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High-spin magnetic states in the two-orbital Hubbard model on a tetrahedron

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Abstract
We present a study of the two-orbital degenerate Hubbard model in which the exact numerical solution on a regular tetrahedron is obtained via suitable implementation of the symmetries generated by the spin, the pairing and the orbital pseudospin operators. In particular, we show that a large variety of high-spin magnetic ground states can develop away from half filling, depending on the values of the electron density and the parameters of the model. As the tetrahedron is the simplest finite-size cluster where hopping processes connect all pairs of sites with constant probability, the study is extended by providing the exact analytical solution of the model on an infinite lattice in the unconstrained hopping limit.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The minimal model able to describe the physics of the transition metals and their oxides is the Hubbard model, which, in its simplest form, contains the local Coulomb interaction between the electrons in a conduction band originating from a single orbital. In spite of its apparent simplicity, such a single-band model has been deeply investigated in the past as an effective model for the analysis, often only qualitative, of some low-energy properties characterizing the behavior of the above mentioned systems. Nevertheless, it is widely accepted that in several 3d and 4d transition metal oxides a consistent description of the experimental observations requires the use of more realistic models which include, at least, orbital degrees of freedom [1]. Moreover, the orbital degeneracy is known to play a crucial role in many correlated electron systems, allowing for the explanation of remarkable properties like colossal magnetoresistance [2], metal–insulator transition [1] and orbital ordering [3]. Typical orbitally degenerate compounds are V_2O_3 [4], whose properties are essentially determined by the electrons in a doubly degenerate d band, and $LaTiO_3$ [5], which exhibits d bands with triple degeneration.

Many theoretical approaches have so far been proposed to describe the effect of the strong Coulomb interaction in systems with two-orbital degeneracy. Among them we quote variational methods [6, 7], Gutzwiller [8, 9], slave-boson methods [10, 11] and Lanczos diagonalization on finite-size clusters [12]. Nevertheless, theoretical advances in the comprehension of these systems are mainly due to the application of the dynamical mean-field theory, which has led to an increased understanding of the correlation effects associated with the Mott metal–insulator transition [13–16]. 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. In the case of subbands with different bandwidths, this gives rise to separate orbital-selective Mott transitions occurring at different Coulomb strengths, eventually merging into a single critical point only under specific conditions [17–19]. Recent remarkable achievements unambiguously confirm these findings, showing that two distinct and successive Mott transitions are found within the two-orbital Hubbard model [20, 21]. Nevertheless,

a fully reliable numerical approach describing multi-band degenerate Hubbard models is probably still lacking, since imaginary time continuation, high computational time and fundamental difficulties at low temperatures still provide severe limits for numerical calculations.

As far as exact results are concerned, we can say that they are at present still more rare. However, it has been recently shown that symmetry features of the ground state at half filling of a generalized two-orbital Hubbard model including the Hund's rule coupling can be obtained in a large range of the parameter space, combining the property of spin reflection positivity and the use of special unitary transformations [22]. In particular, it has been possible to extract relevant symmetry features related to the orbital, spin and η-pairing pseudospin operators, determining, at half filling and for different parameter regimes, the spin, orbital and η-pairing pseudospin quantum numbers in the ground state. Moreover, these results allowed us to show rigorously that (i) at half filling the charge gap is always larger than both the spin-excitation gap and a properly defined orbital gap [23], and (ii) in one and two dimensions the two-orbital Hubbard model does not exhibit orbital order at any filling and at any finite temperature, if narrow conduction bands are considered [24]. Relevant results in this context have also been obtained in connection with the $SU(4)$ symmetry of the n-fold degenerate Hubbard model with inter-orbital Coulomb repulsion, in the absence of the Hund coupling [25].

On more general grounds, 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 us 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 [26]. These approaches also suffer from 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 [27, 28]. Guided by this motivation, we present in this paper the exact solution of the two-orbital Hubbard model on a small cluster having the structure of a regular tetrahedron. Specific features of this kind of cluster are on the one hand the fact that it represents the smallest three-dimensional unit generating the face-centered cubic lattice, and on the other hand the constancy of the hopping amplitude between every possible pair of sites that can be selected within the cluster. We show that the exact solution of the two-orbital Hubbard model on a tetrahedron indicates that complete or weak ferromagnetism appears in the ground state away from half filling, for suitable choices of the local Coulomb repulsion, the Hund coupling and the hopping amplitude.

