Self Consistent RPA applied to the extended Hubbard Model

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Using the extended Hubbard model with the Self Consistent Random Phase Approximation (SCRPA), we study the intersite interaction effect on the dynamics of N electrons. We consider the extended Hubbard model containing intrasite and intersite interactions, and we apply this model to a system of two interacting atoms, where each atom presents one free electron. The resolution of this tow sites problem is done by the SCRPA approximation; our calculations allow as studying the intersite interaction effect on the excitation energies of system. We have showed that the attractive interaction between the electrons of the neighbour's atoms is the origin of supplementary conductivity of the system.
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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. The Hubbard model [1, 2, 10] is one the simplest description of an interacting electrons on a lattice. The standard Hubbard model contains in its simplest form the competition between the coloumb interaction U between electrons on the same site, and the habitual kinetic of electrons. The standard Hubbard Hamiltonian is of the form [14]:

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

Where the first term of the eq (1) represents the kinetic energy of electrons, where 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 $\sigma = \uparrow, \downarrow$. $c^{+}_{i,\sigma}$ 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, where $n_{i,\sigma} = c^{+}_{i,\sigma}.c_{,\sigma}$ are the number operators of electrons at the site i with spin σ.

Recently, the Random Phase Approximation (RPA) [3, 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 work we have considered the extended Hubbard model [9], where we have introduced an intersite coulomb interaction. We apply the SCRPA method to this extended model; our calculations allow studying the intersite interaction effect on the excitation energies of system.

2- The extended Hubbard model:

The standard Hubbard model with intrasite interaction only, explains some important physical phenomena like Mott-transition [11, 12]. To explain other physical phenomena observed in different areas of the solid state physics: magnetic and transport properties of transitions, and H-T_c superconductor [13, 15], 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 given by [9]:

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

U denotes the effective intrasite coloumb interaction. $V^{(1)}_{ij}$ (and $V^{(2)}_{ij}$) describes the effective intersite coloumb interaction between the electrons in the lattice sites i and j, where these electrons have the same spins (and 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 [3]. In this work we will limit ourselves to the simplest case, and will apply the general formalism of SCRPA to the two sites problem at half filling. We consider closed chains in one dimension, with periodic boundary conditions N= 2; so, our physical system is then equivalent to two neighbour atoms; where each one presents a free electron. The Hamiltonian of this physical system writes:

$$H = -t.\sum_{\sigma}(c^{+}_{1,\sigma}.c_{2,\sigma} + c^{+}_{2,\sigma}.c_{1,\sigma}) + U.(n_{1,\uparrow}.n_{1,\downarrow} + n_{2,\uparrow}.n_{2,\downarrow}) + V_1.\sum_{\sigma} n_{1,\sigma}.n_{2,\sigma} + V_2.\sum_{\sigma} n_{1,\sigma}.n_{2,-\sigma} \qquad \textbf{(3)}$$

where $-t = t_{12} = t_{21}$. In order to apply the approximation SCRPA to the Hubbard model, it is necessary in the first step to apply the Hartree-Fock approximation (HF) to the Hubbard model, which allows as to write the Hamiltonian (3) as function of quasiparticles operators, and so, to have an excitation spectre of independent quasiparticles. The states $|HF\rangle$ are defined as $|HF\rangle = a^{+}_{k_i,\uparrow}.a_{k_i,\downarrow}.|vac\rangle$, where $a_{k_i,\downarrow}$ is the annihilation of operator of the mode $|k_i,\sigma\rangle$; $a_{k,\sigma}$ is related to $c_{j,\sigma}$ with the usual Fourier transformation:

$$c_{j,\sigma} = \frac{1}{\sqrt{N}}.\sum_{k,\sigma} a_{k,\sigma}.\exp(-i.\vec{k}.\vec{R}_j) \qquad \textbf{(4)}$$

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

$$H_{HF} = E_{HF} + \sum_{\sigma}(\varepsilon_1.n_{1,\sigma} + \varepsilon_2.n_{2,\sigma}) \qquad \textbf{(5)}$$

This expression shows that in the HF approximation, the physical system has two possible states $|HF\rangle$ and $|HF\rangle^{*}$. $|HF\rangle$ (and $|HF\rangle^{*}$) is the Hartree-Fock ground state (and excited state), with the momenta $k_1 = 0$: 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 [9], 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 figure 1, we plot the excitation energies as function of U for different value of the intersite interaction energies.

