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Numerical study of t_{2g} orbital system with ferromagnetic polarization

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Finite-temperature orbital state in a ferromagnetic Mott insulator with triply degenerate t_{2g} orbital is investigated numerically. We employ the quantum Monte Carlo simulation with the loop algorithm. Indications for conventional staggered-type orbital order are not remarkable down to the lowest temperature to which the present simulation can get access. Physical parameters monitoring the off-diagonal orbital order, which is characterized by a linear combination of the (d_{yz}, d_{zx}, d_{xy}) orbital-wave functions with equal weights, are not conspicuous. It is found that an orbital gaplike behavior appears in the uniform orbital susceptibility. This is supported by a threshold behavior in the staggered correlation function in a calculation with the additional Ising-type interaction. Some rigorous remarks for the long-range orbital order are also presented.

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Orbital degree of freedom and its strong coupling with spin, charge, and lattice bring about a variety of fascinating physical phenomena in transition-metal oxides.¹⁻³ Colossal magnetoresistance effect observed in vicinity of charge- and orbital-ordered state in perovskite manganites is a typical example. Classical aspects of the orbital, e.g., long-range orbital orders accompanied with the Jahn-Teller distortion and their roles on the magnetic exchange interaction have been fully examined and have been almost settled nowadays. On the other hand, quantum aspects of the orbital are still unrevealed and are expected to open a window for a new research field in correlated electron system.

Perovskite titanate $RTiO_3$ (R : rare-earth metal ion) is one of the candidates as a material where quantum orbital physics is realized. A formal valence of Ti ion is 3+, and one $3d$ electron occupies one of the triply degenerate t_{2g} orbitals. In this Brief Report, we denote, for simplicity, the three t_{2g} orbitals (d_{yz}, d_{zx}, d_{xy}) by $(d_\alpha, d_\beta, d_\gamma)$, respectively. Because of a weak Jahn-Teller coupling and the novel symmetry of the t_{2g} orbital-wave functions, quantum aspects of the orbital are expected to become evident.⁴⁻⁶

In particular, a ferromagnetic Mott insulator with the t_{2g} orbital degeneracy attracts attention as a simple orbital system where spin and charge degrees of freedom are quenched.⁷⁻⁹ One representative material is $YTiO_3$, where the isotropic-spin-wave dispersion relation is observed by the inelastic neutron scattering.¹⁰ This result seems to contradict a long-range orbital order confirmed by several experiments.¹¹⁻¹⁴ The t_{2g} orbital Hamiltonian in a ferromagnetic Mott insulator at zero temperature was examined in Ref. 9. Through the analytical calculations, the two kinds of long-range orbital-ordered states¹⁵ were proposed. It was shown that these orders set in only at zero temperature due to strong quantum fluctuation. However, the puzzling spin-orbital properties in $YTiO_3$ still remain an open issue. Even in a pure theoretical viewpoint, finite-temperature (T) orbital states with large quantum fluctuation are unclear.

In this Brief Report, we study the t_{2g} orbital system with ferromagnetic polarization. Our purpose is to examine finite-temperature orbital state in the idealized t_{2g} orbital model by using an unbiased method. We employ the quantum Monte Carlo (MC) (QMC) simulation with the loop algorithm. Down to at least around $T \sim 0.3J$ with the coupling constant J , indications of the conventional staggered-type order, the

off-diagonal orbital order, and the orbital dimerized state are not conspicuous. Instead, the orbital gaplike behaviors are found in the uniform orbital susceptibility below around $0.8J$.

