Extension of Self Consistent RPA method to off-site Hubbard Model

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We are interested in the possibility that a generalization of Self Consistent Random Phase Approximation (SCRPA) to the Extended Hubbard Model can lead us to accurate estimations of the ground state energy, for closed chains in one dimension with periodic boundary conditions: N=2 (two states problem). We have considered an extended Hubbard model including on-site and off-site interactions, we have compared the SCRPA with a Direct Analytical (DA) results for the ground state energy, and have shown that SCRPA solves the two states problem exactly for any value of U (on-site interaction energy), V_2 (off-site interaction energy with opposite spins) and V_1 (off-site interaction energy with same spins).

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I. INTRODUCTION:

In recent decades much attention has been paid to the physics of strongly correlated electron systems: cuprates [1,2], manganites [3,4,5]. The usual Hubbard model [6,7,8] is one of the simplest description of a system interacting electrons on lattice, with only two parameters: a hopping kinetic energy t, and an on-site interaction energy U. In order, to establish a solution of the self-consistent equations taking into account the correlations of type 2p-2h (two particles- two holes), Jemai and al [9] proposed the Self Consistent Random Phase Approximation (SCRPA). They used RPA method [10], and introduced the RPA excitation operators for (p-h), where the vacuum represents the ground state of the system. These
excitation operators are constructed from the linear combinations of pair operators (p-h). The quality of the SCRPA method to solve the usual Hubbard model for finite size system has been investigated in a previous work by Ref. [9], in which, the authors showed the remarkable agreement between the SCRPA and exact results for the usual Hubbard model.

To explain other physical phenomena observed in different areas of the solid state physics like magnetic and transport properties, an extended Hubbard Model is proposed [11,12] taking into account the off-site interaction, with two supplementary parameters: V_2 (off-site interaction energy with opposite spins), and V_1 (off-site interaction energy with same spins).

In this paper, we consider closed chains in one dimension with periodic boundary conditions, where each closed chain is organized alternately of two types of atoms noted "1" and "2". In order to enrich the physics of this system and to study the effect of the off-site interaction on the dynamics of our electrons system, we are interested in the possibility that a generalization of SCRPA method to the Extended Hubbard Model can lead us to accurate estimations of the ground state energy.

This paper is organized as follows. In sec.2, we present the theory and give the details of the calculation based on the minimization of the system energy, which lead us to non linear coupled equations. In sec.3, we present the SCRPA results and compare them with a Direct Analytical results.

II. THE EXTENDED HUBBARD HAMILTONIAN:

The extended Hubbard Hamiltonian is given by [11]:

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

The first term of the Eqs. (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 σ. $c^{+}_{i,\sigma}$ 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 on-site coulomb interaction with energy U, where $n_{i,\sigma}$ is the number operator of electrons at the site i with spin σ. $V_{ij}^{\sigma\sigma'}$ describes the effective off-site coulomb interaction between the electrons in the lattice sites i and j, with spin σ and σ' respectively. The off-site interaction energies $V_{ij}^{\sigma,\sigma}$ and $V_{ij}^{\sigma,-\sigma}$ are not necessary equal. The model (1) 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 [9].

In this work we will limit ourselves to a simplest case, and will apply the general formalism of SCRPA to the two states problem. We consider a closed chains in one dimension, with periodic boundary conditions, where our closed chain is organized with two types of atoms noted “1” and “2”.

The Hamiltonian of this physical system is [12,13]:

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

Where, V_1 is the off-site interaction energy with same spins and V_2 is the off-site interaction energy with opposite spins.

In order to apply the SCRPA method to the Extended Hubbard Model, we define the RPA excitation operator as [12]:

$$Q^{+}_{\nu} = \sum_{\sigma}(x^{\nu}_{\sigma}.J^{+}_{\sigma} - y^{\nu}_{\sigma}.J^{-}_{\sigma}) \quad (3)$$

