correlations in narrow-band systems and has been studied extensively. However, even when the Hubbard model is conceptually very simple, this model is very difficult to solve in general, with few tractable limits. When the bonding dominates, we have the so called weak coupling limit, which leads to a non-interacting electron gas and is therefore fairly well understood. But even in weak coupling there are some surprises. For a bipartite lattice at half-filling, an infinitesimal short-range Coulomb repulsion drives the system through a metal-insulator transition [8], a result which is not contained in the free electron description. Strong-coupling limit is hardly understood at all. At half-filling, the model maps onto an insulating spin-half Heisenberg model [8]. If the charge density is away from half-filling, the behavior remains a mystery.

The Hubbard model has been applied successfully to describe some new electronic phenomena where electronic correlations are very important, such as the metal-insulator transition [9], itinerant magnetism [10], charge density and spin density waves [11] and local pair formation, which may play a significant role in the explanation of the high-Tc superconductors [12, 13] and the superconductivity in heavy fermions systems [14].

In this paper we wish to address the low-density limit, two-electrons in a one-dimensional empty lattice. An analytical solution of this problem for the extended Hubbard Hamiltonian, using a real-space mapping method and the Green function technique, is presented.

The diluted limit of the Hubbard model has been previously studied by analytical and numerical methods [1, 12, 15], including different kinds of disorder in the model [16–18] and also including the bond-charge interaction [2, 19–21].

In Sec. II we give a brief description of the Hamiltonian and the mapping method, we also present in this section the analytical solution for the two particles in an empty lattice. Finally, in Sec. III we summarize our results.

2. Two correlated particles in an empty lattice

The extended Hubbard Hamiltonian may be written in real space as

$$H = \sum_{<i,j>,\sigma} t_{i,j} c^{+}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{<i,j>} n_i n_j, \quad (1)$$

where $< i, j >$ denotes nearest-neighbor sites, $c^{+}_{i,\sigma}$ ($c_{i,\sigma}$) is the creation (annihilation) operator with spin $\sigma =\downarrow \; or \; \uparrow$ at site i, and $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ where $n_{i,\sigma} = c^{+}_{i,\sigma} c_{i,\sigma}$. The transfer integral $t_{i,j}$ is written as $t_{i,j} = t$, which means that all hopping processes have the same probability. It is worth mentioning that in principle, the parameters U and V are positive because they are direct Coulomb integrals. However, U and V could be negative if attractive indirect interactions, through phonons or other bosonic excitations, are included and are stronger than direct Coulombic repulsions.

One of the most common techniques to study the Hubbard model is the mean-field approximation (MFA), used to analyze different problems [12], because the many-body problem can be reduced to a one-body problem in an effective medium. However, it is well known that the MFA is not sufficient to describe electronic correlations, since fluctuations are not included within this approximation. Another useful technique to deal with the Hubbard model is the slave-boson formalism [11, 22]. However, in this formalism the Hilbert space of fermion states is replaced by an enlarged Hilbert space of fermion and boson states where approximations are still necessary. On the other hand, the quantum Monte Carlo techniques [23] provide a natural framework for numerical calculations in strongly interacting electron models, but these techniques have been used only for small clusters. The renormalization group method [24] has been used for very large systems. This method consists in constructing iteratively a variational ground state by dividing the system into many cells. Since for each step only the lowest-lying energy states in each cell are taken into account, sometimes the results are far away from the exact solution. Finally, the exact diagonalization method is the most desirable one. However, this method is applicable only to small systems, since the dimension of the Hamiltonian matrix increases very rapidly with the number of sites and the number of particles [25]. In the following subsection we will describe briefly the mapping method, which allows us to diagonalize exactly the Hubbard Hamiltonian for an infinite lattice and which is very useful in finding analytical solutions for two interacting electrons in a one-dimensional empty lattice.

