Schwinger-Boson Mean-Field Theory of Mixed-Spin Antiferromagnet $L_2BaNiO_5$

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(March 22, 2022)

Abstract

The Schwinger-boson mean-field theory is used to study the three-dimensional antiferromagnetic ordering and excitations in compounds $L_2BaNiO_5$, a large family of quasi-one-dimensional mixed-spin antiferromagnet. To investigate magnetic properties of these compounds, we introduce a three-dimensional mixed-spin antiferromagnetic Heisenberg model based on experimental results for the crystal structure of $L_2BaNiO_5$. This model can explain the experimental discovery of coexistence of Haldane gap and antiferromagnetic long-range order below Néel temperature. Properties such as the low-lying excitations, magnetizations of Ni and rare-earth ions, Néel temperatures of different compounds, and the behavior of Haldane gap below the Néel temperature are investigated within this model, and the results are in good agreement with neutron scattering experiments.

PACS numbers: 75.10.Jm, 75.50.Ee, 75.50.-y

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I. INTRODUCTION

The existence of Haldane gap \[^1\] in the magnetic excitation spectrum has kept the integer-spin one-dimensional (1D) Heisenberg antiferromagnet to be one of the most interesting subjects in condensed matter physics during the past twenty years. The integer-spin Heisenberg antiferromagnetic (AF) chain should have a singlet ground state, exponentially decaying correlations, and a quantum gap, which have been confirmed by numerous theoretical \[^2,3,4,5,6\] and experimental \[^7,8,9,10\] studies. Kennedy and Tasaki have proved that the appearance of Haldane gap in the spin-1 AF chain corresponds to the breaking of a hidden \(Z_2 \times Z_2\) symmetry \[^11\]. The recent discovery of coexistence of Haldane gap and AF long-range order (AF LRO) in rare-earth compounds \(L_2\text{BaNiO}_5\) with \(L=Y, \text{Nd}, \text{Sm}, \text{Eu}, \text{Gd}, \text{Tb}, \text{Dy}, \text{Ho}, \text{Er},\) and \(\text{Tm} \[^{10,12,13,14,15,16}\] has offered an opportunity to investigate the effect of staggered field on the Haldane chain. The polarized and unpolarized inelastic neutron scattering experiments on \(L_2\text{BaNiO}_5 \[^{14,16}\] present that, on the one hand, there are AF interactions between spins of rare-earth and \(\text{Ni}\) ions, which lead to the three-dimensional (3D) AF LRO with Néel temperature \((T_N)\) ranging from 20 – 70K \[^{12,13}\]. On the other hand, these compounds are also characterized by the presence of \(\text{NiO}_6\) octahedron chains along \(a\)-axis. As is anticipated, above the Néel temperature, energy gap has been found in the excitation propagating along \(\text{Ni}\)-chain. Also the Haldane gap is discovered to persist in the 3D AF phase and increase with decreasing temperature below \(T_N \[^{14,15,16}\].

Recently several theoretical works have focused on the quasi-1D Haldane system \(L_2\text{BaNiO}_5 \[^{17,18,19}\]. To describe the coexistence of Haldane gap and AF LRO, the non-linear sigma model in a static staggered magnetic field has been introduced by Maslov and Zheludev \[^17\]. This system has been studied numerically within the density matrix renormalization group method by adopting the model of a 1D spin-1 Heisenberg chain in a static field \[^18\]. In the above studies, the reason for introducing the static staggered field is based on the assumption that there are 3D directly AF exchange interactions between the spins of rare-earth ions, which lead to the AF LRO below \(T_N\). However, it has been pointed out
by some experiments \cite{12,13,14} that spins of Ni ions also play an important role in forming AF LRO, and the two-dimensional mixed-spin Heisenberg model with $s_1 = 1$ and $s_2 = 1/2$ chains staked alternatively has also been adopted for this system \cite{19}.