Where J^{+}_{σ} (J^{-}_{σ}) is the creation (annihilation) operator of pair: particle-hole. The Eqs. (3) shows that the excitation in the ph-RPA is done only by the creation and (annihilation) of pair: particle-hole via the operator J^{+}_{σ} and (J^{-}_{σ}) with the amplitude x^{ν}_{σ} and (y^{ν}_{σ}). The excited states are defined as: $|\nu\rangle = Q^{+}_{\nu}|RPA\rangle$, and the correspondent excitation energy is:

$$\varepsilon_{\nu} = \frac{\langle RPA|\left[Q_{\nu},\left[H,Q^{+}_{\nu}\right]\right]|RPA\rangle}{\langle RPA|\left[Q_{\nu},Q^{+}_{\nu}\right]|RPA\rangle} \quad (4)$$

The minimization of ε_{ν} leads to the usual RPA equations, with the form:

$$\begin{pmatrix} A_{\uparrow\uparrow} & A_{\uparrow\downarrow} & B_{\uparrow\uparrow} & B_{\uparrow\downarrow} \\ A_{\downarrow\uparrow} & A_{\downarrow\downarrow} & B_{\downarrow\uparrow} & B_{\downarrow\downarrow} \\ -B_{\uparrow\uparrow} & -B_{\uparrow\downarrow} & -A_{\uparrow\uparrow} & -A_{\uparrow\downarrow} \\ -B_{\downarrow\uparrow} & -B_{\downarrow\downarrow} & -A_{\downarrow\uparrow} & -A_{\downarrow\downarrow} \end{pmatrix} \begin{pmatrix} x^{\nu}_{\uparrow} \\ x^{\nu}_{\downarrow} \\ y^{\nu}_{\uparrow} \\ y^{\nu}_{\downarrow} \end{pmatrix} = E_{\nu} \begin{pmatrix} x^{\nu}_{\uparrow} \\ x^{\nu}_{\downarrow} \\ y^{\nu}_{\uparrow} \\ y^{\nu}_{\downarrow} \end{pmatrix} \quad (5)$$

Where, the SCRPA matrix elements are given by:

$$A_{\sigma\sigma'} = \frac{1}{\sqrt{1-\langle M_{\sigma}\rangle}\sqrt{1-\langle M_{\sigma'}\rangle}}\left\langle\left[J^{-}_{\sigma},\left[H,J^{+}_{\sigma'}\right]\right]\right\rangle$$

$$B_{\sigma\sigma'} = \frac{1}{\sqrt{1-\langle M_{\sigma}\rangle}\sqrt{1-\langle M_{\sigma'}\rangle}}\left\langle\left[J^{-}_{\sigma},\left[H,J^{-}_{\sigma'}\right]\right]\right\rangle$$

M_{σ} is the total number of quasi-particles. Where the mean values $\langle ... \rangle$ are taken with respect to the RPA vacuum. With the orthonormality relations of the set $\{Q_{\nu};Q^{+}_{\nu}\}$, we have:

$$A_{\uparrow\uparrow} = A_{\downarrow\downarrow} = A \quad , \quad A_{\uparrow\uparrow} = A_{\downarrow\downarrow} = A \quad ,$$

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

With the Hamiltonian (2), we can write the SCRPA matrix elements as: $A = B + 2t$ and $A' = B'$, where:

$$A = 2.t + (U - V).\sqrt{\frac{1-\langle M_{\uparrow}\rangle}{1-\langle M_{\downarrow}\rangle}}.\sum_{\nu} x^{\nu}_{\uparrow}(x^{\nu}_{\downarrow} + y^{\nu}_{\downarrow}) \quad (6)$$

$$A' = \frac{U-V}{2}.\frac{1}{1-\langle M_{\sigma}\rangle} \quad (7)$$

With

$$\langle M_{\sigma}\rangle = \frac{2.\sum_{\nu}\left|y^{\nu}_{\sigma}\right|^2}{1+2.\sum_{\nu}\left|y^{\nu}_{\sigma}\right|^2} \quad (8)$$

The ph-RPA matrix has two positive roots:

$$\varepsilon_1 = 2t\sqrt{\frac{A-A'}{t}-1} \ , \ \varepsilon_2 = 2t\sqrt{\frac{A+A'}{t}-1} \quad (9)$$

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

$$x_1 = -\frac{A-A'+\varepsilon_1}{A-A'-2t}y_1 \ , \ y_1 = -\sqrt{2\left(\frac{A-A'+\varepsilon_1}{A-A'-2t}\right)^2 - 2} \quad (10)$$

$$x_2 = -\frac{A + A' + \varepsilon_2}{A - A' - 2t} y_2 \ , \ y_2 = -\sqrt{2\left(\frac{A + A' + \varepsilon_2}{A - A' - 2t}\right)^2 - 2} \quad (11)$$

