Long-range order in the ground state of spin systems with orbital degeneracy

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We apply the method of infrared bounds to the spin-orbital systems with isotropic and anisotropic interactions to examine the existence of long-range order (LRO) in two or more dimensions. For the isotropic case, we prove the existence of antiferro-spin and antiferro-orbital LRO in three or more dimensions and ferro-spin-orbital LRO in seven or more dimensions. For the anisotropic case, we prove the existence of antiferro-orbital LRO in two or more dimensions. Under some acceptable assumptions we conjecture on the existence of antiferro-spin LRO in three or more dimensions and extend the region where we can show antiferro-orbital LRO in two or more dimensions.

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I. INTRODUCTION

It has been recognized, through a number of experimental and theoretical works, that quantum spin systems with orbital degeneracy exhibit interesting phenomena induced by combined spin-orbital degrees of freedom in addition to spin and orbital ones. In real materials these situations are realized in the Mott insulators of the transitional-metal oxides,[1–4] the dynamical Jahn-Teller ionic or molecular systems with a strong electron-phonon coupling,[5–9] and the heavy fermion systems in the insulating phase.[10–12] One of the typical models for these systems containing spin, orbital, and spin-orbital interactions is described by the Hamiltonian[5,6,10,13–15]

$$\mathcal{H}=I\sum_{\langle x,y\rangle}\mathbf{S}(x)\cdot\mathbf{S}(y)+J\sum_{\langle x,y\rangle}\{\Delta[T_1(x)T_1(y)+T_2(x)T_2(y)]+T_3(x)T_3(y)\}-K\sum_{\langle x,y\rangle}[\mathbf{S}(x)\cdot\mathbf{S}(y)]\{\Delta[T_1(x)T_1(y)+T_2(x)T_2(y)]+T_3(x)T_3(y)\}, \tag{1}$$

where $\mathbf{S}(x)$ and $\mathbf{T}(x)$ are spin-1/2 and pseudospin-1/2 operators representing the spin and orbital degrees of freedom, respectively, and Δ is an anisotropy of orbital interactions. In this paper we are concerned with Hamiltonian (1) on the hypercubic lattice and, in particular, investigate the existence of long-range order (LRO) in the ground state of this Hamiltonian. The orbital LRO (Refs. 16 and 17) and the anisotropy of orbital interactions[18] have been actually observed in some magnetic systems by using resonant x-ray scattering techniques.

In the case of $I=J=1$ and $\Delta=1$, Hamiltonian (1) at $K=-4$ is an ordinary SU(4) symmetric model.[2] On the other hand, in this case Hamiltonian (1) at $K=4$ is a different SU(4) symmetric model[19] introduced by Santoro *et al.*[6]

In one dimension, the model at the SU(4) symmetric point with $K=-4$ is exactly soluble by the Bethe ansatz, and its solution gives three branches of low-energy gapless excitations.[20,21] For the model at the SU(4) symmetric point with $K=4$, according to numerical methods, the ground-state exhibits a spin-Peiels-like dimerization.[19] For the region $K\leqslant 0$, the ground state phase diagram of this model has been investigated by various accurate methods. (See, e.g., Refs. 22 and 23, and references therein.)

In two dimensions, the ground states of both SU(4) symmetric points are considered to be disordered states with finite energy gaps, which has been investigated by a variational method,[2] a spin-wave theory,[24] a Schwinger-boson mean-field theory,[25] and numerical calculations.[26–28] The recent results of approximation methods also suggested that the ground state around the SU(4) symmetric point with $K=-4$ is disordered.[29,30] In particular, a Schwinger-boson mean-field theory predicted that disordered ground states are still stable in three dimensions for some interval in the region $K<0$, $I=J=1$, $\Delta=1$.[30] The two-dimensional system at SU(4) symmetric point with $K=4$ is shown to be a disordered ground state with a gapful energy excitation by the Monte Carlo method;[28] thus the ground state in the vicinity of this SU(4) symmetric point is thought to be disordered. These behaviors are in contrast to the SU(2) antiferromagnetic Heisenberg model having a Néel-ordered ground state in two or more dimensions. However, as was pointed out by some authors, the mean-field-type approximation methods contain an uncontrolled accuracy,[29] and for the numerical studies of two- and three-dimensional systems, those system sizes are not enough compared with those of one-dimensional systems due to the large degrees of freedom of this system[25] and a minus sign problem.[31] Although the above studies have these difficulties, for the two-dimensional systems at both SU(4) symmetric points and around it, almost all the results support the disordered ground state.

In this paper we focus our attention on the region $I=J=1$, $K\geqslant 0$, $0\leqslant\Delta\leqslant 1$, and examine the existence of LRO at zero temperature. The models in this region are potentially realized in the systems expected to show the strong dynamical Jahn-Teller effect in the insulating phase, such as the large body of new molecular compounds based on C_{60} or larger fullerides[7,32] and some two-dimensional copolymers.[8,9] As mentioned above, the ground state is expected to be disordered state with a finite energy gap at $K=4$ and $\Delta=1$ in two dimensions. Therefore, it is interesting whether the ground states at this point and around it are ordered ones or not in three or more dimensions.

In the present paper, we use the method of infrared bounds to establish the existence of LRO in the ground state of Hamiltonian (1). This method was successfully used for the rigorous proof of the existence of LRO in the spin systems with continuous symmetry.[33–35] In the case of the spin-T Heisenberg model, this method is applicable to the antiferromagnetic case $[I=K=0, J>0, \Delta>0$ in our Hamiltonian (1)]. For the isotropic case $(\Delta=1)$ Dyson, Lieb, and Simon (DLS) proved that there exists antiferromagnetic LRO at sufficiently low temperatures for $d\geqslant 3$ and $T\geqslant 1$.[34] By applying the technique of DLS, Jardão Neves and Fernando Perez proved the existence of antiferromagnetic LRO in the ground state for $d\geqslant 2$ and $T\geqslant 1$.[36,37] Kennedy, Lieb, and Shastry (KLS) improved the technique of DLS and proved its existence in the ground state for $d\geqslant 3$ and $T=1/2$.[38] Kubo and Kishi extended the proof to the anisotropic case $(0\leqslant\Delta\neq 1)$,[39] and then, their result was improved by some authors.[40–42] As far as we know, the existence of antiferromagnetic LRO is proved in the region $\Delta\geqslant 0$ for $T\geqslant 1/2$ in three dimensions and $\Delta\geqslant 0$ for $T\geqslant 1$ and $0\leqslant 1/\Delta<0.20$, $1/\Delta>1.66$ for $T=1/2$ in two dimensions. The proof of its existence at the Heisenberg point and around it is still an open problem in the case of $d=2$ and $T=1/2$.

The method of infrared bounds can be applied to the Hamiltonian satisfying so-called reflection positivity. In this paper we show that Hamiltonian (1) satisfies reflection positivity for $I\geqslant 0$, $J\geqslant 0$, $K\geqslant 0$, $\Delta\geqslant 0$, and by using the method of infrared bound, we prove that there exists LRO in the ground state of Hamiltonian (1) for a restricted parameter region within the region $I=J=1$, $K\geqslant 0$, $0\leqslant\Delta\leqslant 1$. In the case of $\Delta\neq 1$ we reexamine the existence of LRO in the region $0\leqslant K\leqslant 4$ under acceptable assumptions.

This paper is organized as follows. In Sec. II, we define some notation used throughout this paper. In Sec. III, we summarize the method of infrared bounds. In Sec. IV, by using the method of infrared bounds with the KLS technique, we prove the existence of LRO at zero temperature in the isotropic case $(\Delta=1)$. In Sec. V, we extend the proof to the anisotropic case and suggest conjectures for the existence of LRO under a few assumptions. In Sec. VI, we summarize and discuss the results of Secs. IV and V.

II. DEFINITION AND SOME NOTATION

We start with the definition of the model. Let $\Lambda\subset Z^d$ be a d-dimensional hypercubic lattice of the form

$$\Lambda=\{x=(x_1,\ldots,x_d)\,|\,-L+1\leqslant x_i\leqslant L\}, \tag{2}$$

where L is an integer. We impose periodic boundary conditions in all directions. For each site $x\in\Lambda$, we associate operators $\mathbf{S}(x)$ and $\mathbf{T}(x)$ with $S(x)=T(x)=1/2$, which denote the degrees of freedom for spin and orbit, respectively. In this paper we use the following matrix representation:

$$S_1=\frac{1}{2}\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix},\quad S_2=\frac{1}{2}\begin{pmatrix}0&-i&0&0\\i&0&0&0\\0&0&0&-i\\0&0&i&0\end{pmatrix},$$

$$S_3=\frac{1}{2}\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix},$$

$$T_1=\frac{1}{2}\begin{pmatrix}0&0&1&0\\0&0&0&1\\1&0&0&0\\0&1&0&0\end{pmatrix},\quad T_2=\frac{1}{2}\begin{pmatrix}0&0&-i&0\\0&0&0&-i\\i&0&0&0\\0&i&0&0\end{pmatrix},$$

$$T_3=\frac{1}{2}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix}. \tag{3}$$

