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Exact diagonalization scheme for the degenerate two-orbital Hubbard model on a ring

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Abstract. The two-orbital degenerate Hubbard model proves to be a powerful tool in the investigation of several $3d$ and $4d$ transition metal oxides where orbital degeneracy is known to play a crucial role. We present here a finite-size cluster study of this model where an exact numerical diagonalization procedure is used, based on the implementation of the symmetries generated by the spin, the pairing and the orbital pseudospin operators. The technique is then applied to the solution of the model on a four-site ring, and an explicit comparison is presented between the behavior of the spin, charge and orbital gaps as the on-site Coulomb repulsion is varied.

1. Introduction

It is well known that in several $3d$ and $4d$ transition metal oxides [1], as well as in alkali-doped fullerides [2], a consistent description of the experimental observations cannot be performed within single-band correlated electron models, but rather requires the use of more realistic models including orbital degrees of freedom. Well-known cases of this type concern the widely studied systems V_2O_3 [3], whose properties are essentially determined by the electrons in a doubly degenerate d-band, and $LaTiO_3$ [4], which exhibits d-bands with triple degeneration.

In the case of two-orbital degeneracy, many theoretical approaches have so far been proposed to describe the effect of the strong Coulomb interaction. Among them we quote variational methods [5, 6, 7], slave-boson methods [8], and, in particular, the dynamical mean-field theory, which has led to an increased understanding of the correlation effects associated with the Mott metal-insulator transition [9, 10, 11, 12]. Indeed, due to the presence of orbital degrees of freedom, the Mott physics contains in this case extra elements of unconventional character associated, for instance, with the possibility of having some of the d orbitals displaying localized spin and orbital degrees of freedom, and others providing itinerant electrons.

On a more general ground, the two-orbital Hubbard model is a typical correlated electron model describing systems where the strength of the interactions between particles is at least comparable with their kinetic energy. Due to the intrinsic non-perturbative nature of the problem, extreme difficulties are encountered to devise theoretical tools allowing to deal with these models in a reliable way. For this reason, a huge amount of work has been devoted in the

last decades to their solution on clusters made of a relatively small number of sites, obtained using exact diagonalization, Lanczos or quantum Monte Carlo methods [13].

These approaches also suffer of several limitations, such as the rapid increase of the computational effort with the cluster size or the unavoidable presence of finite-size effects limiting the possibility of extracting information on the low-energy scale behavior. Nonetheless, in many cases they provide useful indications on the physics of the model and often represent the starting point of powerful approximations where the infinite lattice problem is mapped into a finite-size cluster self-consistently embedded in a suitably defined mean field [14, 15]. Guided by this motivation, we present in this paper an exact diagonalization method which is based on the full implementation of the symmetries generated by the spin, the pairing and the orbital pseudospin operators. As an application, this technique is used here to determine in the case of a four-site ring the exact eigenstates and eigenvalues of the model. The latter are then used to show that the spin, charge and orbital gaps satisfy well defined order relations, in agreement with a theorem recently demonstrated [16].

2. The model and its symmetries

We consider a lattice system with two equivalent orbitals on each site. The corresponding Hamiltonian is

$$H \;=\; H_{\rm kin} \;+\; H_{\rm el-el} \tag{1}$$

where $H_{\rm kin}$ is the kinetic term describing electron hopping between orbitals of the same type on nearest-neighbor sites,

$$H_{\rm kin} \;=\; t \sum_{\langle ij\,\rangle,\,\alpha,\,\sigma} d^{\dagger}_{i\alpha\sigma} d_{j\alpha\sigma} + {\rm h.c.} \quad , \tag{2}$$

