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

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Abstract

Using the SCRPA, 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 SCRPA 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, SCRPA, ph-RPA

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]:

$$H = \sum_{i \neq j,\sigma} t_{ij}.c^{\dagger}_{i,\sigma}.c_{j,\sigma} + U.\sum_{i} n_{i,\uparrow}.n_{i,\downarrow} \tag{1}$$

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 σ. $c^{\dagger}_{i,\sigma}$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 coloumb interaction with energy U, where $n_{i,\sigma}$ is the number operator of electrons at the site i with spin σ .

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 superconductors 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 coloumb repulsion modified by the polaronic effect. The extended Hubbard Hamiltonian is then given by[12, 13]:

$$H = \sum_{i \neq j,\sigma} t_{ij}.c^{\dagger}_{i,\sigma}.c_{j,\sigma} + U.\sum_{i} n_{i,\uparrow}.n_{i,\downarrow} + \frac{1}{2}\sum_{i \neq j,\sigma} V^{(1)}_{ij}.n_{i,\sigma}.n_{j,\sigma} + \frac{1}{2}\sum_{i \neq j,\sigma} V^{(2)}_{ij}.n_{i,\sigma}.n_{j,-\sigma} \tag{2}$$

U denotes the effective intrasite coloumb interaction. $V^{(1)}_{ij}$($V^{(2)}_{ij}$) describes the effective intersite coloumb interaction between the electrons in the lattice sites i and j, with the same spins (opposite spins). $V^{(1)}_{ij}$ and $V^{(2)}_{ij}$ 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:

$$\begin{aligned} H_{II} &= -t\sum_{\sigma}.(c^{\dagger}_{1,\sigma}.c_{2,\sigma} + c^{\dagger}_{2,\sigma}.c_{1,\sigma}) + U.(n_{1,\uparrow}.n_{1,\downarrow} + n_{2,\uparrow}.n_{2,\downarrow}) \\ &\quad + V_1.\sum_{\sigma} n_{1,\sigma}.n_{2,\sigma} + V_2.\sum_{\sigma} n_{1,\sigma}.n_{2,-\sigma} \end{aligned} \tag{3}$$

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, wich allow us to obtain the excitation spectrum of independent quasiparticles. The states $|HF\rangle$ are defined as: $|HF\rangle = a^{\dagger}_{k_i,\uparrow}.a^{\dagger}_{k_i,\downarrow}.|vac\rangle$, where $a^{\dagger}_{k,\sigma}$ is the annihilation operator of the mode (k,σ); $a_{k;\sigma}$ is related to $c_{j;\sigma}$with the usual Fourier transformation:

$$c_{j,\sigma} = \frac{1}{\sqrt{N}}.\sum_{k,\sigma} a_{k,\sigma}.\exp(-i.\overrightarrow{k}.\overrightarrow{R_j}) \tag{4}$$

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 $\exp(-i.\overrightarrow{k}.\overrightarrow{R_j}) = 1$,

which have two solutions in the first Brillouin zone: $k_1 = 0$ and $k_2 = -\pi$. Thus the Hamiltonian is then written as:

$$H_{HF} = E_{HF} + \sum_{\sigma} \{\varepsilon_1.n_{1,\sigma} + \varepsilon_2.n_{2,\sigma}\} \tag{5}$$

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: ε_1 (and ε_2), where $|HF\rangle = a^+_{k_1,\uparrow}.a^+_{k_1,\downarrow}.|vac\rangle$ and $|HF\rangle^* = a^+_{k_2,\uparrow}.a^+_{k_2,\downarrow}.|vac\rangle$. 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:

$$H = H_{HF} + H_{k=0} + H_{k=-\pi} \tag{6}$$

where

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

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

With

$$J^-_{\sigma} = b_{1,\sigma}\, b_{2,\sigma},\ J^{\dagger}_{\sigma} = \left(J^-_{\sigma}\right)^{\dagger},\ \tilde{n}_{k_i,\sigma} = b^{\dagger}_{i,\sigma}\, b_{i,\sigma}$$

$H_{k=0}$ and $H_{k=-\pi}$ take into account the correlation between the number operators of the type: $\tilde{n}_{k_i,\sigma}\tilde{n}_{k_j,\sigma'}$ in the ground state: $k_1 = 0$ (below the Fermi momentum) and between the magnetic momentum operators of the type: $J^{\dagger}_{\sigma}.J^-_{\sigma'}$ 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:

$$Q_v^\dagger = \sum_{p,h} (x_{ph}^v . b_p^\dagger . b_h^\dagger - y_{ph}^v . b_h . b_p) \tag{7}$$