The condition of constant hopping amplitude, which has in the regular tetrahedron its three-dimensional realization, can also be assumed to hold in an infinite lattice. This choice gives rise to the so-called infinite range hopping limit which has been shown in the past to be exactly solvable in the case of several correlated electron models. In the second part of the paper we show that the general approach developed in this context can successfully be applied to the two-orbital Hubbard model too, leading to a particularly simple form for the partition function and all the thermodynamic quantities which can be derived from it.

The paper is organized as follows. In section 2 we introduce the two-orbital Hubbard Hamiltonian. In section 3 we present the exact diagonalization study of the model on a tetrahedron, devoting special attention to the possible occurrence of magnetic ground states for suitable values of the filling and the microscopic parameters of the model Hamiltonian. Section 4 is devoted to the analysis of the exact solution of the same model in the infinite range hopping limit on an infinite lattice. Section 5 contains a summary of the results, together with the conclusions.

2. The model

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

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

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

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

$d^{\dagger}_{j\alpha\sigma}$ being the creation operator for an electron with spin σ at site i in the α orbital ($\alpha = 1, 2$), and $H_{\text{el-el}}$ is the term describing electron–electron interaction [6, 13, 14, 16]:

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

We notice that $H_{\text{el-el}}$ 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 inter-orbital interaction between electrons with the same spin is repulsive[4]. From now on all the energies are expressed in units of the hopping amplitude t.

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

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

[4] A comprehensive discussion on the form of the interaction parameters can be found in [2].

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

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

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 (5), $\boldsymbol{\eta}$ is the pairing operator introduced by Yang [29], extended to the case of two types of electron. 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 $N_{\mathrm{tot}}/2 - N_{\mathrm{s}}$, 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 (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 moves 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 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 [22, 23].

3. The exact solution on a tetrahedron

We present in this section the exact numerical solution of the two-orbital degenerate Hubbard model on a regular tetrahedron. This cluster geometry has often been considered in the past in exact diagonalization studies of the one-band Hubbard model [30–33], in some cases with the motivation that a tetrahedron can be seen as the smallest three-dimensional building block constituting a face-centered cubic lattice. Besides numerical approaches, a complete analytical solution on a tetrahedron has recently been given for the single-orbital Hubbard model including the nearest-neighbor Coulomb correlation and the nearest-neighbor Heisenberg exchange [34].

In our approach the numerical diagonalization of the Hamiltonian has been 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, a size which reaches its maximum value, equal to 1810×1810, in the case of half filling (eight electrons on four sites) for $S_z = \eta_z = T_z = 0$. We notice that when 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. We have devoted special attention to the study of the possible occurrence, for suitable values of the parameters and of the filling, of high-spin ground state configurations. We have

