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Excitation gaps in the orbitally degenerate Hubbard model

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Abstract

The excitation gaps for the two-orbital degenerate Hubbard model are investigated by applying a generalized version of Lieb's spin-reflection positivity. Combining the known exact results on the ground state, and making use of symmetry properties, we rigorously show that, at half-filling, the charge gaps are always larger than the spin-excitation gaps and properly defined orbital gaps.

1. Introduction

It is generally recognized that the Hubbard Hamiltonian is the simplest model for describing strongly interacting many-electron systems. Despite its simplicity, this model is considered to capture the essential physics of several electronic systems, ranging from a metal–insulator transition, and associated antiferromagnetism, to possible d-wave superconductivity and so on [1]. Although most of the real systems displaying these phenomena have orbital degrees of freedom, most of theoretical works have concentrated on the orbitally non-degenerate model for simplicity.

Nevertheless, in real materials, such as the transition metal oxides [2], the magneto-resistive materials [3], the alkali-doped fullerides [4] as well as the spin triplet superconductor Sr_2RuO_4 [5], the orbital degeneracy plays an important role and necessarily has to be taken into account. Therefore, the gaining of some insight into the behaviour of these complex oxides requires the investigation of the orbitally degenerate Hubbard (ODH) model. In this description, key interaction parameters are the Hund coupling and the intra-orbital and inter-orbital Coulomb interactions.

Several theoretical studies have been made up to now on the ODH model, concentrating mainly on the application of the slave-boson mean field approximation [6], the quantum Monte Carlo (QMC) method, and dynamical mean field theory (DMFT). Namely, using the QMC technique, the thermodynamics and spectra for the ODH model in infinite spatial dimensions have been calculated [7]; then, by using DMFT combined with the non-crossing approximation,

the one-particle spectral function and the optical conductivity have been computed [8]. Koga *et al* [9] used the exact diagonalization method to solve the DMFT equations and to obtain two Mott–Hubbard transitions, the so-called orbital-selective Mott–Hubbard transition. Liebsch [10] employed QMC simulations and the iterated perturbation theory to solve the DMFT equations, finding a single first-order Mott–Hubbard transition with similar changes in both bands. Referring to the limits of these procedures, we would like to point out that the QMC is more suitable for addressing the Mott–Hubbard transition, allowing us to identify a gap unambiguously. However, the QMC simulations are restricted to relatively high temperatures and there is a sign problem when the Hund exchange coupling is fully taken into account and not only the Ising component is considered. It is finally worth mentioning the results obtained by employing the most recent advances in the field of QMC simulations for DMFT. In particular, the projective QMC method [11] enables us to address the study of this model also at $T = 0$, and furthermore, a new Hubbard–Stratonovich decoupling [12] allows us to perform the calculations assuming the full $SU(2)$-symmetric Hund exchange and, at the same time, to manage the well-known sign problem.

Apart from these numerical-based works, only a few exact results have been known up to now: we refer to the $SU(4)$ theory presented for the one-dimensional model case [13] and the symmetry properties of the ground state when the model is referenced to a bipartite lattice [14].

The aim of this paper is to provide some new exact results on the ODH model, proving two theorems on the excitation gaps. Indeed, we will derive exact inequalities between the spin, the charge and a properly defined orbital gap. We would like to note that the proof of these theorems strictly follows the elegant procedure outlined and successfully applied to a large variety of strongly correlated electron models proposed in [15]. In particular, in these papers it has been shown that the charge gaps and the quasi-particle gaps are always larger than the corresponding spin gaps, when suitable choices of the filling and a connected bipartite lattice are assumed.

The organization of this paper is as follows. In section 2 we introduce the microscopic ODH model to which we refer, as well as its symmetry properties, in section 3 we state and prove two theorems on the excitation gaps, and finally, in the last section, we supply a summary of the results and concluding remarks.

2. The ODH model and its symmetry properties

The model Hamiltonian to which we refer is built up by different contributions that reproduce the dynamics of electrons in a manifold spanned by two equivalent orbitals on a connected bipartite lattice Γ:

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

The first term in equation (1) is the kinetic operator that defines the hopping between neighbouring sites on the same orbital:

$$H_{\mathrm{kin}} = -t \sum_{ij,\alpha,\sigma} (d^{\dagger}_{i\alpha\sigma} d_{j\alpha\sigma} + \mathrm{h.c.}) \tag{2}$$

where $d^{\dagger}_{i\alpha\sigma}$ is the creation operator for an electron with spin σ at the i site in the α orbital, and the hopping amplitude is assumed to be t for both the orbitals.

