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Spin–spin interaction effect in 2D Extended Hubbard Model

A. Zouhair [a], S. Harir [a,b,*], M. Bennai [a], Y. Boughaleb [a,c,d]

[a] Laboratoire de Physique de la Matière Condensée (URAC10), Faculté des Sciences Ben M'Sik, Université Hassan II-Mohammedia Casablanca, Morocco
[b] Département de Physique-Chimie, Centre Régional des Métiers, de l'éducation et de la Formation, Settat, Morocco
[c] Ecole Normale Supérieure, Université Hassan II, Casablanca, Morocco
[d] Hassan II Academy of Sciences and Technology, Morocco

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ABSTRACT

Using an exact diagonlization for finite square lattice and taking into account the periodic boundary conditions in the two directions, we study the spin–spin interaction effect on some local electronic properties for antiferromagnetic correlated electrons system. We have considered an Extended Hubbard Model (EHM) including on-site coulomb interaction energy U and spin–spin interaction term J. The diagonlization of this 2D EHM model allows us to study J effect on some local properties for finite square lattice. The analysis of the obtained results shows that the introduction of spin–spin interaction induces a supplementary conductivity for antiferromagnetic correlated electrons system, even in the strong on-site interaction regime.

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1. Introduction

To understand the electronic correlations and spin–spin interactions effects in strongly correlated electronic systems, is considered as one of the most challenging problems in condensed matter [1]. In spite of intensive research during the last decades [2–6], there is no consensus on a possible

* Corresponding author at: Laboratoire de Physique de la Matière Condensée (URAC10), Faculté des Sciences Ben M'Sik, Université Hassan II-Mohammedia Casablanca, Morocco. Tel.: +21 2613865489.
E-mail address: harirsaid@gmail.com (S. Harir).

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mechanism for certain new phases that are found from time to time. In this context, the Hubbard model is one of the most fundamental models able to describe some complex phase diagrams observed in solid-state materials [7–9].

In its simplest form, the Usual Hubbard model [10] is based on approximating the electron–electron Coulomb interaction by an on-site repulsion U between electrons of opposite spin. In spite of this severe approximation, the resulting Hamiltonian captures many aspects of strong correlations, including the Mott transition [11] at half filling in 1D and the high superconductivity in 2D [12].

Very recently, many works show that some magnetic and electronic properties of strongly correlated electrons systems are strongly related to spin–spin interactions [13,14]. Moreover, recent experimental studies of electron and spin-excitation spectra using angle-resolved photoemission (ARPES) have revealed an important role of antiferromagnetic (AF) spin excitations in the d-wave pairing in high T_c superconductors [15]. Thus, to explain other magnetic properties observed in different areas of the solid state physics, an EHM is proposed taking into account the spin–spin interaction.

In an earlier work [16], we have studied spin–spin interaction effect on some local magnetic properties of an EHM for 2D ferromagnetic correlated electrons system. Our proposed numerical diagonalization allowed us to discuss the behavior of ground-state energy E_{GS}, spin gap ΔS and spin correlation function f_c as a function of off-site interaction energy V and spin–spin interaction term J. The obtained results showed the existence of competition between Spin Density Wave (SDW) and Charge Density Wave (CDW). Especially, for $J \neq 0$, the spin correlation function decreases with V, where it vanishes at critical value V_c.

In the context of continuing in the same direction, in this actual paper, we purpose to study spin–spin interaction effect on other local electronic properties of 2D antiferromagnetic correlated electrons system. The paper is organized as follows. In Section 2, we present the considered EHM and the diagonalization procedure adapted for it. In Section 3, we present the obtained results for some local electronic properties, where we have discussed the spin–spin interaction effect on our considered system. Finally, in Section 4 we give our conclusions.

2. Model and formalism

To take into account electronic repulsion and spin spin interaction, an Extended Hubbard Model is defined by the second quantized Hamiltonian:

$$H = -t\sum_{\langle i,j\rangle,\sigma} c^{+}_{i,\sigma}c_{j,\sigma} + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow} + J\sum_{\langle i,j\rangle} S_iS_j$$

The first term of this Hamiltonian represents the kinetic energy of electrons, where each electron has a possibility of hopping to nearest neighbor sites with hopping term t. $c^{+}_{i,\sigma}$ and $c_{i,\sigma}$ are the creation and annihilation operators of electron of a lattice site i with spin σ, respectively. Noticing that $\langle i,j\rangle$ runs over nearest neighbor sites. The second term represents local repulsion with on-site coulomb energy U, whereas $n_{i,\sigma} = c^{+}_{i,\sigma}c_{i,\sigma}$ is the number operator of electrons at the site i with spin σ. The last term takes into account the spin spin interaction with exchange energy J. S_i is $S = 1/2$ quantum spin operator on the site i.

The considered system consists of N_e electrons on N_S atomic sites of 2D square lattice at one-eighth filling $\left(\frac{N_e}{N_S} = 1/4\right)$. In the weak concentration case, many experimental studies show that the 2D correlated electrons systems can be grated in regular squares with finite size.

With this manner, one can perform a numerical diagonalization for 4×4 square lattice occupied by four electrons, in first steep. Then, it is possible to generalize this diagonalization to our considered system taking into account the periodic boundary conditions in both directions.

In the case of antiferromagnetic correlated electrons system, we have $S_{tot} = 0$. In this case, three types of particle configuration may occur for each 4×4 square lattice. Firstly, we can have two double occupancies at sites i and j ($i \neq j$). Secondly, we may have a double occupancy at site i and two electrons with opposite spins at sites j and k ($i \neq j \neq k$). Finally, we may have four single occupancies placed on different sites of this 4×4 square lattice. These three possible configurations give $N_d = \frac{16\times15\times16\times15}{4!}$ states. As mentioned in Ref. [17], one can regroup these N_d states in 85 cluster states.