2.1. Mapping method

The mapping method is explained in detail in Ref. [1, 26] for different lattice topologies. In order to present a brief explanation of the mapping method, let us consider the case of two electrons with opposite spins in an N-site chain ($N = 2, 3, 4, \cdots$). For $N = 4$, the state configuration is

$$\begin{aligned}
|1\rangle &= |\pm 000\rangle, \; |2\rangle = |+-00\rangle, \; |3\rangle = |+0-0\rangle, \; |4\rangle = |+00-\rangle, \\
|5\rangle &= |0+0-\rangle, \; |6\rangle = |0+-0\rangle, \; |7\rangle = |0\pm 00\rangle, \; |8\rangle = |-+00\rangle, \\
|9\rangle &= |-0+0\rangle, \; |10\rangle = |0-+0\rangle, \; |11\rangle = |00\pm 0\rangle, \; |12\rangle = |00+-\rangle, \\
|13\rangle &= |000\pm\rangle, \; |14\rangle = |00-+\rangle, \; |15\rangle = |0-0+\rangle, \; |16\rangle = |-00+\rangle, \qquad (2)
\end{aligned}$$

where $+$ and $-$ represent an electron with spin up and spin down, respectively, and 0 represents an empty site. Furthermore, $\pm$ indicates a doubly occupied site. In general, the number of two-electron states is given by N^2.

The states of Eq. (2) have a geometric representation in a square lattice (see Fig. 1), which can be described by a one-body tight-binding effective Hamiltonian with $(3N - 2)$ ordered site-impurities. Among these impurities, N are localized on sites along the principal diagonal of the square lattice with a self-energy U and the others, $2(N - 1)$, are localized on the two next-diagonals with a self-energy V. The new one-body Hamiltonian is written as follows [27]:

$$H = \sum_{i} \epsilon_i b^{+}_i b_i + \sum_{i,j} t_{i,j} b^{+}_i b_j, \qquad (3)$$

where the operator b^{+}_i create the many-body states, $|i\rangle$, given by Eq. (2) and ϵ_i represents the self-energy of the two-electron states (see Fig. 1). Sites in Fig. 1 represent the two-body states and not the usual Wannier wave function.

A simple way to obtain the solution is to take advantage of the translational symmetry of the site-impurities and projecting the two-dimensional lattice of states onto a linear chain of effective states as it is shown in Fig. 1, where $\beta = 2tcos(Ka/\sqrt{2})$, the lattice parameter $a = 1$, and K is the wave vector in the projection direction.

In general, this method maps the original many-body problem onto a one-body one with some ordered site-impurities in an nd-dimensional lattice, n being the number of electrons and d the dimensionality of the original system. In this hyper-space lattice, the on-site (U) and the nearest-neighbor (V) interactions from the original Hubbard Hamiltonian become the self-energies of the site-impurities. So, in order to find a solution for the n-interacting particles we should solve the new effective Hamiltonian given by Eq. (3).

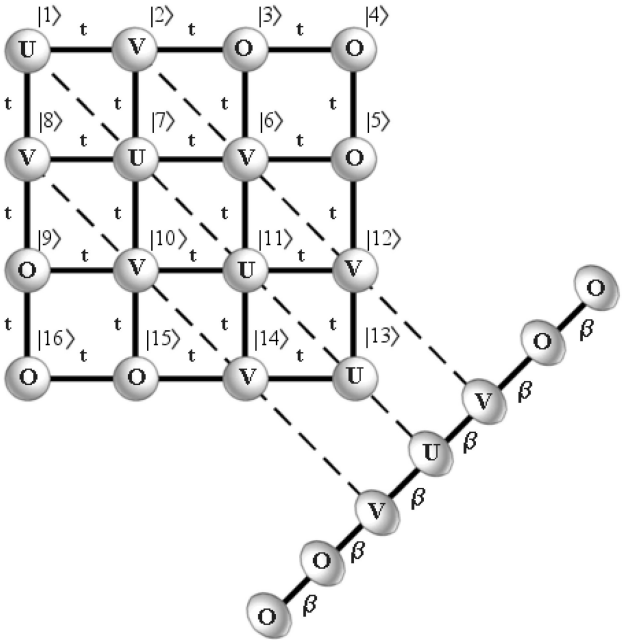

FIGURE 1. Geometric representation of the two-electron states for a chain of four sites. The states are represented by circles with site-energy indicated inside, and the numeration of states is according to Eq. (2). The direction of the projection procedure is shown by dashed lines. The final chain is formed by effective states, represented by ellipses, and the effective hopping parameters β.

