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บทความวิจัย

แฮมิลโทเนียลยังผลสำหรับแบบจำลองฮับบาร์ดชนิดสองออบิทอล

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บทคัดย่อ

ได้ทำการคำนวณแฮมิลโทเนียนยังผลของแบบจำลองฮับบาร์ดชนิดสองออบิทอลที่ไร้สปิน โดยใช้การแปลงแบบบัญญัติ ได้ทำการเลือกตัวกำเนิดของการแปลงนี้เพื่อให้มีการทำลายพจน์ที่ผสมกันระหว่างฐานหลักที่มีอิเล็กตรอนเดี่ยว และฐานหลักที่มีอิเล็กตรอนคู่ หลังจากนั้นได้ใช้เงื่อนไขให้อิเล็กตรอนในระบบมีเพียงครึ่งเดียวและอันตรกิริยากันระหว่างอิเล็กตรอนในตำแหน่งเดียวกันมีสูงมาก จากเงื่อนไขทั้งสองที่กำหนดให้ จะได้แฮมิลโทเนียนยังผลที่เขียนอยู่ในรูปของตัวดำเนินการสปินเทียม จะพบว่าปริภูมิฮิลเบิร์ตของแฮมิลโทเนียนนี้จะมีเฉพาะฐานหลักที่ประกอบไปด้วยอิเล็กตรอนหนึ่งตัวต่อหนึ่งตำแหน่งของแลตทิสเท่านั้น เหตุผลดังกล่าวจะทำให้ขนาดของปริภูมิฮิลเบิร์ตเล็กลงซึ่งจะเป็นผลดีต่อการคำนวณหาสมบัติต่าง ๆที่เกี่ยวข้องกับสถานะพื้นของแบบจำลองนี้โดยวิธีคำนวณเชิงตัวเลข

คำสำคัญ: แบบจำลองฮับบาร์ดชนิดสองออบิทอลที่ไร้สปิน การแปลงแบบบัญญัติ ตัวดำเนินการสปินเทียม

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Effective Hamiltonian for Two-Orbital Hubbard Model

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ABSTRACT

The effective Hamiltonian for spinless two-orbital Hubbard model has been derived using the canonical transformation. The generator is chosen to annihilate the mixing terms between the double occupied and single occupied basis. Furthermore, the limits of half filling and strong on-site Coulomb interaction have been applied. The result is the effective Hamiltonian that is written in term of pseudo-spin operators. The Hilbert space of this Hamiltonian is therefore restricted to only basis states with one electron on each lattice site and the dimension of the Hilbert space is reduced accordingly. This would benefit the numerical methods that will be used to calculate the ground state properties of this model.

Keywords: spinless two-orbital Hubbard model, canonical transformation, pseudo-spin operators

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Introduction

The interest in strongly correlated electronic systems has increased greatly in the last decade. This is mainly because of the discovery of vary rich properties of transition metal oxides such as the high temperature superconductivity and the colossal magnetore-sistance [1, 2]. It is believed that the correlation between the electrons are responsible for such phenomena. It has also been recognised that the orbital degeneracy plays a major role in the strongly correlated electronic systems [3-5]. It is believed to be responsible for an anomalous magnetic behaviour found in lithium nickel oxide [6]. It is also found to be an important ingredient for understanding the physical properties of the manganite compounds $La_{1-x}Ca_xMnO_3$ [3, 5, 7]. Coupled orbital, charge and spin degree of freedoms, produce a fascinating phase diagram in this kind of materials [3]. Though there have been an intensive theoretical studies on this degree of freedom in various complex models for manganite [7 -11], it is still helpful to study the effect of the orbital degree of freedom alone.

In this paper we consider a situation where there is an orbital degeneracy with the absence of the spin degeneracy. The absence of the spin degeneracy is realised in the ordered phase of the system such as magnetite (Fe_3O_4) and the mixed manganese compounds e.g. $La_{0.7}Ca_{0.3}MnO_3$ which are known as manganite. In magnetite, the Pauli exclusion principle prevents the conduction electrons in the t_{2g} bands having their spins parallel to the core octahedral site spins. The conduction electrons in manganite, in an e_g bands, are subjected to a very strong Hund's rule coupling, therefore their spin is forced to be parallel to the core spin. In the ground state or at low temperatures well below the magnetic ordering temperature, the core spins of both magnetite and manganite are well ordered, therefore the conduction electrons of both materials lose their spin degeneracy.

