

# Hubbard model in one dimension with a general bond-charge interaction: Analytical ground-state solution for the pairing of two particles

E. Vallejo and O. Navarro

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

(Received 8 August 2002; revised manuscript received 18 March 2003; published 28 May 2003)

In this work we solve a general Hubbard Hamiltonian for two interacting particles in a periodic and nonperiodic infinite one-dimensional lattice, using a real-space mapping method, the renormalized perturbation expansion (RPE), and the Green-function technique. This Hamiltonian considers a general bond-charge interaction, the on-site interaction, and the general intersite interaction. The real-space method is based on mapping the correlated many-body problem onto an equivalent site- and bond-impurity tight-binding problem in a higher-dimensional space. Analyzing the periodic and the quasiperiodic lattices in this new space, we obtained the analytical solution for the binding condition at the ground state. Our general results for the periodic chain reproduce completely the limit cases of the numerical solution obtained previously and those obtained in reciprocal space

DOI: 10.1103/PhysRevB.67.193105

PACS number(s): 71.10.Fd, 71.10.Li, 71.27.+a

## I. INTRODUCTION

The one-dimensional simple Hubbard model is the prototype of an exactly solvable model for correlated electrons in narrow-band systems,<sup>1,2</sup> 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 of an infinite-dimensional space.<sup>3</sup> The exact solutions, particularly those obtained using the Bethe ansatz, have brought very important progress to 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.<sup>4</sup> For instance, it is difficult to include additional interactions in the Hubbard model so that the resulting Hamiltonian is still integrable.

The Hubbard model<sup>5</sup> is the simplest 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 bonding dominates, we have the so-called weak-coupling limit, which leads to a noninteracting electron gas and is therefore fairly well understood. But even with 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,<sup>6</sup> a result that 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.<sup>6</sup> If the charge density is away from half-filling, the behavior remains a mystery. This model has been applied successfully to describe some new electronic phenomena where electronic correlations are very important, such as the metal-insulator transition,<sup>7</sup> itinerant magnetism,<sup>8</sup> charge-density and spin-density waves,<sup>9</sup> and local pair formation, which may play a significant role in the explanation of the high- $T_c$  superconductors<sup>10,11</sup> and superconductivity in heavy-fermion systems.<sup>12</sup>

The Hubbard Hamiltonian has been widely studied by us-

ing different approximations. One of the most common techniques is the mean-field approximation (MFA), which has been used to analyze different problems,<sup>10</sup> since with this technique 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, because the fluctuations are not included within this approximation. Another useful technique to deal with the Hubbard Hamiltonian is the slave-boson formalism.<sup>9,13</sup> However, since in this formalism the Hilbert space of fermion states is replaced by an enlarged Hilbert space of fermion and boson states, approximations are still necessary. On the other hand, quantum Monte Carlo techniques<sup>14</sup> 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<sup>15</sup> has been used for very large systems. This method consists of 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.<sup>16</sup>

The diluted limit of the Hubbard model has been previously studied by analytical and numerical methods,<sup>10,17,18</sup> including different kinds of disorder<sup>19-21</sup> and also the bond-charge interaction.<sup>22-25</sup> However, a solution for the general Hubbard Hamiltonian has not yet been given, even for the low-density limit.

In this Brief Report we wish to address the low-density limit, two particles in one-dimensional (1D) periodic and quasiperiodic empty lattices. An analytical solution with a general Hubbard Hamiltonian, using a real-space mapping method, the renormalized perturbation expansion (RPE), and the Green-function technique, is presented.

In Sec. II we give a brief description of the Hamiltonian together with the generalization of the mapping method,

which allows us to diagonalize exactly the general Hubbard Hamiltonian, and in Sec. III we present results and a discussion of the analytical solution for two interacting particles in 1D periodic and quasiperiodic empty lattices. Finally, in Sec. IV we summarize our results.