We start from the Hamiltonian for the $(t_{2g})^1$ system with ferromagnetic polarization in an ideal Perovskite lattice. The generalized Hubbard Hamiltonian in a simple-cubic lattice with the triply degenerate t_{2g} orbitals is given as

$$\begin{aligned} \mathcal{H}_0 = & \sum_{\langle ij \rangle \xi \xi' s} (t_{ij}^{\xi \xi'} d_{i\xi s}^\dagger d_{j\xi' s} + \text{H.c.}) + U \sum_{i\xi} n_{i\xi \uparrow} n_{i\xi \downarrow} \\ & + \frac{1}{2} U' \sum_{i\xi \neq \xi'} n_{i\xi} n_{i\xi'} + \frac{1}{2} K \sum_{i\xi \neq \xi' s s'} d_{i\xi s}^\dagger d_{i\xi' s'}^\dagger d_{i\xi s} d_{i\xi' s'} \\ & + I \sum_{i\xi \neq \xi'} d_{i\xi \uparrow}^\dagger d_{i\xi \downarrow}^\dagger d_{i\xi \downarrow} d_{i\xi \uparrow}. \end{aligned} \quad (1)$$

We define the electron annihilation operator $d_{i\xi\sigma}$ with orbital $\xi = (\alpha, \beta, \gamma)$, spin $s = (\uparrow, \downarrow)$ at site i , and the electron transfer integral $t_{ij}^{\xi \xi'}$. A pair of the nearest neighboring (NN) sites is denoted by $\langle ij \rangle$. The intraorbital Coulomb interaction U , the interorbital one U' , the Hund coupling K , and the pair hopping I are introduced. In an atomic limit, there is the relations $U = U' + 2I$ and $K = I$. We also introduce a number operator $n_{i\xi} = \sum_s n_{i\xi s} = \sum_s d_{i\xi s}^\dagger d_{i\xi s}$, which has a conservation $\sum_\xi n_{i\xi} = 1$. When the electron transfer integrals through the O $2p_\pi$ orbitals are only taken into account, the transfer integral is written as a simple form $t_{ij}^{\xi \xi'} = t \delta_{\xi \xi'} (\delta_{a_i \xi} + \delta_{b_i \xi})$. A subscript $l = (x, y, z)$ indicates a direction connecting i and j . We define two ‘‘active’’ orbitals a_l and b_l , with a finite transfer integral, and an ‘‘inactive’’ one c_l , with no transfer integral. That is, $(a_x, b_x, c_x) = (\beta, \gamma, \alpha)$, $(a_y, b_y, c_y) = (\gamma, \alpha, \beta)$, and $(a_z, b_z, c_z) = (\alpha, \beta, \gamma)$. It is convenient to introduce the pseudospin (PS) operator for the active orbitals $\mathbf{T}_i^l = \frac{1}{2} \sum_{s \xi \xi' = (a, b)} d_{i\xi s}^\dagger \sigma_{\xi \xi'}^l d_{i\xi' s}$ with the Pauli matrices σ . The effective Hamiltonian for the $(t_{2g})^1$ system which has strong on-site Coulomb interactions is obtained by the perturbational processes.^{7,9,16} The virtual intermediate states are classified by the irreducible representations for the $(t_{2g})^2$ states, i.e., 1A_1 , 1T_2 , 1E and 3T_1 . The lowest energy state is 3T_1 with the energy of $U' - K$. We assume that spins are saturated in ferromagnetic phase where

3T_1 is only the relevant intermediate state. The Hamiltonian studied in the present Brief Report is

$$\mathcal{H} = -2J \sum_{\langle ij \rangle} \left\{ n_{ia_l} n_{jb_l} + n_{ib_l} n_{ja_l} - (d_{ia_l}^\dagger d_{ib_l} d_{jb_l}^\dagger d_{ja_l} + d_{ib_l}^\dagger d_{ia_l} d_{ja_l}^\dagger d_{jb_l}) + \frac{1}{2} [n_{ic_l} (n_{ja_l} + n_{jb_l}) + (n_{ia_l} + n_{ib_l}) n_{jc_l}] \right\}, \quad (2)$$

where the exchange constant is $J = t^2 / (U' - K)$. This Hamiltonian is rewritten by using the PS operator as $\mathcal{H} = 4J \sum_{\langle ij \rangle} \{ \mathbf{T}_i^l \cdot \mathbf{T}_j^l + (n_{ic_l} n_{jc_l} - 1) / 4 \}$ and is the same Hamiltonian studied in Refs. 7 and 9. In Ref. 9, the authors proposed the two orbital orders where the wave functions are the linear combinations of the $(d_\alpha, d_\beta, d_\gamma)$ orbitals with equal weight,¹⁵ which are called the off-diagonal-type orbital orders in this Brief Report.