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 $b_p^\dagger . b_h^\dagger$ ($b_h . b_p$) with the amplitude x_{ph}^v (y_{ph}^v). The corresponding excited state of this excitation operator is $|v\rangle = Q_v^\dagger . |RPA\rangle$, and the corresponding excitation energy is:

$$E_v = \frac{\langle RPA| \left[Q_v, \left[H, Q_v^\dagger \right] \right] |RPA\rangle}{\langle RPA| \left[Q_v, Q_v^\dagger \right] |RPA\rangle} \tag{8}$$

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 $\left\{ Q_v ; Q_v^\dagger \right\}$, 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.

$$Q_v^\dagger = x_\uparrow^v . k_\uparrow^\dagger + x_\downarrow^v . k_\downarrow^\dagger - y_\uparrow^v . k_\uparrow^- - y_\downarrow^v . k_\downarrow^- \tag{9}$$

With $K_\sigma^\dagger = b_{2,\sigma}^\dagger . b_{1,\sigma}^\dagger / \sqrt{1 - \langle M_\sigma \rangle}$, $K_\sigma^- = b_{1,\sigma} . b_{2,\sigma} / \sqrt{1 - \langle M_\sigma \rangle}$ and $M_\sigma = \widehat{n}_{1,\sigma} + \widehat{n}_{2,\sigma}$, 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:

$$\begin{pmatrix} A_{\uparrow\uparrow} & A_{\uparrow\downarrow} & B^{\uparrow\uparrow} & B_{\uparrow\downarrow} \\ A_{\downarrow\uparrow} & A_{\downarrow\downarrow} & B_{\downarrow\uparrow} & B_{\downarrow\downarrow} \\ -B_{\uparrow\uparrow} & -B_{\uparrow\downarrow} & -A_{\uparrow\uparrow} & -A_{\uparrow\downarrow} \\ -B_{\downarrow\uparrow} & -B_{\downarrow\downarrow} & -A_{\downarrow\uparrow} & -A_{\downarrow\downarrow} \end{pmatrix} . \begin{pmatrix} x_\uparrow^v \\ x_\downarrow^v \\ y_\uparrow^v \\ y_\downarrow^v \end{pmatrix} = E_v . \begin{pmatrix} x_\uparrow^v \\ x_\downarrow^v \\ y_\uparrow^v \\ y_\downarrow^v \end{pmatrix} \tag{10}$$

Where the SCRPA matrix elements are given by:

$$A_{\sigma\sigma'} = \left\langle \left[K_{\sigma}^{-}, \left[H, K_{\sigma'}^{\dagger} \right] \right] \right\rangle$$

and

$$B_{\sigma\sigma'} = \left\langle \left[K_{\sigma}^{-}, \left[H, K_{\sigma'}^{-} \right] \right] \right\rangle$$

The orthonormality relations of the set $\left\{ Q_v; Q_v^{\dagger} \right\}$, give:

$$\begin{array}{ll} A_{\uparrow\uparrow} = A_{\downarrow\downarrow} = A & A_{\uparrow\downarrow} = A_{\downarrow\uparrow} = A' \\ B_{\uparrow\uparrow} = B_{\downarrow\downarrow} = B & B_{\uparrow\downarrow} = B_{\downarrow\uparrow} = B' \end{array}$$

From the Hamiltonian given in eqs(10), we can writte the SCRPA matrix elements as: $A = B + 2.t$, $A' = B'$, where:

$$A = 2.t + (U - V_2) . \sqrt{\frac{1 - \langle M_{\downarrow} \rangle}{1 - \langle M_{\uparrow} \rangle}} . \sum_v x_{\uparrow}^v (y_{\downarrow}^v + x_{\downarrow}^v) \tag{11}$$

$$-\frac{V_1}{2} . \left(\frac{1}{1 - \langle M_{\sigma} \rangle} - \sum_v (x_{\sigma}^v . x_{\sigma}^v + y_{\sigma}^v . y_{\sigma}^v + 2 . x_{\sigma}^v . y_{\sigma}^v) \right) \tag{12}$$

and

$$A' = \frac{U - V_2}{2} . \frac{1}{1 - \langle M_{\sigma} \rangle} \tag{13}$$

where

$$\langle M_{\sigma} \rangle = \frac{2 \sum\limits_{\nu} |y_{\sigma}^{\nu}|^2}{1 + 2 \sum\limits_{\nu} |y_{\sigma}^{\nu}|^2}$$

so, the ph-RPA matrix takes the form:

$$\begin{pmatrix} A & A' & A - 2.t & A' \\ A' & A & A' & A - 2.t \\ 2.t - A & -A' & -A & -A' \\ -A' & 2.t - A & -A' & -A \end{pmatrix} \begin{pmatrix} x_{\uparrow}^v \\ x_{\downarrow}^v \\ y_{\uparrow}^v \\ y_{\downarrow}^v \end{pmatrix} = E_v . \begin{pmatrix} x_{\uparrow}^v \\ x_{\downarrow}^v \\ y_{\uparrow}^v \\ y_{\downarrow}^v \end{pmatrix}$$