## II. THE MODEL AND THE MAPPING METHOD

The Hubbard model is the simplest model that is able to describe electronic correlation in narrow-band systems and was obtained by Hubbard<sup>5</sup> from the general Hamiltonian

$$H = \sum_{\langle i,j \rangle, \sigma} t_{i,j} c_{i,\sigma}^{\dagger} c_{j,\sigma} + \frac{1}{2} \sum_{i,j,k,l,\sigma,\sigma'} \langle ij|v|kl \rangle c_{i,\sigma}^{\dagger} c_{j,\sigma'}^{\dagger} c_{l,\sigma'} c_{k,\sigma}, \quad (1)$$

by making some approximations in the interaction term. This Hamiltonian has been called the general Hubbard Hamiltonian and will be considered here to study the problem of two correlated particles. In Eq. (1),  $c_{i,\sigma}^{\dagger}$  ( $c_{i,\sigma}$ ) is the creation (annihilation) operator with spin  $\sigma = \uparrow$  or  $\downarrow$  at site  $i$ ,  $\langle i,j \rangle$  denote nearest-neighbor sites, and the transfer integral  $t_{i,j}$  is written as  $t_{i,j} = t_{j,i} = t$  for a periodic lattice. The parameter  $\langle ij|v|kl \rangle$  is the matrix element of the Coulomb interaction with respect to the Wannier functions at the sites,  $i, j, k, l$ . It is worth mentioning that in principle, the general two-particle interaction parameter  $\langle ij|v|kl \rangle$  is positive because it is a direct Coulomb integral, but it could be negative if an attractive indirect interaction through phonons or other bosonic excitations is included and is stronger than the direct Coulomb repulsion.

In this work, we will consider the matrix elements of the interaction as

$$\langle ij|v|kl \rangle \equiv \begin{cases} E_{|i-j|} & \text{for } k=i \text{ and } l=j \\ \Delta t_m & \text{for } j=l, \langle i,k \rangle \text{ and } \langle i,l \rangle_m \text{ or } \langle l,k \rangle_m \end{cases}, \quad (2)$$

together with  $\sigma' = -\sigma$ . Taking into account these interactions one obtains the following general Hubbard Hamiltonian:

$$H = t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^{\dagger} c_{j,\sigma} + \frac{1}{2} \sum_{i,j} E_{|i-j|} n_i n_j + \frac{\Delta t_m}{2} \sum'_{\langle i,k \rangle, l, \sigma} c_{i,\sigma}^{\dagger} c_{k,\sigma} n_{l,-\sigma}, \quad (3)$$

where  $n_i = n_{i,\uparrow} + n_{i,\downarrow}$  with  $n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$  and the on-site and the intersite interactions are given by  $E_{|i-j|}$  for  $i=j$  and  $i \neq j$ , respectively.  $\langle i,j \rangle_m$  means that  $i$  and  $j$  are  $m$ th nearest neighbors (when  $m=0$  we have  $i=j$ ). The prime on the third term indicates that terms already considered previously for each  $m$  should be excluded and that  $\Delta t_m$  is limited by Eq. (2).  $\Delta t_m$  is the bond-charge interaction considering many sites, which may be viewed as a general density-dependence hopping. The special case  $E_{|i-j|} = U$  for  $i=j$ ,  $E_{|i-j|} = V$  for  $i$  and  $j$  nearest neighbors and  $\Delta t_m = 0$  corresponds to the

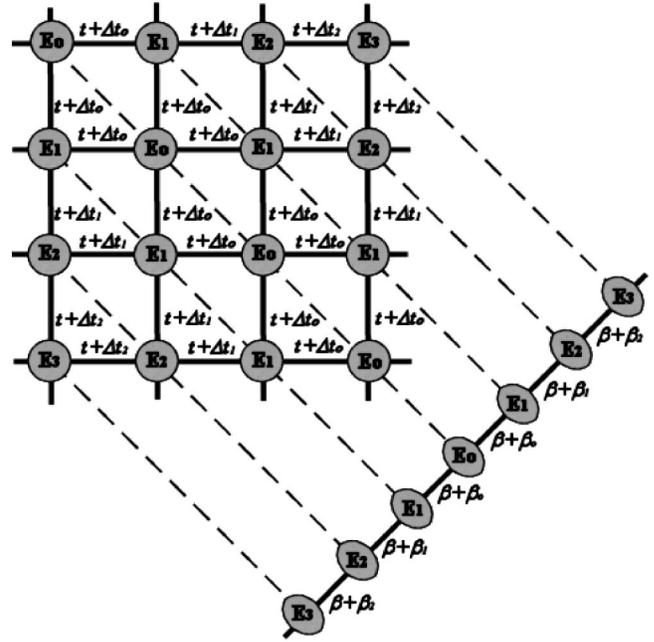


FIG. 1. Geometric representation of the two-particle states for a periodic chain. The states are represented by circles with site energy indicated inside. The direction of the projection procedure is shown by dashed lines. The final chain is formed by effective states, represented by ellipses, and the effective hopping parameters.