Before showing the numerical results, we remark some rigorous results for the orbital order. There is a unique symmetry in this Hamiltonian. In each plane perpendicular to a direction l , an electron number with the inactive orbital c_l , $\Sigma'_l n_{ic_l}$, is conserved.^{6,7,9} The symbol Σ'_l implies a sum of sites in a plane being perpendicular to l . The Hamiltonian is invariant under the two-dimensional $U(1)$ gauge transformation denoted by $U(\theta) = \exp(-i\theta \Sigma'_l n_{ic_l})$. By following the generalized Elitzur's theorem,^{17,18} the physical quantities which are not invariant under this transformation have a vanishing mean value. This is proven from a combination of a theorem about a gauge transformation in a reduced dimension and the Mermin-Wagner theorem.^{17,19} By using the theorem, we prove that the long-range order for the following orbital operator does not appear at finite temperature:

$$O_{\mathbf{p}}^l = \sum_i e^{i\mathbf{p} \cdot \mathbf{r}_i} (C_a d_{ic_l}^\dagger d_{ib_l} + C_b d_{ia_l}^\dagger d_{ic_l} + \text{H.c.}) \quad (3)$$

for $l=(x, y, z)$ with numerical constants C_a and C_b . That is to say, $\langle O_{\mathbf{p}}^l \rangle = 0$ at finite temperature.

To analyze the Hamiltonian in finite temperature by using an unbiased method, we employ the QMC method with the loop algorithm.^{20,21} There is no negative-sign problem. Simulations are performed on L^3 cubic lattices with the periodic-boundary condition. The Suzuki-Trotter decomposition with the Trotter number n is adopted. To check efficiency of the present QMC simulation, we calculate the autocorrelation time²² for the parameter $L^{-3} \sum_i T_{iz}^x$. The autocorrelation time grows up monotonically with decreasing temperature and reaches around 750 MC steps at $T/J = 0.3$. Thus, we adopt, in the following simulation, 2×10^3 MC steps for thermalization and 10^4 MC steps for measurements. We estimate averages and errors for the physical quantities in ten independent simulations. The system size is taken to be $L=6-12$ in a cubic lattice. Numerical data obtained in the Trotter numbers $n=10, 20$, and 30 are extrapolated.

First, we show results for the staggered-type orbital order. We introduce the staggered correlation function along direction l

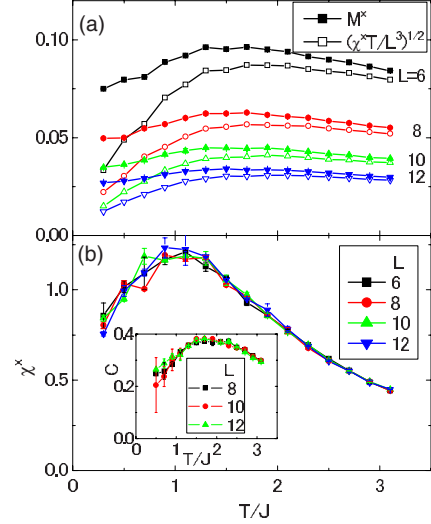


FIG. 1. (Color online) (a) Staggered correlation function M^x for the orbital PS operator T_{iz}^x . (b) Staggered orbital susceptibility χ^x . For comparison, $\sqrt{\chi^x T / L^3}$ is also plotted in (a). The inset of (b) shows specific heat C .