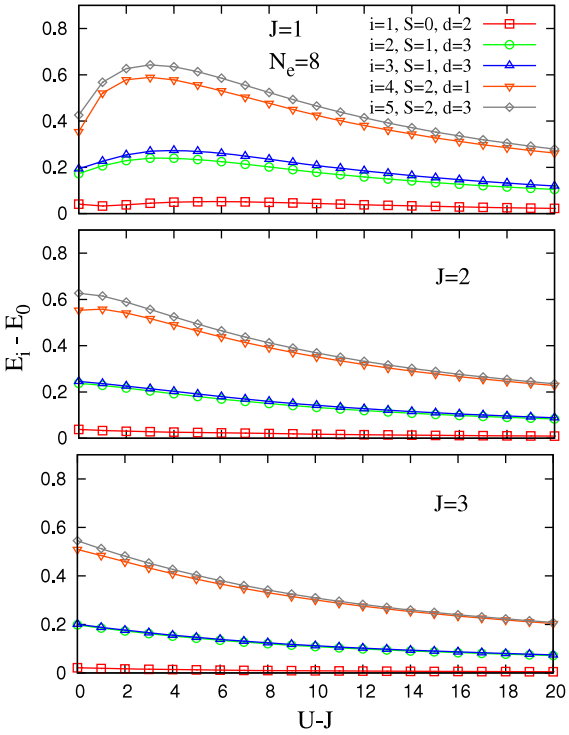

Figure 1. Energies E_i of the first few excited states ($i = 1, \ldots, 5$), measured with respect to the ground state energy E_0, for $N_{\mathrm{e}} = 8$. The specified values of S and d denote the spin quantum number and the number of $(2S + 1)$-plets with a given energy E_i occurring in the spectrum, respectively. For increasing values of J the energy E_1 of the first excited state, though getting closer and closer to E_0, remains separated from it, always leaving the ground state non-degenerate. All the energies are given in units of the hopping amplitude t.

first of all verified that in the case of half filling the ground state is always non-magnetic, in the sense that for any possible value of the parameters t, J and U the electrons minimize the energy, always arranging themselves in zero spin configurations. In figure 1 we report the energies E_i of the first few excited states, evaluated for $J = 1$ and rescaled with respect to the ground state energy E_0. We can see that several non-zero spin states are found among the low-lying excited states, but they all remain well separated from the non-magnetic non-degenerate ground state for every possible choice of the parameters. This result was to some extent expected as the natural generalization to the two-band case of well established results concerning one-band models [35].

A high-spin ground state in contrast appears when one hole is added to the half-filled configuration and positive values of the hopping amplitude t are considered. As one can see from figure 2, in this case the total spin is maximized for sufficiently high values of J and U. In particular, as soon as the Hund's coupling is greater than a critical value J_{c1}, approximately equal to 1.1, a ground state with maximum spin $S = 7/2$ is established only when U exceeds a critical value U_{c} which tends to decrease as J is increased above J_{c1}. In the case considered in figure 2, U_{c} goes to zero for J approximately equal to $J_{\mathrm{c2}} = 5$, indicating that above J_{c2} a maximum spin ground state develops, however small the value of U–J. It should also be noted that when J is greater than

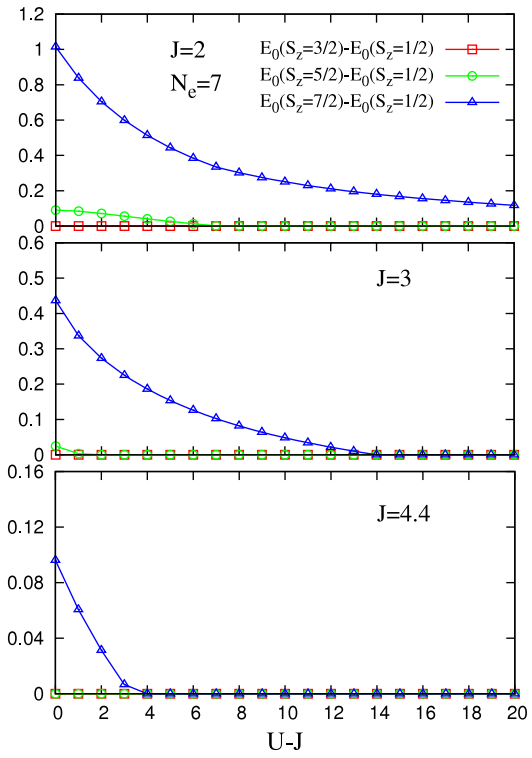

Figure 2. Energy difference between the lowest eigenstates belonging to subspaces with different S_z in the case of seven electrons on a regular tetrahedron.

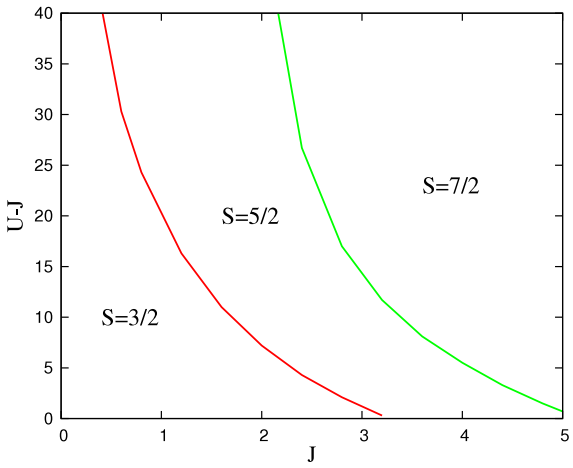

Figure 3. U versus J phase diagram giving the ground state value of the total spin quantum number for $N_e = 7$.