$d^{\dagger}_{j\alpha\sigma}$ being the creation operator for an electron with spin σ at site i in the α orbital ($\alpha = 1, 2$), and $H_{\rm el-el}$ is the term describing electron-electron interaction [5, 9, 10, 12]:

$$\begin{aligned} H_{\rm el-el} \;\;=\;\; & (U+J) \sum_{i,\,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + U \sum_{i,\,\sigma} n_{i1\,\sigma} n_{i2\bar{\sigma}} \\ & + (U-J) \sum_{i,\,\sigma} n_{i1\sigma} n_{i2\sigma} + J \sum_{i,\,\sigma} d^{\dagger}_{i1\sigma} d^{\dagger}_{i2\bar{\sigma}} d_{i1\bar{\sigma}} d_{i2\,\sigma} \quad . \end{aligned} \tag{3}$$

We notice that $H_{\rm el-el}$ contains intra-site interactions only, distinguishing among the cases when electrons belonging to different orbitals have the same spin or opposite spins (here $\bar{\sigma} = -\sigma$). Moreover, with the above choice of the coupling constants the total Hamiltonian is rotationally invariant with respect to the spin and the orbital degrees of freedom. The condition $U > J$ is also assumed (with U and J being both positive), in order to ensure that the total interorbital interaction between electrons with the same spin is repulsive [17].

Let us now introduce the spin, pairing and pseudospin orbital operators, defined respectively as

$$\mathbf{S} \;=\; \frac{1}{2} \sum_{i,\,\sigma,\,\sigma',\,\alpha} d^{\dagger}_{i\alpha\sigma} \left(\boldsymbol{\sigma}\right)_{\sigma\sigma'} d_{i\alpha\sigma'} \tag{4}$$

$$\boldsymbol{\eta} \;=\; \frac{1}{2} \sum_{i,\,\alpha,\,\sigma,\,\sigma'} D^{\dagger}_{i\alpha\sigma} \left(\boldsymbol{\sigma}\right)_{\sigma\sigma'} D_{i\alpha\sigma'} \tag{5}$$

$$\mathbf{T} \;=\; \frac{1}{2} \sum_{i,\,\alpha,\,\alpha',\,\sigma} d^{\dagger}_{i\alpha\sigma} \left(\boldsymbol{\sigma}\right)_{\alpha\alpha'} d_{i\alpha'\sigma} \quad , \tag{6}$$

where $\boldsymbol{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$ is the vector having the Pauli matrices as components, and $\mathbf{D}_{i\alpha}$ is a two-component vector having elements $D_{i\alpha\uparrow} = d_{i\alpha\uparrow}$ and $D_{i\alpha\downarrow} = d^{\dagger}_{i\alpha\downarrow}$.

In Eq.5 $\boldsymbol{\eta}$ is the pairing operator introduced by Yang [18], extended to the case of two types of electrons. The symmetry related to this operator is a kind of hidden symmetry in the particle-hole space, for which the generators are obtained from the usual spin SU(2) ones through an electron-hole transformation involving only one kind of spin. As the operator $\mathbf{S}$ is associated with a symmetry involving spin degrees of freedom, similarly the symmetry generated by the operator $\boldsymbol{\eta}$ is related to the charge degrees of freedom. This is evident from the fact that the z component of $\boldsymbol{\eta}$ is equal to $N_{tot}/2 - N_s$, where N_{tot} is the total number operator and N_s is the number of lattice sites. On the other hand, the orbital operator $\mathbf{T}$ defined in Eq.6 has again properties analogous to those of the spin 1/2 operators. Indeed, on a given site T^+ takes an electron in orbital 2 and move it to orbital 1, T^- produces the reverse process, and T_z has eigenvalues $+1/2$ or $-1/2$ depending on whether an electron is in the orbital 1 or 2, respectively. The operators $\mathbf{S}$, $\boldsymbol{\eta}$ and $\mathbf{T}$ commute with the Hamiltonian (1) and thus correspond to symmetries of the model which can be used to classify eigenstates and eigenvalues [19, 16].