In the theoretical studies of electronic behaviours of this system, many crucial models have been invented. The Hubbard model [12] is one of the popular models that has been used to study strong correlated electronic systems in many systems. When it includes the orbital degree of freedom, it has been called the orbital Hubbard model. Therefore, it has been used to study the effect of orbital occupied by electrons in many conditions; in finite on-site coulomb potential U with full cubic symmetries by Yuan *et al.* [9], in the strong-coupling limit with full cubic symmetries by Horsch *et al.* [11] and in $U \rightarrow \infty$ with finite size in 2D Hamiltonian by C. Srinitiwarawong and G. A. Gerhring [13]. In their work, finite system size was considered as full cubic symmetries and 2D cluster. Moreover, they studied the orbital ordering of the system in each case.

In this paper we will derive the effective Hamiltonian from the spinless orbital Hubbard model in the limits of half filling and large on-site coulomb interaction. The effective Hamiltonian is obtained from the canonical transformation by projecting out the high energy states.

Two-Orbital Hubbard Model

The Hubbard Hamiltonian is written as

$$H = H_{\text{hop}} + H_U. \tag{1}$$

The two terms are the description of opposing tendencies: metallic and insulator phases. The H_U denotes the on-site interaction term, which can be written as

$$H_U = U \sum_i \hat{n}_{ia} \hat{n}_{ib}, \tag{2}$$

where $\hat{n}_{ia(b)}$ is the number operator of an electron in $a(b)$-orbital at site i This term explains the Coulomb repulsion among electrons sharing the same site, with U defines the Coulomb potential energy. This term tends to resist the living of two electrons on the same site and leading to the insulator phase. In contrast,

$$H_{\text{hop}} = \sum_{<ij>} \sum_{\alpha\beta} t_{ij}^{\alpha\beta} c_{i\alpha}^{\dagger} c_{j\beta}, \tag{3}$$

where the Greek indices refer to the orbital quantum numbers, denotes the hopping of one electron to nearest neighbor sites and thus brings about the metallic behaviors. The summation over $\langle ij \rangle$ is taken only over the pair of nearest neighbor sites.

The states of electrons occupying on a particular site i are defined as four basis states in the followings:

$$|0\rangle_i \qquad \text{empty state at site } i \text{ (no electron occupies at site } i), \tag{4}$$

$$|a\rangle_i = c_{ia}^{\dagger}|0\rangle_i \qquad \text{electron occupies } a\text{-orbital at site } i, \tag{5}$$

$$|b\rangle_i = c_{ib}^{\dagger}|0\rangle_i \qquad \text{electron occupies } b\text{-orbital at site } i, \tag{6}$$

$$|d\rangle_i = c_{ia}^{\dagger} c_{ib}^{\dagger}|0\rangle_i \qquad \text{two electrons occupy both } a \text{ and } b\text{-orbital at site } i\ , \tag{7}$$

where $c_{ia(b)}^{\dagger}$ is a creation operator which creates an electron at site i with $a(b)$ orbital.

All possible hopping processes in two-orbital Hubbard Hamiltonian are separated into three parts; creating the doubly occupied site (H^+), annihilating the doubly occupied site (H^-) and the processing that does not change the number of doubly occupied sites (H^0). The Hamiltonian is written as

$$H_{\rm hop} = \sum_{\sigma} \{H^+_{t_{\sigma,\sigma}} + H^+_{t_{\sigma,-\sigma}} + H^-_{t_{\sigma,\sigma}} + H^-_{t_{\sigma,-\sigma}} + H^0_{t_{\sigma,\sigma}} + H^0_{t_{\sigma,-\sigma}}\}, \tag{8}$$

where σ and $-\sigma$ refer to orbital degree of freedoms which the corresponding states are orthogonal and $t_{\sigma,-\sigma}$ refers to the hopping amplitude between orbitals. Terms in the Hamiltonian are written as

