Ground State Energy of Extended Hubbard Model
by Self-Consistent RPA

S.Harir$^1$, M.Bennai$^{1,3}$ and Y.Boughaleb$^{1,2}$

$^1$ Laboratoire de Physiques de la Matière Condensée.
Faculté des Sciences Ben M'Sik, Université Hassan II-Mohammedia Casablanca, Maroc.

$^2$ LPMC, Faculté des Sciences d’Eljadida, Université Chouaib Doukkali, Maroc.

$^3$ Groupement Nationale de Physique des Hautes Energies, Focal point, LabUFR-PHE, Rabat, Morocco.

Abstract

Using the SCRP A, we study the intersite interaction effect on the dynamics of N electrons system. We have considered an extended Hubbard model including intrasite and intersite interactions, and we have applied this model to a system of two neighbouring atoms containing a free electron. The application of SCRP A to this model allows us to study the intersite interaction effect on the ground state and the excitation energies of system. We show that the repulsive interaction between the electrons of the neighbouring atoms is the origin of an supplementary conductivity of the system.

Keywords: extended Hubbard model, SCRP A, ph-RPA

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*Corresponding autor: bennaiidrissi@yahoo.fr, m.bennai@univh2m.ac.ma
†Member of Hassan-II Academy of Sciences and Technology
1 Introduction

The discovery of High-Temperature superconductivity has motivated a considerable effort in physics of strongly correlated electronic systems, and many theoretical models have been proposed[1]. The Hubbard model [2, 3] is one of the simplest and more general description of an interacting electrons system on a lattice. In its simplest form, it includ the usual kinetic energy of electrons and the competition between the on-site electron-electron interaction. The standard Hubbard model is defined by the second quantized Hamiltonian [2, 3]:

$$H = \sum_{i \neq j, \sigma} t_{ij} c_{i, \sigma}^\dagger c_{j, \sigma} + U \sum_i n_{i, \uparrow} n_{i, \downarrow}$$  \hspace{1cm} (1)

The first term of the eqs(1) represents the kinetic energy of electrons, and each electron has a possibility of hopping between different lattice sites. $c_{j, \sigma}$ is the annihilation operator of the electron at a lattice site $j$ with spin index $\sigma$. $c_{i, \sigma}^\dagger$ is the creation operator of the electron at a lattice site $i$, so $t_{ij}$ is the hopping integral from the site $j$ to the site $i$. The second term represents the intrasite coulomb interaction with energy $U$, where $n_{i, \sigma}$ is the number operator of electrons at the site $i$ with spin $\sigma$.

Recently, the Random Phase Approximation (RPA)[4], was used to resolve the standard Hubbard model[5, 6]. The RPA is an approach which treats seriously the correlations of system, and attempt to minimise the system energy. The standard Hamiltonian Hubbard must be developed as function of the creation and annihilation operators of the pair particle-hole(p-h), because our RPA regroups the electrons system on pair: particle-hole. The application of RPA to standard Hubbard gives non linear coupled equations, where the resolution is done by a SCRPA[7, 8]. In this paper, we consider an extended Hubbard model[9], where the intersite coulomb interactions are introduced. This model was shown to describe many interesting properties of high TC superconductor materials [10]. In this work, we apply the SCRPA method to this extended Hubbard model, and study the intersite interaction effect on the ground state and excitation energy of system. We show that the repulsive interaction between the electrons of the neighbouring atoms is the origin of a supplementary conductivity of the system.