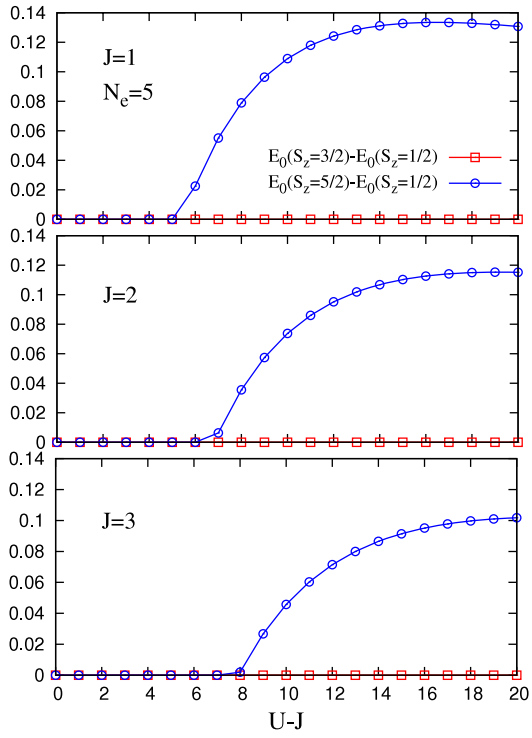

Figure 4. Energy difference between the lowest eigenstates belonging to subspaces with different S_z in the case of five electrons on a regular tetrahedron.

J_{c1} but sufficiently far from J_{c2} the increase of U makes the system approach the maximum spin state passing through two consecutive transitions, the first one at $U = U_{c0} < U_c$ from a state with $S = 3/2$ to a state with $S = 5/2$, and the second one at $U = U_c$ from the latter to the state with maximum spin $S = 7/2$. For the parameter choice considered here, we deduce from figure 2 that the first transition disappears ($U_{c0} \to 0$) for J slightly higher than 3. These results are summarized in the U versus J phase diagram reported in figure 3. As a general comment, we notice that all these results concerning the case of one hole injected within a half-filled configuration present evident analogies with the Nagaoka's theorem [36] for the one-band Hubbard model. The latter states that for $t > 0$ and $N_e = N_s - 1$ (N_e being the number of electrons) the spin in the ground state is maximized for sufficiently high values of U on several kinds of lattice structures, including the face-centered cubic one. We stress, however, that by no means do we intend that our results are consequences or manifestations of Nagaoka's theorem (which, moreover, refers to the single-band case only). The lattice connectivity condition required for the theorem to be valid certainly does not hold on a tetrahedron, so that we can only suggest an analogy implying no direct relationship between our results and the theorem itself.

Always referring to the case of positive hopping amplitude, when a second hole is added to the system ($N_e = 6$), the highest possible spin value, $S = 3$, is reached in the ground state for any possible choice of J and U. In a similar way, for $N_e = 5$ the system is never in the lowest possible spin state $S = 1/2$, but now, as one can see from figure 4, we find a lowering of the total spin from the maximum value $S = 5/2$ to $S = 3/2$ as U is increased, taking place at a critical value of U which grows as increasing values of J are considered. In this respect, it should be noted that the increase of U plays here a role which is opposite compared to the filling $N_e = 7$, in the sense that, while in this latter case it produces a transition towards a maximum spin state, in contrast for $N_e = 5$ it leads to a reduction of **S**. Finally, in the quarter-filled case, $N_e = 4$, we observe a similar effect introduced by the increase of U, but this time the transition at U_c occurs directly from the highest ($S = 2$) to the lowest ($S = 0$) possible spin ground state, with U_c again increasing with J (see figure 5).