We consider the $S=1/2$ spin system with twofold orbital degeneracy described by the Hamiltonian

$$\mathcal{H}_\Lambda=\mathcal{H}_{S\Lambda}+\mathcal{H}_{T\Lambda}-K\mathcal{H}_{X\Lambda}, \tag{4}$$

with

$$\mathcal{H}_{S\Lambda}=\sum_{\langle x,y\rangle}\mathbf{S}(x)\cdot\mathbf{S}(y), \tag{5}$$

$$\mathcal{H}_{T\Lambda}=\sum_{\langle x,y\rangle}\{\Delta[T_1(x)T_1(y)+T_2(x)T_2(y)]+T_3(x)T_3(y)\}, \tag{6}$$

$$\begin{aligned}\mathcal{H}_{X\Lambda}&=\sum_{\langle x,y\rangle}[\mathbf{S}(x)\cdot\mathbf{S}(y)]\{\Delta[T_1(x)T_1(y)+T_2(x)T_2(y)]\\&\quad+T_3(x)T_3(y)\}\\&=\sum_{\langle x,y\rangle}\sum_{l,m=1}^{3}[\Delta X_{lm}(x)X_{lm}(y)(1-\delta_{3m})\\&\quad+X_{lm}(x)X_{lm}(y)\delta_{3m}],\end{aligned} \tag{7}$$

where the summation is over all nearest-neighbor pairs $\langle x,y\rangle$ in Λ, $X_{lm}(x)=S_l(x)T_m(x)$, and δ_{lm} is Kronecker's δ satisfying 1 for $l=m$ and 0 for $l\neq m$. This Hamiltonian corresponds to the case of $I=J=1$ in Hamiltonian (1). By straightforward calculations, we find that the operators appearing in Hamiltonian (4) satisfy the following commutation relations:

$$[S_l(x),S_m(y)]=i\epsilon_{lmn}S_n(x)\delta_{xy}, \tag{8}$$

$$[T_l(x),T_m(y)]=i\epsilon_{lmn}T_n(x)\delta_{xy}, \tag{9}$$

$$[S_l(x),T_m(y)]=0, \tag{10}$$

$$[S_l(x),X_{mp}(y)]=i\epsilon_{lmn}X_{np}(x)\delta_{xy}, \tag{11}$$

$$[T_p(x),X_{lq}(y)]=i\epsilon_{pqr}X_{lr}(x)\delta_{xy}, \tag{12}$$

$$[X_{lp}(x),X_{mq}(y)]=\left(\frac{i}{4}\epsilon_{lmn}S_n(x)\delta_{pq}+\frac{i}{4}\epsilon_{pqr}T_r(x)\delta_{lm}\right)\delta_{xy}, \tag{13}$$

where ϵ_{lmn} is the Levi-Civita symbol satisfying 0 if any pair of subscripts are equal, $+1$ if l,m,n is an even permutation of 1,2,3, and -1 if l,m,n is an odd permutation of 1,2,3. The commutation relation (13) holds only in the case of $S=T=1/2$. In this paper we consider the region $K\geqslant 0$ and $0\leqslant\Delta\leqslant 1$, where we can use the method of infrared bounds. The reason why the method of infrared bound is applicable to such parameter region will become clear in Sec. III.

We describe three types of LRO parameters in the ground state of Hamiltonian (4) as follows. The antiferro-spin LRO (AFSLRO) parameter is defined by

$$m_S^2=\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\left\langle\left[\frac{1}{|\Lambda|}\sum_{x\in\Lambda}(-1)^{|x|}S_3(x)\right]^2\right\rangle_{\Lambda\beta}, \tag{14}$$

the antiferro-orbital LRO (AFOLRO) parameter by

$$m_T^2=\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\left\langle\left[\frac{1}{|\Lambda|}\sum_{x\in\Lambda}(-1)^{|x|}T_3(x)\right]^2\right\rangle_{\Lambda\beta}, \tag{15}$$

and the ferro-spin-orbital LRO (FSOLRO) parameter by

$$m_X^2=\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\left\langle\left(\frac{1}{|\Lambda|}\sum_{x\in\Lambda}X_{33}(x)\right)^2\right\rangle_{\Lambda\beta}, \tag{16}$$

where $|\Lambda|$ is the number of sites in Λ, $|x|\equiv\Sigma_{i=1}^d|x_i|$ for $x=(x_1,\ldots,x_d)$, and $\langle A\rangle_{\Lambda\beta}$ denotes the thermal average of A at inverse temperature β:

$$\langle A\rangle_{\Lambda\beta}=\frac{\mathrm{Tr}\,e^{-\beta\mathcal{H}_\Lambda}A}{Z}, \tag{17}$$

with

$$Z=\mathrm{Tr}\,e^{-\beta\mathcal{H}_\Lambda}. \tag{18}$$

For use later, we define the Duhamel two-point function by

$$(A,B)=Z^{-1}\int_0^1\mathrm{Tr}(e^{-t\beta\mathcal{H}_\Lambda}Ae^{-(1-t)\beta\mathcal{H}_\Lambda}B)dt, \tag{19}$$

and the Fourier transform of $S_l(x)$, $T_l(x)$, and $X_{lm}(x)$ by

$$S_l(k)=\frac{1}{\sqrt{|\Lambda|}}\sum_{x\in\Lambda}e^{-ik\cdot x}S_l(x), \tag{20}$$

$$T_l(k)=\frac{1}{\sqrt{|\Lambda|}}\sum_{x\in\Lambda}e^{-ik\cdot x}T_l(x), \tag{21}$$

$$X_{lm}(k)=\frac{1}{\sqrt{|\Lambda|}}\sum_{x\in\Lambda}e^{-ik\cdot x}X_{lm}(x), \tag{22}$$

respectively, where $k=(k_1,\ldots,k_d)$ is in a reciprocal lattice Λ^*.

III. SUMMARY OF THE DERIVATION OF INFRARED BOUNDS

A. Correlation functions and sum rules

In this subsection we summarize the method of infrared bounds.[34–36,38]

Let us define the Fourier transform of the two-point correlation functions by

$$g_S(k)=\langle S_3(k)S_3(-k)\rangle_{\Lambda\beta}, \tag{23}$$

$$g_T(k)=\langle T_3(k)T_3(-k)\rangle_{\Lambda\beta}, \tag{24}$$

$$g_X(k)=\langle X_{33}(k)X_{33}(-k)\rangle_{\Lambda\beta}, \tag{25}$$

and the interaction energies per site in the ground state by

$$e_{\mathcal{H}\Lambda}=-\frac{1}{|\Lambda|}\lim_{\beta\to\infty}\langle\mathcal{H}_\Lambda\rangle_{\Lambda\beta},\quad e_{\mathcal{H}}=\lim_{\Lambda\to\infty}e_{\mathcal{H}\Lambda}, \tag{26}$$

$$e_{S\Lambda}=-\frac{1}{|\Lambda|}\lim_{\beta\to\infty}\langle\mathcal{H}_{S\Lambda}\rangle_{\Lambda\beta},\quad e_S=\lim_{\Lambda\to\infty}e_{S\Lambda}, \tag{27}$$

$$e_{T\Lambda}=-\frac{1}{|\Lambda|}\lim_{\beta\to\infty}\langle\mathcal{H}_{T\Lambda}\rangle_{\Lambda\beta},\quad e_T=\lim_{\Lambda\to\infty}e_{T\Lambda}, \tag{28}$$

$$e_{X\Lambda}=\frac{1}{|\Lambda|}\lim_{\beta\to\infty}\langle\mathcal{H}_{X\Lambda}\rangle_{\Lambda\beta},\quad e_X=\lim_{\Lambda\to\infty}e_{X\Lambda}. \tag{29}$$

For the discussion of the anisotropic case ($\Delta\neq 1$), we also define the following:

$$\varepsilon_{l\Lambda}^T=-\frac{1}{|\Lambda|}\lim_{\beta\to\infty}\sum_{\langle x,y\rangle}\langle T_l(x)T_l(y)\rangle_{\Lambda\beta},\quad \varepsilon_l^T=\lim_{\Lambda\to\infty}\varepsilon_{l\Lambda}^T, \tag{30}$$

$$\varepsilon_{m\Lambda}^X=\frac{1}{|\Lambda|}\lim_{\beta\to\infty}\sum_{\langle x,y\rangle}\langle X_{lm}(x)X_{lm}(y)\rangle_{\Lambda\beta},\quad \varepsilon_m^X=\lim_{\Lambda\to\infty}\varepsilon_{m\Lambda}^X, \tag{31}$$

for $l,m=1,2,3$. From the definitions (27), (28), and (29), $e_{\mathcal{H}\Lambda}$ is written as

$$e_{\mathcal{H}\Lambda}=e_{S\Lambda}+e_{T\Lambda}+Ke_{X\Lambda}, \tag{32}$$

and from the definitions (30) and (31), $e_{T\Lambda}$ and $e_{X\Lambda}$ as

$$e_{T\Lambda}=2\Delta\varepsilon_{1\Lambda}^T+\varepsilon_{3\Lambda}^T, \tag{33}$$

$$e_{X\Lambda}=6\Delta\varepsilon_{1\Lambda}^X+3\varepsilon_{3\Lambda}^X, \tag{34}$$

where we used the relations $\varepsilon_{1\Lambda}^T=\varepsilon_{2\Lambda}^T$ and $\varepsilon_{1\Lambda}^X=\varepsilon_{2\Lambda}^X$, which come from the symmetry of Hamiltonian.