$$H^0_{t_{\sigma,\sigma}} = -\sum_{<ij>}\sum_{\sigma} t_{\sigma,\sigma}\{\hat{n}_{i,-\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}\hat{n}_{j,-\sigma} + (1-\hat{n}_{i,-\sigma})c^{\dagger}_{i\sigma}c_{j\sigma}(1-\hat{n}_{j,-\sigma}) + H.c.\}, \tag{9}$$

$$\begin{aligned} H^0_{t_{\sigma,-\sigma}} = -\sum_{<ij>}\sum_{\sigma} t_{\sigma,-\sigma}\{&\hat{n}_{i,-\sigma}c^{\dagger}_{i\sigma}c_{j,-\sigma}\hat{n}_{j\sigma} + (1-\hat{n}_{i,-\sigma})c^{\dagger}_{i\sigma}c_{j,-\sigma}(1-\hat{n}_{j\sigma}) \\ &+ \hat{n}_{j\sigma}c^{\dagger}_{j,-\sigma}c_{i\sigma}\hat{n}_{i,-\sigma} + (1-\hat{n}_{j\sigma})c^{\dagger}_{j,-\sigma}c_{i\sigma}(1-\hat{n}_{i,-\sigma})\}. \end{aligned} \tag{10}$$

$$H^-_{t_{\sigma,\sigma}} = -\sum_{<ij>}\sum_{\sigma} t_{\sigma,\sigma}\{(1-\hat{n}_{i,-\sigma})c^{\dagger}_{i\sigma}c_{j\sigma}\hat{n}_{j,-\sigma} + H.c.\}, \tag{11}$$

$$H^-_{t_{\sigma,-\sigma}} = -\sum_{<ij>}\sum_{\sigma} t_{\sigma,-\sigma}\{(1-\hat{n}_{i-\sigma})c^{\dagger}_{i\sigma}c_{j,-\sigma}\hat{n}_{j\sigma} + (1-\hat{n}_{j\sigma})c^{\dagger}_{j,-\sigma}c_{i\sigma}\hat{n}_{i,-\sigma}\}. \tag{12}$$

$$H^+_{t_{\sigma,\sigma}} = -\sum_{<ij>}\sum_{\sigma} t_{\sigma,\sigma}\{\hat{n}_{i,-\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}(1-\hat{n}_{j,-\sigma}) + H.c.\}, \tag{13}$$

$$H^+_{t_{\sigma,-\sigma}} = -\sum_{<ij>}\sum_{\sigma} t_{\sigma,-\sigma}\{\hat{n}_{i-\sigma}c^{\dagger}_{i\sigma}c_{j,-\sigma}(1-\hat{n}_{j\sigma}) + \hat{n}_{j\sigma}c^{\dagger}_{j,-\sigma}c_{i\sigma}(1-\hat{n}_{i,-\sigma})\}, \tag{14}$$

Derivation of the Effective Hamiltonian

When the strongly correlated electrons system are considered, the mixed states between the two subbands, doubly occupied and singly occupied subbands, will appear due to the hopping Hamiltonian; creating and annihilating the doubly occupied states respectively as shown in Eqs. (11) -(12) and (13) -(14). We need to separate these mix states and therefore, the canonical transformation method [14, 15] is introduced to solve this problem. The unmixed states can be found by rotating to such a new suitable basis. According to (8) the two-orbitals Hubbard Hamiltonian can be written as

$$\begin{aligned} H \;=\; & H^+_{t_{aa}} + H^+_{t_{ab}} + H^+_{t_{ba}} + H^+_{t_{bb}} + H^-_{t_{aa}} + H^-_{t_{ab}} + H^-_{t_{ba}} + H^-_{t_{bb}} \\ + \; & H^0_{t_{aa}} + H^0_{t_{ab}} + H^0_{t_{ba}} + H^0_{t_{bb}} + H_U, \end{aligned} \tag{15}$$

or in short

$$H = H_t^+ + H_t^- + H_t^0 + H_U. \tag{16}$$

The effective Hamiltonian is written as

$$\begin{aligned} H_{\text{eff}} &= e^{iS} H e^{-iS} = H + i[S,H] + \frac{i^2}{2}[S,[S,H]] + ..., && (17) \\ &= H_U + H_t^+ + H_t^- + H_t^0 + i[S,H_U] \\ &+ i[S, H_t^+ + H_t^- + H_t^0] + \frac{i^2}{2}[S,[S,H]] + ... && (18) \end{aligned}$$