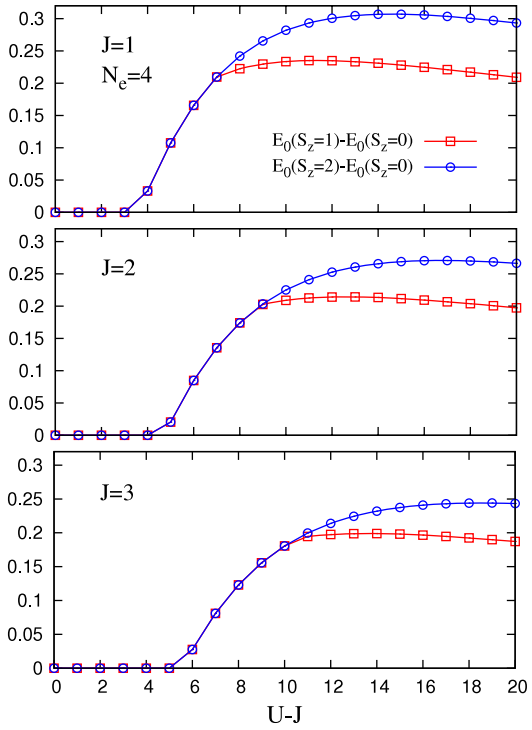

Figure 5. Energy difference between the lowest eigenstates belonging to subspaces with different S_z in the case of four electrons on a regular tetrahedron.

We stress once more that the results discussed so far all refer to the case of positive hopping amplitude. For $t < 0$, in contrast, the ground state always corresponds to the lowest possible spin state, for all electron densities going from half filling down to quarter filling. However, the same kind of high-spin ground states just found for $N_e < 2N_s$ and $t > 0$ symmetrically develop for $N_e > 2N_s$ and $t < 0$ due to the electron–hole symmetry exhibited by the Hamiltonian (3). Since creating an electron amounts to destroying a hole (and vice versa), we can introduce fermionic hole operators $h_{i\alpha\sigma}, h^{\dagger}_{i\alpha\sigma}$ such that $d^{\dagger}_{i\alpha\sigma} = h_{i\alpha\sigma}$. Then one can show that on a given lattice of N_s sites the spectrum of the Hamiltonian $H_e \equiv H(-|t|, d_{i\alpha\sigma}, d^{\dagger}_{i\alpha\sigma})$ for N_e electrons with negative hopping amplitude is related to the spectrum of the Hamiltonian $H_h \equiv H(|t|, h_{i\alpha\sigma}, h^{\dagger}_{i\alpha\sigma})$ for $N_h = 4N_s - N_e$ holes with positive hopping amplitude by the relation

$$H_h = H_e - 3U\,(N_e - 2N_s). \tag{7}$$

Thanks to this symmetry, for $t < 0$ and a given number N_e of electrons, we have a ground state characterized by the same spin value occurring for $t > 0$ and an equal number of holes ($N_h = N_e$). This is the reason why in table 1, where the possible ground states emerging from our two-orbital model on a tetrahedron are summarized, we confine ourselves to electron fillings going from $N_e = 4$ to 8.

As a final comment, we point out that we have also performed the same kind of numerical calculations referring to a slightly different form of the two-orbital Hubbard model, based on a fully invariant Hamiltonian differing from the one considered here by a coupling constant between

Table 1. The nature of the ground state of the degenerate two-orbital Hubbard model on a tetrahedron for different choices of the total electron number. U and J are expressed in units of the hopping amplitude t.

N_e	Sign of t	Type of ground state	Comments
4	+	$S = 2$ for $U < U_c(J)$ $S = 0$ for $U > U_c(J)$	U_c increases with J
4	−	$S = 0$ (arbitrary U, J)	
5	+	$S = 5/2$ for $U < U_c(J)$ $S = 3/2$ for $U > U_c(J)$	U_c increases with J
5	−	$S = 1/2$ (arbitrary U, J)	
6	+	$S = 3$ (arbitrary U, J)	
6	−	$S = 0$ (arbitrary U, J)	
7	+	$S = 3/2$ for $0 < U < U_{c1}(J)$ $S = 5/2$ for $U_{c1}(J) < U < U_{c2}(J)$ $S = 7/2$ for $U > U_{c2}(J)$ (provided that $J > J_{c1}$)	U_{c1} and U_{c2} decrease with J
7	−	$S = 1/2$ (arbitrary U, J)	
8	±	$S = 0$ (arbitrary U, J)	