The second term in H stands for the local Coulomb interactions between electrons in the same, or in different, orbitals. Since the two orbitals are equivalent, they can be interchanged by a properly chosen canonical transformation and the wavefunction can be assumed to be real [16]. These conditions impose a constraint on the set of interaction parameters, leading to

$U = U' + J$ [17], where U (U') is the intra(inter)-orbital Coulomb repulsion and J is the Hund coupling. Thus, $H_{\mathrm{el-el}}$ assumes the following expression:

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

where $n_{\mathbf{i}\alpha\sigma}$ is the on-site charge operator for spin σ and for the α orbital. Moreover, we have used the simplified notation $\overline{\sigma} = -\sigma$.

Hereafter, we will use the condition that U and J are positive[3].

Let us now discuss the symmetry properties of the ODH Hamiltonian. We introduce the following operators:

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

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

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

where $\hat{\boldsymbol{\sigma}}$ are the Pauli matrices and $\varepsilon(i) = \pm 1$ is a form factor depending to which of the two subparts of the bipartite lattice Γ the site i belongs.

The operators defined above are the usual total spin operator, the pairing operator, and the pseudospin orbital operator, respectively.

We point out that the $\boldsymbol{\eta}$ operator in equation (5) extends the definition originally introduced by Yang [19] within the Hubbard model to the case of two equivalent electrons, and it generates an $SU(2)$ algebra which, on each site, has the doubly occupied state and the empty state as basis vectors. The $\mathbf{T}$ operator exhibits the same properties of the usual spin-half operator, implying that it generates an $SU(2)$ algebra too. Moreover, T^z_i at each site assumes the values $1/2$ and $-1/2$, corresponding to the occupied $\alpha = 1$ and $\alpha = 2$ orbitals, respectively, whereas T^+_i (T^-_i) moves an electron sitting at the orbital 2 (1) to the orbital 1 (2), located at the same lattice site.

It is easily checked that H commutes with the total spin operator $\mathbf{S}$, and, since there is no hopping between different orbitals in H_{kin}, also with $\mathbf{T}$. Moreover, η^2 and its third component η^z also commute with H, implying that the eigenstates of H can be classified in terms of the eigenvalues of all these operators. We would like to point out that, although T^- and T^+ commute with H, implying that the states belonging to the same T-multiplet have the same energy, this property does not hold for the η^+ and η^- operators. This circumstance means that states belonging to the same η-multiplet are not degenerate in energy.

The algebras generated by these operators are not independent, but can be related to each other by means of an orbital-type transformation $\mathbf{W}$ and an extended hole–particle transformation $\mathbf{V}$ [14]. Indeed, the spin operator $\mathbf{S}$ is mapped into the $\mathbf{T}$ operator by means of the unitary transformation $\mathbf{W}$:

$$\mathbf{W}\mathbf{S}\mathbf{W}^{-1} = \mathbf{T}, \tag{7}$$

while $\mathbf{V}$ maps the total spin operator into the orbital pseudospin operator

$$\mathbf{V}\mathbf{S}\mathbf{V}^{-1} = \boldsymbol{\eta}. \tag{8}$$

For completeness, we observe that the Hamiltonian H under $\mathbf{W}$ is transformed as follows:

$$\mathbf{W}H\mathbf{W}^{-1} = \tilde{H}_W, \tag{9}$$

[3] A detailed description of the interaction parameters can be found in [18].

where $\tilde{H}_W = H(t, U, J \Rightarrow -J)$, i.e. $\tilde{H}_W$ is obtained from H, replacing J with $-J$. Analogously, we have

$$\mathbf{V}H\mathbf{V}^{-1} = \tilde{H}_V, \tag{10}$$

where $\tilde{H}_V = H(t, U \Rightarrow -U, J \Rightarrow -J)$, meaning that $\tilde{H}_V$ is obtained from H, replacing U and J with $-U$ and $-J$, respectively. Besides, equations (9) and (10) suggest that the eigenvalues and eigenvectors of H and the unitary-transformed Hamiltonian $\tilde{H}_i$ $(i = V, W)$ are linked to each other.

Under the simultaneous application of $\mathbf{V}$ and $\mathbf{W}$ transformations, the Hamiltonian H becomes:

$$(\mathbf{WV})H(\mathbf{WV})^{-1} = \tilde{H}, \tag{11}$$

where

$$\tilde{H} = -t \sum_{\langle i,j\rangle\alpha\sigma} d^{\dagger}_{i\alpha\sigma} d_{j\alpha\sigma} - (U - J) \sum_{i,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} - U \sum_{i,\sigma} n_{i1\sigma} n_{i2\overline{\sigma}} - (U + J) \sum_{i,\sigma} n_{i1\sigma} n_{i2\sigma} - J \sum_{i,\sigma} d^{\dagger}_{i1\sigma} d_{i1\overline{\sigma}} d^{\dagger}_{i2\overline{\sigma}} d_{i2\sigma}. \tag{12}$$