Depending on the experimental finding of crystal structure, we introduce a more suitable 3D mixed-spin AF Heisenberg model to describe the magnetic properties of compounds $L_2\text{BaNiO}_5$. In this model we define $s_1 = 1$ for the spins of Ni ions, and investigate different members of this family by changing the spin value $s_2$ of rare-earth ions correspondingly. We use the Schwinger-boson mean-field (SBMF) \cite{20,21,22} theory to study this 3D mixed-spin model. The SBMF theory has been successful to the study of spin-integer Heisenberg chains \cite{20,21}, and has also been extended to cases with magnetic ordering by identifying the magnetization with the Bose condensation of the Schwinger bosons \cite{20,21,22}. Within this model, we could explain the experimental discovery of coexistence of Haldane gap and AF LRO. The interactions between spins of Ni and rare-earth ions are proved to be very important in forming the AF LRO. Properties such as the magnetization, Haldane gap and Néel temperatures are also discussed for cases with different $s_2$. Comparing our results with neutron scattering experiments, we find that our findings could explain some experimental discoveries.

The paper is organized as follows: In Sec. II we introduce the 3D mixed-spin Heisenberg model and Schwinger-boson mean-field theory. Our results of the magnetic properties of $L_2\text{BaNiO}_5$ compounds are presented in Sec. III. Finally, we conclude our findings in Sec. IV.

II. MIXED-SPIN HEISENBERG MODEL AND SCHWINGER-BOSON MEAN-FIELD THEORY

The crystal structures of $L_2\text{BaNiO}_5$ compounds have been investigated extensively by neutron scattering experiments \cite{12,13,14}. They belong to the orthorhombic system, having approximate cell Parameters around $a = 3.8\text{Å}, b = 5.8\text{Å}$ and $c = 11.3\text{Å}$. In all members
of this compounds, as figure 1(b) shown, strings of distorted NiO$_6$ octahedron share apical oxygen and form Haldane chains along the $a$-axis. The intrachain Ni-O-Ni AF superexchange coupling is about 200-300K [12][13][14], which is the strongest magnetic interaction in the compound. While in the $bc$ plane, as figure 1(a) shown, there is one oxygen between the Ni and rare-earth (L)ions, and thus the Ni-O-L interactions establish links between individual Ni chains. This coupling is of the order of tens of Kelvin (10-30K). Figure 1(a) also shows that there are L-O-L AF interactions between rare-earth ions, which is of the order of 1K or less.

Based on the experimental discovery of the crystal structure of compounds $L_2$BaNiO$_5$, we introduce a 3D mixed-spin AF Heisenberg model expressed by the Hamiltonian

$$H = J_1 \sum_{i, \eta_a} S_{1,i} \cdot S_{1,i+\eta_a} + J_2 \sum_{i, \eta_b, \eta_c} S_{1,i} \cdot S_{2,i+\eta_b+\eta_c} + J_3 \sum_j S_{2,j} \cdot S_{2,j+\eta_0},$$

where $S_1$ and $S_2$ are the spin operators of Ni and rare-earth ions respectively. $\eta_b$ and $\eta_c$ denote a sum over nearest-neighbor (NN) bonds in the $bc$ plane, and so is $\eta_a$ for the NN bonds along the $a$-axis. The AF superexchange couplings along the Ni chain, between $L$ and Ni ions, and among the rare-earth $L$ ions are represented as $J_1$, $J_2$, and $J_3$ respectively as figure 1(a) shown.

The Schwinger-boson theory introduces $S_i = \frac{1}{2} b^\dagger_{i\alpha} \sigma_{\alpha,\beta} b_{i\beta} (\alpha \text{ or } \beta = \uparrow, \downarrow)$ [20][21], and the spin degrees of freedom are mapped to the boson degrees of freedom. Meanwhile the original spin Hilbert space corresponds to a boson Hilbert subspace in which $b^\dagger_{i\uparrow} b_{i\uparrow} + b^\dagger_{i\downarrow} b_{i\downarrow} = 2s_i$. These constraints to the boson Hilbert space are imposed in the Hamiltonian (1) by introducing two kinds of Lagrangian multipliers $\lambda_1(i)$ and $\lambda_2(j)$. In addition, we define the bond operators as $Q_a(i, \eta_a) = b_{i\uparrow}b_{i+\eta_a\uparrow} - b_{i\downarrow}b_{i+\eta_a\downarrow}$, $Q_h(i, \eta_b, \eta_c) = b_{i\uparrow}b_{i+\eta_b+\eta_c\uparrow} - b_{i\downarrow}b_{i+\eta_b+\eta_c\downarrow}$, and $Q_c(j, \eta_0) = b_{2j\uparrow}b_{2(j+\eta_0)\downarrow} - b_{2j\downarrow}b_{2(j+\eta_0)\uparrow}$. The Hamiltonian (1) can be rewritten as

