

# Long-range order in gapped magnetic systems induced by Bose-Einstein condensation

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We study the Heisenberg antiferromagnet with single-ion anisotropy in two and three dimensions and present self-consistent intuitive theory to show the Bose-Einstein condensation-induced long-range order in the gapped magnetic systems, when the energy gap is tuned to zero by changing the physical parameters or by applying an external magnetic field. The recent experimental results on  $\text{NiCl}_2 \cdot 4\text{SC}(\text{NH}_2)_2$  are interpreted by the theory. Many other gapped magnetic systems share the same physical picture. The theory is also helpful in understanding the superfluid-Mott insulator transition observed in the system of ultracold atoms in the optical lattice.

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## I. INTRODUCTION

Quantum spin systems have received considerable attention from both theoretical and experimental points of view. Many magnetic systems show a singlet ground state and a triplet excitation gap. When the energy gap, changing with the physical parameters, goes to zero, a quantum phase transition (QPT) occurs. On the other hand, an external magnetic field can lower one of the Zeeman-split triplet components, and at a critical magnetic field, may result in long-range magnetic order. Several low-dimensional materials, for example,  $S=1$  antiferromagnetic chains,<sup>1</sup> antiferromagnetic spin dimers,<sup>2</sup> even-leg spin ladders,<sup>3</sup> and  $S=\frac{1}{2}$  alternating chains or frustrated spin systems,<sup>4</sup> were reported to exhibit field-induced magnetic ordering in the plane perpendicular to the applied field.

Although the QPT in low-dimensional systems has been studied extensively, experimental results in three-dimensional systems are rare and intuitive theory to describe such systems is still absent. Very recently,  $\text{NiCl}_2 \cdot 4\text{SC}(\text{NH}_2)_2$ , which was regarded as lying in the three-dimensional large- $D$  phase, were experimentally studied and the field-induced magnetic ordering was found.<sup>5</sup> In this paper, we give theoretical analysis of this system and obtain a region of field-induced Néel order in the plane perpendicular to the applied field, which coincides well with the experiments. At the same time, we present a universal description of QPT from the gapped singlet state to the gapless ordered state with the idea of Bose-Einstein condensation (BEC) of magnons,<sup>6</sup> which has been used to study the magnetic-field effects on various magnetic systems.<sup>7-11</sup>

Concerning the experimental results on  $\text{NiCl}_2 \cdot 4\text{SC}(\text{NH}_2)_2$ , we study the  $S=1$  Heisenberg antiferromagnetic model with a single-ion anisotropy in two and three dimensions:

$$H = \frac{1}{2} J \sum_{\vec{r}, \vec{\delta}} (S_{\vec{r}}^x S_{\vec{r}+\vec{\delta}}^x + S_{\vec{r}}^y S_{\vec{r}+\vec{\delta}}^y + R S_{\vec{r}}^z S_{\vec{r}+\vec{\delta}}^z) + D \sum_{\vec{r}} (S_{\vec{r}}^z)^2 - g \mu_B B \sum_{\vec{r}} S_{\vec{r}}^z, \quad (1)$$

where  $\sum_{\vec{r}, \vec{\delta}}$  sums over the nearest neighbors and an external

magnetic field is applied with  $\mu_B$  the Bohr magneton. In one dimension, the model (1) with  $R=1$  was extensively studied in connection with Haldane's fascinating conjecture.<sup>12</sup> During  $D_{c1}(\sim -0.29) < D < D_{c2}(\sim 0.93)$ , the system is in the Haldane phase. While when  $D > D_{c3}(\sim 1.01)$ , the system is in the large- $D$  phase<sup>13,14</sup> with a singlet ground state and an excitation gap; its difference from the Haldane phase can be found from the symmetry consideration.<sup>15</sup> The field-induced long-range order in the  $S=1$  antiferromagnetic chain was investigated with the exact diagonalization of finite chains.<sup>16</sup> The models in higher dimensions are less studied. When  $D=0$ , the system is in the Néel state<sup>17</sup> and when  $J=0$ , the system is in the large- $D$  phase. There is a critical  $D_c$  denoting the transition from the large- $D$  phase to the Néel phase. With a coupled-cluster expansion, Wong *et al.*<sup>18</sup> obtained critical points in various lattices. In the following, we use the bond operator formalism to study this model in two and three dimensions. In Sec. II we give the self-consistent equations on the  $S=1$  Heisenberg model with single-ion anisotropy and then in Secs. III and IV, we study the phase transitions induced by changing the physical parameters and by applying an external magnetic field, respectively. The experimental results on  $\text{NiCl}_2 \cdot 4\text{SC}(\text{NH}_2)_2$  are interpreted in Sec. IV. A summary is given in Sec. V.

