Spin-charge-orbital ordering on triangle-based lattices

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Abstract

We investigate the ground-state property of an $e_g$-orbital Hubbard model at quarter filling on a zigzag chain by exploiting the density matrix renormalization group method. When two orbitals are degenerate, the zigzag chain is decoupled to a double-chain spin system to suppress the spin frustration due to the spatial anisotropy of the occupied orbital. On the other hand, when the level splitting is increased and the orbital anisotropy disappears, a characteristic change in the spin incommensurability is observed due to the revival of the spin frustration.

Preprint submitted to Elsevier Science 23 March 2022

Key words: Geometrical frustration, Orbital ordering, Spin incommensurability, Density matrix renormalization group method

PACS: 75.10.-b; 71.10.Fd; 75.30.Et

The magnetic property of frustrated spin systems has been one of the central issues for many years in the research field of condensed matter physics [1]. For example, it is well known that in the antiferromagnetic (AFM) Ising model on a triangular lattice, there occurs macroscopic degeneracy for possible spin configurations in the ground state [2]. In general, however, such high degeneracy is lifted to suppress the spin frustration, since the lattice is deformed to lower the lattice symmetry due to the spin-lattice coupling.

On the other hand, recently there has been a rapid increase of interest in the effect of the interplay of spin and orbital degrees of freedom [3]. It has been emphasized that the orbital anisotropy plays a significant role to cause a variety of cooperative phenomena in realistic materials. In particular, in geometrically frustrated lattices, it is expected that orbital ordering occurs to affect the spin frustration due to the spin-orbital coupling, since the orbital anisotropy leads to the non-uniform exchange interactions.

In this paper, to clarify the key role of the orbital anisotropy in geometrically frustrated lattices, we investigate an $e_g$-orbital degenerate model [5]. The Hamiltonian considered here is given by

$$ H = \sum_{\gamma,\rho,\sigma} t_{\gamma\rho} \rho_{\gamma\sigma} \rho_{\gamma'\sigma} - (\Delta/2) \sum_{\gamma} (\rho_{\gamma a} - \rho_{\gamma b}) + U \sum_{\gamma} \rho_{\gamma a} \rho_{\gamma b} + U' \sum_{\gamma} \rho_{\gamma a} \rho_{\gamma b}, \tag{1} $$

where $d_{\gamma\sigma} (d^\dagger_{\gamma\sigma})$ is the annihilation operator for an electron with spin $\sigma$ in the $3z^2-r^2 (x^2-y^2)$ orbital at site $1$, $\rho_{\gamma a} = d_{\gamma a} d_{\gamma\sigma}$, and $\rho_{\gamma} = \sum_{\sigma} \rho_{\gamma\sigma}$. $t_{\gamma\gamma'}$ is nearest-neighbor hopping between $\gamma$ and $\gamma'$ orbitals along the $a$ direction. Note that the zigzag chain is considered as a double chain connected by a zigzag path. The hopping amplitudes are given by $t_{\gamma a} = t/4$, $t_{\gamma b} = -t\sqrt{3}/4$, $t_{\gamma b} = 3t/4$ for the double-chain direction and $t_{\gamma a} = t/4$, $t_{\gamma b} = t\sqrt{3}/8$, $t_{\gamma b} = 3t/16$ along the zigzag path. Hereafter, $t$ is taken as the energy unit. $\Delta$ is the level splitting between $3z^2-r^2$ and $x^2-y^2$ orbitals, $U$ is the intraorbital Coulomb interaction, and $U'$ is the interorbital Coulomb interaction.

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the state is also changed. To clarify this point, it is convenient to reduce the present model to a spin system
on the orbital-ordered background. Then, the present
system is described by the zigzag spin chain, in which
the spin correlation has a commensurate peak at $q = \pi$
for $0 \leq J_2/J_1 \leq 1/2$, but the peak is gradually changed to
an incommensurate one for $J_2/J_1 \geq 1/2$, and eventually,
we find the incommensurate peak at $q = \pi/2$ for infinite
$J_2/J_1$ [8,9]. In Fig. 1(c), we show our DMRG result
of the spin correlation $S(q) = \sum_{i,j} e^{i q (i-j)} \langle S_i^z S_j^z \rangle / N^2$
with $S_i^z = \sum_\sigma (\rho_{\gamma \uparrow} - \rho_{\gamma \downarrow})/2$ for $\Delta = 0$. We find a clear
peak at $q = \pi/2$, consistent with that of the zigzag spin
chain with large $J_2/J_1$, since $J_2/J_1 = 64^2$ for $\Delta = 0$. On
the other hand, as shown in Fig. 1(d), the peak position
for $\Delta = 1$ changes from $q = \pi/2$ toward $q = \pi$, expected by
analogy with the zigzag spin chain, since we estimate
$J_2/J_1 = 1.61$ for $\Delta = 1$. The detail of the $\Delta$ dependence
will be discussed elsewhere in future.

Finally, let us consider how the orbital state changes
in the intermediate region. In Fig. 1(e), we show the $\Delta$
dependence of the electron densities $n_i = \sum_j \rho_{\gamma j} / N$
in $3z^2-r^2$ and $x^2-y^2$ orbitals. With increasing $\Delta$, elec-
trons are forced to accommodate in the lower $3z^2-r^2$
level, but the electron density in each orbital is found
to change gradually without any singularity. To under-
stand this behavior, we evaluate the electron densities
for the optimal orbitals. As shown in Fig. 1(f), it is
found that one of the optimal orbitals is occupied irre-
pective of $\Delta$ and the fluctuation is very small even in
the intermediate region. Namely, the present system is
always regarded as a one-orbital system, although we have
considered the multi-orbital system.

In summary, for $\Delta = 0$, the $3z^2-r^2$ orbital is selec-
tively occupied to suppress the spin frustration and the
zigzag chain is decoupled to a double-chain spin sys-
tem due to the orbital anisotropy. In fact, the ratio of
the AFM exchange interaction along the double-chain
direction $J_2$ to that along the zigzag path $J_1$ is esti-
mated as $J_2/J_1 = 64^2$. On the other hand, for $\Delta = 1$,
lower-energy $3z^2-r^2$ orbital is favorably occupied, as
shown in Fig. 1(b). Note that when the $3z^2-r^2$ orbital
is fully occupied for infinite $\Delta$, the orbital anisotropy
disappears in the $xy$ plane, i.e., $J_2/J_1 = 1$, and the spin
frustration becomes effective.

In accordance with the variation in the orbital shape,