As in the case of the antiferromagnetic Heisenberg model, we have the following KLS-type sum rule:[38]

$$\frac{1}{|\Lambda|}\lim_{\beta\to\infty}\sum_{k\in\Lambda^*} g_S(k)\left(\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right)=-\frac{e_{S\Lambda}}{3d}, \quad (35)$$

$$\frac{1}{|\Lambda|}\lim_{\beta\to\infty}\sum_{k\in\Lambda^*} g_T(k)\left(\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right)=-\frac{\varepsilon_{3\Lambda}^T}{d}, \quad (36)$$

$$\frac{1}{|\Lambda|}\lim_{\beta\to\infty}\sum_{k\in\Lambda^*} g_X(k)\left(\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right)=\frac{\varepsilon_{3\Lambda}^X}{d}. \quad (37)$$

By using the above sum rules, the three types of order parameters (14), (15), and (16) are written as

$$m_S^2=\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\frac{1}{|\Lambda|}g_S(Q)=\frac{e_S}{3d}-G_S, \quad Q=(\pi,\ldots,\pi), \quad (38)$$

$$m_T^2=\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\frac{1}{|\Lambda|}g_T(Q)=\frac{\varepsilon_3^T}{d}-G_T, \quad (39)$$

$$m_X^2=\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\frac{1}{|\Lambda|}g_X(P)=\frac{\varepsilon_3^X}{d}-G_X, \quad P=(0,\ldots,0), \quad (40)$$

with

$$G_S=\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\frac{1}{|\Lambda|}\sum_{k\neq Q} g_S(k)\left(-\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right), \quad (41)$$

$$G_T=\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\frac{1}{|\Lambda|}\sum_{k\neq Q} g_T(k)\left(-\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right), \quad (42)$$

$$G_X=\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\frac{1}{|\Lambda|}\sum_{k\neq P} g_X(k)\left(\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right). \quad (43)$$

In order to prove that the order parameters take finite values in the ground state, we evaluate lower bounds for e_S, ε_3^T, and ε_3^X and upper bounds on G_S, G_T, and G_X. To obtain those upper bounds, we estimate infrared bounds, i.e., upper bounds on the correlation functions $g_S(k)$ with $k\neq Q$, $g_T(k)$ with $k\neq Q$, and $g_X(k)$ with $k\neq P$.

B. Infrared bounds

In the following, we describe the derivation of infrared bounds on the two-point correlation functions.

Theorems 3.2 and 5.1 in the paper of DLS (Ref. 34) applied to Hamiltonian (4) assures that

$$g_S(k)\leqslant\frac{1}{2}\sqrt{B_S(k)C_{S\beta}(k)}\coth\left(\frac{1}{2}\beta\sqrt{\frac{C_{S\beta}(k)}{B_S(k)}}\right), \quad k\neq Q, \quad (44)$$

if we can estimate $B_S(k)$ and $C_S(k)$ satisfying

$$(S_3(k),S_3(-k))\leqslant\beta^{-1}B_S(k), \quad k\neq Q, \quad (45)$$

and

$$\langle[[S_3(k),\mathcal{H}_\Lambda],S_3(-k)]\rangle_{\Lambda\beta}\leqslant C_{S\beta}(k). \quad (46)$$

In the limit $\beta\to\infty$, the hyperbolic cotangent factor of the right-hand side of inequality (44) drops off and an infrared bound is given by[34,36]

$$\lim_{\beta\to\infty} g_S(k)\leqslant\frac{1}{2}\sqrt{B_S(k)C_S(k)}, \quad k\neq Q, \quad (47)$$

where $C_S(k)=\lim_{\beta\to\infty}C_{S\beta}(k)$.

When Hamiltonian satisfies reflection positivity, we can estimate $B_S(k)$ as described below. Let us define

$$\tilde{S}_1(x)=U_S^\dagger S_1(x)U_S, \quad \tilde{T}_1(x)=U_T^\dagger T_1(x)U_T,$$

$$\tilde{S}_2(x)=U_S^\dagger iS_2(x)U_S, \quad \tilde{T}_2(x)=U_T^\dagger iT_2(x)U_T,$$

$$\tilde{S}_3(x)=U_S^\dagger S_3(x)U_S, \quad \tilde{T}_3(x)=U_T^\dagger T_3(x)U_T, \quad (48)$$

and

$$\tilde{X}_{lm}(x)=\tilde{S}_l(x)\tilde{T}_m(x), \quad (49)$$

with $U_S=\exp[i\pi\Sigma_{x\in\Lambda_{\text{odd}}}S_2(x)]$ and $U_T=\exp[i\pi\Sigma_{x\in\Lambda_{\text{odd}}}T_2(x)]$, where Λ_{odd} is a collection of sites x with odd $|x|$. Let $h_m(x)$ $(m=1,\ldots,d)$ be a real-valued function on the site x. Then we consider the following Hamiltonian dependent on $h=\{h_m(x)|m=1,\ldots,d,x\in\Lambda\}$:

$$\tilde{\mathcal{H}}_\Lambda^S(h)=\tilde{H}_\Lambda^S(h)+\tilde{H}_\Lambda^T(0)+\tilde{H}_\Lambda^X(0), \quad (50)$$

with

$$\tilde{H}_\Lambda^S(h)=\frac{1}{2}\sum_{x\in\Lambda}\sum_{m=1}^{d}\Bigg[[\tilde{S}_1(x)-\tilde{S}_1(x+\delta_m)]^2+[\tilde{S}_2(x)-\tilde{S}_2(x+\delta_m)]^2+[\tilde{S}_3(x)-\tilde{S}_3(x+\delta_m)+h_m(x)]^2-\frac{1}{2}\Bigg], \quad (51)$$

$$\tilde{H}_\Lambda^T(h)=\frac{1}{2}\sum_{x\in\Lambda}\sum_{m=1}^{d}\Bigg\{\Delta\{[\tilde{T}_1(x)-\tilde{T}_1(x+\delta_m)]^2+[\tilde{T}_2(x)-\tilde{T}_2(x+\delta_m)]^2\}+[\tilde{T}_3(x)-\tilde{T}_3(x+\delta_m)+h_m(x)]^2-\frac{1}{2}\Bigg\}, \quad (52)$$

$$\tilde{H}_\Lambda^X(h)=\frac{1}{2}K\sum_{x\in\Lambda}\sum_{m=1}^{d}\left[\Delta\sum_{p,q=1}^{3}[\tilde{X}_{pq}(x)-\tilde{X}_{pq}(x+\delta_m)]^2(1-\delta_{3q})+[\tilde{X}_{13}(x)-\tilde{X}_{13}(x+\delta_m)]^2+[\tilde{X}_{23}(x)-\tilde{X}_{23}(x+\delta_m)]^2+[\tilde{X}_{33}(x)-\tilde{X}_{33}(x+\delta_m)+h_m(x)]^2-\frac{1}{8}\right], \tag{53}$$

where δ_m denotes the unit vector in the m direction. We note that

$$\tilde{\mathcal{H}}_\Lambda^S(0)=U_T^\dagger U_S^\dagger \mathcal{H}_\Lambda U_S U_T. \tag{54}$$

For $\tilde{\mathcal{H}}_\Lambda^S(h)$ we can easily check the following facts: the matrix elements of all matrices appearing in $\tilde{\mathcal{H}}_\Lambda^S(h)$ are real, and the coefficients of all the nearest-neighbor spin interaction terms are negative and those of nearest-neighbor orbital interaction and spin-orbital interaction terms are nonpositive for $K\geqslant 0$ and $\Delta\geqslant 0$ (in this paper $K\geqslant 0$ and $0\leqslant\Delta\leqslant 1$). These conditions are required so as to satisfy reflection positivity. Thus, following Sec. IV and theorem 6.1 in the paper of DLS,[34] we have

$$\tilde{Z}_S(h)\leqslant\tilde{Z}_S(0), \tag{55}$$

with

$$\tilde{Z}_S(h)=\mathrm{Tr}\exp[-\beta\tilde{\mathcal{H}}_\Lambda^S(h)], \tag{56}$$

and then inequality (55) leads to

$$\frac{\mathrm{Tr}\exp\left\{-\beta\left[\tilde{\mathcal{H}}_\Lambda^S(0)+\sum_{x\in\Lambda}\eta(x)\tilde{S}_3(x)\right]\right\}}{\tilde{Z}_S(0)}\leqslant\exp\left(\frac{\beta}{2}\sum_{x\in\Lambda}\sum_{m=1}^{d}|h_m(x)|^2\right), \tag{57}$$

with $\eta(x)=\Sigma_{m=1}^d[h_m(x+\delta_m)-h_m(x)]$. We also follow theorem 4.2 in the paper of DLS; then we have

$$\left(\sum_{x\in\Lambda}\eta(x)^*\tilde{S}_3(x),\sum_{x\in\Lambda}\eta(x)\tilde{S}_3(x)\right)\leqslant\frac{1}{\beta}\sum_{x\in\Lambda}\sum_{m=1}^{d}|h_m(x)|^2, \tag{58}$$

where we should note that $h_m(x)$ is extended to a complex-valued function.