2 Extended Hubbard Model

The standard Hubbard model with intrasite interaction explains some important physical phenomena like High-Temperature superconductivity [3], Mott-transition[11]. To explain other physical phenomena observed in different areas of the solid state physics like magnetic and transport properties, it is convenient to take into account also the intersite interaction resulting from original coulomb repulsion modified by the polaronic effect. The extended Hubbard Hamiltonian is then given by[12, 13]:

$$H = \sum_{i \neq j, \sigma} t_{ij} c_{i, \sigma}^\dagger c_{j, \sigma} + U \sum_i n_{i, \uparrow} n_{i, \downarrow} + \frac{1}{2} \sum_{i \neq j, \sigma} V_{ij}^{(1)} n_{i, \sigma} n_{j, \sigma} + \frac{1}{2} \sum_{i \neq j, \sigma} V_{ij}^{(2)} n_{i, \sigma} n_{j, -\sigma}$$  \hspace{1cm} (2)

$U$ denotes the effective intrasite coulomb interaction. $V_{ij}^{(1)}$ and $V_{ij}^{(2)}$ describes the effective intersite coulomb interaction between the electrons in the lattice sites $i$ and $j$, with the same spins (opposite spins). $V_{ij}^{(1)}$ and $V_{ij}^{(2)}$ are not necessary equal. The model(2) cannot be solved in a general case. There is however, a special but non trivial case of finite number of sites, which possesses exact analytical solution[5].

In this work we will limit ourselves to a simple case, and will apply the general formalism of SCRPA to the two sites problem. We consider a closed chain in one dimension, with periodic boundary conditions
$N = 2$. Our physical system is then equivalent to two neighbouring atoms containing a free electron. The Hamiltonian of the system is:

$$
H_{HF} = -t \sum_{\sigma} (c_{1,\sigma}^\dagger c_{2,\sigma} + c_{2,\sigma}^\dagger c_{1,\sigma}) + U \sum_{\sigma} (n_{1,\uparrow} n_{1,\downarrow} + n_{2,\uparrow} n_{2,\downarrow}) + V_1 \sum_{\sigma} n_{1,\sigma} n_{2,\sigma} + V_2 \sum_{\sigma} n_{1,\sigma} n_{2,-\sigma}
$$

where $t = -t_{12} = -t_{21}$.

In order to apply the approximation SCRPA to the Hubbard model, it is necessary, first, to apply the Hartree-Fock approximation (HF) to the Hubbard model. In the HF method, we write the Hamiltonian (3) as function of quasiparticles operators, which allow us to obtain the excitation spectrum of independent quasiparticles. The states $|HF\rangle$ are defined as: $|HF\rangle = a_{k_1,\uparrow}^\dagger a_{k_2,\downarrow}^\dagger |\text{vac}\rangle$, where $a_{k,\sigma}^\dagger$ is the annihilation operator of the mode $(k, \sigma)$; $a_{k,\sigma}$ is related to $c_{j,\sigma}$ with the usual Fourier transformation:

$$
c_{j,\sigma} = \frac{1}{\sqrt{N}} \sum_{k,\sigma} a_{k,\sigma} \exp(-i \cdot \vec{k} \cdot \vec{R}_j)
$$

$k$ is the momentum of state $|k, \sigma\rangle$. The periodic boundary conditions suppose that $c_{N+j,\sigma} = c_{j,\sigma}$. With this condition, eqs (4) gives $\exp(-i \cdot \vec{k} \cdot \vec{R}_j) = 1$, which have two solutions in the first Brillouin zone: $k_1 = 0$ and $k_2 = -\pi$. Thus the Hamiltonian is then written as:

$$
H_{HF} = E_{HF} + \sum_{\sigma} \{\varepsilon_1 n_{1,\sigma} + \varepsilon_2 n_{2,\sigma}\}
$$

This expression shows that in the HF approximation, the physical system has two possible states $|HF\rangle$ and $|HF\rangle^*$, $|HF\rangle$ ($|HF\rangle^*$ ) is the Hartree-Fock ground state (excited state), with the momentum: $k_1 = 0$; below (and $k_2 = -\pi$; above ) the Fermi momentum, and the excitation energy: $\varepsilon_1$ (and $\varepsilon_2$), where $|HF\rangle = a_{k_1,\uparrow}^\dagger a_{k_2,\downarrow}^\dagger |\text{vac}\rangle$ and $|HF\rangle^* = a_{k_2,\uparrow}^\dagger a_{k_1,\downarrow}^\dagger |\text{vac}\rangle$. As in ref [13], we define the HF quasiparticle operators by: $b_{1,\sigma} = a_{k_1,\sigma}$ and $b_{2,\sigma} = a_{k_2,\sigma}$. We have then $b_{k,\sigma} |HF\rangle = 0$, for all $k$.