## II. SELF-CONSISTENT EQUATIONS ON THE $S=1$ HEISENBERG MODEL WITH SINGLE-ION ANISOTROPY

For a single  $S=1$  spin, there are three eigenstates  $|\pm 1\rangle$  and  $|0\rangle$ . Along the same line as the  $S=\frac{1}{2}$  spins,<sup>19</sup> three boson operators were introduced to denote the three eigenstates:<sup>20</sup>

$$|1\rangle = u^\dagger |v\rangle, \quad |0\rangle = t_z^\dagger |v\rangle, \quad |-1\rangle = d^\dagger |v\rangle, \quad (2)$$

where  $|v\rangle$  is the vacuum state. With a constraint  $u^\dagger u + d^\dagger d + t_z^\dagger t_z = 1$ , the spin operators can be represented by

$$S^+ = \sqrt{2}(t_z^\dagger d + u^\dagger t_z), \quad S^- = \sqrt{2}(d^\dagger t_z + t_z^\dagger u),$$

$$S^z = u^\dagger u - d^\dagger d. \quad (3)$$

Substituting the above boson representation into the original Hamiltonian (1) and assuming the  $t_z$  bosons are condensed,  $\langle t_z \rangle = \langle t_z^\dagger \rangle = t$ , we get

$$H = \frac{1}{2} J \sum_{\vec{r}, \vec{\delta}} [t^2 (d_{\vec{r}}^\dagger d_{\vec{r}+\vec{\delta}} + u_{\vec{r}+\vec{\delta}}^\dagger u_{\vec{r}} + u_{\vec{r}} d_{\vec{r}+\vec{\delta}} + d_{\vec{r}}^\dagger u_{\vec{r}+\vec{\delta}}^\dagger + \text{H.c.}) + R(u_{\vec{r}}^\dagger u_{\vec{r}} - d_{\vec{r}}^\dagger d_{\vec{r}})(u_{\vec{r}+\vec{\delta}}^\dagger u_{\vec{r}+\vec{\delta}} - d_{\vec{r}+\vec{\delta}}^\dagger d_{\vec{r}+\vec{\delta}})] + D \sum_{\vec{r}} (u_{\vec{r}}^\dagger u_{\vec{r}} + d_{\vec{r}}^\dagger d_{\vec{r}}) - h \sum_{\vec{r}} (u_{\vec{r}}^\dagger u_{\vec{r}} - d_{\vec{r}}^\dagger d_{\vec{r}}) - \sum_{\vec{r}} \mu_{\vec{r}} (u_{\vec{r}}^\dagger u_{\vec{r}} + d_{\vec{r}}^\dagger d_{\vec{r}} + t^2 - 1), \quad (4)$$

where  $h = g\mu_B B$  and a temperature-dependent chemical potential  $\mu_{\vec{r}}$  is introduced to impose the constraint condition of single occupancy. By a mean-field approximation, we replace the local constraint by a global one and let  $\mu_{\vec{r}} = \mu$ . It is pointed out that  $\mu$  is still temperature dependent. We let  $J = 1$  in the following calculations. Making mean-field decoupling to the four operator terms

$$\begin{aligned} & (u_{\vec{r}}^\dagger u_{\vec{r}} - d_{\vec{r}}^\dagger d_{\vec{r}})(u_{\vec{r}+\vec{\delta}}^\dagger u_{\vec{r}+\vec{\delta}} - d_{\vec{r}+\vec{\delta}}^\dagger d_{\vec{r}+\vec{\delta}}) \\ &= \frac{1}{2} (1 - t^2 + m)(u_{\vec{r}}^\dagger u_{\vec{r}} + u_{\vec{r}+\vec{\delta}}^\dagger u_{\vec{r}+\vec{\delta}}) \\ &+ \frac{1}{2} (1 - t^2 - m)(d_{\vec{r}}^\dagger d_{\vec{r}} + d_{\vec{r}+\vec{\delta}}^\dagger d_{\vec{r}+\vec{\delta}}) \\ &- p(u_{\vec{r}} d_{\vec{r}+\vec{\delta}} + d_{\vec{r}} u_{\vec{r}+\vec{\delta}} + \text{H.c.}) - \frac{1}{2} (1 - t^2)^2 - \frac{1}{2} m^2 + 2p^2 \end{aligned} \quad (5)$$