Now we choose

$$h_m(x)=\frac{1}{\sqrt{|\Lambda|}}\{\exp[ik\cdot(x-\delta_m)]-\exp(ik\cdot x)\}; \tag{59}$$

then inequality (58) becomes

$$\beta(S_3(k),S_3(-k))\leqslant\frac{1}{2E(k-Q)}=B_S(k),\quad k\neq Q, \tag{60}$$

with

$$E(k)=\sum_{m=1}^{d}(1-\cos k_m). \tag{61}$$

Combining inequalities (47) and (60), we have

$$\lim_{\beta\to\infty}g_S(k)\leqslant\frac{1}{\sqrt{8E(k-Q)}}\sqrt{C_S(k)},\quad k\neq Q. \tag{62}$$

We can obtain infrared bounds on $g_T(k)$ and $g_X(k)$ by following a similar process of the derivation of an infrared bound on $g_S(k)$. In the case of $g_T(k)$, we have

$$\lim_{\beta\to\infty}g_T(k)\leqslant\frac{1}{\sqrt{8E(k-Q)}}\sqrt{C_T(k)},\quad k\neq Q, \tag{63}$$

with

$$\lim_{\beta\to\infty}\langle[[T_3(k),\mathcal{H}_\Lambda],T_3(-k)]\rangle_{\Lambda\beta}\leqslant C_T(k) \tag{64}$$

in the region satisfying reflection positivity, $K\geqslant 0$ and $\Delta\geqslant 0$.

On the other hand, for an infrared bound on $g_X(k)$, we have

$$\lim_{\beta\to\infty}g_X(k)\leqslant\frac{1}{2}\sqrt{B_X(k)C_X(k)},\quad k\neq P, \tag{65}$$

with

$$(X_{33}(k),X_{33}(-k))\leqslant\beta^{-1}B_X(k),\quad k\neq P, \tag{66}$$

and

$$\lim_{\beta\to\infty}\langle[[X_{33}(k),\mathcal{H}_\Lambda],X_{33}(-k)]\rangle_{\Lambda\beta}\leqslant C_X(k). \tag{67}$$

In order to evaluate $B_X(k)$, we discuss the Hamiltonian defined by

$$\tilde{\mathcal{H}}_\Lambda^X(h)=\tilde{H}_\Lambda^S(0)+\tilde{H}_\Lambda^T(0)+\tilde{H}_\Lambda^X(h), \tag{68}$$

and then we have

$$\left(\sum_{x\in\Lambda}\eta(x)^*\tilde{X}_{33}(x),\sum_{x\in\Lambda}\eta(x)\tilde{X}_{33}(x)\right)\leqslant\frac{1}{\beta K}\sum_{x\in\Lambda}\sum_{m=1}^{d}|h_m(x)|^2. \tag{69}$$

Noting that $\tilde{X}_{33}(x_{\mathrm{odd}})=U_T^\dagger U_S^\dagger X_{33}(x_{\mathrm{odd}})U_S U_T=X_{33}(x_{\mathrm{odd}})$ $(x_{\mathrm{odd}}\in\Lambda_{\mathrm{odd}})$, from this inequality, we obtain

$$\beta(X_{33}(k),X_{33}(-k))\leqslant\frac{1}{2KE(k)}=B_X(k),\quad k\neq P, \tag{70}$$

corresponding to inequality (60) in the region $K>0$ and $\Delta\geqslant 0$. From inequalities (65) and (70), an infrared bound on $g_X(k)$ is evaluated as

$$\lim_{\beta\to\infty} g_X(k) \leqslant \frac{1}{\sqrt{8KE(k)}}\sqrt{C_X(k)}, \quad k\neq P. \tag{71}$$

In the following sections, we will estimate upper bounds on $C_S(k)$, $C_T(k)$, and $C_X(k)$ and lower bounds for e_S, ε_3^T, and ε_3^X for each case.

IV. CASE OF AN ISOTROPIC INTERACTION, $\Delta=1$

A. Antiferro-spin and antiferro-orbital long-range order

In this subsection, we prove the existence of AFSLRO and AFOLRO in the ground state of Hamiltonian (4) with SU(2)⊗SU(2) symmetry ($\Delta=1$), i.e., $m_S^2=m_T^2>0$ within the region $0\leqslant K<4$.

First, we consider a lower bound on e_S. We label two of the four eigenstates of S_3 and T_3 in the matrix representation (3) on each site as

$$|\uparrow+\rangle=\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad |\downarrow-\rangle=\begin{pmatrix}0\\0\\0\\1\end{pmatrix}. \tag{72}$$

If we take the following trial state with a two-sublattice structure,

$$(\otimes_{x\in\Lambda_{\mathrm{odd}}}|\uparrow+\rangle_x)\otimes(\otimes_{x\in\Lambda_{\mathrm{even}}}|\downarrow-\rangle_x) \tag{73}$$

(here $\Lambda_{\mathrm{even}}=\Lambda\setminus\Lambda_{\mathrm{odd}}$), then we obtain

$$e_{\mathcal{H}}=e_S+e_T+Ke_X\geqslant\left(\frac{K}{16}+\frac{1}{2}\right)d. \tag{74}$$

We now consider the Bogoliubov inequality in a stronger form[34]

$$|\langle[A,B]\rangle_{\Lambda\beta}|^2\leqslant\beta(B^\dagger,B)\langle[[A,\mathcal{H}_\Lambda],A^\dagger]\rangle_{\Lambda\beta}. \tag{75}$$

Noting $(B^\dagger,B)\geqslant0$, we see

$$\lim_{\beta\to\infty}\langle[[A,\mathcal{H}_\Lambda],A^\dagger]\rangle_{\Lambda\beta}\geqslant0. \tag{76}$$

Setting $A=X_{33}(Q)$ in inequality (76), we obtain

$$e_{S\Lambda}\geqslant\frac{4}{3}e_{X\Lambda}, \quad 0\leqslant K<4, \tag{77}$$

$$e_{S\Lambda}\leqslant\frac{4}{3}e_{X\Lambda}, \quad K>4, \tag{78}$$

where we have used $e_{S\Lambda}=e_{T\Lambda}$. Combining inequalities (74) and (77), we obtain

$$e_S\geqslant d\left(\frac{K}{16}+\frac{1}{2}\right)\left(\frac{3}{4}K+2\right)^{-1} \tag{79}$$

for $0\leqslant K<4$.

Second, to evaluate an upper bound on G_S through inequality (62), we estimate an upper bound on the double commutator $C_S(k)$. After some straightforward calculations, the left-hand side of inequality (46) is reduced to

$$\lim_{\beta\to\infty}\langle[[S_3(k),\mathcal{H}_\Lambda],S_3(-k)]\rangle_{\Lambda\beta}=\frac{4}{3d}(e_{S\Lambda}+Ke_{X\Lambda})E(k). \tag{80}$$

By using inequality (77), an upper bound $C_S(k)$ on the expectation value of double commutator (80) at zero temperature is evaluated as

$$C_S(k)=\frac{1}{d}\left(K+\frac{4}{3}\right)e_{S\Lambda}E(k). \tag{81}$$

From inequality (62) and Eq. (81), we have

$$\lim_{\beta\to\infty}g_S(k)\leqslant\sqrt{\frac{E(k)}{E(k-Q)}}\sqrt{\frac{e_{S\Lambda}}{8d}\left(K+\frac{4}{3}\right)}. \tag{82}$$

Thus, we obtain the following bound on G_S:

$$G_S\leqslant\sqrt{\frac{e_S}{8d}\left(K+\frac{4}{3}\right)}\Gamma_{\mathrm{I}}^+(d), \tag{83}$$

with

$$\Gamma_{\mathrm{I}}^+(d)=\frac{1}{(2\pi)^d}\int_{-\pi}^{\pi}d^dk\sqrt{\frac{E(k)}{E(k-Q)}}\left\{-\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right\}_+, \tag{84}$$

where

$$\{F\}_+=\begin{cases}F & \text{if } F\geqslant0,\\ 0 & \text{otherwise}\end{cases} \tag{85}$$

TABLE I. The results of the numerical calculations for $\Gamma_{\mathrm{I}}^+(d)$, $\Gamma_{\mathrm{II}}^+(d)$, and $\Gamma_{\mathrm{III}}(d)$.

d	$\Gamma_{\mathrm{I}}^+(d)$	$\Gamma_{\mathrm{II}}^+(d)$	$\Gamma_{\mathrm{III}}(d)$
2	0.646 . . .	0.457 . . .	1.393 . . .
3	0.349 . . .	0.202 . . .	1.157 . . .
4	0.253 . . .	0.126 . . .	−
5	0.206 . . .	0.0923 . . .	−
6	0.177 . . .	0.0725 . . .	−
7	0.157 . . .	0.0597 . . .	−

We have evaluated $\Gamma_{\mathrm{I}}^+(d)$ numerically and have summarized the results in Table I. Applying inequality (83) to Eq. (38), we obtain the following lower bound for m_S^2:

$$m_S^2\geqslant\sqrt{\frac{e_S}{d}}\left(\frac{1}{3}\sqrt{\frac{e_S}{d}}-\sqrt{\frac{1}{8}K+\frac{1}{6}}\Gamma_{\mathrm{I}}^+(d)\right). \tag{86}$$

We also apply inequality (79) to the right-hand side of this inequality; then it is bounded from below by

$$\sqrt{\frac{e_S}{d}}\left[\frac{1}{3}\sqrt{\left(\frac{1}{16}K+\frac{1}{2}\right)\left(\frac{3}{4}K+2\right)^{-1}}-\sqrt{\frac{1}{8}K+\frac{1}{6}}\Gamma_{\mathrm{I}}^+(d)\right]. \tag{87}$$

TABLE II. For $0\leqslant K<4$, the region where we have shown the existence of AFSLRO and AFOLRO in d dimensions from inequality (88).

