ANALYTICAL SOLUTION FOR TWO CORRELATED PARTICLES IN A HUBBARD MODEL*

E. Vallejo, O. Navarro

Instituto de Investigaciones en Materiales, UNAM
Apartado Postal 70-360, 04510 Méxii D.F., Méxii, Mexico

and J.E. Espinosa

Facultad de Ciencias Físico-Matemáticas (Posgrado en Optoelectrónica) BUAP
Puebla Pue., México, Mexico

(Received July 10, 2002)

The extended Hubbard Hamiltonian is solved analytically for the case of two-particles in an infinite one-dimensional lattice, using a real-space mapping method and the Green function technique. The results obtained are in agreement with the numerical solution previously reported by O. Navarro and C. Wang *Solid State Commun.* **83**, 473 (1992).

PACS numbers: 71.10.Fd, 71.10.Li, 71.27.+a

1. Introduction

The Hubbard model [2] is the simplest one used to describe correlations in narrow-band systems and have been studied extensively. However, even when the Hubbard model is conceptually very simple, this model is very difficult to solve in general, but there are 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. Strong-coupling limit, is hardly understood at all. In this paper we wish to address the low-density limit [3,4], two-electrons in a one-dimensional empty lattice. We found the analytical solution of this problem for the extended Hubbard Hamiltonian, using a real-space mapping method and the Green function technique. In Section 2. we present the analytical solution for the two particles in an empty lattice, Section 3. summarize our results.

* Presented at the International Conference on Strongly Correlated Electron Systems, (SCES 02), Cracow, Poland, July 10–13, 2002.

2. Two correlated particle in an empty lattice

The extended Hubbard Hamiltonian may be written in real space as

$$H = \sum_{\langle i,j\rangle,\sigma} t_{i,j} c^{+}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{\langle i,j\rangle} n_i n_j \,, \tag{1}$$

where $\langle i,j\rangle$ 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 $t_{i,j}$ will be written as $t_{i,j} = t$, which means that all the hopping process 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 interaction through phonons or other bosonic excitations are included and are stronger than the direct Coulomb repulsion.

We analyzed the Hubbard model by using the mapping method previously reported [1], which allows us to diagonalize exactly the Hubbard Hamiltonian for an infinite lattice and which will be very useful to find the analytical solution of two interacting electrons in a one-dimensional empty lattice.

In general, this method will map 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 equation

$$H = \sum_{i} \varepsilon_i b^{+}_i b_i + \sum_{i,j} t_{i,j} b^{+}_i b_j \,, \tag{2}$$

where the operator b^{+}_i create the many-body states, $|i\rangle$, and ε_i represents the self-energy of the two-electron states [5]. Sites represent the two-body states and not the usual Wannier wave function.

3. Analytical solution

To find the ground-state analytical solution of the two-interacting electrons in a one-dimensional lattice, we should find the solution of the impurity chain [5], using the new effective tight-binding Hamiltonian.

The one-dimensional impurity chain has three impurities, one at the central site with energy $\varepsilon_1 = U$ and two at the nearest-neighbors with energies $\varepsilon_2 = V$ (at the position $l = 1$) and $\varepsilon_3 = V$ (at the position $l = -1$). Let

us analyze each of these cases for the ground state $K = 0$ ($\beta = 2t$) and find the binding energy.

(a) The first case corresponds to the central impurity with energy $\varepsilon_1 = U$ and the other two impurities $\varepsilon_2 = \varepsilon_3 = 0$. The binding energy $\Delta \equiv -(B+E)$ is given by

$$\Delta = B\left(\sqrt{1+\left(\frac{U}{B}\right)^2}-1\right). \tag{3}$$

for $U < 0$, $B = |2\beta|$ is the semi-band width for the case of two particles within the independent particle approximation 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 $\varepsilon_1 = U$ and a second impurity at the position $l = 1$ with energy $\varepsilon_2 = V$ and the third impurity $\varepsilon_3 = 0$, we obtain the binding energy for our system

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

Eq. (4) 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 general case, it means, a system with three impurities: one impurity at the central site with energy $\varepsilon_1 = U$, a second impurity with energy $\varepsilon_2 = V$ at the position $l = 1$ and a third impurity with energy $\varepsilon_3 = V$ at the position $l = -1$, we obtain the binding energy $\Delta = -B(1-x)$.

$$x = \frac{1}{6v}\left(C_2 + \frac{-4v^3u+10v^2+4v^2u^2+v^4-8vu+1}{C_2}+v^2+4vu-1\right) \tag{5}$$

for $v \leq 0$, and

$$\begin{aligned} x = & -\frac{1}{12v}\left(C_2+\frac{-4v^3u+10v^2+4v^2u^2+v^4-8vu+1}{C_2}+2-8vu-2v^2\right) \\ & -\frac{1}{12v}i\sqrt{3}\left(C_2-\frac{-4v^3u+10v^2+4v^2u^2+v^4-8vu+1}{C_2}\right) \end{aligned} \tag{6}$$

for $v > 0$, where

$$x = \frac{E}{B}, \qquad u = \frac{U}{B}, \qquad v = \frac{2V}{B}, \tag{7}$$

which is valid for $E^2 > B^2$. The coefficients C_1 and C_2 are given by

$$C_1 = 6v\left(-3u^2 - 42v^2u^2 + 42vu + 36vu^3 - 3v^4u^2 + 12v^3u^3 - 12v^2u^4 + 3v^4 + 33v^2 - 6v^3u - 3\right)^{1/2}, \quad (8)$$

$$C_2 = \left(-6v^5u + 12v^4u^2 - 42v^3u + 15v^4 + 39v^2 - 8v^3u^3 + 24v^2u^2 + v^6 + 12vu - 1 + C_1\right)^{1/3}. \quad (9)$$

The condition for pairing in our limit of low concentration is

$$\sqrt{(1+u)(1+v)} - 1 < 0\,. \quad (10)$$

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].

4. Conclusions

In this paper we studied the diluted 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.

REFERENCES

[1] O. Navarro, C. Wang, *Solid State Commun.* **83**, 473 (1992); O. Navarro, C. Wang, *Rev. Mex. Fís.* **38**, 553 (1992).

[2] J. Hubbard, *Proc. R. Soc.* **A276**, 238 (1963).

[3] F. Marsiglio, J.E. Hirsch, *Physica C* **171**, 554 (1990).

[4] J.E. Espinosa, O. Navarro, M. Avignon, *Eur. Phys. J.* **B18**, 9 (2000).

[5] E. Vallejo, O. Navarro, J.E. Espinosa, submitted to *Rev. Mex. Fís.*