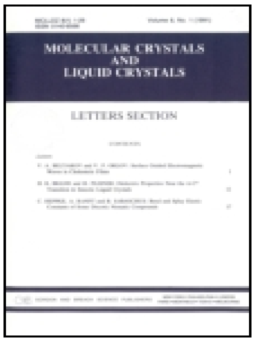

Molecular Crystals and Liquid Crystals

ISSN: 1542-1406 (Print) 1563-5287 (Online) Journal homepage: http://www.tandfonline.com/loi/gmcl20

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MOL. CRYST. LIQ. CRYST.
2016, VOL. 628, 162–166
http://dx.doi.org/10.1080/15421406.2015.1137123

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Charge and magnetic properties of 2D extended Hubbard model

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ABSTRACT
The ground state of the two-dimensional Extended Hubbard Model is studied within an exact analytical diagonalization. The Charge and magnetic properties are determined by analyzing the behaviour of charge gap and spin gap as a function of on-site coulomb interaction energy *U* and spin-spin interaction term *J*. The obtained results showed that the introduction of long-range off-site interactions induces a vanishing of charge gap and a *J* independency of spin gap.

KEYWORDS
Extended Hubbard model; Spin-spin interaction; off-site coulomb interaction

1. Introduction

The Hubbard model is one of the most fundamental models in condensed matter physics. It offers simple way to get insight into how the interactions between electrons can give rise to insulating [1–4], magnetic [5, 6[, and high T_c superconducting [7–9] effects in a solid.

The Hubbard model was originally proposed to describe correlations between d-electrons in transition metals Hubbard [10, 11]. In its usual Hamiltonian, the Hubbard model exhibits the competition between localization and non-localization terms.

$$H_0 = \sum_{i,j,\sigma} t_{ij} c^{+}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

The first term in H_0 represents the kinetic energy of electrons, where, each electron has a possibility of hopping between different lattice sites. In second quantized, $c_{\mathrm{i},\sigma}{}^{+}$and $c_{\mathrm{i},\sigma}$ are, respectively, the creation and annihilation operators of electrons at a lattice site i with spin σ, whereas t_{ij} is the hopping term from the site j to the site i. For correlated electrons system, t_{ij} decreases rapidly with intersite distance. Thus, one can suppose that $\mathrm{t}_{\mathrm{i}\,\mathrm{j}} = -\mathrm{t}$ for nearest neighbour sites and $t_{ij} = 0$ otherwise. The second term represents the on-site coulomb interaction with energy U, where $n_{i,\sigma} = c^{+}_{i,\sigma} c_{j,\sigma}$ is the number operator of electrons at the site i with spin σ.

In spite of its simple description of describing electrons system dynamic, the model can capture many interesting properties of strongly correlated systems. For instance, at half-filling,

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the competition between t and U gives a possibility to have a phase transition between conductor and insulator phases at a critical value $U_c = 2t$ and $U_c = 4t$for $1D$ and $2D$electrons system, respectively.

To explain some other phenomena manifested in correlated electrons system, many extensions of Hubbard model was proposed in the last three decades. For instance, an extension of Hubbard Model with long-range coulomb interaction allowed describing $2D$ high T_c superconductivity. Whereas, an extension of Hubbard model with spin-spin interaction allowed describing the low-energy spin excitations in correlated electronic systems [12, 13, 14].

In this paper we study some magnetic and charge properties of the $2D$ Extended Hubbard Model at one-eighth filling using an exact diagonalization for finite square lattice with periodic boundary conditions. The remainder of the paper is organized as follows. The considered model and the diagonalization procedure are presented in Sec. II. The behaviours of charge gap and spin gap are given in Sec. 3. Finally, the main results are summarized in the conclusion.

2. Model and formalism

As mentioned in the introduction, we will consider an Extended Hubbard Model with taking into account two types of long-range interactions

$$H = H_0 + J\sum_{\langle i,j\rangle} S_i S_j + \sum_{i,j,\sigma} V_{ij} n_{i,\sigma} n_{i,\sigma}$$

The term $J\sum_{\langle i,j\rangle} S_i S_j$ takes into account the spin-spin interaction with exchange energy J, where S_i is $S = \frac{1}{2}$ quantum spin operator at the site i. The last term of the Hamiltonian takes into account the nonlocal repulsive interaction, where V_{ij} denotes the interaction energy between two electrons in the lattice sites i and j. This nonlocal repulsive interaction is purely coulombic, we can pu

$V_{ij} = \frac{V}{|\overrightarrow{R_i} - \overrightarrow{Rj}|}$, where V is the interaction energy between the first nearest neighboring sites and $\overrightarrow{R_i} - \overrightarrow{Rj}$ is the intersite distance.