$$M^{l2} = \frac{4}{6n(L^3)^2} \left\langle \left\{ \sum_{\tau} \left\{ \sum_i (-1)^i T_{iz}^l(\tau) \right\}^2 \right\} \right\rangle \quad (4)$$

and the staggered orbital susceptibility

$$\chi^l = \frac{4}{(6n)^2 L^3 T} \left\langle \left\{ \sum_{\tau} \sum_i (-1)^i T_{iz}^l(\tau) \right\}^2 \right\rangle, \quad (5)$$

where τ is an imaginary time, $T_{iz}^l(\tau)$ is the z component of the PS operator at τ , and $\langle \dots \rangle$ implies the QMC average. In the classical limit, M^l should be identical to $\sqrt{\chi^l T / L^3}$. Numerical results of M^x are presented in Fig. 1(a). We have checked that three M^l for $l=(x, y, z)$ coincide with each other within numerical errors. In $L=6$ case, M^x shows a broad peak around $T/J=1.5$. This peak is, however, smeared out with increasing L . All obtained values are less than 10% of the maximum value, i.e., 1. For comparison, $\sqrt{\chi^x T / L^3}$ is also plotted in the same figure. In high temperatures, M^x and $\sqrt{\chi^x T / L^3}$ merge together for all L as expected. A deviation between the two is remarkable below $T/J \sim 1$ where the quantum effect starts to be effective. In both the two quantities, there are no divergent behaviors at $T=0$. Around $T/J \sim 1.5$, reduction in the specific heat is also seen [the inset of Fig. 1(b)]. As shown in Fig. 1(b), numerical data of χ^x for all system size L are scaled by a single curve in a whole temperature range. This implies that the correlation function $\sum_{ij\tau\tau'} (-1)^{i+j} \langle T_{iz}^l(\tau) T_{jz}^l(\tau') \rangle$ in Eq. (5) is of the order of L^3 . That is to say, this correlation is rather short ranged down to at least $0.3J$. The obtained χ^x remains to be finite down to the lowest temperature.

This decrease in M^l and χ^l below $T/J \sim 1$ may be explained by a scenario that the orbital order of the off-diagonal operator proposed in Ref. 9 is developed in low temperatures; in both the two wave functions claimed in Ref. 9, the correlation function $\langle T_{iz}^l T_{jz}^l \rangle$ for every NN pairs of sites i and j vanishes. To examine this possibility, we calculate the

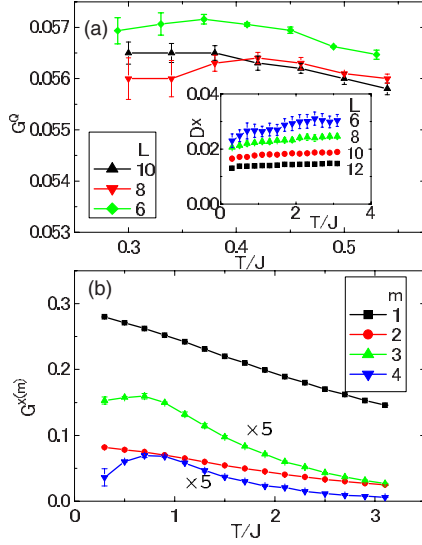


FIG. 2. (Color online) (a) Correlation function G^Q for the off-diagonal orbital operator Q_i . (b) Correlation function $G^{l(m)}$ for the orbital PS operator T_{iz}^x . The system size in (b) is taken to be $L=10$. Results in $G^{x(3)}$ and $G^{x(4)}$ are multiplied by 5. The inset of (a) shows the dimer order parameter D^x .

physical quantities for the off-diagonal orbital operator. In general, thermal average of the two-point function for an off-diagonal operator may be calculated by utilizing the improved estimator in the loop algorithm.^{20,21} In the present QMC simulation, however, this method is not realistic. This is because a value of the improved estimator depends on a shape of the loop since the orbital interaction explicitly depends on the bond direction. Instead, the NN correlation functions for the off-diagonal operators are able to be calculated, when these operators are included in the Hamiltonian explicitly. We calculate the following correlation function for the off-diagonal operator $Q_i \equiv \sum_{l=(x,y,z)} T_{ix}^l$ defined by

$$G^Q = \frac{1}{z6nL^3} \left\langle \sum_{\tau} \sum_{\langle ij \rangle} Q_i(\tau) Q_j(\tau) \right\rangle, \quad (6)$$

where $z=6$. For the orbital-ordered states proposed in Ref. 9, $G^Q=0.22$ and 0.16 for the type-I and type-II orders, respectively. Numerical results of G^Q presented in Fig. 2(a) show weak size dependence and do not show remarkable increase with decreasing temperature. The obtained values are about 35% of the values expected from the ideal off-diagonal orbital orders.