$$H = -\frac{1}{2} J_1 \sum_{i, \eta_a} \{Q^+_{a}(i, \eta_a)Q_a(i, \eta_a) - 2s^2_i\} - \frac{1}{2} J_2 \sum_j \{Q^+_{h}(j, \eta_b, \eta_c)Q_h(j, \eta_b, \eta_c) - 2s^2\}$$

$$-\frac{1}{2} J_3 \sum_{i, \eta_b, \eta_c} \{Q^+_{c}(j, \eta_0)Q_c(j, \eta_0) - 2s_1s_2\}$$

$$+ \sum_i \lambda_1(i) \left\{b^\dagger_{i\uparrow}b_{i\uparrow} + b^\dagger_{i\downarrow}b_{i\downarrow} - 2s_i\right\} + \sum_j \lambda_2(j) \left\{b^\dagger_{2j\uparrow}b_{2j\uparrow} + b^\dagger_{2j\downarrow}b_{2j\downarrow} - 2s_2\right\}. \quad (2)$$
Next, we make a Hartree-Fock decomposition of Eq. (2) by taking the average values of the bond operators and Lagrange multipliers to be uniform and static as \( \langle Q_a(i, \eta_a) \rangle = Q_a \), \( \langle Q_h(i, \eta_b, \eta_c) \rangle = Q_h \), \( \langle Q_c(j, \eta_0) \rangle = Q_c \), \( \langle \lambda_1(i) \rangle = \lambda_1 \), and \( \langle \lambda_2(j) \rangle = \lambda_2 \). Under the Fourier transformation, we obtain the following mean-field Hamiltonian in the momentum space

\[
H_{MF} = \sum_k 2Z_k \left\{ b_{1k\uparrow}b_{1(-k)\downarrow} - b_{1k\downarrow}b_{1(-k)\uparrow} + h.c \right\} + \sum_k 4D_k \left\{ b_{1k\uparrow}b_{2(-k)\downarrow} - b_{1k\downarrow}b_{2(-k)\uparrow} + h.c \right\}
+ \sum_k 2\chi_k \left\{ b_{2k\uparrow}b_{2(-k)\downarrow} - b_{2k\downarrow}b_{2(-k)\uparrow} + h.c \right\} + \sum_{k\sigma} \left\{ 4\lambda_1 b_{1k\sigma}^+ b_{1k\sigma} + 8\lambda_2 b_{2k\sigma}^+ b_{2k\sigma} \right\}
+ 2N \left\{ J_1 Q_a^2 + 4J_2 Q_h^2 + J_3 Q_c^2 - 4\lambda_1 s_1 + 2J_1 s_1^2 + 8J_2 s_1 s_2 + 2J_3 s_2^2 - 8\lambda_2 s_2 \right\},
\]

(3)

where \( Z_k = J_1 Q_a \cos(k_x a_0) \), \( \chi_k = J_3 Q_c \cos(k_x c_0) \), and \( D_k = 2J_2 Q_h \cos(k_x c_0) \cos(k_y b_0) \).

Diagonalizing \( H_{MF} \) in Eq. (3) by the Bogoliubov transformation, we obtain

\[
H_{MF} = 2 \sum_k \left\{ E_k^+ \left( \alpha_{1k\sigma}^+ \alpha_{1k\sigma} + \alpha_{2k\sigma}^+ \alpha_{2k\sigma} \right) + E_k^- \left( \beta_{1k\sigma}^+ \beta_{1k\sigma} + \beta_{2k\sigma}^+ \beta_{2k\sigma} \right) \right\} + E_0
\]