To study the charge and spin gap of the $2D$ Extended Hubbard Model at one-eight filling, we diagonalize the model for square supercells of $4 \times L_y$. In order to probe correlations at long range, our largest system size simulated in this diagonalization is $N_s = 4096$.

In the case of ferromagnetic correlated electrons system, all possible states can be described by the configuration $|a\rangle = \prod_{i=1}^{N_S/4} c^{+}_{i,\sigma}|0\rangle$ where $|0\rangle$ represents the vacuum state with no electrons present. Whereas, in the case of antiferromagnetic correlated electrons system, the possible states can be described by three types of configuration $|b\rangle$, $|c\rangle$and $|d\rangle$ (For more details, see Ref. [15].).

Finally, we define the matrix energy as: $E_{nm} = \langle n|H|.m\rangle$. where $|n\rangle$ and $|n\rangle$ are two vectors of the r-space basis engendered by the family of states$|a\rangle$, $|b\rangle$, $|c\rangle$ and $|d\rangle$. The diagonalization of the matrix energy allows us to determine, numerically, the eigenvalues and the eigenvectors of this matrix.

3. Results and discussion

To analyse the spin–spin interaction effect on charge properties of our considered system, we define the charge gap as the difference between the first excited state energy E^* and the ground

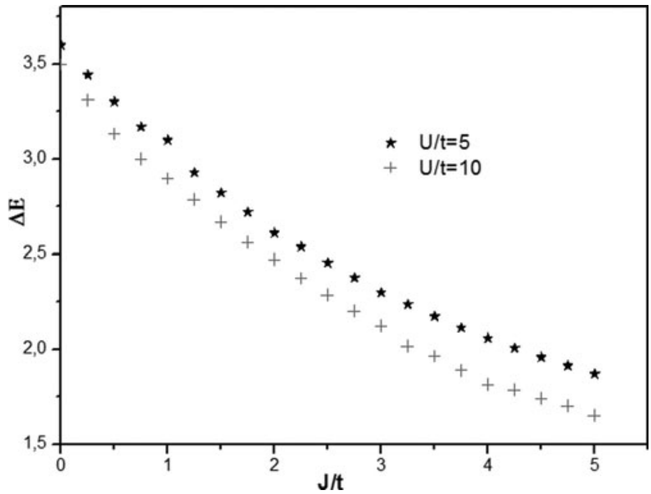

Figure 1. Charge gap ΔE as a function of *J/t* for two values of *U/t*.

state energy E_{GS}.

$$\Delta E = E^* - E_{GS}$$

First, we neglect the off-site interactions, and, we plot the variations of charge gap ΔE as a function of the exchange energy J for different values of U with $V = 0$ (See Fig. 1).

At a fixed value of U, the curves show that the charge gap decreases with$J$. Thus, the introduction of spin–spin interactions induces a supplementary conductivity of this $2D$ electrons sytem. Moreover, the fitting of the curves confirms that the charge gap has an exponential J dependency,

$$\Delta E = \Delta E_0 e^{-J/J_C}$$

The characteristic parameter J_c is proportional to the system's temperature T ($J_c \propto T$). The comparison between different values of J_c for the two curves shows that J_c decreases with U. Thus, we can deduce that the repulsive on-site interaction becomes more important at low temperatures.

Then, we plot, the variations of charge gap ΔE as a function of the exchange energy J for pure Nearest-Neighbor (NN) interaction case and more than NN interactions case.

At a fixed value of J, the introduction of off-site interactions induces an important reduction of charge gap ΔE, where it tends to a constant value Δ_0. Especially, with long-range off-site interactions, the charge gap vanishes ($\Delta_0 = 0$) even for intermediate values of J. Thus, the repulsive off-site interaction increases the conductivity of system. Moreover, with interactions exceeding NN distances in range, this gap vanishes, where each electron can jump between different sites without any loss of energy.

In order to study some magnetic properties of the considered system, one can define the spin gap as:

$$\Delta S = E_{GS}\,(N_e;\, S_{tot} = N_e/2) - E_{GS}\,(N_e;\, S_{tot} = 0)$$

Where $E_{GS}(N_e;\, S_{tot} = N_e/2)$ and $E_{GS}(N_e;\, S_{tot} = 0)$ are, respectively, the ground state energy of N_e electrons system with total spin $N_e/$ 2and 0.

In Fig. 3, the variations of spin gap ΔS are shown as a function of the spin-spin interaction J at intermediate on-site interaction site ($U/t = 5$) for three cases.

