Effect of Hund’s rule coupling on SU(4) spin-orbital system

Hiroaki Onishi *, Takashi Hotta

Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan

Received 5 July 2006

Abstract

We investigate the ground-state property of a one-dimensional two-orbital Hubbard model at quarter filling by numerical techniques such as the density-matrix renormalization group method and the exact diagonalization. When the Hund’s rule coupling $J$ is zero, the model is SU(4) symmetric. In fact, both spin and orbital correlations have a peak at $q=\pi/2$, indicating an SU(4) singlet state with a four-site periodicity. On the other hand, with increasing $J$, it is found that the peak position of the orbital correlation changes to $q=\pi$, while that of the spin correlation remains at $q=\pi/2$. We briefly discuss how the SU(4) symmetry is broken by $J$.

PACS: 75.45.+j; 75.10.-b; 75.40.Mg

Keywords: SU(4) spin-orbital system; Hund’s rule coupling; density-matrix renormalization group

It has been widely recognized that the interplay of spin and orbital degrees of freedom plays a significant role in the emergence of exotic magnetism in strongly correlated electron systems with orbital degeneracy. In this context, the highest symmetric SU(4) spin-orbital model has been one of the subjects of much interests from a theoretical viewpoint. In particular, the one-dimensional model is Bethe ansatz solvable [1], and the combined quantum effects of spin and orbital have been revealed by analytical and numerical investigations [2,3,4]. Indeed, it is characteristic of an SU(4) singlet state that correlation functions show critical behavior with a four-site periodicity and the elementary excitation is gapless.

The highest SU(4) symmetry originates in the situation, where electrons hop only between the same types of orbitals with equal amplitude and the Hund’s rule coupling is ignored in a two-orbital Hubbard model. In a more realistic situation, however, the Hund’s rule coupling should break the SU(4) symmetry down to SU(2)$_\text{spin}$×U(1)$_\text{orbital}$ [3,5,6]. To clarify the effect of such symmetry breaking, Lee et al. have studied an SU(4) Hubbard model perturbed by the Hund’s rule coupling by means of renormalization-group and bozonization methods, and proposed that the spin gap opens for an arbitrarily small Hund’s rule coupling [5].

In this paper, we investigate spin and orbital correlations in a one-dimensional two-orbital Hubbard model with one electron per site. The Hamiltonian is given by

$$
H = t \sum_{i,\tau,\sigma} (d_{i\tau\sigma}^\dagger d_{i+1\tau\sigma} + \text{h.c.}) + U \sum_{i,\tau} \rho_{i\tau\uparrow} \rho_{i\tau\downarrow} \\
+ U' \sum_{i,\tau,\sigma,\sigma'} \rho_{i\tau\sigma} \rho_{i\tau\sigma'} + J \sum_{i,\tau,\sigma} d_{i\tau\sigma}^\dagger d_{i\tau\sigma'}^\dagger d_{i\tau\sigma'} d_{i\tau\sigma} \\
+ J' \sum_{i,\tau,\tau' \neq \tau} d_{i\tau\uparrow}^\dagger d_{i\tau'\uparrow}^\dagger d_{i\tau'\downarrow} d_{i\tau\downarrow},
$$

(1)

where $d_{i\tau\sigma}$ is the annihilation operator for an electron with spin $\sigma$ in orbital $\tau (=\alpha, \beta)$ at site $i$, $\rho_{i\tau\sigma} = d_{i\tau\sigma}^\dagger d_{i\tau\sigma}$, and $t$ is the hopping amplitude. Hereafter, $t$ is taken as the energy unit. $U$, $U'$, $J$, and $J'$ denote intra-orbital Coulomb, inter-orbital Coulomb, exchange (Hund’s rule coupling), and pair hopping interactions, respectively. Note that $U=U'+J+J'$ due to the rotational invariance in the local orbital space, and $J=J'$ due to the reality of the wavefunction [7]. When the Hund’s rule coupling is zero, i.e., $U=U'$ and $J=J'=0$, the system possesses the SU(4) symmetry.

We analyze the model with 32 sites ($N=32$) in the open boundary condition by the density-matrix renormalization group method [8]. The finite-system algorithm is employed with keeping 400 states per block and the truncation error is estimated to be $5 \times 10^{-6}$ at most. We also use the Lanczos method for the analysis of a four-site periodic chain. In this paper, we set $U'-J=20$ to consider the strong-coupling region, and investigate the dependence on $J$.

In Fig. 1, we show our DMRG results for the spin and orbital structure factors, defined by

* Corresponding author.

Email address: onishi.hiroaki@jaea.go.jp (Hiroaki Onishi).