Finally, we define the ground state energy as: $E_{SCRPA} = \langle RPA | H | RPA \rangle$. With, the condition $Q_v | RPA \rangle = 0$, one can find that:

$$E_{SCRPA} = E_{HF} + t\sum_{\sigma} \langle M_{\sigma} \rangle + (-\frac{U}{2} + V).\langle (J_{\uparrow}^{-} + J_{\uparrow}^{+})(J_{\downarrow}^{-} + J_{\downarrow}^{+}) \rangle \quad (12)$$

Where

$$\langle J_{\sigma'}^{+} J_{\sigma}^{-} \rangle = \sqrt{\langle 1 - M_{\sigma'} \rangle . \langle 1 - M_{\sigma} \rangle} \sum_{v} y_{\sigma'}^{v} . y_{\sigma}^{v} \quad (13)$$

$$\langle J_{\sigma'}^{-} J_{\sigma}^{+} \rangle = \sqrt{\langle 1 - M_{\sigma'} \rangle . \langle 1 - M_{\sigma} \rangle} \sum_{v} x_{\sigma'}^{v} . x_{\sigma}^{v} \quad (14)$$

$$\langle J_{\sigma'}^{+} J_{\sigma}^{+} \rangle = \sqrt{\langle 1 - M_{\sigma'} \rangle . \langle 1 - M_{\sigma} \rangle} \sum_{v} y_{\sigma'}^{v} . x_{\sigma}^{v} \quad (15)$$

$$\langle J_{\sigma'}^{-} J_{\sigma}^{-} \rangle = \sqrt{\langle 1 - M_{\sigma'} \rangle . \langle 1 - M_{\sigma} \rangle} \sum_{v} x_{\sigma'}^{v} . y_{\sigma}^{v} \quad (16)$$

In order to analyze the behaviour of E_{SCRPA} as function of the local parameters of our system: U, V_1 and V_2, it is necessary to solve a system of fourteen coupled equations (Eqs. 6, 7, ….,16). Thus, we solve this system of coupled equations numerically by iteration leading to a SCRPA solution.

III. RESULTS AND DISCUSSIONS:

In this section, we present our SCRPA results for the ground state energy and compare them with a Direct Analytical ground state energy given by [15]:

$$E_{DA} = (-2t + \frac{V_1}{2}).\cos(2\phi) + \frac{U}{2}(1 - \sin(2\phi)) + \frac{V_2}{2}(1 + \sin(2\phi)) \quad (17)$$

Where

$$\phi = \arctan(\frac{U - V_2}{4t + \sqrt{(U - V_2)^2 + 16t^2}})$$

In Fig.1 the ground state energy of the SCRPA and the DA methods are shown as function of the on-site interaction energy U for $V_1 = V_2 = 0$ (case of usual Hubbard model). In Ref [4], the authors show that the agreement between the SCRPA and exact results is very good for any value of U. They deduce that the SCRPA method solves exactly the Usual Hubbard Model for the two states problem.

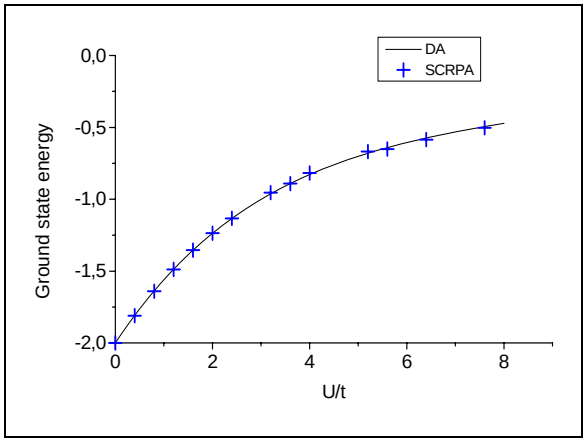

FIG.1: Ground state energy of SCRPA and DA methods as function of on-site interaction energy for $V_1 = V_2 = 0$

In order to test the efficiency of the SCRPA method in the resolution of the extended Hubbard model with off-site interaction, we compare in the following the variation of SCRPA and DA results for the ground state energy as function of V_1 and V_2. In Fig.2 (Fig.3) we take $V_1 = 0$ ($V_2 = 0$), and we plot the variation of SCRPA and exact results for the ground state energy as function of V_2 (V_1) at $U = 2.t$.