(4)

with

\[
E_k^\pm = \sqrt{\frac{A \pm \sqrt{A^2 - 4B}}{2}}
\]

\[
A = \lambda_1^2 + 4\lambda_2^2 - \left( Z_k^2 + \lambda_k^2 + 2D_k^2 \right)
\]

\[
B = 4\lambda_1 \lambda_2 \left( \lambda_1 \lambda_2 - D_k^2 \right) - \lambda_k^2 \lambda_1^2 - 4Z_k^2 \lambda_2^2 + \left( \chi_k Z_k - D_k \right)^2
\]

\[
E_0 = 2N \left\{ J_1 Q_a^2 + 4J_2 Q_h^2 + J_3 Q_c^2 + 2J_1 s_1^2 + 8J_2 s_1 s_2 + 2J_3 s_2^2 \right\}
- 8N \lambda_1 \left( \frac{s_1 + 1}{2} \right) - 16N \lambda_2 \left( \frac{s_2 + 1}{2} \right).
\]

(5)

Furthermore, the mean-field free energy is given by

\[
F_{MF} = \frac{8}{\beta} \sum_k \ln \left\{ \left( 2 \sinh \left( \frac{\beta E_k^+}{2} \right) \right) + \ln \left( 2 \sinh \left( \frac{\beta E_k^-}{2} \right) \right) \right\} + E_0.
\]

(6)

The mean-field equations are obtained by differentiating \( F_{MF} \) with respect to the parameters \( Q_a, Q_h, Q_c, \lambda_1, \) and \( \lambda_2 \) as

\[
\frac{\partial F_{MF}}{\partial Q_a} = \frac{\partial F_{MF}}{\partial Q_h} = \frac{\partial F_{MF}}{\partial Q_c} = \frac{\partial F_{MF}}{\partial \lambda_1} = \frac{\partial F_{MF}}{\partial \lambda_2} = 0.
\]

(7)

Thus we obtain five self-consistent equations to determine the average values of the bond operators and Lagrange multipliers.
III. MEAN-FIELD SOLUTIONS

In this section, we present the solutions of the SBMF theory. The experimental discovery of coexistence of Haldane gap and AF LRO below $T_N$ are obtained by our study. As equation (5) shown, there are two branches of the magnetic excitations $E_k^+$ and $E_k^-$, which have quite different behaviors below $T_N$. On the one hand, the magnetic excitation $E_k^+$ has an energy gap in the whole temperature region, and below $T_N$ this energy gap increases with decreasing temperature. On the other hand, within the temperature region from zero to $T_N$, $E_k^-$ keeps to be gapless and has its minimal value $E_k^- = 0$ at $k = 0$. Under this condition, the Schwinger-boson condensation occurs and leads to the AF LRO in this system. In our calculation, we introduce the Schwinger-boson condensation into the self-consistent mean-field equations, and obtain the temperature dependence of the magnetizations of $Ni$ ($M_1$) and rare-earth ($M_2$) ions below $T_N$ respectively. The magnetizations $M_1$ and $M_2$ are expressed as

$$M_1 = \langle S_1^z \rangle = \frac{1}{2N} \sum_i (b_{1i\uparrow}^+ b_{1i\uparrow} - b_{1i\downarrow}^+ b_{1i\downarrow})$$

$$M_2 = \langle S_2^z \rangle = \frac{1}{2N} \sum_j (b_{2j\uparrow}^+ b_{2j\uparrow} - b_{2j\downarrow}^+ b_{2j\downarrow}).$$

We choose the AF superexchange interactions as $J_1 = J$, $J_2 = 0.1J$ and $J_3 = 0.01J$ ($J > 0$) according to the experimental studies of the magnetic properties of compounds $L_2BaNiO_5$ [12,13,14]. The AF interactions between $Ni$ ions has been estimated as $2J = 200 - 300K$ by the neutron scattering experiments [12,14]. To make it simple and clear, in our calculation we choose $J = 100K$.