d	K
2	–
3	$0\leqslant K<0.342$
4	$0\leqslant K<1.342$
5	$0\leqslant K<2.264$
6	$0\leqslant K<3.148$
7	$0\leqslant K<4$

Therefore the LRO parameters m_S^2 and m_T^2 take finite values in d dimensions if parameter K satisfies

$$0\leqslant K<\overline{K}(d), \tag{88}$$

where $\overline{K}(d)$ is given by

$$\overline{K}(d)=\frac{1+\sqrt{324[\Gamma_{\mathrm{I}}^{+}(d)]^4+324[\Gamma_{\mathrm{I}}^{+}(d)]^2+1}}{27[\Gamma_{\mathrm{I}}^{+}(d)]^2}-2. \tag{89}$$

Since $\Gamma_{\mathrm{I}}^{+}(d)$ is monotonously decreasing in d,[43] $\overline{K}(d)$ is monotonously increasing in d. Then, in $d+1$ or more dimensions, there is LRO in the region where we can prove the existence of LRO in d dimensions. The results for $3\leqslant d\leqslant 7$ are summarized in Table II. In two dimensions, there is no region where we can prove $m_S^2=m_T^2>0$ from inequality (87). This result is consistent with the paper of KLS (Ref. 38) as follows. As we described in section I, KLS could prove the existence of AFSLRO (Néel order) in the ground state of spin-1/2 Heisenberg antiferromagnets on a simple cubic lattice, but could not on a square lattice, and this problem has been unresolved. At $K=0$, our Hamiltonian is divided into the two independent antiferromagnetic Heisenberg models, and we find that inequality (86) at $K=0$ becomes equivalent to inequality (4) in their paper (but they impose $m_S^2=0$ for the way of their discussion). We can easily see that the part within the brackets of lower bound (87) takes its maximal value at $K=0$. Thus, if we cannot prove the existence of AFSLRO at $K=0$, then there is no region for which we can prove its existence for $0<K<4$ from the lower bound (87). For this reason, noting the results of the paper of KLS described above, we can see that we have no region where we can prove it for $0<K<4$ in two dimensions.

B. Long-range order at $K=4$

In this subsection, we focus on the case of $K=4$ and $\Delta=1$, where the system satisfies a class of SU(4) symmetry.[19] Indeed, we can see that

$$[\mathcal{H}_\Lambda,S_l^{\mathrm{tot}}]=[\mathcal{H}_\Lambda,T_m^{\mathrm{tot}}]=[\mathcal{H}_\Lambda,X_{pq}^{\mathrm{tot}}]=0, \tag{90}$$

where

$$S_l^{\mathrm{tot}}=\sum_{x\in\Lambda} S_l(x), \tag{91}$$

$$T_m^{\mathrm{tot}}=\sum_{x\in\Lambda} T_m(x), \tag{92}$$

$$X_{pq}^{\mathrm{tot}}=2\sum_{x\in\Lambda}(-1)^{|x|}X_{pq}(x), \tag{93}$$

which generate a SU(4) Lie algebra.

We introduce the unitary operator defined by

$$V_X=\exp\left(\frac{\pi}{2}iX_{33}^{\mathrm{tot}}\right). \tag{94}$$

By using this unitary operator, we have

$$V_X^{\dagger}S_1(x)V_XV_X^{\dagger}S_1(y)V_X=-4X_{23}(x)X_{23}(y). \tag{95}$$

Noting Eq. (95) and the rotational invariance of $\mathcal{H}_\Lambda$ with respect to the spin and pseudospin, we obtain the relations

$$\frac{1}{15}e_{\mathcal{H}\Lambda}=\frac{1}{3}e_{S\Lambda}=\frac{1}{3}e_{T\Lambda}=\frac{4}{9}e_{X\Lambda} \tag{96}$$

and

$$m_S^2=m_T^2=4m_X^2. \tag{97}$$

By using Eq. (96), Eqs. (38) and (80) are written as

$$m_S^2=\frac{e_{\mathcal{H}}}{15d}-G_S \tag{98}$$

and

$$\lim_{\beta\to\infty}\langle[[S_3(k),\mathcal{H}_\Lambda],S_3(-k)]\rangle_{\Lambda\beta}=\frac{16}{15}\frac{e_{\mathcal{H}\Lambda}}{d}E(k)=C_S(k), \tag{99}$$

respectively. Combining Eqs. (62) and (99), we have

$$G_S\leqslant\sqrt{\frac{2}{15}\frac{e_{\mathcal{H}}}{d}}\Gamma_{\mathrm{I}}^{+}(d). \tag{100}$$

Thus, by applying this inequality to Eq. (98), we have a lower bound for m_S^2, and also applying inequality (74) to that lower bound, we find

$$\begin{aligned} m_S^2&\geqslant\sqrt{\frac{e_{\mathcal{H}}}{15d}}\left(\sqrt{\frac{e_{\mathcal{H}}}{15d}}-\sqrt{2}\Gamma_{\mathrm{I}}^{+}(d)\right)\\ &\geqslant\sqrt{\frac{e_{\mathcal{H}}}{15d}}\left(\sqrt{\frac{1}{20}}-\sqrt{2}\Gamma_{\mathrm{I}}^{+}(d)\right). \end{aligned} \tag{101}$$

By using the numerical results in Table I and noting Eq. (97), we show that

$$m_S^2=m_T^2=4m_X^2\geqslant\sqrt{\frac{e_{\mathcal{H}}}{105}}\left(\sqrt{\frac{1}{20}}-\sqrt{2}\Gamma_{\rm I}^+(7)\right)$$
$$=(0.000161\dots)\sqrt{\frac{e_{\mathcal{H}}}{105}}>0. \qquad (102)$$

Since $\Gamma_{\rm I}^+(d)$ is monotonously decreasing in d, we proved that three types of LRO parameters simultaneously take finite values in the ground state in seven or more dimensions.

C. Ferro-spin-orbital long-range order

In this subsection, we prove the existence of FSOLRO in the ground state of Hamiltonian (4) with isotropic interaction $(\Delta=1)$ within the region $K>4$. For the proof, we consider Eq. (40). In the case of $\Delta=1$, since the pseudospin part of Hamiltonian (4) also possesses SU(2) symmetry, Eq. (40) is written as

$$m_X^2=\frac{e_X}{9d}-G_X. \qquad (103)$$

Let us evaluate a lower bound for e_X. We combine inequalities (74) and (78), then we have

$$e_X\geqslant d\left(\frac{K}{16}+\frac{1}{2}\right)\left(K+\frac{8}{3}\right)^{-1}. \qquad (104)$$

In order to obtain an upper bound on $g_X(k)$, we evaluate $C_X(k)$. The left-hand side of inequality (67) takes the following form:

$$\lim_{\beta\to\infty}\langle[[X_{33}(k),\mathcal{H}_\Lambda],X_{33}(-k)]\rangle_{\Lambda\beta}$$
$$=\frac{2}{3}e_{S\Lambda}+\frac{2}{9}Ke_{X\Lambda}$$
$$+\left(\frac{K}{6}e_{S\Lambda}+\frac{8}{9}e_{X\Lambda}\right)\frac{1}{d}\sum_{m=1}^{d}\cos k_m=C_X(k). \qquad (105)$$

From the above equation and inequality (71), we obtain

$$\lim_{\beta\to\infty}g_X(k)\leqslant\sqrt{\frac{I_{1\Lambda}\left\{\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right\}+I_{2\Lambda}}{E(k)}}, \qquad (106)$$

with

$$I_{1\Lambda}=\frac{1}{48}e_{S\Lambda}+\frac{1}{9K}e_{X\Lambda}, \qquad (107)$$

$$I_{2\Lambda}=\frac{1}{12K}e_{S\Lambda}+\frac{1}{36}e_{X\Lambda}. \qquad (108)$$

Then we have

$$\lim_{\beta\to\infty}\frac{1}{|\Lambda|}\sum_{k\neq P}g_X(k)\left(\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right)$$
$$\leqslant\frac{1}{|\Lambda|}\sum_{k\neq P}\sqrt{\frac{I_{1\Lambda}\left\{\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right\}_+ +I_{2\Lambda}}{E_k}}$$
$$\times\left\{\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right\}_+. \qquad (109)$$

Applying inequality (78) to Eqs. (107) and (108), we obtain

$$I_{1\Lambda}\leqslant\left(\frac{1}{36}+\frac{1}{9K}\right)e_{X\Lambda}, \qquad (110)$$

$$I_{2\Lambda}\leqslant\left(\frac{1}{36}+\frac{1}{9K}\right)e_{X\Lambda}, \qquad (111)$$

for $K>4$. From inequalities (109), (110), and (111), we have

$$G_X\leqslant\sqrt{\left(\frac{1}{36}+\frac{1}{9K}\right)e_X}\Gamma_{\rm II}^+(d), \qquad (112)$$

where

$$\Gamma_{\rm II}^+(d)=\frac{1}{(2\pi)^d}\int_{-\pi}^{\pi}d^dk\sqrt{\frac{\left\{\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right\}_+ +1}{E_k}}$$
$$\times\left\{\frac{1}{d}\sum_{m=1}^{d}\cos k_m\right\}_+. \qquad (113)$$

We calculate numerically $\Gamma_{\rm II}^+(d)$, and the results are listed in Table I. By applying inequalities (104) and (112) to Eq. (103), we obtain

$$m_X^2\geqslant\sqrt{e_X}\left(\frac{1}{9d}\sqrt{e_X}-\sqrt{\frac{1}{36}+\frac{1}{9K}}\Gamma_{\rm II}^+(d)\right)$$
$$\geqslant\sqrt{e_X}\left[\frac{1}{9d}\sqrt{d\left(\frac{K}{16}+\frac{1}{2}\right)\left(K+\frac{8}{3}\right)^{-1}}\right.$$
$$\left.-\sqrt{\frac{1}{36}+\frac{1}{9K}}\Gamma_{\rm II}^+(d)\right]. \qquad (114)$$

Consequently, in seven dimensions FSOLRO parameter takes a finite value for

$$K>4.023. \qquad (115)$$

In six or less dimensions, we cannot draw a conclusion about the existence of FSOLRO from inequality (114).