This ph-RPA matrix has two positive roots:

$$\varepsilon_1 = 2.t.\sqrt{\frac{A-A'}{t}-1} \quad \text{and} \quad \varepsilon_2 = 2.t.\sqrt{\frac{A+A'}{t}-1} \tag{14}$$

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

$$x_1 = -\frac{A-A'+\varepsilon_1}{A-A'-2.t}.y_1 \quad ; \quad x_2 = -\frac{A+A'+\varepsilon_1}{A+A'-2.t}.y_1 \tag{15}$$

and

$$y_1 = -\sqrt{2.\left(\frac{A-A'+\varepsilon_1}{A-A'-2.t}\right)^2-2} \quad ; \quad y_2 = -\sqrt{2.\left(\frac{A+A'+\varepsilon_2}{A+A'-2.t}\right)^2-2} \tag{16}$$

So, like the HF approximation, in ph-RPA, our system have tow excitation energies $\varepsilon_1$and ε_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 th evolution of the ground state and excited energies in term of the interaction V_1 and V_2.

In figure1 we plot the variation of the ground state energy $E_{SCRPA} = \langle 0 | H | 0 \rangle$ as 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} become more important when we introduce the intersite interaction with the opposite spins: V_2. This results can be explained by the fact that the SCRPA include only, for the fundamental state, the correlations between the particles with different spins**:** $|0\rangle = \left(c_0^1 + c_1^1 J_\uparrow^+ . J_\downarrow^+\right)|HF\rangle$

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

The results show that, when U increases, the gap $\Delta = \varepsilon_2 - \varepsilon_1$ between the two excitation energies increases too, and so, the jump of electrons between

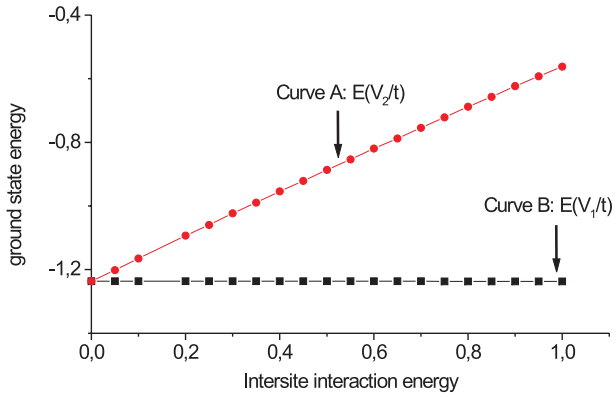

Figure 1: Ground state energy of SCRPA as function of the two parametrs of the intersite interaction V_1/t and V_2/t for $U/t = 2$

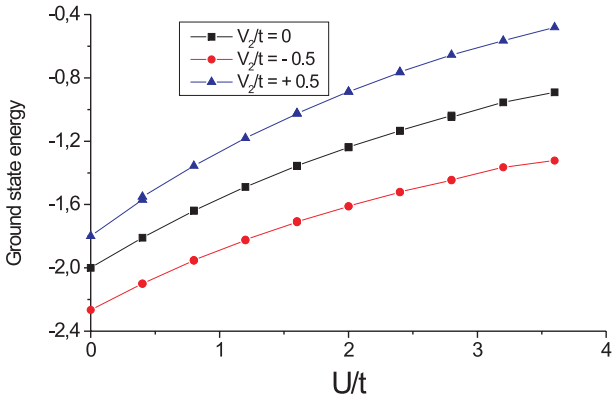

Figure 2: Ground state energy of SCRPA as function of the intersite interaction U/t for differents values of V_2/t, with $V_1/t = 0$

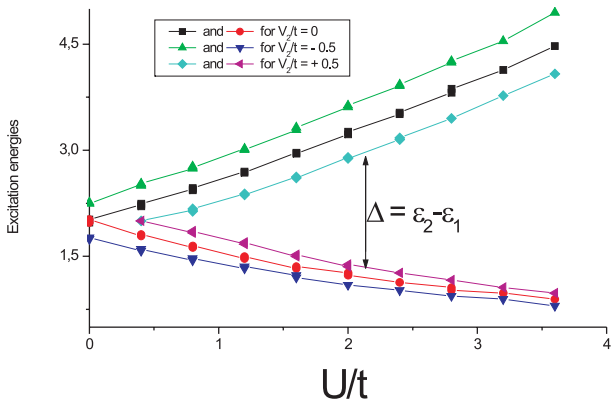

Figure 3: Excitation energies of SCRPA as function of the intersite interaction U/t for differents values of V_2/t, with $V_1/t = 0$

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 Δ 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 excact 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: $(\Delta = \varepsilon_2 - \varepsilon_1)$ 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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