2.2. Analytical solution

As already explained, to find the ground-state analytical solution of the two-interacting electrons in a one-dimensional lattice, we must find the solution of the impurity chain represented by ellipses in Fig. 1, but using now the new effective tight-binding Hamiltonian. The Hamiltonian for the sites impurities can be written as

$$H = H_0 + \sum_{i=1}^{n} H_i, \tag{4}$$

where

$$H_0 = \epsilon_0 \sum_m |m\rangle \langle m| + \beta \sum_{<n,m>} |n\rangle \langle m| \tag{5}$$

and

$$H_i = |i\rangle \, \epsilon_i \, \langle i| \, . \tag{6}$$

H_0 gives the Hamiltonian for a periodic lattice (without impurities) in the Dirac representation and H_i represents the perturbation associated to the site impurities.

For the n-site impurity problem the Green operator is [28]

$$G_n = G_{n-1} + \frac{G_{n-1} |n\rangle \, \epsilon_n \, \langle n| G_{n-1}}{1 - \epsilon_n \langle n| G_{n-1} |n\rangle}, \tag{7}$$

where $\langle n| G_{n-1} |n\rangle$ represents all matrix elements of the Green operator at the site of the impurity n with energy ϵ_n. Equation (7) is valid for systems having at least one impurity.

The poles of Eq. (7) give the eigenvalues of the Hamiltonian [28]. So, in order to find the energy (E) associated to the impurities we must solve equation

$$\langle n| G_{n-1} |n\rangle = \frac{1}{\epsilon_n}. \tag{8}$$

The one-dimensional impurity chain (see Fig. 1) has three impurities, one at the central site with energy $\epsilon_1 = U$ and two at the nearest-neighbors with energies $\epsilon_2 = V$ (at the position $l = 1$) and $\epsilon_3 = V$ (at the position $l = -1$). Let us analyze all three possible cases for the ground state $K = 0$ ($\beta = 2t$) and find the corresponding binding energies.

(a) The first case corresponds to the central impurity with energy $\epsilon_1 = U$ and the other two impurities $\epsilon_2 = \epsilon_3 = 0$. The Green function for the perfect linear chain is given by [28]

$$\langle p| G_0 |q\rangle = G_0(p, q; E) = \frac{1}{\sqrt{E^2 - B^2}} \rho^{|p-q|}, \tag{9}$$

where

$$\rho = \frac{E}{B} - \sqrt{\left(\frac{E}{B}\right)^2 - 1}, \tag{10}$$

and $B = |2\beta|$ is the semi-band width for the case of two particles within the independent particle approximation. However, using Eq. (8) for the central impurity and evaluating Eq. (9) at the central site a relationship for U is obtained:

$$\langle 0| G_0 |0\rangle = \frac{1}{\sqrt{E^2 - B^2}} = \frac{1}{U}; \quad \text{for } E^2 > B^2. \tag{11}$$

Hence, the binding energy $\Delta \equiv |E| - B$ is given by

$$\Delta = B \left(\sqrt{1 + \left(\frac{U}{B}\right)^2} - 1 \right); \quad \text{for } U < 0. \tag{12}$$

This is the binding energy for a two-interacting electrons in a one-dimensional lattice with an attractive on-site interaction U and a nearest-neighbor interaction $V = 0$ [1].

(b) The second case corresponds to the system with a central impurity with energy $\epsilon_1 = U$ and a second impurity at the position $l = 1$ with energy $\epsilon_2 = V$ and the third impurity $\epsilon_3 = 0$. The Green function of a linear chain having a central impurity with energy U is given by

$$\langle p| G_1 |q\rangle = G_1(p, q; E) = \frac{\rho^{|p-q|}}{\sqrt{E^2 - B^2}} + \frac{U \rho^{|q|} \rho^{|p|}}{\sqrt{E^2 - B^2} \left(\sqrt{E^2 - B^2} - U \right)}. \tag{13}$$

Using Eq. (8) for the impurity with energy $\epsilon_2 = V$ and evaluating Eq. (13) at the position $l = 1$, it means for $p = q = 1$, we obtain

$$\langle 1| G_1 |1\rangle = \frac{B^2 + 2U\sqrt{E^2 - B^2} - 2EU}{B^2 \left(\sqrt{E^2 - B^2} - U \right)} = \frac{1}{V}; \quad \text{for } E^2 > B^2. \tag{14}$$

So, the binding energy for our system is

$$\Delta = B\left(\frac{2UV\left(U+V\right)-\left(2UV-B^2\right)\sqrt{\left(U-V\right)^2+B^2}}{B\left(B^2-4UV\right)}-1\right). \tag{15}$$

Equation (15) is valid for $U, V < 0$ and the cases $U > 0$, $V < 0$ or $U < 0$, $V > 0$ are limited to $UV + B(U + V)/2 < 0$.