electrons in the same orbital equal to $U + 2J$, rather than $U + J$, and by the presence of a pair hopping term $J\sum_i[d^{\dagger}_{i1\uparrow}d^{\dagger}_{i1\downarrow}d_{i2\downarrow}d_{i2\uparrow} + \text{h.c.}]$ describing inter-orbital transfer of electron pairs [7, 8, 17, 19–21]. The results obtained in this case show only small quantitative deviations from the ones reported here, so that all the conclusions drawn in this section also remain valid for this different version of the two-orbital model.

4. The infinite range hopping limit

In the previous section we provided the exact solution of the degenerate two-orbital Hubbard model on a tetrahedron, i.e. a tridimensional four-site cluster where the distance between all possible pairs of sites is a constant. In this situation the usual tight-binding choice of a hopping amplitude being non-vanishing only between nearest-neighbor sites becomes equivalent to the assumption that all possible hopping processes are equally likely to occur. In this way, the case of the tetrahedron can be seen as the finite size three-dimensional realization of the so-called infinite range hopping limit, in which the itinerancy of the electrons is realized through unconstrained intersite processes. We are thus naturally led to the analysis of the two-orbital Hubbard model in this limit, applied to the case of an infinite lattice. Though rather artificial as far as its possible applications to real systems are concerned, this limit has its main virtue in its tractability, so that it has often been studied in the past in connection with several correlated electron models, such as the Hubbard model [37], the t–J model [38], the Kondo lattice model [39] and the Anderson lattice model [40].

If the hopping amplitude is equal to a constant t for all possible pairs of sites that one can consider on the lattice, then it immediately follows that

$$\varepsilon_{\vec{k}} = t\,N_s\,\delta_{k,0} \tag{8}$$

where

$$\varepsilon_{\vec{k}} = \frac{1}{N_s} \sum_{ij} t_{ij} e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)}. \tag{9}$$

The peculiar form of $\varepsilon_{\vec{k}}$, which is made of a single contribution with $\vec{k} = 0$, allows us to obtain the non-local part $H_{\rm kin}$ of the total Hamiltonian in the simple form

$$H_{\rm kin} = N_s\, t \sum_{\sigma\alpha} d^{\dagger}_{\vec{k}=0,\alpha\sigma} d_{\vec{k}=0,\alpha\sigma}. \tag{10}$$

Moreover, this result implies that in the thermodynamic limit $H_{\rm kin}$ commutes with $H_{\text{el-el}}$, as a consequence of the fact that the latter is the sum of many contributions with all possible values of $\vec{k}$, among which the one at $\vec{k} = 0$ can be neglected with an error of order of N_s^{-1}, going to zero in the limit $N_s \to \infty$. It is thus possible to diagonalize $H_{\rm kin}$ and $H_{\text{el-el}}$ separately and write down the partition function in the form $Z = [Z(H_{\rm kin})Z(H_{\text{el-el}})]^{N_s}$, where $Z(H_{\rm kin})$ is simply equal to $\exp(-4\beta t)$, with $\beta = 1/k_B T$, while $Z(H_{\text{el-el}})$ has the form

$$Z(H_{\text{el-el}}) = \sum_{i=1}^{16} e^{-\beta(E_i - \mu N_i)}, \tag{11}$$

with E_i being the eigenvalues of $H_{\text{el-el}}$ and N_i the corresponding eigenvalues of the total number operator. The explicit expression of $Z(H_{\text{el-el}})$ is

$$\begin{aligned} Z(H_{\text{el-el}}) &= 1 + 4z + 3(e^{-\beta(U-J)} + e^{-\beta(U+J)})z^2 \\ &\quad + 4e^{-3\beta U} z^3 + e^{-6\beta U} z^4 \end{aligned} \tag{12}$$