V. CASE OF AN ANISOTROPIC ORBITAL INTERACTION, $0\leqslant\Delta<1$

A. Antiferro-orbital long-range order

In this subsection, we examine the existence of AFOLRO in the ground state for $0\leqslant\Delta<1$.

When we know the relations among the nearest-neighbor correlations in the ground state, e.g., inequalities (77) and (78), and Eq. (96) in the case of $\Delta=1$, the KLS-type sum rule (36) well works. In the case of $\Delta\neq 1$, we need to know the relations among $e_{S\Lambda}/3$, $\varepsilon^T_{1\Lambda}$, $\varepsilon^T_{3\Lambda}$, $4\varepsilon^X_{1\Lambda}$, and $4\varepsilon^X_{3\Lambda}$ due to the symmetry lowering of the pseudospin interaction. However, as we will see in Sec. V D, we cannot find those relations enough to work the KLS-type sum rule. Thus, in this subsection, in order to prove the existence of AFOLRO in the ground state, we use the sum rule

$$\frac{1}{|\Lambda|}\sum_{k\in\Lambda^*} g_T(k)=\frac{1}{4} \tag{116}$$

instead of the KLS-type sum rule.

By using the above sum rule, order parameter m_T^2 can be written as

$$m_T^2=\frac{1}{4}-\hat{G}_T, \tag{117}$$

with

$$\hat{G}_T=\lim_{\Lambda\to\infty}\lim_{\beta\to\infty}\frac{1}{|\Lambda|}\sum_{k\neq Q} g_T(k). \tag{118}$$

In order to obtain a lower bound for m_T^2, we evaluate an upper bound on $\hat{G}_T$.

We recall that an upper bound on $g_T(k)$ in the ground state is given by the right-hand side of inequality (63). We have evaluated $B_T(k)$ in Sec. III B; thus we have only to estimate $C_T(k)$ in this subsection.

Let us estimate $C_T(k)$. The expectation value of double commutator (64) is written as

$$\begin{aligned}\lim_{\beta\to\infty}&\langle[[T_3(k),\mathcal{H}_\Lambda],T_3(-k)]\rangle_{\Lambda\beta}\\ &=\frac{4\Delta}{d}(\varepsilon^T_{1\Lambda}+3K\varepsilon^X_{1\Lambda})E(k)\\ &=\frac{4\Delta}{d}\left(-\frac{1}{2}\lim_{\beta\to\infty}\langle\mathbf{T}(x)\cdot\mathbf{T}(y)\rangle_{\Lambda\beta}d\right.\\ &\qquad\left.-\frac{1}{2}\varepsilon^T_{3\Lambda}+3K\varepsilon^X_{1\Lambda}\right)E(k).\end{aligned} \tag{119}$$

Here, we use the Anderson bound[44] (reproduced in Appendix of Ref. 34)

$$\lim_{\beta\to\infty}\langle\mathbf{T}(x)\cdot\mathbf{T}(y)\rangle_{\Lambda\beta}d\geq-\frac{1}{4}(d+1) \tag{120}$$

and the Chaucy-Schwarz inequality

$$-\varepsilon^T_{3\Lambda}=\lim_{\beta\to\infty}\langle T_3(x)T_3(y)\rangle_{\Lambda\beta}d\leq\frac{d}{4}, \tag{121}$$

$$\varepsilon^X_{1\Lambda}=\lim_{\beta\to\infty}\langle S_l(x)T_1(x)S_l(y)T_1(y)\rangle_{\Lambda\beta}d\leq\frac{d}{16}. \tag{122}$$

TABLE III. The region where we have proved the existence of AFOLRO from inequality (127).

K	$d=2$	$d=3$
0.0	$\Delta<0.205$	$\Delta<0.319$
0.5	$\Delta<0.158$	$\Delta<0.241$
1.0	$\Delta<0.128$	$\Delta<0.194$
1.5	$\Delta<0.108$	$\Delta<0.162$
2.0	$\Delta<0.0935$	$\Delta<0.139$
2.5	$\Delta<0.0823$	$\Delta<0.122$
3.0	$\Delta<0.0735$	$\Delta<0.109$
3.5	$\Delta<0.0664$	$\Delta<0.0983$
4.0	$\Delta<0.0605$	$\Delta<0.0894$
4.5	$\Delta<0.0556$	$\Delta<0.0820$
5.0	$\Delta<0.0514$	$\Delta<0.0758$

Then, the right-hand side of Eq. (119) is bounded from above by

$$C_T(k)=\Delta\left(1+\frac{1}{2d}+\frac{3}{4}K\right)E(k). \tag{123}$$

Combining Eq. (123) and inequality (63), $g_T(k)$ in the ground state is bounded as

$$\lim_{\beta\to\infty}g_T(k)\leq\sqrt{\Delta\left(\frac{1}{8}+\frac{1}{16d}+\frac{3}{32}K\right)}\sqrt{\frac{E(k)}{E(k-Q)}},\quad k\neq Q, \tag{124}$$

and an upper bound on $\hat{G}_T$ is given by

$$\hat{G}_T\leq\sqrt{\Delta\left(\frac{1}{8}+\frac{1}{16d}+\frac{3}{32}K\right)}\Gamma_{\mathrm{III}}(d), \tag{125}$$

with

$$\Gamma_{\mathrm{III}}(d)=\frac{1}{(2\pi)^d}\int_{-\pi}^{\pi}d^dk\sqrt{\frac{E(k)}{E(k-Q)}}. \tag{126}$$

We have estimated $\Gamma_{\mathrm{III}}(2)$ and $\Gamma_{\mathrm{III}}(3)$ numerically and have summarized the results in table I. From Eq. (117) and inequality (125), we conclude that m_T^2 takes a nonzero value if

$$0\leq\Delta<\frac{2d}{[d(4+3K)+2][\Gamma_{\mathrm{III}}(d)]^2}. \tag{127}$$

The results for some values of K are listed in Table III.

B. Conjecture for antiferro-spin long-range order

In this and next subsections, in order to discuss the existence of AFSLRO and AFOLRO in the ground state with the KLS-type sum rule, we introduce a few assumptions on the relations among the nearest-neighbor correlations in the ground state. The discussion based on the KLS-type sum rule has the advantage of adopting the variational method which, in the ground state, gives the better results than that based on the sum rule (116).

In this subsection we examine the existence of AFSLRO in the ground state under the following natural assumptions:

$$\frac{1}{3}e_{S\Lambda}\leqslant\varepsilon_{3\Lambda}^{T}, \tag{128}$$

$$4\varepsilon_{3\Lambda}^{X}\leqslant\varepsilon_{3\Lambda}^{T}, \tag{129}$$

$$4\varepsilon_{1\Lambda}^{X}\leqslant\varepsilon_{3\Lambda}^{T}, \tag{130}$$

for $0\leqslant K\leqslant 4$ and $0\leqslant\Delta\leqslant 1$. We will discuss the validities of these assumptions in Sec. V D. Under the assumptions (128), (129), and (130), we evaluate an lower bound for m_S^2. As in Sec. IV, we estimate a lower bound for $e_{S\Lambda}$ and an upper bound on G_S to obtain a lower bound for m_S^2.

Let us estimate a lower bound for $e_{S\Lambda}$. Taking a variational state (73) for Hamiltonian (4), we have

$$e_{S\Lambda}+2\Delta\varepsilon_{1\Lambda}^{T}+\varepsilon_{3\Lambda}^{T}+K(6\Delta\varepsilon_{1\Lambda}^{X}+3\varepsilon_{3\Lambda}^{X})\geqslant\left(\frac{1}{2}+\frac{1}{16}K\right)d. \tag{131}$$

As we will see in Sec. V D [see inequality (150)], we have

$$\varepsilon_{3\Lambda}^{T}+3K\varepsilon_{3\Lambda}^{X}\geqslant\varepsilon_{1\Lambda}^{T}+3K\varepsilon_{1\Lambda}^{X}, \tag{132}$$

for $0\leqslant\Delta<1$. Applying inequalities (129) and (132) to (131), we obtain

$$e_{S\Lambda}\geqslant-(2\Delta+1)\left(1+\frac{3}{4}K\right)\varepsilon_{3\Lambda}^{T}+\left(\frac{1}{2}+\frac{K}{16}\right)d. \tag{133}$$

To evaluate an upper bound on G_S, we need to estimate $C_S(k)$. The expectation value of double commutator (46) is expressed as

$$\lim_{\beta\to\infty}\langle[[S_3(k),\mathcal{H}_\Lambda],S_3(-k)]\rangle_{\Lambda\beta}=\frac{4}{3d}(e_S+Ke_X)E(k). \tag{134}$$

We apply the inequalities (128), (129), and (130) to the right-hand side of Eq. (134); then it is bounded from above by

$$C_S(k)=\frac{1}{d}[4+K(2\Delta+1)]\varepsilon_3^{T}E(k). \tag{135}$$

Combining inequalities (62) and Eq. (135), we have an upper bound on G_S:

$$G_S\leqslant\sqrt{\frac{4+K(2\Delta+1)}{8d}\varepsilon_3^{T}}\Gamma_{\mathrm{I}}^{+}(d). \tag{136}$$

From inequalities (133) and (136), a lower bound for m_S^2 is evaluated as

$$m_S^2\geqslant\frac{1}{3}\left[-(2\Delta+1)\left(1+\frac{3}{4}K\right)\frac{\varepsilon_3^{T}}{d}+\frac{1}{2}+\frac{K}{16}\right] -\sqrt{\frac{4+K(2\Delta+1)}{8}\frac{\varepsilon_3^{T}}{d}}\Gamma_{\mathrm{I}}^{+}(d). \tag{137}$$

Thus we can conclude $m_S^2>0$ if ε_3^{T} satisfies

TABLE IV. For $0\leqslant K\leqslant 4$, the region where we have shown the existence of AFSLRO in three dimensions from inequality (145) obtained under assumptions (128), (129), and (130).