$t$ - $U$ - $V$  extended Hubbard model, which has been studied intensively by analytical and numerical methods.

In order to find an analytical solution of Eq. (3) we will use the mapping method, previously introduced and explained in detail in Refs. 17, 26 for different lattice topologies. The states associated with our Hamiltonian given by Eq. (3) have a geometric representation in a periodic square lattice (see Fig. 1), which can be described by a one-body tight-binding effective Hamiltonian with ordered site and bond impurities. This new one-body Hamiltonian is written as follows:<sup>27</sup>

$$H = \sum_i E_i b_i^{\dagger} b_i + \sum_{i,j} T_{i,j} b_i^{\dagger} b_j, \quad (4)$$

where the operator  $b_i^{\dagger}$  creates the many-body states,  $E_i$  represents the self-energy of the two-particle states (see Fig. 1), and  $T_{i,j}$  is the hopping amplitude between nearest-neighbor two-particle states. 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 and bond impurities and project the two-dimensional lattice of states onto a linear chain of effective states as is shown in Fig. 1, where  $\beta = 2t \cos(Ka/\sqrt{2})$  and  $\beta_i = 2\Delta t_i \cos(Ka/\sqrt{2})$ , the lattice parameter  $a=1$  and  $K$  is the wave vector in the projection direction.

## III. RESULTS AND DISCUSSIONS FOR TWO CORRELATED PARTICLES

### A. Analytical solution for a periodic chain

In order to obtain the ground-state analytical solution for two interacting particles in a one-dimensional periodic lat-

tice, we will use the renormalized perturbation expansion<sup>28</sup> to solve the new effective tight-binding Hamiltonian given by Eq. (4) and the impurity chain represented by ellipses in Fig. 1.

Let us consider, in the impurity linear chain represented by ellipses in Fig. 1, the nearest-neighbor interaction, which give us the following case:

$$\beta_i = E_i = 0 \quad \text{for } i \geq 2. \quad (5)$$

The Green function for the effective linear chain (Fig. 1) at the central site is given by

$$BG(0,0;x) = \frac{1}{x - \epsilon_0 - \frac{\frac{1}{2}(1+k_0)^2}{x - \frac{1}{2}\epsilon_1 - \frac{1}{2}(1+k_1)^2(x \pm \sqrt{x^2-1})}} \quad (6)$$

where  $x = E/B$ ,  $\epsilon_0 = E_0/B$ ,  $\epsilon_i = 2E_i/B$  (valid for  $i > 0$ ), and  $k_i = \beta_i/\beta$ . Here, we have written  $\epsilon_0$ ,  $\epsilon_i$ , and  $k_i$  in a general way in order to include all the cases we will study below. For the ground state we have  $B = 2\beta$ , with  $\beta = 2t$  and  $\beta_i = 2\Delta t_i$ .

Finding the poles of Eq. (6) for  $x^2 > 1$  and  $t < 0$ , we can obtain the condition for binding particles

$$\sqrt{(1+\epsilon_0)(1+\epsilon_1) + (1+\epsilon_0)[1 - (1+k_1)^2]} - 1 < k_0. \quad (7)$$

The limit case  $k_1 = 0$  in Eq. (7) gives the binding condition obtained by Marsiglio and Hirsch.<sup>22</sup> The same condition was found within the BCS theory for a constant density of states model in the low-density limit.

Including the next-nearest-neighbor interaction, the condition in our impurity linear chain (Fig. 1) is

$$\beta_i = E_i = 0 \quad \text{for } i \geq 3. \quad (8)$$

For this case, we can obtain the following condition for binding particles in this interaction regime:

$$\sqrt{(1+\epsilon_0)(1+\epsilon_1) + (1+\epsilon_0)\left(1 - \frac{(1+k_1)^2}{2+\epsilon_2 - (1+k_2)^2}\right)} - 1 < k_0. \quad (9)$$

From this equation, the binding condition given in Eq. (7) can be obtained by using  $\epsilon_2 = k_2 = 0$ .