where $z = \exp(\beta\mu)$ is the fugacity. From the grand-canonical potential $\Omega = -\beta^{-1} \ln Z$, fundamental thermodynamical quantities, such as the total electron density $n = N/N_s$ and the total energy density $e = E/N_s$, can be derived. We obtain

$$\begin{aligned} n &= -\frac{1}{N_s}\frac{\partial\Omega}{\partial\mu} = -\frac{1}{\beta}\left[\frac{\partial}{\partial\mu}\ln Z(H_{\rm kin}) + \frac{\partial}{\partial\mu}\ln Z(H_{\text{el-el}})\right] \\ &= Z(H_{\text{el-el}})^{-1}\left[4z + 6(e^{-\beta(U-J)} + e^{-\beta(U+J)})z^2\right. \\ &\quad \left. + 12e^{-3\beta U} z^3 + 4e^{-6\beta U} z^4\right] \end{aligned} \tag{13}$$

and

$$\begin{aligned} e &= \mu n + \frac{1}{N_s}\frac{\partial}{\partial\beta}(\beta\Omega) \\ &= \mu n + 4t + Z(H_{\text{el-el}})^{-1}\{-4\mu z + 3[(U - J - 2\mu) \\ &\quad \times e^{-\beta(U-J)} + (U + J - 2\mu)\, e^{-\beta(U+J)}]z^2 \\ &\quad + 12(U - \mu)\, e^{-3\beta U} z^3 + (6U - 4\mu)\, e^{-6\beta U} z^4\}. \end{aligned} \tag{14}$$

From (13) we recover at low temperatures the expected stepwise behavior of n as a function of μ, with the transitions between two subsequent integer values of n becoming smoother and smoother as T is increased. This is shown in figure 6 for $U = 2$, $J = 0.5$ and three different choices of the temperature, $T = 0.02, 0.2, 0.5$, all the parameters being from now on expressed in electronvolts.

The expression of the energy density given in (13) also allows us to obtain the dependence of the fugacity on the total electron density. Once $z(n)$ is substituted in (14), the zero-temperature limit of the total energy can be studied for fixed values of n. In particular, we get

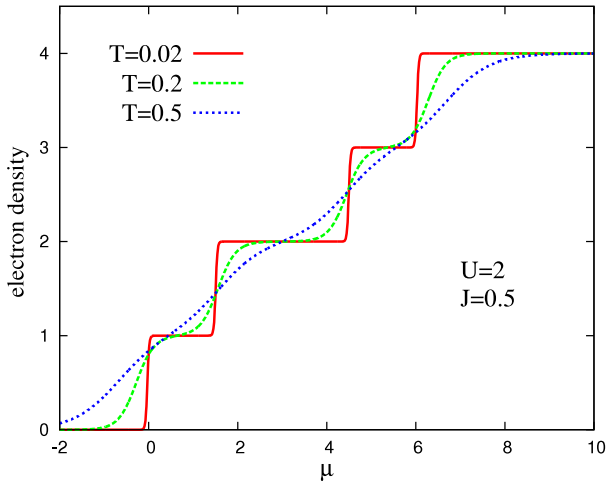

Figure 6. Total electron density as a function of the chemical potential in the infinite range hopping limit for three different values of the temperature.

$$\begin{aligned} \left.\frac{de_G}{dn}\right|_{n\to 1^-} &= 0 \\ \left.\frac{de_G}{dn}\right|_{n\to 1^+} = \left.\frac{de_G}{dn}\right|_{n\to 2^-} &= U - J \\ \left.\frac{de_G}{dn}\right|_{n\to 2^+} = \left.\frac{de_G}{dn}\right|_{n\to 3^-} &= 2U + J \\ \left.\frac{de_G}{dn}\right|_{n\to 3^+} = \left.\frac{de_G}{dn}\right|_{n\to 4^-} &= 3U. \end{aligned} \tag{15}$$

It is worth noting that these values coincide, as expected, with the values of μ at which the electron density jumps at low temperatures from a given integer value to the subsequent one.

