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A Study of the Mixed Valence in a Generalized Hubbard Model

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Abstract:

The mixed valence a generalized version of the Hubbard model is used to study materials where ions of the same element exhibit different oxidation states or valencies within the same crystal structure and it considers two types of spinless formions with different masses to explain the properties of these materials. In mixed valence compounds a particular element exists in multiple oxidations states within the same compound. For example, in the compound Eu203, the Europium (Eu) ion can exist in both +2 and +3 oxidation states. To capture the characteristics of mixed valence systems the Hubbard model is extended to include two or more types of fermions with different masses allowing for the descriptions of different oxidations states within the same lattice.

The generalized Hubbard model is useful for understanding the electronic and magnetic properties of mixed valence materials including their insulating to metallic transitions charge transfer and magnetism.

Hubbard model based on exact results or controlled approximate solutions in various limits for which there is a suitable small parameter. Our primary focus is on the ground state properties of the system on various lattices in two spatial dimensions although both lower and higher dimensions are discussed as well. Finally, we highlight some of the important outstanding open questions.

In the present paper, it is proposed to put some salient feature and highlight in our new generation of a study of the mixed valence in a generalized Hubbard model.

Keywords: Mixed Valence, Crystal Lattice, Formions, Oxidations, Electronic, Insulating, Transitions, Parameter, Dimensions, Diagram, Hybridization, Magnetization

Introduction:

The Hubbard model is a theoretical model in solid state physics that describes the behaviour of electron in a lattic, particularly focusing on the interplay between electron hopping (kinetic energy) and one-site Coulomb repulsion (interaction energy).

A generalized Hubbard model involving two kinds of spinless fermious with different masses is proposed to explain the properties of mixed valence compounds. An equivalence between the proposed model and an effective an isotropic antiferromagnetic Heisenberg model with external field is established in the strong interaction limit. The groundstate energy and partition function are obtained analytically using generalized mean field theory which for bipartite lattices, allows the system to be reduced to an equivalent two site problem. The analystic behaviour of the valence and compressibility under variation of pressure and the phase diagram in the ground state and at finite temperature are investigated. The conditions for a first-order transition depending on the position of the f band are obtained, taking into account the effect of local hybridization between the s and f states. The anomalies in the behaviour of n_f and x in mixed-valence systems are interpreted in analogy with the magnetization and susceptibility in the corresponding pseudospin model.

The mixed valence Hubbard model, a generalized version of the Hubbard model, is used to study materials where an atom can exist in multiple oxidation states, by introducing different bandwidths and allowing for hybridization between different bands.

There are following explanation points:

1. Hubbard Model:

The Hubbard model is a theoretical model in condensed matter physics that describes the electronic properties of interacting electrons in a solid, particularly the transition between metallic and insulating states. It considers two key aspects electron hopping between neighbouring lattice sites and on-site Coulomb repulsion.

2. Mixed-Valence:

In mixed-valence compounds, an element can exist in different oxidation states simultaneously within the same material. For example in a compound like S_mS, the samarium (S_m) ion can exist in both +2 and +3 oxidation states.

3. Generalized Hubbard Model:

To describe these mixed valence systems, the Hubbard model is extended to include two or more bands with different bandwidths, allowing for the possibility of electrons hopping between different bands. This allows for the model to capture the effects of different oxidation states and their interactions.

Key Features of the Generalized Hubbard Model:

1. Multiple bands:

The model considers multiple bands, each representing a different oxidation state or electronic configuration.

2. Hybridization:

Electrons can hop between different bands, allowing for charge transfer and mixing of different oxidation states.

3. Interactions:

The model retains the on-site Coulomb replusion, which is crucial for understanding the insulating behaviour of correlated electron systems.

Applications:

The generalized Hubbard model is used to study various phenomena in mixed valence materials, including:

1. Phase Transitions:

Understanding the transitions between different electronic phase (e.g., metallic to insulating) under pressure or temperature.

2. Charge Ordering:

Investigating the tendency of mixed valence systems to form ordered charge distributions.

3. Magnetic Properties:

Studying the magnetic behaviour of mixed valence materials, which can be complex due to the interplay of different oxidation states.