The generator S is chosen in such away that H_{eff} does not connect different subbands. Therefore the largest cross-terms, H_t^+ and H_t^-, should be eliminated. They are cancelled from the commuted term, $i[S,H_U]$. This condition will be brought to find the suitable generator S. Note that terms with orders of t higher than 2 are also neglected.

The generator S is separated into two parts being $S = S' + S''$. We will let S' and S'' be in the order of t and t^2 respectively where t is the hopping amplitude in all cases of an electron hopping between two sites. The operator S' can be chosen to be

$$S' = \frac{-i}{U}(H_t^+ - H_t^-). \tag{19}$$

Term of $i[S,H_U]$ replaced by $S = S' + S''$, becomes

$$i[S,H_U] = i[S',H_U] + i[S'',H_U], \tag{20}$$

whereas

$$i[S',H_U] = -(H_t^+ + H_t^-), \tag{21}$$

and

$$i[S'',H_U] = -\frac{1}{U}[H_t^+ - H_t^-, H_t^0]. \tag{22}$$

Moreover, we get

$$i[S, H_t^+ + H_t^- + H_t^0] = i[S', H_t^+ + H_t^- + H_t^0] + i[S'', H_t^+ + H_t^- + H_t^0]. \tag{23}$$

The first term of the right-hand side which is the order of t^2 can be separated into two parts

i.e.

$$i[S', H_t^+ + H_t^-] = \frac{2}{U}[H_t^+, H_t^-], \tag{24}$$

and

$$i[S', H_t^0] = \frac{1}{U}[H_t^+ - H_t^-, H_t^0], \tag{25}$$

where Eq. (25) is cancelled by Eq. (22). Moreover, the second term of the right hand side in Eq. (23) has disappeared because it is of the order t^3.

Besides, the term $\frac{i^2}{2}[S,[S,H_U]]$ can be written as

$$\frac{i^2}{2}[S,[S,H_U]] = -\frac{1}{U}[H_t^+, H_t^-]. \tag{26}$$

Finally, substituting Eqs. (21), (22), (24), (25) and (26) into Eq. (18), the effective Hamiltonian to the order of t^2 can be written as

$$\begin{aligned} H_{\text{eff}} &= H_{t_{aa}}^0 + H_{t_{ab}}^0 + H_{t_{ba}}^0 + H_{t_{bb}}^0 + H_U \\ &+ \frac{1}{U}[H_{t_{aa}}^+ + H_{t_{ab}}^+ + H_{t_{ba}}^+ + H_{t_{bb}}^+, H_{t_{aa}}^- + H_{t_{ab}}^- + H_{t_{ba}}^- + H_{t_{bb}}^-]. \end{aligned} \tag{27}$$

In the conditions of large onsite coulomb interaction and half-filling, the term of H_t^0 and H_U , which are up against these conditions, are neglected. We need to calculate the last term on the right hand side of equation (27). For convenience, the suitable tool so-called the Hubbard operators [15] will be used for this calculation. The hopping process that take electron from orbital a to orbital b on the same site j is written as

$$X_j^{b\leftarrow a} = |b\rangle_{jj}\langle a|. \tag{28}$$

Using this notation, the last terms in equation (27) are written as

$$H_t^+ = H_{t_{aa}}^+ + H_{t_{ab}}^+ + H_{t_{ba}}^+ + H_{t_{bb}}^+, \tag{29}$$

$$\begin{aligned} H_t^+ &= -\sum_{<ij>}\sum_{\sigma}\{t_{\sigma\sigma}\eta(\sigma)(X_i^{d\leftarrow -\sigma}X_j^{0\leftarrow\sigma} + X_j^{d\leftarrow -\sigma}X_i^{0\leftarrow\sigma}) \\ &+ t_{\sigma-\sigma}(\eta(\sigma)X_i^{d\leftarrow -\sigma}X_j^{0\leftarrow -\sigma} + \eta(-\sigma)X_j^{d\leftarrow\sigma}X_i^{0\leftarrow\sigma})\}, \end{aligned} \tag{30}$$