© 2022 Elsevier B.V. All rights reserved.
we observe a peak at $q=\pi/2$, clearly indicating an SU(4) singlet state with a four-site periodicity, which is consistent with the previous numerical work for the SU(4) spin-orbital model [3]. On the other hand, $S(q)$ and $T(q)$ exhibit distinct behavior with increasing $J$, as shown in Figs. 1(b) and 1(c). It is observed that the peak position of $T(q)$ changes from $q=\pi/2$ to $q=\pi$, since $T(\pi/2)$ is suppressed, while $T(\pi)$ is enhanced due to the effect of $J$. As for the spin correlation, the peak position of $S(q)$ remains at $q=\pi/2$ even for finite values of $J$, since the magnitude of $S(\pi/2)$ increases in sharp contrast to the case of $T(q)$.

To obtain intuitive understanding for the changes in $S(q)$ and $T(q)$, it is useful to consider a four-site system, which is a minimal model to form the SU(4) singlet ground state at $J=0$ [9]. The SU(4) singlet state is expressed as

$$|\text{SU}(4)\rangle = (1/\sqrt{24}) \sum_{i\neq j \neq k \neq l} d_{i\alpha_1}^{\dagger} d_{j\alpha_2}^{\dagger} d_{k\beta_1}^{\dagger} d_{l\beta_2}^{\dagger} |0\rangle,$$

where $|0\rangle$ is the vacuum state and the summation is taken over all permutations for site indices. Note that $|\text{SU}(4)\rangle$ consists of 24 states with the same weight for each state. For finite $J$, however, the ground state is not represented by $|\text{SU}(4)\rangle$ itself. As shown in Figs. 2(a)-(c), the 24 states are split into three classes with eight states for each according to the weight in the spin-singlet ground state [6]. Note that each class is characterized by the peak positions of $S(q)$ and $T(q)$, denoted by $(q_{\text{spin}}, q_{\text{orbital}})$: $(\pi/2, \pi)$ for the class $a$, $(\pi/2, \pi/2)$ for the class $b$, and $(\pi, \pi/2)$ for the class $c$.

In Fig. 2(d), we show the $J$ dependence of the weight of each class $m$ in the ground state,

$$w_m = \sum_{i \in m} |\langle \phi_i | \psi_G \rangle|^2,$$

where $\psi_G$ is the ground state and $\phi_i$ denotes the basis. At $J=0$, three classes contribute to the ground state with equal weight. With increasing $J$, the weight of the class $a$ increases, while those of the class $b$ and $c$ decrease and the total weight of the three classes does not change. In the class $a$, as shown in Fig. 2(a), partly spin ferromagnetic (FM) alignment appears due to the Hund’s rule coupling, and an antiferro-orbital (AFO) configuration is favored to avoid the energy loss in the hopping process due to the intra-orbital Coulomb interaction, indicating the instability to a FM/AFO state due to the Hund’s rule coupling. Thus, the correlations of $S(\pi/2)$ and $T(\pi)$ are enhanced, leading to the change of the peak position of $T(q)$, as shown in Fig. 1. We note that with further increasing $J$, the ground state is changed to a FM/AFO state.

We have tried to understand how the spin gap $\Delta_s$ of the present model (1) is affected by $J$, but it is a difficult task to estimate $\Delta_s$ with precision, because of charge, spin, and orbital degrees of freedom. To clarify the behavior of $\Delta_s$ in the thermodynamic limit, it would be appropriate to investigate an effective spin-orbital model in the strong-coupling limit, which is an interesting future issue.

In summary, at $J=0$, $S(q)$ and $T(q)$ agree with each other and have a peak at $q=\pi/2$ due to the SU(4) singlet ground state. On the other hand, with increasing $J$, we observe the transition of the peak position of $T(q)$ to $q=\pi$ in accordance with the change of relevant spin-orbital configuration.

We thank K. Ueda for useful discussions. T.H. is supported by the Japan Society for the Promotion of Science and by the Ministry of Education, Culture, Sports, Science, and Technology of Japan.

References

[1] B. Sutherland, Phys. Rev. B 12 (1975) 3795.
[2] Y. Q. Li, M. Ma, D. N. Shi, and F. C. Zhang, Phys. Rev. B 60 (1999) 12781.
[3] Y. Yamashita, N. Shibata, and K. Ueda, Phys. Rev. B 58 (1998) 9114.
[4] B. Frischmuth, F. Mila, and M. Troyer, Phys. Rev. Lett. 82 (1999) 835.
[5] H. C. Lee, P. Azaria, and E. Boulat, Phys. Rev. B 69 (2004) 155109.
[6] J. C. Xavier, H. Onishi, T. Hotta, and E. Dagotto, Phys. Rev. B 73 (2006) 014405.
[7] E. Dagotto, T. Hotta, and A. Moreo, Phys. Rep. 344 (2001) 1.
[8] S. R. White, Phys. Rev. Lett. 69 (1992) 2863.
[9] Y. Q. Li, M. Ma, D. N. Shi, and F. C. Zhang, Phys. Rev. Lett. 81 (1998) 3527.