The solution for the general case, or the general impurity linear chain shown in Fig. 1, can also be obtained. The general condition is given by

$$\beta_i = E_i = 0 \quad \text{for } i \geq n+1, \quad (10)$$

where  $n$  is the  $n$ th-nearest-neighbor interaction that has been considered. The Green function for this general impurity linear chain at the central site is

$$BG(0,0;x) = \frac{1}{x - \epsilon_0 - \frac{\frac{1}{2}(1+k_0)^2}{x - \frac{1}{2}\epsilon_1 - \frac{\frac{1}{4}(1+k_1)^2}{x - \frac{1}{2}\epsilon_2 - \frac{\frac{1}{4}(1+k_2)^2}{\vdots}}}} \quad (11)$$

$$x - (1/d)\epsilon_n - (m/2)(1+k_n)^2(x \pm \sqrt{x^2-1})$$

Here,  $d = 1$ ,  $m = 2$  for  $n = 0$ , and  $d = 2$ ,  $m = 1$  for  $n > 0$ .

### B. Analytical solution for a Fibonacci chain

A Fibonacci sequence consists of two letters  $A$  and  $B$ , and the entire sequence is generated by successive application of the substitution rule. The first few generations are  $G_0 = B$ ,  $G_1 = A$ ,  $G_2 = AB$ ,  $G_3 = ABA$ ,  $G_4 = ABAAB, \dots$ ,  $G_i = G_{i-1}G_{i-2}$  for  $i \geq 2$ , where  $G_i$  indicates the generation  $i$ . In a Fibonacci chain, the letters  $A$  and  $B$  from the Fibonacci sequence may denote two different atoms (site model) or two different bonds separating identical atoms (transfer model). In this work we will study the transfer model, where the hopping integrals take two values  $t_L$  and  $t_S$  corresponding to a large bond ( $L$ ) and a short bond ( $S$ ), respectively. In the transfer model the number of large bonds is  $N_L(n)$  and the number of short bonds is  $N_S(n)$ . The total number of bonds in a generation  $n$  is represented by  $N(n)$ . These numbers are related by

$$N(n) = N(n-1) + N(n-2),$$

$$N_L(n) = N(n-1), \quad (12)$$

$$N_S(n) = N(n-2).$$

In the quasiperiodic limit ( $n \rightarrow \infty$ ), the ratio  $N_L(n)/N_S(n)$  converges toward the golden mean  $\sigma = (\sqrt{5} + 1)/2$ .

To study the electronic correlation of two particles with antiparallel spins in a Fibonacci chain, we use the general Hubbard model and the real-space mapping method described above to obtain all the state configuration as was done for the periodic chain. Here, the states have a geometric representation in a square lattice with bond-quasiperiodic symmetry in different directions, which can be described by a one-dimensional tight-binding effective Hamiltonian. For the ground state we can approximate the projection of the two-dimensional lattice of states onto a chain of effective

states, similar to the projection given in Fig. 1 for the periodic chain. In the ground state of the extended Hubbard Hamiltonian, for the above chain of effective states we have  $E_0=U$ ,  $E_1=V$ ,  $E_i=0$  for  $i>1$ ,  $\beta_i=0$ , and  $\beta=2t_S[(f\sigma+1)/(\sigma+1)]$  with  $t_L=ft_S$  (see Fig. 1). In our limit of low concentration, the condition for pairing is

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

where  $u=U/B$  and  $v=2V/B$  with  $B=2\beta$ . The effects of quasiperiodicity, in the analytical expression for the pairing condition, are introduced through the effective hopping parameter  $\beta$ , which reproduces the results for the periodic chain when  $f=1$ , or  $t_L=t_S$ .