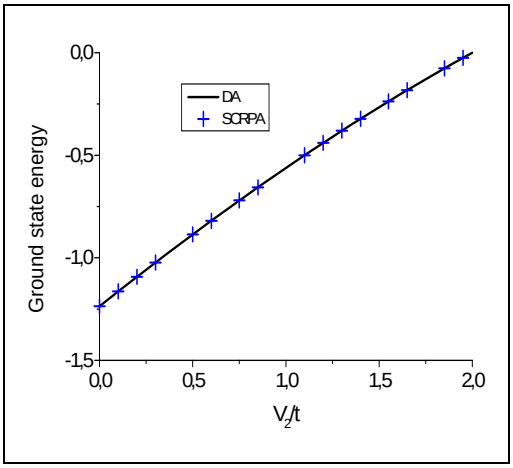

FIG.2: Ground state energy of SCRPA and DA methods as function of off-site interaction energy V_2 / t for $U / t = 2$ and $V_1 = 0$

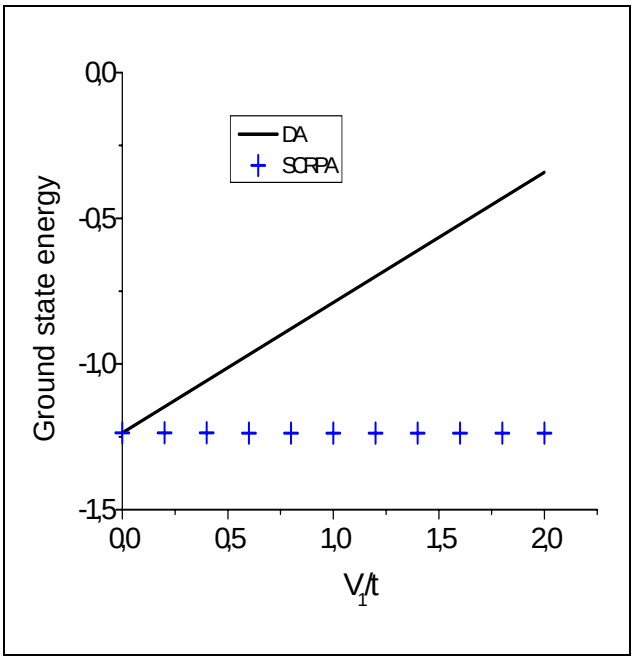

FIG.3: Ground state energy of SCRPA and DA methods as function of off-site interaction energy V_1 / t for $U / t = 2$ and $V_2 = 0$

The SCRPA and the DA ground state energy are practically equal for any value of V_2 . But, if we take into account the off-site interaction with same spins ($V_1 \neq 0$), we will have a dramatic divergence between the SCRPA and the DA method. The DA ground state energy increases with V_1, whereas the SCRPA ground state energy remains practically constant for any value of V_1. Thus, we can conclude that the SCRPA is more rigorous than the DA method, knowing that the half- filled Hubbard Model in 1D have always an anti-ferromagnetic nature: $\langle n_{1\uparrow} n_{2\uparrow} \rangle \neq 0$, since the hopping between neighbouring sites is inhibited by the Pauli principle if the electronic spins on these two sites are pointing in the same direction. Therefore, the third term of the Hamiltonian 2 hasn't practically any effect on the dynamics of electrons and thus the ground state energy of our system is U independent.

IV- CONCLUSION:

In this work, the SCRPA approximation is used to solve the Extended Hubbard Model given in Eqs. 1, we are interested in the possibility that a generalization of SCRPA to the Extended Hubbard Model can lead us to accurate estimations of the ground state energy, for closed chains in one dimension with periodic boundary conditions for the two states problem. We have compared the SCRPA results with ones obtained by an exact analytical approach, we have shown that the SCRPA method solves the two states problem exactly for any value of U (on-site interaction energy), V_2 (off-site interaction energy with opposite spins) and V_1 (off-site interaction energy with same spins). In future work, we propose to solve the 4-sites case for the two dimensional Extended Hubbard Model and discuss the V effect on the dynamics of this system 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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