In normal ordering of $b_{1,\sigma}$ and $b_{2,\sigma}$, the Hamiltonian (3) becomes:

$$
H = H_{HF} + H_{k=0} + H_{k=-\pi}
$$

where

$$
H_{k=0} = \frac{U + V_2}{2} (\tilde{n}_{k_2,\downarrow} - \tilde{n}_{k_1,\downarrow}) (\tilde{n}_{k_2,\downarrow} - \tilde{n}_{k_1,\downarrow}) + \frac{V_1}{4} \sum_{\sigma} (\tilde{n}_{k_2,\sigma} - \tilde{n}_{k_1,\sigma})^2
$$

$$
H_{k=-\pi} = -\frac{U - V_2}{2} (J_{\uparrow}^\dagger + J_{\uparrow}^\dagger)(J_{\downarrow}^\dagger + J_{\downarrow}^\dagger) - \frac{V_1}{4} \sum_{\sigma} (J_{\sigma}^\dagger + J_{\sigma}^\dagger)^2
$$

With

$$
J_{\sigma} = b_{1,\sigma} b_{2,\sigma}, \quad J_{\sigma}^\dagger = (J_{\sigma}^\dagger)^\dagger, \quad \tilde{n}_{k,\sigma} = b_{1,\sigma}^\dagger b_{1,\sigma}
$$

$H_{k=0}$ and $H_{k=-\pi}$ take into account the correlation between the number operators of the type: $\tilde{n}_{k_1,\sigma} \tilde{n}_{k_1,\sigma'}$ in the ground state: $k_1 = 0$ (below the Fermi momentum) and between the magnetic momentum operators of the type: $J_{\sigma}^\dagger J_{\sigma}^\dagger$ in the excited state: $k_2 = -\pi$ (above the Fermi momentum).
3 Self Consistent Random Phase Approximation

3.1 Formalism

In order to apply the Formalism of SCRPA to the Hubbard model, it is convenient to use the particle-hole (ph-RPA) approximation, which regroup the physical system on pair. We can then define the RPA excitation operator as:

$$Q^i_v = \sum_{p,h} (x^i_{ph} \hat{b}^i_p \hat{b}^i_h - y^i_{ph} \hat{b}^i_h \hat{b}^i_p)$$  \hspace{1cm} (7)

Where $h$ (and $p$) are the momentum below (and above) the Fermi momentum. Eqs(7) shows that the excitation in the ph-RPA is done only by the creation or (annihilation) of pair: particle-hole via the operator $\hat{b}^i_p \hat{b}^i_h (\hat{b}^i_h \hat{b}^i_p)$ with the amplitude $x^i_{ph} (y^i_{ph})$. The corresponding excited state of this excitation operator is $|v\rangle = Q^i_v |RPA\rangle$, and the corresponding excitation energy is:

$$E_v = \frac{\langle RPA | [Q_v, [H, Q^i_v]] | RPA \rangle}{\langle RPA | Q_v Q^i_v | RPA \rangle}$$  \hspace{1cm} (8)

Where $|RPA\rangle$ is the vacuum of this RPA excitation operator: $Q_v |RPA\rangle = 0$

The minimization of $E_v$ leads to usual RPA equations of type:

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} x^v \\ y^v \end{pmatrix} = E_v. \begin{pmatrix} x^v \\ y^v \end{pmatrix}$$

With the relations of the orthonormality conditions of the set $\{Q_v; Q^i_v\}$, we can express the elements of $A$ and $B$ by the RPA-amplitudes, and therefore we have a completely closed system of equations for amplitudes $x$ and $y$. For our problem, we consider only the excitation operators, which conserve the spin, where the excitation is done only by the creation or annihilation of the pair: particle-hole with the same spin.

