The atomic method for the Hubbard dimer

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Abstract

The single-band Hubbard Hamiltonian [1] is the simplest model of interacting electrons in a lattice. It was developed by John Hubbard, who introduced the model to take into account the local electronic correlations in narrow energy bands. The model has a kinetic term that allows hopping of electrons between atomic sites and a term that considers the on-site interaction between electrons. This model is largely used in solid state physics to study magnetic properties of solids, insulator-metal transition (Mott transition) and high temperature superconductors. However, this is a problem that has exact analytical solution in a very few limiting cases and must be treated approximately or numerically.

In this work, we propose a new methodology to analytically solve the Hubbard Hamiltonian, mapping it into a two-site model (the Hubbard dimer). To obtain the Green’s function for the lattice, we employed the cumulant expansion technique, using as a ‘seed’ the exact two-site Green’s function (the atomic method) [2]. From the Green’s function, we obtained the density of states [DOS] and the occupation numbers as functions of the external parameters of the model, and compared the results with the Hubbard I approximation [1].

Introduction

The microscopic model consists of two parts: a kinetic term describing the hopping of electrons and a second term which approximates the Coulomb interaction among them. From the original Hubbard work [1] we know that the Hamiltonian to model a lattice including the electron correlations is given by

$$H = \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} + \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow}$$

In this work we study the Hubbard dimer, which is modeled by the Hubbard Hamiltonian with only two sites. Each site might be empty (0), occupied by a spin up electron (↑) or a spin down electron (↓), or by two electrons with opposite spins (↑↓). These states generate a Fock space for the dimer.

This problem treats a non-trivial interacting electronic system that has exact analytical solution. The Hamiltonian used to model this problem is [2]:

$$H = \sum_{i=1,2} \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{i,j=1,2} \sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i=1,2} \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} + \sum_{i=1,2} \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma}$$

where $t$ is the kinetic hopping energy of the electrons, which represents the possibility of an electron hopping from a site to another; $u$ denotes the

Figure 1. The interactions in the Hubbard model
Coulomb interaction between two electrons on the same site; $\varepsilon_0$ is the local energy of an electron.

### Methods and Results

Calculating the sums and rewriting the Hamiltonian in the basis of the dimer states one gets a $16 \times 16$ matrix and by calculating its eigenvectors and eigenvalues, the complete solution of the model for the dimer can be found (table 1). From this solution, it is possible to identify the transitions on the dimer and the energy variation associated with these (table 2).

#### Table 1. The exact solution of the model for the dimer

<table>
<thead>
<tr>
<th>State</th>
<th>Eigenenergies ($E_i$)</th>
<th>Eigenvalue $E_i$</th>
<th>$n$</th>
<th>$S_z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$E_{12} &gt; E_{14} &gt; E_{24} &gt; E_{13} &gt; E_{34}$</td>
<td>$E_{3} &gt; 0$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>$E_{12} &gt; E_{14} &gt; E_{24} &gt; E_{13} &gt; E_{34}$</td>
<td>$E_{3} = 0 + i t$</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>3</td>
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<td>$E_{3} = 0 - i t$</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>4</td>
<td>$E_{12} &gt; E_{14} &gt; E_{24} &gt; E_{13} &gt; E_{34}$</td>
<td>$E_{3} = 0$</td>
<td>0</td>
<td>0</td>
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<tr>
<td>5</td>
<td>$E_{12} &gt; E_{14} &gt; E_{24} &gt; E_{13} &gt; E_{34}$</td>
<td>$E_{3} = - \varepsilon_0$</td>
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<tr>
<td>6</td>
<td>$E_{12} &gt; E_{14} &gt; E_{24} &gt; E_{13} &gt; E_{34}$</td>
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<td>8</td>
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<td>$E_{3} = - \varepsilon_0$</td>
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<td>0</td>
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</table>

The sixteen eigenvectors $v_i(r)$ have energies $E_i$; being $n$ the number of electrons, $r$ the state of the dimer with $n$ electrons and $S_z$ the total spin in the z direction. Also, $a = \sqrt{2 \left( \frac{1}{\varepsilon_0} + 1 \right)}$, $b = \sqrt{2 \left( \frac{1}{\varepsilon_0} + 1 \right)}$ and $c = \sqrt{16b^2 + 4}$. 