and

$$H_t^- = H_{t_{aa}}^- + H_{t_{ab}}^- + H_{t_{ba}}^- + H_{t_{bb}}^-, \tag{31}$$

$$\begin{aligned} H_t^- &= -\sum_{<ij>}\sum_{\sigma}\{t_{\sigma\sigma}\eta(\sigma)(X_i^{\sigma\leftarrow 0}X_j^{-\sigma\leftarrow d} + X_j^{\sigma\leftarrow 0}X_i^{-\sigma\leftarrow d}) \\ &+ t_{\sigma-\sigma}(\eta(-\sigma)X_i^{\sigma\leftarrow 0}X_j^{\sigma\leftarrow d} + \eta(\sigma)X_j^{-\sigma\leftarrow 0}X_i^{-\sigma\leftarrow d})\}, \end{aligned} \tag{32}$$

where $\eta(\sigma)$ is

$$\eta(\sigma) = \begin{cases} +1 & if\ \sigma = a \\ -1 & if\ \sigma = b. \end{cases} \tag{33}$$

The important term in the large-U limit and half-filling of H_{eff} is $\frac{1}{U}[H_t^+, H_t^-] = \frac{1}{U}[H_t^+ H_t^- - H_t^- H_t^+]$. Since we are interested in half filling, the Hilbert space of the effective Hamiltonian will contain only single occupied states. The $H_t^+ H_t^-$ term is absent since the value of it operating on these single occupied state will be zero. So, the remaining term which becomes the effective Hamiltonian is only $H_t^+ H_t^-$. The effective Hamiltonian in the form of Hubbard operators is written as

$$\begin{aligned}
-\frac{1}{U} H_t^- H_t^+ &= \sum_{<ij>} \{ -\sum_\sigma \frac{t_{\sigma\sigma}^2}{U} X_i^{-\sigma\leftarrow-\sigma} X_j^{\sigma\leftarrow\sigma} + \sum_\sigma \frac{t_{\sigma\sigma} t_{\sigma-\sigma}}{U} X_i^{-\sigma\leftarrow\sigma} X_j^{\sigma\leftarrow\sigma} \\
&- \sum_\sigma \frac{t_{\sigma-\sigma} t_{\sigma\sigma}}{U} X_i^{-\sigma\leftarrow-\sigma} X_j^{-\sigma\leftarrow\sigma} + \sum_\sigma \frac{t_{\sigma-\sigma}^2}{U} X_i^{-\sigma\leftarrow\sigma} X_j^{-\sigma\leftarrow\sigma} \\
&+ \sum_\sigma \frac{t_{-\sigma-\sigma} t_{\sigma\sigma}}{U} X_i^{\sigma\leftarrow-\sigma} X_j^{-\sigma\leftarrow\sigma} - \sum_\sigma \frac{t_{-\sigma-\sigma} t_{\sigma-\sigma}}{U} X_i^{\sigma\leftarrow\sigma} X_j^{-\sigma\leftarrow\sigma} \\
&+ \sum_\sigma \frac{t_{-\sigma\sigma} t_{\sigma\sigma}}{U} X_i^{\sigma\leftarrow-\sigma} X_j^{\sigma\leftarrow\sigma} - \sum_\sigma \frac{t_{-\sigma\sigma} t_{\sigma-\sigma}}{U} X_i^{\sigma\leftarrow\sigma} X_j^{\sigma\leftarrow\sigma} \\
&- \sum_\sigma \frac{t_{\sigma\sigma}^2}{U} X_i^{\sigma\leftarrow\sigma} X_j^{-\sigma\leftarrow-\sigma} + \sum_\sigma \frac{t_{\sigma\sigma} t_{\sigma-\sigma}}{U} X_i^{\sigma\leftarrow\sigma} X_j^{-\sigma\leftarrow\sigma} \\
&+ \sum_\sigma \frac{t_{\sigma-\sigma} t_{\sigma\sigma}}{U} X_i^{\sigma\leftarrow\sigma} X_j^{\sigma\leftarrow-\sigma} - \sum_\sigma \frac{t_{\sigma-\sigma}^2}{U} X_i^{\sigma\leftarrow\sigma} X_j^{\sigma\leftarrow\sigma} \\
&+ \sum_\sigma \frac{t_{-\sigma-\sigma} t_{\sigma\sigma}}{U} X_i^{-\sigma\leftarrow\sigma} X_j^{\sigma\leftarrow-\sigma} - \sum_\sigma \frac{t_{-\sigma-\sigma} t_{\sigma-\sigma}}{U} X_i^{-\sigma\leftarrow\sigma} X_j^{\sigma\leftarrow\sigma} \\
&- \sum_\sigma \frac{t_{-\sigma\sigma} t_{\sigma\sigma}}{U} X_i^{-\sigma\leftarrow\sigma} X_j^{-\sigma\leftarrow-\sigma} + \sum_\sigma \frac{t_{-\sigma\sigma} t_{\sigma-\sigma}}{U} X_i^{-\sigma\leftarrow\sigma} X_j^{-\sigma\leftarrow\sigma} \}.
\end{aligned} \tag{34}$$