#### IV. CONCLUSIONS

In this Brief Report we studied the dilute limit of the general Hubbard model, including a general bond-charge interaction and general intersite interactions, by using a real-

space mapping method, the renormalized perturbation expansion, and the Green-function technique. We obtained the ground-state analytical solution for the pairing condition of two interacting particles in an infinite one-dimensional periodic and nonperiodic empty lattice. In order to find the solution for the general Hubbard Hamiltonian, a generalization of the mapping method has been done. In the periodic case, the general expression for the pairing condition obtained in this paper reproduces completely the limit cases: the numerical results and those coming from the reciprocal space. The non-periodic case analyzed in this paper was the Fibonacci chain, where an analytical solution for the pairing condition of two interacting particles is also given.

#### ACKNOWLEDGMENT

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

- 
- <sup>1</sup>E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).  
<sup>2</sup>See reprints in *Exactly Solvable Models of Strongly Correlated Electrons*, edited by V. E. Korepin and F. H. L. Ebler (World Scientific, Singapore, 1994).  
<sup>3</sup>W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).  
<sup>4</sup>A. M. Tsvelick and P. B. Wiegmann, Adv. Phys. **32**, 453 (1983); A. A. Aligia, C. A. Balseiro and C. R. Proetto, Phys. Rev. B **33**, 6476 (1986).  
<sup>5</sup>J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963); M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963).  
<sup>6</sup>E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).  
<sup>7</sup>N. F. Mott, *Metal-Insulator Transition*, 2nd. ed. (Taylor & Francis, London, 1990).  
<sup>8</sup>P. W. Anderson, Solid State Phys. **14**, 99 (1963).  
<sup>9</sup>S. Caprara, M. Avignon and O. Navarro, Phys. Rev. B **61**, 15 667 (2000).  
<sup>10</sup>R. Micnas, J. Ranninger and S. Robaszkiewicz, Rev. Mod. Phys. **62**, 113 (1990).  
<sup>11</sup>A. S. Blaer, H. C. Ren and O. Tchernyshyov, Phys. Rev. B **55**, 6035 (1997).  
<sup>12</sup>S. Fujimoto, Phys. Rev. B **64**, 085102 (2001).  
<sup>13</sup>G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986).  
<sup>14</sup>S. R. White, D. J. Scalapino, R. L. Sugar, and N. E. Bickers, Phys. Rev. Lett. **63**, 1523 (1989).  
<sup>15</sup>J. E. Hirsch, Phys. Rev. B **22**, 5259 (1980).  
<sup>16</sup>F. López-Urías and G. M. Pastor, Phys. Rev. B **59**, 5223 (1999).  
<sup>17</sup>O. Navarro and C. Wang, Rev. Mex. Fis. **38**, 553 (1992); O. Navarro, C. Wang, Solid State Commun. **83**, 473 (1992); L. A. Pérez, O. Navarro and C. Wang, Phys. Rev. B **53**, 15389 (1996).  
<sup>18</sup>M. W. Long and R. Fehrenbacher, J. Phys.: Condens. Matter **2**, 10 343 (1990).  
<sup>19</sup>A. S. Alexandrov, S. V. Traven, and P. E. Kornilovitch, J. Phys.: Condens. Matter **4**, L89 (1992).  
<sup>20</sup>D. L. Shepelyansky, Phys. Rev. Lett. **73**, 2607 (1994).  
<sup>21</sup>R. Oviedo-Roa, C. Wang, and O. Navarro, J. Low Temp. Phys. **105**, 651 (1996).  
<sup>22</sup>F. Marsiglio and J. E. Hirsch, Physica C **171**, 554 (1990).  
<sup>23</sup>H. Q. Lin and J. E. Hirsch, Phys. Rev. B **52**, 16 155 (1995).  
<sup>24</sup>M. Airoidi and A. Parola, Phys. Rev. B **51**, 16 327 (1995).  
<sup>25</sup>J. E. Espinosa, O. Navarro, and M. Avignon, Eur. Phys. J. B **18**, 9 (2000).  
<sup>26</sup>O. Navarro, *Introducción a la Superconductividad* (Aula Magna UAS, Culiacán, 1997), Vol. 11.  
<sup>27</sup>S. A. Trugman, in *Applications of Statistical and Field Theory Method to Condensed Matter*, edited by D. Baeriswy *et al.*, (Plenum Press, New York, 1990), p. 252.  
<sup>28</sup>E. N. Economou, *Green's Functions in Quantum Physics*, 2nd ed. Springer Series in Solid State Sciences (Springer, Berlin, 1993), Vol. 7.