#### Table 2. Energy differences of the possible dimer transitions

<table>
<thead>
<tr>
<th>Energy variation</th>
<th>Transition</th>
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<tbody>
<tr>
<td>$\omega = \epsilon - i$</td>
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</tr>
</tbody>
</table>

Using a conduction band with a square shape, the Green’s function for the lattice becomes:

$$G(\omega) = \frac{1}{2D} \int_{-D}^{D} dt \frac{M_{1\sigma}(\omega)}{1 - e^{\omega\mu} M_{1\sigma}(\omega)}$$

This relation is exact, but the exact cumulants are unknown. The main approximation for the model is made here: the first order cumulant and the dimer solution are used as an approximation for the exact cumulants. Then, we obtain

$$G(\omega) = \frac{1}{2D} \ln \left[ \frac{1 + DM_{1\sigma}(\omega)}{1 - DM_{1\sigma}(\omega)} \right]$$
From the Green’s functions for the lattice, the density of states [DOS] is obtained. A comparison between the DOS in the Hubbard I approximation and in our cumulant approach can be seen in the figure 2:

![Figure 2](image)

**Figure 2.** The density of states as a function of the electronic correlation \( U \) for the Hubbard I approximation (blue) and our cumulant approach (red) taking into consideration both the single site cumulant and the dimer cumulant.

We can also obtain the occupation numbers of the model through the relations:

\[
n = \left( \frac{1}{\pi} \right) \int_{-\infty}^{\infty} dz n_F(z) \text{Im} \left( G^\sigma(z) \right),
\]

\[
n_d = \left( \frac{1}{\pi} \right) \int_{-\infty}^{\infty} dz n_F(z) \text{Im} \left( \Gamma^\sigma(z) \right),
\]

\[
\langle \langle n_i \sigma^\sigma c_i^\dagger c_j^\sigma \rangle \rangle \omega \equiv \Gamma^\sigma_{ij}(\omega),
\]

\[
n_{\text{vac}} = \left( \frac{1}{\pi} \right) \int_{-\infty}^{\infty} dz \left( 1 - n_F \right) \text{Im} \left( G^\sigma(z) \right),
\]

\[
n_s = n - n_d.
\]

Such that

\[
C = n_{\text{vac}} + n_s + n_d = 1.
\]

Where \( n, n_d, n_{\text{vac}}, n_s \) and \( C \) are, respectively, the single plus double occupation, the double occupation, the vacuum occupation, the single occupation and the completeness.

A comparison between occupation numbers of the model in different approaches can be seen in figures 3 and 4:

![Figure 3](image)

**Figure 3.** The occupation numbers of the model in the Hubbard I approximation.

![Figure 4](image)

**Figure 4.** The occupation numbers of the model in the cumulant approach taking into consideration both the single site cumulant and the dimer cumulant.

**Discussion**

The atomic method was implemented successfully to the Hubbard model, using the exact one site and two site solutions as a ‘seed’ for a cumulant expansion. The DOS and the occupation numbers for the model were obtained.

As a result of using both the first order cumulant and the dimer cumulant, the particle-hole symmetry for high values of electronic correlation was recovered, as can be seen by the analysis of the band areas on the DOS and by the analysis of the occupation numbers of the model for different values of the chemical potential.

In all the calculations we consider a square band of semi-width \( D=1 \) in a particle-hole symmetry case. \( E_0=-0.5D \) is the local energy, \( U=1.0D \) is the electron correlation and the temperature is \( T=0.0001D \).

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In figure 2 we represent the DOS in a typical particle-hole symmetric case, and we observe that the Hubbard I approximation does not fulfill this symmetry whereas our cumulant approach practically recovers this symmetry.

In figures 3 and 4 we plot the occupation numbers as functions of the chemical potential. The loss of the particle-hole symmetry in the Hubbard I approximation is reflected in the occupation number of the lower Hubbard band, which is equal to 0.4 as indicated in figure 3. On the other hand, in figure 4 we obtain the occupation number 0.5, which is consistent with the particle-hole symmetry of the present cumulant approach.

At the moment, we are developing a computational iterative algorithm to solve the Hubbard Hamiltonian for a cluster of 1, 2, 3, ..., N sites using this cumulant Green's function method and combine the solutions in order to improve the results. Also, by developing this algorithm, we would like to establish an alternative to the dynamical mean-field theory [DMFT] to solve the Hubbard Hamiltonian.

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References:


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