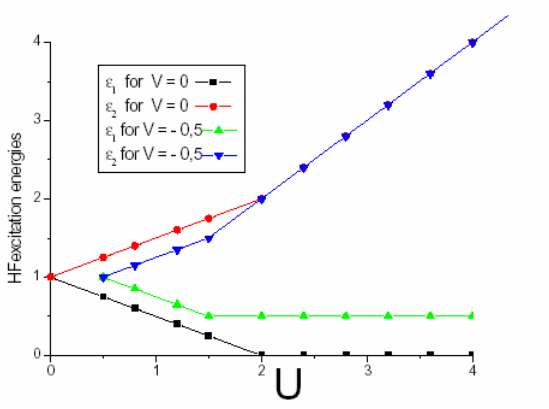

Figure 1: The excitation energies of HF as function of the intrasite interaction U for tow values of the intersite interaction (V = 0 and V = - 0.5.t, where $V=V_1+V_2$ and t=1)

The variation of the excitation energies shows that, for U= V= 0, the system has one energy level ($\varepsilon_1=\varepsilon_2$), so, in this limit our model is equivalent to the free electron model. For $U \succ 0$, the excitation of energy is splitting in to two energy levels: in this case, each electron jumps between the two energies levels, only for $U \leq 2.t$; but, when U becomes important, the jumping of electron becomes more difficult, so, each electron remains linked to its atom, but if the dynamic of the electron system is governed by an attractive intersite interaction $V \succ 0$, the jumping of electron between the sites becomes more favourable.

3- SCRPA applied to the extended Hubbard model:

3-1- Formalism of SCRPA:

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

$$Q_v^+ = \sum_{p,h} (x_{ph}^v . b_p^+ . b_h^+ - y_{ph}^v . b_h . b_p) \quad \textbf{(6)}$$

Where h (and p) are momenta below (and above) the Fermi momentum. The eq (6) shows that the excitation in the ph-RPA is done only by the creation or (annihilation) of pair: particle-hole via the operator $b_p^+ . b_h^+$ ($b_h . b_p$) with the amplitude x_{ph}^v (x_{ph}^v). The correspondent excited state to this excitation operator is $|v\rangle = Q_v^+ . |\mathrm{RPA}\rangle$, and the corresponding excitation energy is:

$$E_v = \frac{\langle RPA | \left[Q_v , \left[H , Q_v^+ \right] \right] | RPA \rangle}{\langle RPA | \left[Q_v , Q_v^+ \right] | RPA \rangle} \quad \textbf{(7)}$$

Where $|RPA\rangle$ is the vacuum of this RPA excitation operator: $Q_v |RPA\rangle = 0$. The minimisation of E_v gives the equations of the usual RPA 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 $\{Q_v, Q_v^+\}$, 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 work only with the $|RPA\rangle$ 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.

$$Q_v^+ = x_\uparrow^v . k_\uparrow^+ + x_\downarrow^v k_\downarrow^+ - y_\uparrow^v k_\uparrow^- - y_\downarrow^v k_\downarrow^- \quad \textbf{(8)}$$

With $k_\sigma^+ = \frac{b_{2,\sigma}^+ . b_{1,\sigma}^+}{\sqrt{1 - \langle M_\sigma \rangle}}$ and $k_\sigma^- = \frac{b_{1,\sigma} . b_{2,\sigma}}{\sqrt{1 - \langle M_\sigma \rangle}}$ where the mean values $\langle ... \rangle$ are taken with respect to the RPA vacuum: $Q_v |RPA\rangle = 0$. The obtained SCRPA system can be written in the form:

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

(9)

where the SCRPA matrix elements are given by:

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

and

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

With the orthonormality relations of the set $\{Q_v, Q_v^+\}$, we have:

$$A_{\uparrow\uparrow} = A_{\downarrow\downarrow} = A \quad \text{and} \quad A_{\downarrow\uparrow} = A_{\uparrow\downarrow} = A'$$
$$B_{\uparrow\uparrow} = B_{\downarrow\downarrow} = B \quad \text{and} \quad B_{\downarrow\uparrow} = B_{\uparrow\downarrow} = B'$$

3.2 Intersite interaction effect on dynamics:

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

$$H = H_{HF} + H_{k=0} + H_{k=-\pi} \quad \textbf{(10)}$$

where

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

The first term H_{HF} in eq (10) presents the Hamiltonian of our system in the HF approximation, where the HF ground state energy of system is $E_{HF} = -2.t + \frac{U + V_1 + V_2}{2}$, ε_1 and ε_2 are the excitation energies. The remain tem of (10) take into account

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

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

the correlation between the number operators of the type: $n_{k_i,\sigma} . n_{k_j,\sigma'}$ in the ground state: $k = 0$ (below the Fermi momentum) and between the magnetic moment operators of the type: $J_{\sigma}^{\pm} J_{\sigma'}^{\pm}$ in the excited state: $k = -\pi$ (above the Fermi momentum) where: $J_{\sigma}^{-} = b_{1,\sigma} . b_{2,\sigma}$, $J_{\sigma}^{+} = \left(J_{\sigma}^{-}\right)^{+}$ and $n_{k_i,\sigma} = b_{i,\sigma}^{+} . b_{i,\sigma}$

With the Hamiltonian given in eq (10), the SCRPA matrix elements are written as: $A = B + 2.t$, $A' = B'$, where:

$$A = 2.t + \left(U - V_2\right) . \sqrt{\frac{1 - \langle M_{\uparrow} \rangle}{1 - \langle M_{\downarrow} \rangle}} . \sum_{v} x_{\uparrow}^{v} (x_{\downarrow}^{v} + y_{\downarrow}^{v}) - \frac{V_1}{2} . \left(\frac{1}{1 - \langle M_{\uparrow} \rangle} - \sum_{v} \left((x_{\uparrow}^{v})^2 + (y_{\uparrow}^{v})^2 + 2 . x_{\uparrow}^{v} . y_{\uparrow}^{v} \right) \right)$$

and

(11)

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

where,

$$\langle M_{\sigma} \rangle = \frac{2 . \sum_{v} \left| y_{\sigma}^{v} \right|^2}{1 + 2 . \sum_{v} \left| y_{\sigma}^{v} \right|^2}$$

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 tow positive roots:

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

$$\varepsilon_2 = 2.t . \sqrt{\frac{A + A'}{t} - 1} \quad \textbf{(12)}$$

The corresponding eigenvectors are: $V_1 = \left[x_1, -x_1, y_1, -y_1\right]$] and $V_2 = \left[x_2, -x_2, y_2, -y_2\right]$, respectively ; where:

$$x_1 = -\frac{A - A' + \varepsilon_1}{A - A' - 2.t} y_1 \ ,$$

$$x_2 = -\frac{A + A' + \varepsilon_2}{A - A' - 2.t} y_2 \quad \textbf{(13)}$$

$$y_1 = -\sqrt{2 . \left(\frac{A - A' + \varepsilon_1}{A - A' - 2.t} \right)^2 - 2}$$

$$\text{and} \quad y_2 = -\sqrt{2 . \left(\frac{A + A' + \varepsilon_2}{A - A' - 2.t} \right)^2 - 2} \quad \textbf{(14)}$$

So, like the HF approximation; in ph-RPA approximation, our system has tow excitation energies ε_1 and ε_2, but they are coupled. It is necessary to construct a system of equations which must be solved numerically by iterations, leading to a SCRPA solutions which are quasi identical to the exact result. In figure 2 and 3 we plot the variation of the excitation energies as function of the repulsive intrasite

interaction U for different values of the intersite interaction V.