The neutron scattering experimental results of $Nd_2BaNiO_5$ obtained by Yokoo et al. [15] are shown in Fig. 2(a) and 2(b) (open circles). The solid lines in Fig. 2(a) and 2(b) show fits to the above experimental results by our numerical calculations for the case with $s_2 = 3/2$ respectively. The temperature dependence of magnetizations $M_1/s_1$ and $M_2/s_2$ for the cases of $s_2 = 1/2, 1, 3/2, 2, 5/2, 3$ are shown in figure 2(c) and 2(d) respectively. As temperature increases, the thermal fluctuation in the system becomes stronger, and the magnetizations decrease rapidly and drop to zero at the Néel temperatures. Therefore, we
could also determine the Néel temperatures $T_N$ for all members of the $L_2BaNiO_5$ family through our calculation.

In figure 3, we plot the Néel temperature $T_N$ as a function of spin value $s_2$ (filled circles and dotted line). For comparison, the Néel temperatures of compounds $Ho_2BaNiO_5$ ($T_N = 53K$) \cite{12}, $Nd_2BaNiO_5$ ($T_N = 48K$) \cite{13} and $Pr_2BaNiO_5$ ($T_N = 24K$) \cite{14} obtained by the neutron scattering experiments are also shown in Fig. 3 (filled triangles). Our theoretical results roughly agree with the experimental results. We also obtain that the Néel temperature $T_N$ increases monotonously with the increasing of $s_2$. As the spin value of the rare-earth ions $s_2$ equal to 1/2 and 3, we get that the minimize and maximum Néel temperature are $T_N^{\text{Min}} \approx 0.207J$ and $T_N^{\text{Max}} \approx 0.872J$ respectively. Our result of the Néel temperature region is approximately from 20.7K to 87.2K when $J = 100K$, which is in good agreement with the experimental estimation of $T_N$ region 20 − 70K \cite{12,13}.

The two branches of the magnetic excitation $E_k^+$ and $E_k^-$ represent the spin fluctuations along the a-axis and within $bc$ plane respectively. In the exactly one-dimensional case ($J_2 = J_3 = 0$), the excitation $E_k^-$ vanishes and the energy gap of $E_k^+$ is just the Haldane gap of AF Heisenberg chain, which is closely related to the breaking of a hidden $Z_2 \times Z_2$ symmetry \cite{11}. We obtain that the coexistence of Haldane gap and AF LRO below $T_N$ is a common feather of all members of compounds $L_2BaNiO_5$ except $Y_2BaNiO_5$. The neutron scattering experiments have discovered that, below the Néel temperature, the Haldane gap increases as the temperature decreases \cite{14,15,16}. The temperature dependences of the Haldane gap $\Delta$ for the cases of $s_2 = 1/2, 1, 3/2, 2, 5/2$ and 3 are also investigated by the SBMF theory and the behaviors are shown in figure 4(a) respectively. The temperature dependence of the energy gap $\Delta$ obtained by our calculation is found to agrees with the experimental discovery.

Our calculation also implies that the effect of the staggered magnetization on the magnetic excitation is to widen the Haldane gap. Below $T_N$, the effective internal magnetic field $H_{\text{eff}}$ imposed on the Haldane chain is assumed approximately as the magnetization $M_1$ of Ni ions. This field is found to increase with the decreasing of temperature and the increasing of spin value $s_2$ because of the thermal fluctuation being weakened and the AF
ordering being enhanced. In figure 4(b), we plot the energy gap $\Delta$ of zero temperature as a function of $H_{\text{eff}}$, and we find that $H_{\text{eff}}$ has strong effect to widen the Haldane gap.

In addition, based on the 3D mixed-spin model, we obtain that AF LRO below the Néel temperature is not constructed only by the rare-earth ions. Our results support the suggestion that Ni ions also play an important role in forming the AF LRO. We plot in figure 5 the Néel temperature as a function of AF coupling $J_2$ in the cases with $s_2 = 1/2$, $J_1 = J$, and $J_3 = 0.01J$. In compounds $L_2BaNiO_5$, the effective interactions between individual Ni chains rely on the AF coupling $J_2$ between $Ni^{2+}$ and rare-earth $L^{3+}$. We obtain that the Néel temperature rises rapidly with the increase of $J_2$ as shown in figure 5, so the coupling $J_2$ are important in forming the AF LRO. Besides, as $J_2 = 0$, there are no interactions between Ni chains and thus the Néel temperature drops to zero. The Haldane excitation energy $E_k^+$ in 3D and 1D cases are shown in figure 6(a) and 6(b) respectively. Here we choose $s_2 = 1/2$, $J_1 = J$, $J_2 = 0.01J$, $J_3 = 0.01J$, and $k_x = k_y = 0$ for the 3D case, and obtain that the corresponding Néel temperature is $T_N = 0.206J$. To compare the behaviors of magnetic excitations below and above the Néel temperature, we study two conditions of $T = 0.1$ (solid lines) and $T = 0.4J$ (dotted lines) respectively for both 1D and 3D cases. In the 3D case, we find, in figure 6(a), that the energy gap below the Néel temperature is obviously bigger than that above the Néel temperature, which is in opposition with the behavior for pure 1D case (shown in figure 6(b)). In addition, we obtain that the thermal fluctuation has strong effect to destroy the 3D spin correlations in the compounds, as a result the behaviors in 3D case is the same as that in 1D case when temperature is above the Néel temperature.