(c) The most general case corresponds to a system with three impurities: one impurity at the central site with energy $\epsilon_1 = U$, a second impurity with energy $\epsilon_2 = V$ at the position $l = 1$ and a third impurity with energy $\epsilon_3 = V$ at the position $l = -1$. The associated Green function of a linear chain with two impurities, one at the central site with energy U and the second with energy $\epsilon_2 = V$ at the position $l = 1$ is given by

$$\begin{aligned}\langle p|\,G_2\,|q\rangle &= G_2(p,q;E)=\frac{\rho^{|p-q|}}{\sqrt{E^2-B^2}}+\frac{U\rho^{|q|}\rho^{|p|}}{\sqrt{E^2-B^2}\left(\sqrt{E^2-B^2}-U\right)}\\ &+\frac{V\left(\dfrac{\rho^{|1-q|}}{\sqrt{E^2-B^2}}+\dfrac{U\rho^{|q|}\rho}{\sqrt{E^2-B^2}\left(\sqrt{E^2-B^2}-U\right)}\right)\left(\dfrac{\rho^{|p-1|}}{\sqrt{E^2-B^2}}+\dfrac{U\rho\rho^{|p|}}{\sqrt{E^2-B^2}\left(\sqrt{E^2-B^2}-U\right)}\right)}{1-V\left(\dfrac{1}{\sqrt{E^2-B^2}}+\dfrac{U\rho^2}{\sqrt{E^2-B^2}\left(\sqrt{E^2-B^2}-U\right)}\right)}\end{aligned} \tag{16}$$

Finding the poles of Eq. (8) for the impurity with energy $\epsilon_3 = V$ and evaluating Eq. (16) at the position $l = -1$, it means for $p = q = -1$, we obtain

$$\langle -1|\,G_2\,|-1\rangle = \frac{B^4+2UB^2\left(\sqrt{E^2-B^2}-E\right)-4V\left(E-U\right)\left(\sqrt{E^2-B^2}-E\right)^2}{B^2\left(B^2\left(\sqrt{E^2-B^2}-U-V\right)+2UV\left(E-\sqrt{E^2-B^2}\right)\right)}=\frac{1}{V}, \tag{17}$$

which is valid for $E^2 > B^2$.

The solution of Eq. (17), give us a binding energy $\Delta = -B(1 - |x|)$, with x given by

$$x=\frac{1}{6v}\left(C_2+\frac{-4v^3u+10v^2+4v^2u^2+v^4-8vu+1}{C_2}+v^2+4vu-1\right), \quad \text{for} \quad v\lessapprox 0; \tag{18}$$

and

$$\begin{aligned}x &= -\frac{1}{12v}\left(C_2+\frac{-4v^3u+10v^2+4v^2u^2+v^4-8vu+1}{C_2}+2-8vu-2v^2\right)\\ &-\frac{1}{12v}i\sqrt{3}\left(C_2-\frac{-4v^3u+10v^2+4v^2u^2+v^4-8vu+1}{C_2}\right), \quad \text{for} \quad v>0;\end{aligned} \tag{19}$$

where

$$x=\frac{E}{B},\ u=\frac{U}{B} \quad \text{and} \quad v=\frac{2V}{B}. \tag{20}$$

The coefficients C_1 and C_2 are given by

$$C_1 = 6v\sqrt{-3u^2-42v^2u^2+42vu+36vu^3-3v^4u^2+12v^3u^3-12v^2u^4+3v^4+33v^2-6v^3u-3}, \tag{21}$$

$$C_2 = \left(-6v^5u+12v^4u^2-42v^3u+15v^4+39v^2-8v^3u^3+24v^2u^2+v^6+12vu-1+C_1\right)^{1/3}. \tag{22}$$

In our limit of low concentration, the pairing condition is

$$\sqrt{(1+u)(1+v)}-1<0. \tag{23}$$

This is the analytical solution for the binding energy of two-interacting electrons in a one-dimensional infinite lattice with an on-site interaction U and a nearest-neighbor interaction V. The analytical expression is in complete agreement with the numerical solutions obtained previously in real space [1].