K	Δ	K	Δ
0.0	$\Delta<1.000$	2.5	$\Delta<0.0679$
0.5	$\Delta<0.792$	3.0	$\Delta<0.0137$
1.0	$\Delta<0.432$	3.5	–
1.5	$\Delta<0.252$	4.0	–
2.0	$\Delta<0.142$		

$$\frac{\varepsilon_3^{T}}{d}-\xi_+>0, \tag{138}$$

where ξ_+ is the larger solution of the following quadratic equation for ξ:

$$a\xi^2+b\xi+c=0, \tag{139}$$

with

$$a=(2\Delta+1)^2\left(1+\frac{3}{4}K\right)^2, \tag{140}$$

$$b=-(2\Delta+1)\left(1+\frac{3}{4}K\right)\left(1+\frac{K}{8}\right) -\frac{36+9K(2\Delta+1)}{8}[\Gamma_{\mathrm{I}}^{+}(d)]^2, \tag{141}$$

$$c=\left(\frac{1}{2}+\frac{K}{16}\right)^2. \tag{142}$$

In order to obtain a lower bound for ε_3^{T}, we combine inequalities (128) and (133). Then we have

$$\varepsilon_3^{T}\geqslant\frac{(8+K)d}{64+32\Delta+12K(2\Delta+1)}. \tag{143}$$

Applying inequality (143) to the left-hand side of inequality (138), we obtain

$$\frac{\varepsilon_3^{T}}{d}-\xi_+\geqslant\frac{8+K}{64+32\Delta+12K(2\Delta+1)}-\xi_+>0. \tag{144}$$

Therefore, we obtain the region where we can evaluate $m_S^2>0$ for $0\leqslant K\leqslant 4$ as follows:

$$0\leqslant\Delta <-\frac{3K^2+16K+8}{6K^2+8K}+\frac{\sqrt{6K^3+56K^2+64K+64[\Gamma_{\mathrm{I}}^{+}(d)]^2}}{(6K^2+8K)\Gamma_{\mathrm{I}}^{+}(d)}. \tag{145}$$

The results in three dimensions for some values of K are summarized in Table IV. In two dimensions, there is no region where we can conjecture $m_S^2>0$ from inequality (145).

TABLE V. The region where we have conjectured the existence of AFOLRO under assumptions (128) and (129) within $0\leqslant K\leqslant 4$.

K	$d=2$	$d=3$
0.0	$\Delta<0.378$	$\Delta<1.000$
0.5	$\Delta<0.346$	$\Delta<0.915$
1.0	$\Delta<0.269$	$\Delta<0.721$
1.5	$\Delta<0.220$	$\Delta<0.595$
2.0	$\Delta<0.185$	$\Delta<0.507$
2.5	$\Delta<0.160$	$\Delta<0.442$
3.0	$\Delta<0.141$	$\Delta<0.392$
3.5	$\Delta<0.125$	$\Delta<0.352$
4.0	$\Delta<0.113$	$\Delta<0.320$

C. Conjecture for antiferro-orbital long-range order

In this subsection, we reexamine the region where we can show $m_T^2>0$ in the ground state under assumptions (128) and (129).

Let us estimate a lower bound for the right-hand side of Eq. (39). Applying inequalities (132) and (129) to the expectation value of double commutator (64) in the ground state [see also (119)], we have

$$\frac{4\Delta}{d}(\varepsilon_{1\Lambda}^T+3K\varepsilon_{1\Lambda}^X)E(k)\leqslant\frac{\Delta}{d}(4+3K)\varepsilon_{3\Lambda}^T E(k)=C_T(k). \tag{146}$$

By using this $C_T(k)$ and inequality (63), we obtain

$$G_T\leqslant\sqrt{\frac{\varepsilon_3^T}{d}}\sqrt{\frac{\Delta}{8}(4+3K)}\Gamma_{\rm I}^+(d). \tag{147}$$

Then, a lower bound for m_T^2 is given by

$$\begin{aligned} m_T^2 &\geqslant \frac{\varepsilon_3^T}{d}-\sqrt{\frac{\varepsilon_3^T}{d}}\sqrt{\frac{\Delta}{8}(4+3K)}\Gamma_{\rm I}^+(d)\\ &\geqslant\sqrt{\frac{\varepsilon_3^T}{d}}\left(\sqrt{\frac{8+K}{64+32\Delta+12K(2\Delta+1)}}\right.\\ &\qquad\left.-\sqrt{\frac{\Delta}{8}(4+3K)}\Gamma_{\rm I}^+(d)\right), \end{aligned} \tag{148}$$

where we used inequality (143). Here we should note that inequality (143) can be derived from only two assumptions (128) and (129). From lower bound (148), we can conclude that m_T^2 takes a finite value in the region

$$0\leqslant\Delta<-\frac{3K+16}{12K+16}+\frac{\sqrt{16(K+8)+(3K+16)^2(\Gamma_{\rm I}^+(d))^2}}{4(3K+4)\Gamma_{\rm I}^+(d)} \tag{149}$$

for $0\leqslant K\leqslant 4$. These results are summarized in Table V.

D. Validties of assumptions in Sec. V B and V C

In Secs. V B and V C, we used assumptions (128), (129), and (130) to prove the existence of LRO. In this subsection, we discuss the validities of these assumptions.

The reason for which we introduced these assumptions is as follows. In the isotropic case, we found $e_{S\Lambda}=e_{T\Lambda}$ and $\varepsilon_{1\Lambda}^X=\varepsilon_{3\Lambda}^X$. Thus, in the Ising-like region $(0\leqslant\Delta<1)$, it is natural to assume that $\varepsilon_{3\Lambda}^T\geqslant e_{S\Lambda}/3\geqslant\varepsilon_{1\Lambda}^T$ and $\varepsilon_{3\Lambda}^X\geqslant\varepsilon_{1\Lambda}^X$. Then, assumption (128) may hold. We should note that $e_{S\Lambda}\geqslant 4e_{X\Lambda}/3$ for $0\leqslant K\leqslant 4$, in the case of $\Delta=1$ [recall inequality (77) and Eq. (96)]. From these relations, it is acceptable to assume $\varepsilon_{3\Lambda}^T\geqslant 4\varepsilon_{3\Lambda}^X\geqslant 4\varepsilon_{1\Lambda}^X$ (note also $\varepsilon_{m\Lambda}^X=e_{X\Lambda}/9$ in the case of $\Delta=1$). Thus, assumptions (129) and (130) also may hold.

By using inequality (76) and numerical calculations, we discuss the validities of these assumptions in more detail.

Let us set $A=T_1(P)$ in inequality (76). Then, this inequality leads to

$$\varepsilon_{3\Lambda}^T+3K\varepsilon_{3\Lambda}^X\geqslant\varepsilon_{1\Lambda}^T+3K\varepsilon_{1\Lambda}^X \tag{150}$$

for $0\leqslant\Delta<1$, and also do $A=X_{11}(Q)$ and $A=X_{33}(Q)$; then we have

$$\frac{1}{3}e_{S\Lambda}+\frac{1}{2}\varepsilon_{3\Lambda}^T\geqslant 6\varepsilon_{1\Lambda}^X \tag{151}$$

at $K=4\Delta$ for $0\leqslant\Delta<1$ and

$$\frac{1}{3}e_{S\Lambda}+\Delta\varepsilon_{1\Lambda}^T\geqslant 4\varepsilon_{3\Lambda}^X+4\Delta\varepsilon_{1\Lambda}^X \tag{152}$$

for $0\leqslant K<4$, respectively. Assumptions (128), (129), and (130) do not contradict these inequalities. Noting that we consider $\varepsilon_{3\Lambda}^T\geqslant\varepsilon_{1\Lambda}^T$ ($\varepsilon_{3\Lambda}^T\geqslant e_{S\Lambda}/3\geqslant\varepsilon_{1\Lambda}^T$) in the above, we find that this relation combined with assumption (129) satisfies rigorous inequality (150).