Theorem: The Hubbard model describes itinerant, interacting electrons of spin $-\frac{1}{2}$ hopping on a set $\wedge$ of spatially localized orbitals. The Hamiltonian is written as:

$$H = -\sum_{i,j \in \wedge} \sum_{\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i \in \wedge} c^{+}_{i\uparrow} c^{+}_{i\downarrow} c_{i\downarrow} c_{i\uparrow}.$$

Where the hopping t_{ij} is often restricted to nearest-neighbor sites.

i.e., $t_{ij} = t_{j*i} = t\,\delta_{|i-j|,1}$,

but eralizations can include further neighbor hopping and Peicrls phase factors to account for non-zero magnetic flux. Unless explicitly noted, we confine our attention to the zero flux case. Furthermore, we consider only regular, connected lattices, we do not consider the effects of disorder. The electron filling is defined to be $n \equiv N/|\wedge|$ where $|\wedge|$ is the total number of sites and N is the number of electrons. The half-filled band, with one electron per site, corresponds to $n = 1$.

Methodology:

Many phenomena in heavy-fermion compounds high-Tc superconductors, quantum crystals etc. We have been modeled either with a single-band Hubbard model or a spinless Falicov-Kimball model. These models are also often used to explain phase diagram anomalies and interesting valence behaviour in mixed-valence compounds under change of temperature and pressure. Aside from some details of electron structure these two models can be studied together as particular cases of a more general model.

$$H_{GM} = -t_1 \sum_{ij} c_{i\uparrow}^{+} c_{j\uparrow} - t_2 \sum_{ij} c_{i\downarrow}^{+} c_{j\downarrow} + U \sum_{i} c_{i\uparrow}^{+} c_{i\uparrow} c_{i\downarrow}^{+} c_{i\downarrow}$$
$$- \frac{H}{2} \sum_{i} \left(c_{i\uparrow}^{+} c_{i\uparrow} - c_{i\downarrow}^{+} c_{i\downarrow} \right)$$

Which includes hopping terms and intrasite repulsion ($U > 0$) for two different kinds of particles. For $t_1 = t_2$ it is, of course, a Hubbard model with an applied magnetic field. Although above equation general model is written in the language of electron creation operators with spin indices, an equivalent Hamiltonion could be written using band or orbital indices, as in the Falicov-Kimball model. In other words, the $c_{\uparrow}^{+}$, $c_{\downarrow}^{+}$ operators in above equation can be replaced with creation operators f^{+}, a^{+} representing spinless fermions in the f and s bands. The field strength H in this case represents the energy difference between the centers of the two bands, which in mixed-valence materials can be changed with pressure. For $t_1 = 0$, this is equivalent to the Falicov-Kimball model. In the strong interaction limit $U \to \infty$ the general model reveals some interesting relations between the two models and helps to explain the connections between such phenomena as super-fluity and excitonic insulators, antiferromagnetism and valence density wave, ferromagnetism and pure integer valency. In addition, viewed as a generalization of the Falicov-Kimball model. There are significant advantages to using above general model equation for describing mixed-valence compounds. In the pure Falicov-Kimball, for example, mixed-valence states can appear only as a spatially periodic lattice of ions, with $n_f = 0$ or 1, a kind of orbital antiferromagnetism. The generalized model, however, also permits a liquidlike state of uniform, non-integer valence, as has been seen experimentally and it correctly predicts the first order transitions seen in those materials under change of temperature and pressure.

Discussion and Result:

In spite of the fact that the exact solution of the 2D Heisenberg-Ising model is not know, it is possible to reach some conclusions about the ground-state properties and correlation function behaviour even in this case. For example, at low temperatures the bounds obtained in rule out the possibility of excitonic condensation in 2D lattices, but allow power-law-like decay for excitonic correlations in the general model, which can be of the Kosterlitz-Thouless type, whenever t_1 or t_2 is different from zero.

Conclusion:

In this research paper we have tried to provide a study of the mixed valence in a generalized Hubbard model Hamiltonian, Heisenberg, Falicov-Kimball and some of its condensed matter elementary physics.

The mixed-valence, a generalized version of the Hubbard model is used to study materials where an atom can exist in multiple oxidation states, by introducing different bandwidths and allowing for hybridization between different bands.

The Hubbard model was investigated in the large U limit at half filling. The effective Hamiltonian corresponding to the anisotropic Heisenberg model was derived and the effective antiferromagnetic interaction was discussed. A phase separation phenomenon was considered in the ground state of the asymmetric Hubbard model.

It is known that there are possible phase separations at low temperature in the case of the Falicov-Kimball model and in the general case of the asymmetric Hubbard model. Beside the segregated phases, the long range antiferromagnetic type ordering is possible at low temperature.

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