Using the pseudo-spin operators, the effective Hamiltonian becomes

$$\begin{aligned}
H_{\text{eff}} &= \sum_{<ij>} \{ \frac{2}{U}(t_{aa}^2 + t_{bb}^2)(\hat{\tau}_i^z \hat{\tau}_j^z - \frac{\hat{n}_i \hat{n}_j}{4}) - \frac{2(t_{ab}^2 + t_{ba}^2)}{U}(\hat{\tau}_i^z \hat{\tau}_j^z + \frac{\hat{n}_i \hat{n}_j}{4}) \\
&+ \frac{2t_{ab} t_{ba}}{U}(\hat{\tau}_i^+ \hat{\tau}_j^+ + \hat{\tau}_i^- \hat{\tau}_j^-) + \frac{2t_{aa} t_{bb}}{U}(\hat{\tau}_i^+ \hat{\tau}_j^- + \hat{\tau}_i^- \hat{\tau}_j^+) \\
&+ 2(\frac{t_{aa} t_{ab}}{U} - \frac{t_{bb} t_{ba}}{U})(\hat{\tau}_i^z \hat{\tau}_j^+ + \hat{\tau}_i^z \hat{\tau}_j^-) \\
&+ 2(\frac{t_{aa} t_{ba}}{U} - \frac{t_{bb} t_{ab}}{U})(\hat{\tau}_i^+ \hat{\tau}_j^z + \hat{\tau}_i^- \hat{\tau}_j^z) \},
\end{aligned} \tag{35}$$

where $\hat{\tau}^z_{i(j)}$, $\hat{\tau}^+_{i(j)}$ and $\hat{\tau}^-_{i(j)}$ are the pseudo-spin operators at site $i(j)$ defined by

$$\begin{aligned}
\hat{\tau}^z &= \frac{1}{2}(c^\dagger_{ia}c_{ia} - c^\dagger_{ib}c_{ib}), \\
\hat{\tau}^+ &= c^\dagger_{ia}c_{ib}, \\
\hat{\tau}^- &= c^\dagger_{ib}c_{ia}, \\
\hat{n}_i &= c^\dagger_{ia}c_{ia} + c^\dagger_{ib}c_{ib}.
\end{aligned} \tag{36}$$

Conclusion

We have derived the effective Hamiltonian in the limits of half filling and large onsite coulomb interactions from the spinless orbital Hubbard model. The canonical transformation has been used to separate the high energy states from the low energy states. As a result, the terms in Hamiltonian that mix between double occupied subband and single occupied subband have been eliminated. The Hamiltonian is then written in the form of pseudo-spin operators which is similar to those used in the Heisenberg Hamiltonian. This effective Hamiltonian can be used to calculate the ground state properties. The dimension of the Hilbert space of this Hamiltonian is greatly reduced and thus benefits the finite-site calculations such as the exact diagonalisation or the density matrix renormalisation group methods.

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