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Hubbard pair cluster in the external fields. Studies of the polarization and susceptibility

T. Balcerzak, K. Szałowski *

Department of Solid State Physics, Faculty of Physics and Applied Informatics, University of Łódź, ulica Pomorska 149/153, 90-236 Łódź, Poland

HIGHLIGHTS

- Magnetoelectric effect is discussed in Hubbard model for a dimer (pair cluster).
- Exact diagonalization method is applied within grand canonical ensemble.
- Magnetic and electric polarization are investigated in external electric and magnetic field.
- Anomalous behaviour of polarizations vs. temperature near the critical magnetic field is shown.
- Discontinuous transitions caused by the fields are found at the ground state.

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ABSTRACT

The electric and magnetic polarizations as well as the electric and magnetic susceptibilities of the Hubbard pair-cluster embedded in the external fields were studied by the exact method. Based on the grand canonical ensemble for open system, the numerical calculations were performed for the electron concentration corresponding to the half-filling case. It has been found that the electric and magnetic properties are strictly interrelated, what constitutes a manifestation of a magnetoelectric effect, and the detailed explanation of such behaviour was given. In particular, near the ground state where the transitions are induced by the external fields, discontinuous changes of the studied quantities have been found. They have been associated with the occurrence of the singlet–triplet transitions. An anomalous behaviour of the electric and magnetic polarizations as a function of the temperature, occurring below the critical magnetic field, was illustrated. In the presence of the competing electric and magnetic fields, the influence of Coulombic repulsion on the studied properties was discussed.

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1. Introduction

The Hubbard model, since its formulation [1–4], has been intensively studied by the solid state physicists. Being the first model capable to describe the metal–insulator (Mott) transition, it has also been studied in relation to such problems as the magnetic phase transitions, high-temperature superconductivity, optical lattices and graphene properties [5–47].

Despite numerous theoretical efforts, the rigorous solutions to the Hubbard model for infinite systems have been obtained in very few cases only. The exact results include, for instance, the solution for one-dimensional (1D) system [11,12,31,32] as well as several rigorous theorems, to mention Mermin–Wagner theorem in 2D systems [36,37,43] or Lieb theorems for the ground state [30].

* Corresponding author.
E-mail addresses: t_balcerzak@uni.lodz.pl (T. Balcerzak), kszalowski@uni.lodz.pl (K. Szałowski).

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At the same time, it has been noticed that the exact solutions to the model can be obtained for small clusters, consisting of several lattice sites [48–83]. Intensive investigations of such systems have been carried out both from the point of view of static properties [48–50,52,58,62,64,66,67,70–72,74–79,81,82,84–88], as well as for dynamical description [54,59,61,69,80,83]. In case of very small atomic clusters, exact results for the Hubbard model have been obtained by analytical methods [48–50,52,54,62,66,67,70,72–74,78,79,81,83,84]. However, for larger clusters the numerical techniques turned out to be indispensable [58,64,65,71,75–77,82]. It is worth mentioning that theoretical studies of finite clusters are becoming increasingly important for the development of experimental nanophysics and nanotechnology.

The simplest system, for which the Hubbard model can be solved analytically, is a two-site atomic cluster (dimer). Despite many theoretical works, the system has not been fully examined yet. For instance, this concerns the case when the two-site cluster is simultaneously embedded in two external fields: magnetic and electric one, and is able to exchange the electrons with its environment. Such a system can model a physical situation where the atomic dimer is deposited on the surface and interacts both with the surface and the external fields. The influence of the electric field, acting as a control factor, on the magnetic properties of the cluster constitutes a manifestation of magnetoelectric effect and is very interesting from the point of view of possible application, for instance, in spintronics and/or memory devices. Some examples can be recalled here, mainly to mention the molecular dimer systems. Among them molecular mixed-valence dimers [89–94] or κ-(BEDT-TTF) [95] focus particular attention and appear highly promising; however, also some non-molecular systems such as dimers on graphene surface [96] also attract the interest.

The theoretical studies of two-atomic Hubbard cluster, treated as a thermodynamic open system and placed simultaneously in two external fields, have been initiated in the papers [66,67]. In Ref. [66] the main formalism has been presented and thorough investigations of the chemical potential have been carried out. On this basis, in the paper [67] the studies have been extended to magnetic properties, concentrating mainly on the phase diagrams, cluster magnetization, spin–spin correlation functions and mean hopping energy.