$$Q^i_v = x^i_v.\hat{k}^i_1 + x^i_v.\hat{k}^i_\uparrow - y^i_v.\hat{k}^i_\uparrow - y^i_v.\hat{k}^i_\downarrow$$  \hspace{1cm} (9)

With $K^i_\sigma = b^i_{1,\sigma} b^i_{1,\sigma}/\sqrt{1-(M_\sigma)}$, $K^i_\uparrow = b^i_{1,\sigma} b^i_{1,\sigma}/\sqrt{1-(M_\sigma)}$ and $M_\sigma = \hat{n}_{1,\sigma} + \hat{n}_{2,\sigma}$, where the mean values $\langle...\rangle$ are taken with respect to the RPA vacuum ($Q_v |RPA\rangle = 0$). The SCRPA equation can then be written in the form:

$$\begin{pmatrix} A_{1\uparrow} & A_{1\downarrow} & B_{1\uparrow} & B_{1\downarrow} \\ A_{1\downarrow} & A_{1\uparrow} & B_{1\downarrow} & B_{1\uparrow} \\ -B_{1\uparrow} & -B_{1\downarrow} & A_{1\uparrow} & A_{1\downarrow} \\ -B_{1\downarrow} & -B_{1\uparrow} & A_{1\downarrow} & A_{1\uparrow} \end{pmatrix} \begin{pmatrix} x^i_\uparrow \\ x^i_\downarrow \\ y^i_\uparrow \\ y^i_\downarrow \end{pmatrix} = E_v \begin{pmatrix} x^i_\uparrow \\ x^i_\downarrow \\ y^i_\uparrow \\ y^i_\downarrow \end{pmatrix}$$  \hspace{1cm} (10)

Where the SCRPA matrix elements are given by:

$$A_{\sigma\sigma'} = \langle [K^i_\sigma, [H, K^j_\sigma']] \rangle$$

and

$$B_{\sigma\sigma'} = \langle [K^i_\sigma, [H, K^j_\sigma'-]] \rangle$$

The orthonormality relations of the set $\{Q_v; Q^i_v\}$, give:
From the Hamiltonian given in eqs (10), we can write the SCRP matrix elements as: 

\[ A = B + 2t, \quad A' = B' \]

where:

\[
A = \begin{pmatrix}
A & A' \\
A' & A
\end{pmatrix}
\]

\[
B = \begin{pmatrix}
B & B' \\
B' & B
\end{pmatrix}
\]

From the Hamiltonian given in eqs (10), we can write the SCRP matrix elements as: 

\[ A = B + 2t, \quad A' = B' \]

where:

\[
A = 2t + (U - V_2) \cdot \sqrt{\frac{1 - \langle M_\sigma \rangle}{1 - \langle M_\tau \rangle}} \sum_x x_1^\uparrow (y_1^\uparrow + x_1^\uparrow)
\]

\[
-\frac{V_1}{2} \left( \frac{1}{1 - \langle M_\sigma \rangle} - \sum_x (x_\sigma^\uparrow x_\sigma^\downarrow + y_\sigma^\uparrow y_\sigma^\downarrow + 2x_\sigma^\uparrow y_\sigma^\downarrow) \right)
\]

and

\[
A' = \frac{U - V_2}{2} \cdot \frac{1 - \langle M_\sigma \rangle}{1 - \langle M_\tau \rangle}
\]

so, the ph-RPA matrix takes the form:

\[
\begin{pmatrix}
A & A' & A - 2t & A' \\
A' & A & A' & A - 2t \\
2t - A & -A' & -A & -A' \\
-A' & 2t - A & -A' & -A
\end{pmatrix}
\begin{pmatrix}
x_1^\uparrow \\
x_1^\downarrow \\
x_2^\uparrow \\
x_2^\downarrow
\end{pmatrix}
= E_{v_1}
\begin{pmatrix}
x_1^\uparrow \\
x_1^\downarrow \\
x_2^\uparrow \\
x_2^\downarrow
\end{pmatrix}
\]

This ph-RPA matrix has two positive roots:

\[ \varepsilon_1 = 2t \sqrt{\frac{A - A'}{t} - 1} \quad \text{and} \quad \varepsilon_2 = 2t \sqrt{\frac{A + A'}{t} - 1} \]

The corresponding eigenvectors are: \( V_1 = [x_1, -x_1, y_1, -y_1] \) and \( V_2 = [x_2, -x_2, y_2, -y_2] \), respectively.