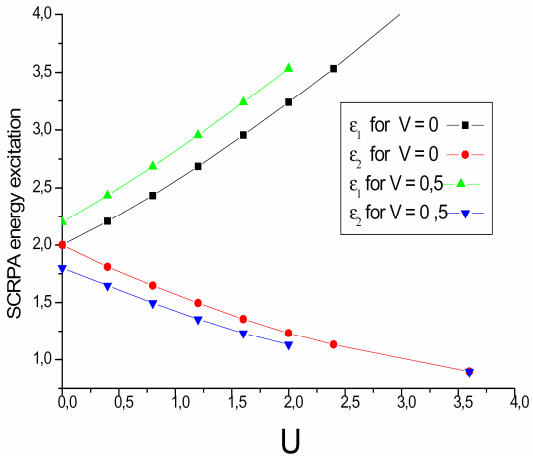

Figure 2: Excitation energies of SCRPA as function of intrasite interaction U for tow values of intersite interaction **V=0** and **V = + 0.5.t** (repulsive intersite interaction), where V = V_1+V_2 and **t =1**.

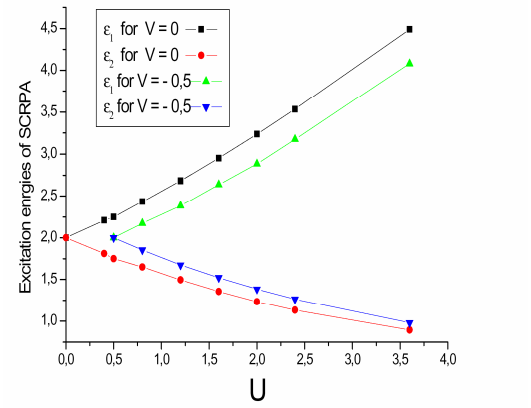

Figure 3: Excitation energies of SCRPA as function of intrasite interaction U for tow values of intersite interaction **V=0** and **V = - 0.5.t** (attractive intersite interaction), where V = V_1+V_2 and **t =1.**

The result shows that, when U increases, the gap $\Delta = \varepsilon_2 - \varepsilon_1$ between the two excitation energies increases, and so, the electrons have a more difficulties to jump between these two sites. These figures shows also, the intersite interaction effect on dynamics of electrons; for a fixed value of U, while the intersite interaction is repulsive (attractive), the gap Δ becomes more (less) important. These remarks allow supposing that the attractive interaction between the electrons of the neighbour's atoms is the origin of supplementary conductivity of the system.

4- Conclusion and perspectives:

In this work, the SCRPA approximation is used to resolve the extended Hubbard model given in eq (3). The SCRPA is extended to study the intersite interaction effects on dynamics of the electrons in the tow sites problem at half filling, with $\langle n_{i,\uparrow} \rangle = \langle n_{i,\downarrow} \rangle$. We showed that the gap between the excitation energies $\Delta = \varepsilon_2 - \varepsilon_1$ is correlated with the intersite interaction energy V_1 and V_2. When, we introduce a repulsive intersite interaction the gap $\Delta = \varepsilon_2 - \varepsilon_1$ becomes more important, but it becomes less important, when the intersite interaction is attractive. These results allow as supposing that the attractive interaction intersite (between the electrons of the neighbour's atoms) is the origin of a supplementary conductivity of the system, where, each electron help the other electrons to jump between different lattice sites. In future work, we propose to resolve this tow sites problem but with $\langle n_{i,\uparrow} \rangle \neq \langle n_{i,\downarrow} \rangle$ in order to exhibit the magnetic aspect of the extended Hubbard model on superconducting phenomena.

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