Before proceeding to the numerical calculations, in order to find that some of the assumptions hold in the special case of our Hamiltonian, we consider the relations among the nearest-neighbor correlations in the ground state in four cases $K=0$, $\Delta=0$, $K=4\Delta$, and $K=4$. At $K=0$, from inequality (150), we have $\varepsilon_{3\Lambda}^T\geqslant\varepsilon_{1\Lambda}^T$ [but we cannot show assumption (128)]. At $\Delta=0$, we have $e_S/3\geqslant 4\varepsilon_{3\Lambda}^X$ from inequality (152). Combining this inequality and assumption (128), we can prove assumption (129). Next, we consider the case of $K=4\Delta$. Combining assumption (128) and inequality (151), we can derive assumption (130). Furthermore, at $K=4$, we can find that

$$[\mathcal{H}_\Lambda,S_i^{\rm tot}]=[\mathcal{H}_\Lambda,T_3^{\rm tot}]=[\mathcal{H}_\Lambda,X_{33}^{\rm tot}]=0 \tag{153}$$

for $\Delta\neq 1$. By using these relations as in Sec. IV B, we have

$$\frac{1}{3}e_{S\Lambda}=4\varepsilon_{3\Lambda}^X, \tag{154}$$

$$\varepsilon_{1\Lambda}^T=4\varepsilon_{1\Lambda}^X. \tag{155}$$

If we use Eq. (154), then the assumption (128) is equivalent to (129). Thus, it is sufficient if we put either assumption in this case. Combining Eq. (155) and the assumption (130), we have $\varepsilon_{1\Lambda}^{T} \leqslant \varepsilon_{3\Lambda}^{T}$. Therefore the assumptions at $K=4$ can be replaced by $\varepsilon_{1\Lambda}^{T} \leqslant e_S/3 \leqslant \varepsilon_{3\Lambda}^{T}$.

Next, we directly calculate $e_{S\Lambda}/3$, $\varepsilon_{1\Lambda}^{T}$, $\varepsilon_{3\Lambda}^{T}$, $4\varepsilon_{1\Lambda}^{X}$, and $4\varepsilon_{3\Lambda}^{X}$ to confirm that the assumptions are established on lattices with two, four (a single square), and eight (a single cube) sites. By using exact diagonalization, we have estimated the nearest-neighbor correlations for some values of K and Δ in $0 \leqslant K \leqslant 4$ and $0 \leqslant \Delta \leqslant 1$, and have confirmed that the results satisfy the relations $\varepsilon_{3\Lambda}^{T} \geqslant e_{S\Lambda}/3 \geqslant \varepsilon_{1\Lambda}^{T}$ and $\varepsilon_{3\Lambda}^{T} \geqslant 4\varepsilon_{3\Lambda}^{X} \geqslant 4\varepsilon_{1\Lambda}^{X}$. We also have found that relations (154) and (155) hold at $K=4$. These results suggest that assumptions (128), (129), and (130) are valid.

VI. SUMMARY

We have constructed upper bounds on the correlation functions $g_S(k)$ $(k \neq Q)$, $g_T(k)$ $(k \neq Q)$, and $g_X(k)$ $(k \neq P)$ in the finite system within the region satisfying reflection positivity, i.e., $K \geqslant 0$ and $0 \leqslant \Delta \leqslant 1$. If the correlation function for the mode k in the finite system is bounded from above by a finite value independent of the lattice size, the LRO parameter for that mode is vanishing in the infinite system. It should be noted that we could not construct upper bounds on the spin and orbital two-point correlation functions for the mode Q and the spin-orbital correlation function for the mode P. Thus we can determine the kind of LRO which would be realized in an infinite system if it exists; i.e., candidates for LRO are AFSLRO, AFOLRO, and FSOLRO in the thermodynamic limit in the considered parameter region. Indeed, we have used these upper bounds to examine the existence of three types of LRO and have proved or conjectured that m_S^2, m_T^2, and m_X^2 take positive values under some conditions.

In the isotropic case $(\Delta=1)$, for the region $0 \leqslant K < 4$, we have proved that AFSLRO and AFOLRO coexist for $0 \leqslant K < \overline{K}(d)$. These results are summarized in Table II. At $K=4$ [SU(4) symmetric point], by using the SU(4) symmetry of the Hamiltonian, we have shown that $m_S^2 = m_T^2 = 4m_X^2$, and these order parameters take positive values in seven or more dimensions. We cannot prove the existence of LRO for $2 \leqslant d \leqslant 6$. In two dimensions, this result does not contradict the result of Monte Carlo simulations.[28] For the region $K > 4$, we have proved that FSOLRO exist for $K > 4.023$ in seven dimensions.

In the anisotropic case $(0 \leqslant \Delta < 1)$, we have proved the existence of AFOLRO in the region given by inequality (127) in two and three dimensions. The results are summarized in Table III. For the region $0 \leqslant K \leqslant 4$, we have also conjectured on the existence of AFSLRO and AFOLRO in the region determined by inequalities (145) and (149), respectively. These results are listed in Tables IV and V for some values of K.

These conjectures are based on a few assumptions. By using the rigorous relations among the nearest-neighbor correlations and the results of the exact diagonalization for the finite-size clusters, we have discussed the validities of the assumptions in Sec. V D. In particular, at $K=4\Delta$, we could prove assumption (130). At $\Delta=0$, we also could prove assumption (129). At $K=4$, we found $e_{S\Lambda}/3 = 4\varepsilon_{3\Lambda}^{X}$ and $\varepsilon_{1\Lambda}^{T} = 4\varepsilon_{1\Lambda}^{X}$. By using these relations, we could replace the assumptions by $\varepsilon_{1\Lambda}^{T} \leqslant e_S/3 \leqslant \varepsilon_{3\Lambda}^{T}$. This assumption is quite natural in the Ising-like region. All the considerations in Sec. V D imply that all assumptions in Secs. V B and V C are valid, and we expect that the results of Secs. V B and V C are fairly reliable.

In conclusion, we have established the proof and conjecture for the existence of three types of LRO, i.e., AFSLRO, AFOLRO, and FSOLRO, in fairly wide parameter regions, and have first presented reliable results in higher-dimensional systems where mean-field-type approximations or numerical calculations suffer from various difficulties, such as uncontrolled accuracy or too large degrees of freedom. The present results for $0 \leqslant K \leqslant 4$ in three dimensions are summarized in Fig. 1. This figure shows that the proof

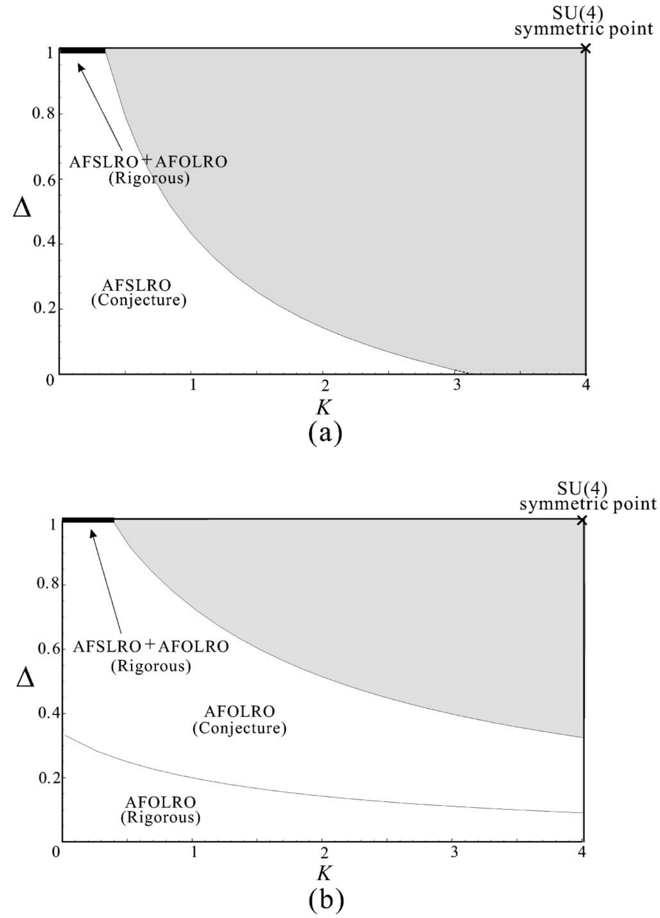

FIG. 1. The regions we have proved or conjectured on the existence of LRO in three dimensions. The region AFSLRO +AFOLRO (rigorous) $(0 \leqslant K < 0.342,\ \Delta=1)$ is determined by inequality (88). (a) The region AFSLRO (conjecture) is determined by inequality (145). (b) The regions AFOLRO (rigorous) and AFOLRO (conjecture) are determined by inequalities (127) and (149), respectively. We cannot conclude anything in the shaded regions.

and the conjecture of LRO become difficult as SU(4) symmetric point is approached in the K-Δ plane. For the region $K>4$, the right-hand side of inequality (102), giving a lower bound for the FSOLRO parameter, is also decreasing as K approaches this point. These tendencies probably imply the increase of quantum fluctuations. Here, we should note that, as we described in Sec. I, the existence of the antiferromagnetic LRO in the ground state of the spin-S Heisenberg antiferromagnet on the d-dimensional hypercubic lattice was proved except for the case of $d=2$ and $S=1/2$, and quantum fluctuations in this case are considered to be the strongest in two or more dimensions. In three dimensions, our results left the possibility of the existence of the disordered ground state at SU(4) symmetric point and its vicinity. We hope that this problem will be explored by other techniques.

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