Where

\[
x_1 = \frac{A - A' + \varepsilon_1}{A - A' - 2t} y_1 \quad ; \quad x_2 = \frac{A + A' + \varepsilon_1}{A + A' - 2t} y_1
\]

and

\[
y_1 = -\sqrt{2 \left( \frac{A - A' + \varepsilon_1}{A - A' - 2t} \right)^2 - 2} \quad ; \quad y_2 = -\sqrt{2 \left( \frac{A + A' + \varepsilon_2}{A + A' - 2t} \right)^2 - 2}
\]

So, like the HF approximation, in ph-RPA, our system have tow excitation energies \( \varepsilon_1 \) and \( \varepsilon_2 \), but they are coupled. Thus in this work, we solve a system of a coupled equations numerically by iteration leading to a SCRPQ solution which are quasi identical to the exact result.
3.2 Results and discussion

To show the effect of intersite interaction on the energy of the system, we have studied the evolution of the ground state and excited energies in terms of the interaction $V_1$ and $V_2$.

In figure 1, we plot the variation of the ground state energy $E_{SCRPA} = \langle 0 | H | 0 \rangle$ as a function of the two parameters of the intersite interaction $V_1$ and $V_2$. The result shows that the ground state energy is quasi-independent on $V_1$ but, the variation of $E_{SCRPA}$ becomes more important when we introduce the intersite interaction with the opposite spins: $V_2$. This result can be explained by the fact that the SCRPA includes only, for the fundamental state, the correlations between the particles with different spins: $|0\rangle = (c_0 J_{\uparrow}^+ J_{\downarrow}^+ + c_1 J_{\uparrow}^- J_{\downarrow}^-) |HF\rangle$

Thus the only type of interaction which is of interest is $V_2$. In the following we analyse the $V_2$ effect on the dynamics of the system. In figure 2 and 3, we plot the variation of the ground state energy and the excitation energies of SCRPA, respectively, as a function of the repulsive intrasite interaction $U$ for different values of the intersite interaction $V_2$. 

Figure 1:
Figure 2:

Figure 3:
The results show that, when $U$ increases, the gap $\Delta = \epsilon_2 - \epsilon_1$ between the two excitation energies increases too, and so, the jump of electrons between these two states becomes more difficult. Thus, we can conclude, that for a fixed value of $U$, while the intersite interaction is repulsive (attractive), the gap $\Delta$ becomes less (more) important. These remarks allow us to assume that repulsive interaction between the electrons of the neighbouring atoms is the origin of supplementary conductivity of the system.

4 Conclusion

In this paper, the SCRPA approximation was used to solve the extended Hubbard model given in Eqs(3). The quality of the SCRPA method has been investigated in a previous work by Jemai[5], in which he has shown a remarkable agreement between SCRPA method and exact results for the standard Hubbard model. In our work, we have extended this technic to study the intersite interaction effects on the dynamics of the electrons in the two sites with $\langle n_{i,\uparrow} \rangle = \langle n_{i,\downarrow} \rangle$. We have shown that the gap between the excitation energies: $\langle \Delta = \epsilon_2 - \epsilon_1 \rangle$ are correlated with the intersite interaction energy $V_2$. This result allow us to suppose that the repulsive intersite interaction (between the electrons of the neighbouring atoms) is the origin of a supplementary conductivity of the system. In future work[14], we propose to solve the 4-sites case (plaquette), which may be very important for the explanation of high $T_c$ superconductivity, by considering the many plaquette configurations in 2D.

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