Conversely, applying $\mathbf{V}$ and $\mathbf{W}$, H is mapped into $\hat{H}$, given by

$$\hat{H} = -t \sum_{\langle i,j\rangle\alpha\sigma} d^{\dagger}_{i\alpha\sigma} d_{j\alpha\sigma} - (U - J) \sum_{i,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} - U \sum_{i,\sigma} n_{i1\sigma} n_{i2\overline{\sigma}} - (U + J) \sum_{i,\sigma} n_{i1\sigma} n_{i2\sigma} - J \sum_{i,\sigma} d^{\dagger}_{i1\sigma} d_{i1\overline{\sigma}} d^{\dagger}_{i2\overline{\sigma}} d_{i2\sigma} \equiv \tilde{H}.$$

As a final consideration, we want to stress that, when H describes *real* physical systems, U is always larger than Hund's coupling energy and this condition implies that all the interaction strengths in $\tilde{H}$ and $\hat{H}$ are negative (see footnote 3). This consideration is essential, since it allows for application of the Lieb argument on the spin reflection positivity and hence for establishing the symmetry properties of the ground-state vector [20].

3. Excitation gaps

In order to prove the theorems claimed in the introduction, let us now introduce the definitions of the excitation gaps.

The spin-excitation gap is defined as

$$\Delta_S \equiv E_G(\eta = 0, T = 0, S = 1; H) - E_G(\eta = 0, T = 0, S = 0; H);$$

the charge excitation gap is given by

$$\Delta_C \equiv E_G(\eta = 1, T = 0, S = 0; H) - E_G(\eta = 0, T = 0, S = 0; H);$$

while the orbital gap is defined by

$$\Delta_T \equiv E_G(\eta = 0, T = 1, S = 0; H) - E_G(\eta = 0, T = 0, S = 0; H).$$

Here $E_G(\eta = j, T = t, S = s; H)$ is the lowest eigenvalue of the corresponding Hamiltonian H in the subspace with quantum numbers $\eta = j$, $T = t$ and $S = s$.

Now we have all the ingredients to state the following theorems:

Theorem 1. *For the Hamiltonian H introduced in equation (1) at half-filling, the charge gap and the corresponding spin gap satisfy the following inequality:*

$$\Delta_C \geqslant \Delta_S. \tag{13}$$

Theorem 2. *For the Hamiltonian H introduced in equation (1) at half-filling, the charge gap and the corresponding orbital gap satisfy the following inequality*

$$\Delta_C \geqslant \Delta_T. \tag{14}$$

In order to prove these theorems, we will make use of the following inequality:

$$E_G(N; H) \geqslant E_G(N; \tilde{H}), \tag{15}$$

where $E_G(N; H)$ and $E_G(N; \tilde{H})$ are the ground-state energies for the Hamiltonian H and $\tilde{H}$, respectively, at a specified even number of electrons with the condition $N \leqslant 4N_0$, with N_0 denoting the number of lattice sites. We want to stress that the inequality equation (15) can be easily proven using the method adopted by Tian [15], noticing that, under the unitary transformation **WV**, the Fock space $F(N)$ of H is mapped into the new Fock space $F(2N_0)$ of $\tilde{H}$.

Now, let us start with an even number of particles $N = 2N_0 + 2$. Applying the above-reported inequality equation (15), we have:

$$E_G(2N_0 + 2; H) \geqslant E_G(2N_0 + 2; \tilde{H}).$$

We notice that the state whose energy is $E_G(2N_0 + 2; \tilde{H})$ has the following quantum numbers, $S = 0$, $T = 0$ and $\eta = 1$, for the spin, the pseudospin orbital and pseudospin operator, respectively.

Since the unitary transformation **WV** maps the spin operator **S** into $\boldsymbol{\eta}$ operator, we also have

$$\begin{aligned} E_G(2N_0 + 2; \tilde{H}) &= E_G(2N_0 + 2; S = 0, T = 0, \eta = 1; \tilde{H}) \\ &= E_G(2N_0; S = 1, T = 0, \eta = 0; H), \end{aligned}$$

where the quantum numbers of the ground state have been written explicitly. Therefore, we can write

$$E_G(2N_0 + 2; H) \geqslant E_G(2N_0; S = 1, T = 0, \eta = 0; H).$$

On the other hand, we known from the definition of $E_G(2N_0 + 2; H)$ and pseudospin operator $\boldsymbol{\eta}$ that

$$E_G(2N_0; S = 0, T = 0, \eta = 1; H) \geqslant E_G(2N_0 + 2; H),$$

implying that, if $E_G(2N_0; S = 0, T = 0, \eta = 0; H)$ is subtracted from the above reported inequalities, we deduce

$$\begin{aligned} &E_G(2N_0; S = 0, T = 0, \eta = 1; H) - E_G(2N_0; S = 0, T = 0, \eta = 0; H) \\ &\quad \geqslant E_G(2N_0; S = 1, T = 0, \eta = 0; H) - E_G(2N_0; S = 0, T = 0, \eta = 0; H) \end{aligned} \tag{16}$$

which corresponds to the proof of equation (13), i.e. to theorem 1.