Further information for the off-diagonal orbital order is obtained by the staggered correlation as a function of distance,

$$G^{l(m)} = \frac{4}{6nL^3} \left\langle \sum_{\tau} \sum'_{\langle ij \rangle_l} (-1)^{i+j} T_{iz}^l(\tau) T_{jz}^l(\tau) \right\rangle, \quad (7)$$

where $\sum'_{\langle ij \rangle_l}$ represents a sum for the m th NN sites i and j along direction l . We calculate $G^{l(m)}$'s for $l=x$ up to $m=4$ [see Fig. 2(b)]. With decreasing temperature, $G^{x(1)}$ and $G^{x(2)}$ monotonically increase even below $T/J \sim 1$ where M^l and χ^l in Fig. 1 start to decrease. On the other hand, reductions are

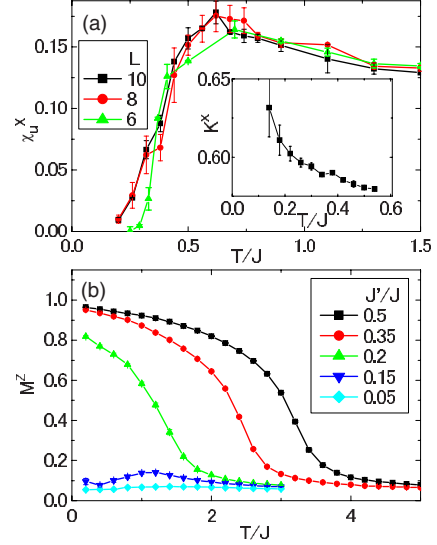


FIG. 3. (Color online) (a) Uniform susceptibility for the orbital PS operator T_{iz}^x . (b) Correlation function M^z calculated in the Hamiltonian $\mathcal{H} + \mathcal{H}'$. The system size and the Trotter number in (b) are chosen to be $L=8$ and $n=10$, respectively. The inset of (b) shows the correlation function K^x for NN PS operators.

seen in $G^{x(3)}$ and $G^{x(4)}$ around $T/J=0.8$. That is, the decreases in M^l and χ^l are attributed to those in the long-range correlations of T_{iz}^l , and short-range correlations still remain to grow up. The obtained result also suggests that the decreases in M^l and χ^l are not attributed to development of the off-diagonal orbital correlation; when the correlation for the off-diagonal operator Q_i grows up at low temperature, reduction in $G^{l(m)}$ should be remarkable in short range. That is, $G^{l(1)}$ and $G^{l(2)}$, instead of $G^{l(3)}$ and $G^{l(4)}$, are expected to be reduced. This expectation is in contrast to the numerical results in Fig. 2(b).

Development of the short-range orbital correlation shown above suggests a kind of the valence-bond state in low-dimensional quantum magnets.²³ However, we are able to exclude a simple orbital dimer state. We calculate the dimer order parameter defined as

$$D^l = \frac{16}{6n(L^3)^2} \left\langle \sum_{\tau} \left\{ \sum_i T_{iz}^l(\tau) T_{i+\mathbf{e}_l}^l(\tau) \right\}^2 \right\rangle \quad (8)$$

with a unit vector \mathbf{e}_l along direction l . Results of D^l show monotonic decreases with decreasing temperature and increasing the system size, as shown in the inset of Fig. 2(a).

The following results indicate that the low-temperature orbital state shows a gaplike feature. The calculated uniform orbital susceptibility defined by

$$\chi_u^l = \frac{4}{(6n)^2 L^3 T} \left\langle \left\{ \sum_{\tau} \sum_i T_{iz}^l(\tau) \right\}^2 \right\rangle, \quad (9)$$