IV. SUMMARY

In conclusion, we have introduced a 3D mixed-spin AF Heisenberg model based on the experimental results of the crystal magnetic structure of compounds $L_2BaNiO_5$, and studied this model with the SBMF theory. The experimental discovery of coexistence of Haldane gap and AF LRO below $T_N$ has been deduced by our calculation. Properties such as the low-
lying excitations, magnetizations of Ni and rare-earth ions, Néel temperatures of different members of this family and behavior of Haldane gap below $T_N$ have also been investigated within this model.

We have obtained two branches of the magnetic excitations $E_k^+$ and $E_k^-$, of which $E_k^+$ has an energy gap and $E_k^-$ is gapless below $T_N$. The theoretical result of the Néel temperature region is approximately from 20.7$K$ to 87.2$K$, which is in good agreement with the experimental estimation of the region 20$-70K$. We have also obtained that Haldane gap increases with decreasing temperature, and the effect of the magnetization is to widen the Haldane gap. Our results are in good agreement with the experimental discoveries. Our findings also support the suggestion that the AF LRO below $T_N$ is not constructed only by the rare-earth ions, and Ni ions also play an important role in forming the AF LRO.

**ACKNOWLEDGMENTS**

We thank Dr. Xintian Wu for helpful discussions. This work was supported by the National Natural Science Foundation of China under Grant Nos. 10125415, 10074007, and 90103024.
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FIGURES

FIG. 1. (a) Structural relation between $Ni$ and rare-earth sites in the $bc$ plane, and (b) $Ni$ and apical oxygen form the Haldane chain along the $a$-axis.

FIG. 2. The temperature dependence of the ordered moment on the $Ni$ (a) and $Nd$ (b) sites in $Nd_2BaNiO_5$ sample taken from Ref. 14 (open circles), and the solid lines show fits to the experimental discovery by our numerical results of the case with $s = 3/2$ respectively; Magnetizations $M_1/s_1$ (c) and $M_2/s_2$ (d) as functions of temperature below $T_N$ for cases of $s_2 = 1/2, 1, 3/2, 2, 5/2$, and 3 respectively.

FIG. 3. Néel temperatures of the compounds $L_2BaNiO_5$ for the cases with different spin value $s_2$. The circles represent the theoretical results, and the triangles are experimental findings of compounds $Nd_2BaNiO_5$, $Pr_2BaNiO_5$ and $Ho_2BaNiO_5$ taken from Ref. 11-13.

FIG. 4. (a) The temperature dependence of Haldane gap for cases of $s_2 = 1/2, 1, 3/2, 2, 5/2$ and 3 below the Néel temperatures respectively; (b) The Haldane gap as a function of the effective internal magnetic field $H_{eff}$.

FIG. 5. Néel temperature as a function of AF coupling $J_2$ between $Ni^{2+}$ and $L^{3+}$ ions of case $s_2 = 1/2$, $J_1 = J$, and $J_3 = 0.01J$.

FIG. 6. The branch of Haldane excitation $E_k^+$ as a function of $k_z$ in (a) 3D with $s_2 = 1/2$, $J_1 = J$, $J_3 = 0.01J$ and (b) pure 1D cases. The solid lines show results of temperature $T = 0.1J$, and the dotted lines present results of $T = 0.4J$. 

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