Now, let us consider theorem 2. To this end, we notice that, under the transformation **VW**, the Hamiltonian in equation (1) is transformed into $\hat{H}$, inequality equation (15) holds, and thus we can apply a proof similar to the one adopted to prove theorem 1. Indeed, let us start by choosing a special filling $N = 2N_0 + 2$ and, considering equation (15), we get

$$E_G(2N_0 + 2; H) \geqslant E_G(2N_0 + 2; \tilde{H}).$$

We know that the quantum numbers of the eigenstate corresponding to the energy $E_G(2N_0 + 2; \tilde{H})$ are $S = 0$, $T = 0$ and $\eta = 1$. Since the unitary transformation **VW** maps the operator **T** into $\boldsymbol{\eta}$ operator, we can write

$$\begin{aligned} E_G(2N_0 + 2; \tilde{H}) &= E_G(2N_0 + 2; S = 0, T = 0, \eta = 1; \tilde{H}) \\ &= E_G(2N_0; S = 0, T = 1, \eta = 0; H). \end{aligned}$$

Therefore, we get

$$E_G(2N_0+2;\,H) \geqslant E_G(2N_0;\,S=0,T=1,\eta=0;\,H).$$

On the other hand, it is well known that

$$E_G(2N_0;\,S=0,T=0,\eta=1;\,H) \geqslant E_G(2N_0+2;\,H),$$

so that, by subtracting the quantity $E_G(2N_0;\,S=0,T=0,\eta=0;\,H)$ from both sides of the above inequality, we finally get the following relationship:

$$\begin{aligned} &E_G(2N_0;\,S=0,T=0,\eta=1;\,H) - E_G(2N_0;\,S=0,T=0,\eta=0;\,H) \\ &\qquad \geqslant E_G(2N_0;\,S=0,T=1,\eta=0;\,H) - E_G(2N_0;\,S=0,T=0,\eta=0;\,H), \end{aligned} \tag{17}$$

which successfully concludes the proof of theorem 2.

4. Conclusions

By exploiting the partial particle–hole symmetry of the ODH model at half-filling and applying a generalized version of Lieb's spin-reflection positivity method, we have established some exact inequalities between the ground-state energies of this relevant strongly correlated electron model. The method that is applied follows a previously adopted procedure introduced by Tian [15] to prove analogous inequalities for relevant strongly correlated electron models such as the Hubbard model, the periodic Anderson model and the Kondo model. As a direct corollary of the derived inequalities, we have proven that the charge gap of the model is always larger than the spin-excitation gap. Moreover, introducing the orbital charge gap as the energy difference between ground-state energies which differ by one in the orbital quantum number T, we have also shown that the charge gap is higher than the orbital gap. We want to stress that the following conditions have to be fulfilled for the validity of the results obtained above: (i) the number of electrons is equal to twice the number of sites in the lattice (half-filling condition); (ii) the numbers of lattice sites belonging to the two sublattices forming the bipartite lattice Γ are equal; (iii) the hopping amplitude is different from zero only for the charge transfer between orbitals of the same type.

We notice that, as far as the Anderson model is concerned, the inequality equation (13) between the charge gap and the spin gap was observed firstly in numerical calculations performed on small-size clusters [21]. Therefore, it would be worth studying the present ODH model on clusters. However, to overcome problems related to finite size effects which make the charge gap strongly parity dependent, it is necessary to redefine this quantity. This has been done by Nishino [22], who showed that one can introduce a new charge gap that is indeed much less parity dependent than the usual charge gap. Subsequently, Tian and Wang [23] proved rigorously that the Nishino gap is always positive and a lower bound exists for this quantity when the half-filled Hubbard model, the periodic Anderson model and the Kondo lattice model are considered. In this respect, we plan the study of the ODH model on finite-size clusters in the near future, with the aim of linking the numerical solutions to the exact results.

As a final remark, we would like to note that some exact non-trivial results are known on generalized one-band Hubbard models [24], but no extensions of these results are available for the multi-orbital Hubbard model. Investigation into the direction of determining, within the method outlined in [24], the exact ground-state wavefunction and energy of ODH in some physically relevant parameter regime is in progress.

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