Some information about the conduction properties of the ground state can be obtained from the so-called Mattis criterion [41]. Introducing the quantities

$$\mu^- = E_G(N) - E_G(N-1) \tag{16}$$

$$\mu^+ = E_G(N+1) - E_G(N), \tag{17}$$

where $E_G(N)$ is the ground state energy for a number of particles equal to N, we say that the system is in a metallic state when $\Delta\mu = \mu^+ - \mu^- = 0$ and in an insulating state when $\Delta\mu = \mu^+ - \mu^- > 0$. Considering that $E_G(0) = E_G(1) = 0$, $E_G(2) = U - J$, $E_G(3) = 3U$ and $E_G(4) = 6U$, we have a kink in the chemical potential ($\mu^+ > \mu^-$) at quarter, half and three-quarter filling, indicating that in these cases the system behaves as an insulator, whereas it is metallic for all other possible electron densities. This result presents strong analogies with what has been found in a study of the same model in the limit of large lattice connectivity [13].

Finally, defining the spin, charge and orbital gaps as

$$\begin{aligned} \Delta_S &= E_G(S = 1, \eta = 0, T = 0) \\ &\quad - E_G(S = 0, \eta = 0, T = 0) \end{aligned} \tag{18}$$

$$\Delta_C = E_G(S=0,\eta=1,T=0) - E_G(S=0,\eta=0,T=0) \quad (19)$$

$$\Delta_T = E_G(S=0,\eta=0,T=1) - E_G(S=0,\eta=0,T=0), \quad (20)$$

where $E_G(S,\eta,T)$ is the lowest eigenvalue of the Hamiltonian in the subspace with quantum numbers S,η,T, it is immediately shown that $\Delta_S = -2J$, $\Delta_C = 2U + J$ and $\Delta_T = 2J$, so that we have $\Delta_S < \Delta_T < \Delta_C$, in agreement with a theorem recently demonstrated [23].

5. Summary and conclusions

We have performed a study of the two-orbital degenerate Hubbard model, widely used to explain the physical properties of many transition metal oxides, in the limit of constant hopping amplitude. The model has been exactly diagonalized on a tetrahedron, which besides representing a cluster realization of the unconstrained hopping hypothesis can also be seen as the elementary three-dimensional unit generating the face-centered cubic lattice. The analysis has been focused in particular on the ground state properties, showing that a large variety of high-, intermediate-and low-spin ground states are established, depending on the relative values of the model parameters. These features have also been shown to persist in a slightly different form of the model considered here, including an intra-site inter-orbital pair hopping term.

Some general properties of the exact analytical solution in the infinite lattice case have also been deduced by extension of a method which has been applied in the past to several other correlated electron models. It relies on the fact that when the hopping is allowed to occur to any lattice site with equal transition rate, the kinetic and the interaction parts of the Hamiltonian commute with each other and can thus be diagonalized independently. Some relevant information has in particular been obtained (i) on the dependence of the total energy on the filling, and (ii) on the occurrence of metal–insulator transitions at quarter, half and three-quarter filling.

In closing this section we would like to briefly comment on the high-spin ground states analyzed in our study. First of all, we notice that ferromagnetism in correlated electron systems is a remarkable phenomenon for which the research activity is still very intense. Standard theories on its origin mainly stem on the one hand from the Heisenberg exchange interaction picture, and on the other hand from the Stoner criterion derived from the Hartree–Fock approximation for band electrons. Nevertheless, it is not completely understood whether these theories really explain the appearance of ferromagnetism in a system of electrons belonging to different orbitals and interacting via spin-independent Coulomb interactions. In this context, one of the motivations of the present study has been to provide exact results for the degenerate two-orbital Hubbard model, which, despite referring to an idealized situation, could be of some help in clarifying some aspect of this debated issue. As we saw in section 3, the occurrence of high-spin ground states strongly depends on the sign and the magnitude of the hopping term, as well as on the values of the Hund coupling and the local Coulomb repulsion. In particular, relevant results found here concern the cases of one and two holes injected within a half-filled configuration. In the first case evident analogies are found with the predictions of Nagaoka's theorem for the one-band Hubbard model, with a finite critical value of the local Coulomb repulsion needed to stabilize the maximum spin state, whereas in the second case the spin in the ground state is found to be maximized for all possible choices of the model parameters.

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