[see in Fig. 3(a)] starts to decrease around $T/J=0.7$ and tends to vanish at low temperatures. Size dependence is seen below $T/J \sim 0.3$, but a global gaplike feature in χ_u^l is not sensitive to the system size. The temperature, where χ_u^l starts to decrease, i.e., $T \sim 0.7J$, almost coincides to the tempera-

ture where the staggered susceptibility χ^x and the short-range correlation functions $G^{x(3)}$ and $G^{x(4)}$ have broad peaks, as shown in Figs. 1(b) and 2(b). We also calculate the following correlation function between the NN PS operators:

$$K^l = -\frac{1}{6nL^3} \left\langle \sum_{\tau} \sum_i \{ \mathbf{T}_i^l(\tau) \cdot \mathbf{T}_{i+\mathbf{e}_l}^l(\tau) - n_i^l(\tau) n_{i+\mathbf{e}_l}^l(\tau) \} \right\rangle \quad (10)$$

with $n_i^l = n_{ia_l} + n_{ib_l}$. Increasing of the correlation function with decreasing T , shown in the inset of Fig. 3(a), suggests a singlet formation between NN PSs. This gaplike feature is also confirmed by the following calculation. We add the Ising-type interaction term into the Hamiltonian (2). This is given by

$$\mathcal{H}' = 2J' \sum_{\langle ij \rangle} (4T_{iz}^c T_{jz}^c - n_{i\alpha} n_{j\alpha} - n_{i\beta} n_{j\beta}), \quad (11)$$

where J' is a positive coupling constant. This term promotes the staggered-type orbital order characterized by M^z . Results are shown in Fig. 3(b) for several values of J'/J . A threshold value for J'/J seems to exist; an increase in M^z in low temperatures is not seen for $J'/J=0.05$ and 0.15 . This is consistent with finite values of χ^x at low temperatures shown in Fig. 1(b). These results indicate a possibility that a quantum gapped state is broken by the Ising-type interaction as well known in the quantum critical issue.

In summary, we present a numerical study of the finite-temperature t_{2g} orbital state in a ferromagnetic Mott insulator. Remarkable developments are not seen in the staggered orbital correlation and the NN correlation for the off-

diagonal orbital operator at least down to $T/J \sim 0.3$. Short-range correlation remains to grow up in low temperatures, but a possibility of the dimerized state is excluded. It is found that the uniform orbital susceptibility shows a gaplike feature below $T/J \sim 0.7$. This result is supported by a calculation in the model where the Ising-type interaction is added. One possible scenario for the low-temperature orbital state is a short-range singlet state where singlet pairs are randomly distributed in a crystal and/or where rearrangement of pairs occurs dynamically. A singlet wave function between sites i and j is $(|d_{ia_l} d_{jb_l}\rangle - |d_{ib_l} d_{ja_l}\rangle) / \sqrt{2}$ where concerning orbitals depend on the bond direction l , i.e., a directional singlet pair. We suppose that the present orbital gaplike feature implies a qualitatively different orbital state realized at low T from the long-range orbital order proposed in Ref. 9; due to the gapless zero-energy mode, the long-range order in Ref. 9 is possible only at $T=0$. To clarify a lower-temperature orbital state in more detail, QMC simulations in large cluster sizes with efficient algorithms are necessary. A variational-type approach based on the above directional singlet assumption may be also helpful.

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¹⁵The two off-diagonal-type orbital orders proposed in Ref. 9 consist of four orbital sublattices in a simple-cubic lattice. The wave functions are given by $|\psi_i^I\rangle = (C_i^\alpha |d_{yz}\rangle + C_i^\beta |d_{zx}\rangle + C_i^\gamma |d_{xy}\rangle) / \sqrt{3}$, for the type I, and $|\psi_i^{II}\rangle = (C_i^\alpha e^{i2\pi/3} |d_{yz}\rangle + C_i^\beta e^{-i2\pi/3} |d_{zx}\rangle + C_i^\gamma |d_{xy}\rangle) / \sqrt{3}$, for the type II, in the classical limit. Subscript $i(i=1-4)$ denotes the four sublattices and coefficients are $(C_i^\alpha, C_i^\beta, C_i^\gamma) = (1, 1, 1)$ for $i=1$, $(-1, -1, 1)$ for $i=2$, $(-1, 1, -1)$ for $i=3$, and $(1, -1, -1)$ for $i=4$.

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