3. Conclusions

In this paper we studied the dilute limit of the Hubbard model, using a real-space mapping method and the Green function technique. In the case of two-interacting particles using an extended Hubbard Hamiltonian in an infinite one-dimensional empty lattice we have carried out the analytical solution for the ground state binding energy. The results are in agreement with the numerical solution obtained previously [1]. It is worth mentioning that one of the advantages of our study is that we have worked in real space, so we could be able to analyze electronic correlation in non-periodic lattices or disorder systems.

Acknowledgement

This work was partially supported by grants from CONACyT México 33630-E, from UNAM through IN106600 and by DGEP-UNAM.

1. O. Navarro and C. Wang, *Rev. Mex. Fís.*, **38** (1992) 553; O. Navarro, C. Wang, *Solid State Commun*. **83** (1992) 473; L.A. Perez, O. Navarro and C. Wang, *Phys. Rev. B* **53** (1996) 15389.
2. F. Marsiglio and J.E. Hirsch, *Physica C* **171** (1990) 554.
3. E.H. Lieb and F.Y. Wu, *Phys. Rev Lett.* **20** (1968) 1445.
4. See reprints in *Exactly Solvable Models of Strongly Correlated Electrons*, edited by V.E. Korepin and F.H.L. Ebler (World Scientific, Singapore, 1994).
5. W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **62** (1989) 324.
6. A.M. Tsvelick and P.B. Wiegmann, *Adv. Phys.* **32** (1983) 453; A.A. Aligia, C.A. Balseiro and C.R. Proetto, *Phys. Rev. B* **33** (1986) 6476.
7. J. Hubbard, *Proc. R. Soc. London Ser. A* **276** (1963) 238; M.C. Gutzwiller, *Phy. Rev. Lett.* **10** (1963) 159.
8. E.H. Lieb, *Phys. Rev. Lett.* **62** (1989) 1201.
9. N.F. Mott, *Metal-Insulator Transition* (Taylor & Francis Inc., London, Second Edition 1990).
10. P.W. Anderson, *Solid State Physics* **14** (1963) 99.
11. S. Caprara, M. Avignon and O. Navarro, *Phys. Rev. B* **61** (2000) 15667.
12. R. Micnas, J. Ranninger and S. Robaszkiewicz, *Rev. Mod. Phys.* **62** (1990) 113.
13. A.S. Blaer, H.C. Ren and O. Tchernyshyov, *Phys. Rev. B* **55** (1997) 6035.
14. S. Fujimoto, *Phys. Rev. B* **64** (2001) 85102.
15. M.W. Long and R. Fehrenbacher, *J. Phys.: Condens. Matter* **2** (1990) 10343.
16. A.S. Alexandrov, S.V. Traven and P.E. Kornilovitch, *J. Phys.: Condens. Matter* **4** (1992) L89.
17. D.L. Shepelyansky, *Phys. Rev. Lett.* **73** (1994) 2607.
18. R. Oviedo-Roa, C. Wang and O. Navarro, *J. Low Temp. Phys.* **105** (1996) 651.
19. H.Q. Lin and J.E. Hirsch, *Phys. Rev. B* **52** (1995) 16155.
20. M. Airoldi and A. Parola, *Phys. Rev. B* **51** (1995) 16327.
21. J.E. Espinosa, O. Navarro and M. Avignon, *Eur. Phys. J. B* **18** (2000) 9.
22. G. Kotliar and A.E. Ruckenstein, *Phys. Rev. Lett.* **57** (1986) 1362.
23. S. R. White, D. J. Scalapino, R. L. Sugar, and N. E. Bickers, *Phys. Rev. Lett.* **63** (1989) 1523.
24. J. E. Hirsch, *Phys. Rev. B* **22** (1980) 5259.
25. F. López-Urías and G.M. Pastor, *Phys. Rev. B* **59** (1999) 5223.
26. O. Navarro, *Introducción a la Superconductividad*, Aula Magna UAS, Vol. **11** (1997).
27. S.A. Trugman, in *Applications of Statistical and Field Theory Method to Condensed Matter*, Ed. by D. Baeriswyl, *et al.*, (Plenum Press, New York, 1990) p.252.
28. E. N. Economou, *Green's Functions in Quantum Physics* (Springer Series in Solid State Sciences, Vol.7, Second Edition, 1993).