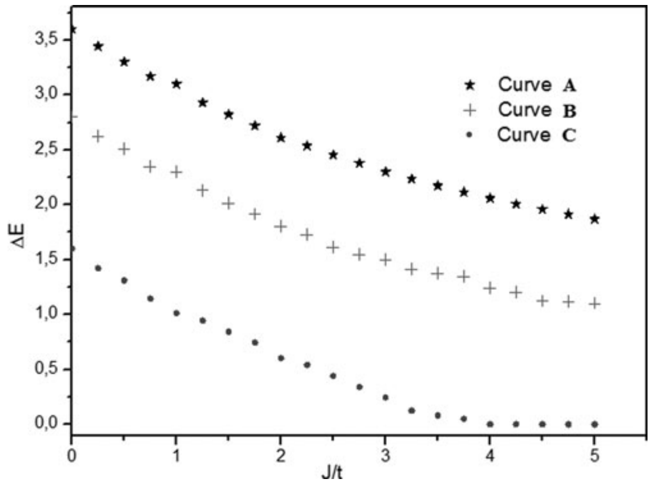

Figure 2. Charge gap ΔE as a function J/t at $U/t = 5$ and $V/t = 1$ (Curve A: without off-site interaction, Curve B: with NN off-site interaction, Curve C: with more than NN off-site interactions).

First, we neglect the off-site interactions $V/t = 0$, the corresponding curve (curve A) shows that the spin gap has a linear J dependency. The fitting of this curve gives $\Delta S \cong \alpha J + \beta$, where $\alpha = 0.2004$ and $\beta = 1.5121$. We deduce that the exchange energy J induces supplementary spin fluctuations of the considered system. Then, we introduce the first off-site interaction $(V \succ 0)$, and we plot the curve B which gives the variation of spin gap ΔS as a function of J with the nearest-neighbour (NN) off-site interactions only. The obtained result shows that the J effect becomes less remarkable, since the fitting of this curve gives $\Delta S \cong \alpha' \, J + \beta'$, where $\alpha' = 0.1214 \prec \alpha$ and $\beta\prime = 1.4215 \prec \beta$. Finally, in the third case, we plot the variation of spin gap ΔS as a function of J with more than NN off-site interactions. The corresponding curve (curve C) shows that ΔS becomes J independent, where it equal to $\Delta S \cong 1.39$ for any value of J. Thus, we deduce that the off-site interactions exceeding NN distances in range allow to the spin fluctuations become J independent.

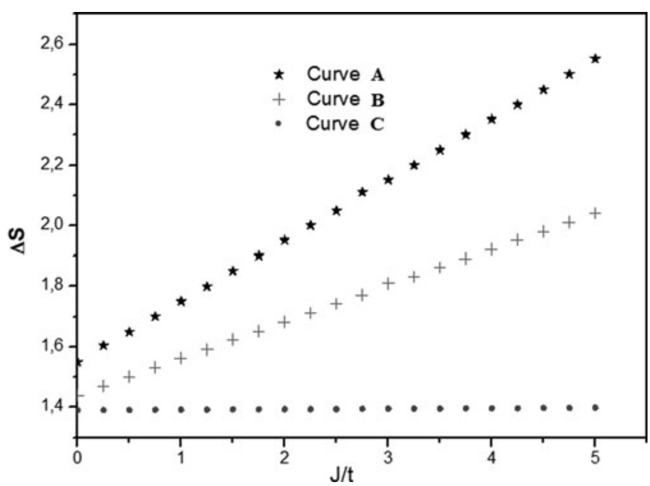

Figure 3. Spin gap ΔS as a function of J/t at $U/t = 5$ and $V/t = 1$ (Curve A: without off-site interaction, Curve B: with NN off-site interaction, Curve C: with more than NN off-site interactions).

4. Conclusion

In the present paper, we have studied the charge and magnetic properties of the t-U-V-J extended Hubbard model at one eight-filling by using an exact diagonalization for square supercells of $N_s = 4 \times L_y$ sites, where, our largest system size simulated in this diagonalization has $N_s = 4096$ sites. The behaviors of charge and spin gaps have been determined in the parameter space of the on-site Coulomb repulsion U, long-range Coulomb interactions V_{ij} and spin-spin interaction energy J.

For usual Hubbard model with on-site interaction only ($V_{ij} = 0$), the obtained results have shown that the charge gap ΔS has an exponential J dependency. The analysis of this dependency allowed us to deduce that the on-site interaction energy U decreases with the temperature of the considered electrons system. But, for an extended Hubbard model with long-range off-site interactions ($V_{ij} \neq 0$) we have found that the charge gap decreases rapidly with J where it vanishes from $J = 4t$. Finally, the magnetic properties of our considered system are studied by analyzing the behaviour of spin gap ΔS as a function of J. The obtained results showed that ΔS has a linear J dependency for usual Hubbard model. Whereas, it becomes J independent for extended Hubbard model with long-range off-site interactions.

In conclusion, the vanishing of ΔE means that the off-site interactions exceeding NN distances in range induces a supplementary conductivity of the considered electrons system, where each electron can jump between different sites without any loss of energy. Moreover, the J independency of ΔS means that spin fluctuations become quasi-inexistent after taking into account this long-range off-site interactions.

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