3. The solution on a four-site ring and the excitation gaps

In our approach the numerical diagonalization of the Hamiltonian is performed in Fock subspaces specified by the values of the third component of the operators $\mathbf{S}$, $\boldsymbol{\eta}$ and $\mathbf{T}$. The implementation of these symmetries leads to a significant reduction of the size of the matrices to be diagonalized. When we refer to a four-site ring, for instance, this size reaches its maximum value, equal to 1810×1810, in the case of half filling (eight electrons) for $S_z = \eta_z = T_z = 0$. On the other hand, if the orbital symmetry is neglected, the largest size of the matrices that one has to diagonalize is 4900×4900, implying that the simultaneous application of spin, charge and orbital symmetries considerably reduces the dimension of the Fock space. The situation is summarized in Table 1 for a total number of electrons N going from 8 (half filling) to 4 (quarter filling), in the cases $S_z = \eta_z = 0$ for even N, and $S_z = \eta_z = 1/2$ for odd N.

We point out that this diagonalization scheme cannot be applied to a slightly more general fully invariant two-orbital degenerate Hamiltonian, differing from the one considered here by a coupling constant between electrons in the same orbital equal to $U + 2J$, rather than $U + J$, and by the presence of a pair hopping term $J \sum_i \left[d^\dagger_{i1\uparrow} d^\dagger_{i1\downarrow} d_{i2\downarrow} d_{i2\uparrow} + h.c. \right]$ describing inter-orbital transfer of electron pairs [6, 7, 20, 21]. Actually, the presence of the pair hopping term breaks the T_z symmetry, and thus the splitting of the Fock space into subspaces specified by the value of T_z turns out to be of no use in the diagonalization procedure.

Table 1. Dimensions of the Fock subspaces for a four-site cluster at fixed values of T_z, for an electron number N going from 8 to 4. The values of S_z and η_z are the lowest possible ones compatible with the value of N.

T_z	S_z	η_z	$N=8$	$N=6$	$N=4$	T_z	S_z	η_z	$N=7$	$N=5$
0	0	0	1810	1184	328	±1/2	1/2	1/2	1316	552
±1	0	0	1184	768	192	±3/2	1/2	1/2	552	208
±2	0	0	328	192	36	±5/2	1/2	1/2	88	24
±3	0	0	32	16		±7/2	1/2	1/2	4	
±4	0	0	1							
generic	0	0	4900	3136	784	generic	1/2	1/2	3920	1568

Let us now introduce the spin, charge and orbital excitation gaps, defined respectively as

$$\Delta_S = E_G(S=1,\eta=0,T=0) - E_G(S=0,\eta=0,T=0) \quad (7)$$

$$\Delta_C = E_G(S=0,\eta=1,T=0) - E_G(S=0,\eta=0,T=0) \quad (8)$$
$$\Delta_T = E_G(S=0,\eta=0,T=1) - E_G(S=0,\eta=0,T=0) \quad (9)$$

where $E_G(S,\eta,T)$ is the lowest eigenvalue of the Hamiltonian in the subspace with quantum numbers S,η,T.

As an application, we have evaluated the above introduced gaps at half filling ($N=8$) and presented their behavior in Fig.1 as functions of U, for a fixed value of J. We stress that these results are in agreement with a theorem rigorously demonstrated in Ref. [16], according to which at half-filling the charge gap is always larger than both the spin-excitation gap and orbital gap.

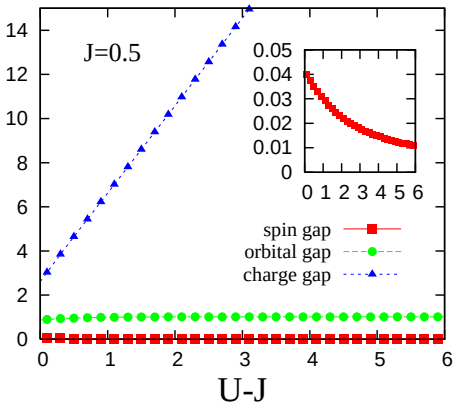

Figure 1. Spin, charge and orbital gaps as functions of $U-J$ at half filling, for $J=0.5$ (bare units). The inset shows the behavior of the spin gap on a different scale.

A more detailed cluster investigation of the two-orbital degenerate Hubbard model, in particular as concerns other ground-state properties such as the possible occurrence of high-spin magnetic states, is under way and will be the subject of a forthcoming paper.

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