The aim of the present work is a continuation of these studies, basing on the formalism developed in Ref. [66], towards elucidation of interesting interrelations between magnetic and electric properties for the Hubbard dimer exhibiting a non-trivial magnetoelectric behaviour. In particular, the electric polarization of the cluster, as well as the electric susceptibility in the external fields will be studied. Simultaneously, the magnetic polarization and magnetic susceptibility will be analysed. A comparison of the magnetic and electric properties will be done, which seems interesting not only from the purely theoretical point of view for this model. In our opinion, the magnetoelectric correlations existing between the described measurable quantities may be also of practical interest, giving the possibility of controlling the magnetic state of the cluster by the electric potential.

The paper is organized as follows: In the theoretical Section 2 the model is briefly presented and the basic quantities, important for numerical calculations, are defined. In the successive Section 3 the numerical results are illustrated in figures and discussed. An extensive comparison of magnetic and electric properties is performed there. The last Section 4 is devoted to a brief summary of the results and concluding remarks. The Appendix collects the expressions for the eigenenergies corresponding to the quantum states with two electrons per dimer and shows the behaviour of these states as a function of the electric and magnetic field.

2. Theoretical model

The Hamiltonian of the Hubbard pair-cluster (dimer) consisting of (a, b) atoms and interacting with the external fields is assumed in the form:

$$\begin{aligned}\mathcal{H}_{a,b} = &-t\sum_{\sigma=\uparrow,\downarrow}\left(c^{+}_{a,\sigma}c_{b,\sigma}+c^{+}_{b,\sigma}c_{a,\sigma}\right)+U\left(n_{a,\uparrow}n_{a,\downarrow}+n_{b,\uparrow}n_{b,\downarrow}\right)\\ &-H\left(S^{z}_{a}+S^{z}_{b}\right)-V\left(n_{a}-n_{b}\right),\end{aligned} \tag{1}$$

where $t > 0$ is the hopping integral and $U \geq 0$ is the on-site Coulomb repulsion parameter. The symbol $H = -g\mu_{\mathrm{B}}H^{z}$ stands for an external uniform magnetic field H^{z} oriented along z-direction. The term with V introduces the potential energy of the atoms a and b in the electric field. For such potential distribution the external electric field E is oriented along the pair and is equal to $E = 2V/(|e|d)$ with d being the interatomic distance, whereas e is the electron charge. For the sake of simplicity, we assume that the hopping integral is a constant parameter, independent on the external fields.

In Hamiltonian (1), $c^{+}_{\gamma,\sigma}$ and $c_{\gamma,\sigma}$ are the electron creation and annihilation operators, respectively, and σ denotes the spin state. The on-site occupation number operators for given spin, $n_{\gamma,\sigma}$, are expressed by $n_{\gamma,\sigma} = c^{+}_{\gamma,\sigma}c_{\gamma,\sigma}$. The z-component of the electron spin on given atom, S^{z}_{γ}, is then defined as $S^{z}_{\gamma} = \left(n_{\gamma,\uparrow} - n_{\gamma,\downarrow}\right)/2$. In turn, the total occupation number operators n_{γ} for site $\gamma = a, b$, are defined as a sum of occupation operators for given spin, $n_{\gamma} = n_{\gamma,\uparrow} + n_{\gamma,\downarrow}$.

Because of treating the pair-cluster as an open electron system within the formalism of grand canonical ensemble, the Hamiltonian should be extended by the chemical potential term, i.e., $\mathcal{H}_{a,b} - \mu\left(n_{a} + n_{b}\right)$ is considered, where μ is the chemical potential. The exact analytical diagonalization of the extended Hamiltonian has been performed in Ref. [66]. As a result, not only the statistical, but also thermodynamic properties can be calculated exactly. In particular, the grand thermodynamic potential $\Omega_{a,b}$ has been obtained in the form:

$$\Omega_{a,b} = -k_{\mathrm{B}}T\ln\mathcal{Z}_{a,b} = -k_{\mathrm{B}}T\ln\{\mathrm{Tr}_{a,b}\,\exp[-\beta\left(\mathcal{H}_{a,b} - \mu\left(n_{a}+n_{b}\right)\right)]\}, \tag{2}$$

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