with  $\langle d_{\vec{r}}^\dagger u_{\vec{r}+\vec{\delta}}^\dagger \rangle = \langle d_{\vec{r}} u_{\vec{r}+\vec{\delta}} \rangle = p$  and  $m = \langle u_{\vec{r}}^\dagger u_{\vec{r}} \rangle - \langle d_{\vec{r}}^\dagger d_{\vec{r}} \rangle$ , and after a Fourier-Bogoliubov transformation, we get the diagonalized Hamiltonian

$$H = \sum_k (\omega_k^{(1)} \alpha_k^\dagger \alpha_k + \omega_k^{(2)} \beta_k^\dagger \beta_k) + \sum_k (\omega_k - \Lambda_k) + C, \quad (6)$$

with

$$\begin{aligned} \omega_k^{(1)} &= \omega_k - h + \frac{1}{2} Z R m, \\ \omega_k^{(2)} &= \omega_k + h - \frac{1}{2} Z R m, \\ \omega_k &= \sqrt{\Lambda_k^2 - \Delta_k^2}, \\ \Lambda_k &= -\mu + D + \frac{1}{2} Z R (1 - t^2) + Z t^2 \gamma_k, \\ \Delta_k &= (t^2 - R p) Z \gamma_k, \\ \gamma_k &= \frac{1}{l} \sum_{\vec{\delta}} \cos(\vec{k} \cdot \vec{\delta}), \end{aligned}$$

$$C = \mu N (1 - t^2) - \frac{1}{4} N Z R (1 - t^2)^2 - \frac{1}{4} N Z R m^2 + N Z R p^2, \quad (7)$$

where  $l$  is the number of the dimension and for the square and simple cubic lattices,  $Z = 2l$ .  $\alpha_k = \chi_k u_k + \rho_k d_{-k}^\dagger$ ,  $\beta_k = \chi_k d_{-k} + \rho_k u_k^\dagger$  with  $\chi_k^2 = \frac{1}{2}(1 + \Lambda_k / \omega_k)$  and  $\rho_k^2 = \frac{1}{2}(-1 + \Lambda_k / \omega_k)$ . The energy gap occurs at  $\vec{k} = \vec{\pi}$ ,  $\Delta = \omega_{\vec{\pi}}$ . The ground state energy per site is  $e_0 = (1/N) \sum_k (\omega_k - \Lambda_k) + (1/N) C$ . The Gibbs free energy  $G = N e_0 - (1/\beta) \sum_k \ln[1 + n(\omega_k^{(1)})] - 1/\beta \sum_k \ln[1 + n(\omega_k^{(2)})]$  with  $n(\omega_k) = 1/(e^{\beta \omega_k} - 1)$  and  $\beta = 1/k_B T$ .  $p$ ,  $t^2$ ,  $\mu$ , and  $m$  can be obtained by the saddle-point equations

$$\begin{aligned} p &= -\frac{1}{2N} \sum_k \frac{\Delta_k}{\omega_k} \gamma_k [1 + n(\omega_k^{(1)}) + n(\omega_k^{(2)})], \\ 2 - t^2 &= \frac{1}{N} \sum_k \frac{\Lambda_k}{\omega_k} [1 + n(\omega_k^{(1)}) + n(\omega_k^{(2)})], \\ \mu &= \frac{Z}{N} \sum_k \frac{\Lambda_k - \Delta_k}{\omega_k} \gamma_k [1 + n(\omega_k^{(1)}) + n(\omega_k^{(2)})], \\ m &= \frac{1}{N} \sum_k [n(\omega_k^{(1)}) - n(\omega_k^{(2)})]. \end{aligned} \quad (8)$$

### III. QUANTUM PHASE TRANSITIONS IN THE ABSENCE OF MAGNETIC FIELD

We first study the case of  $h = 0$ . Without the external magnetic field, the magnetization  $m$  is zero. In two- and three-dimensional cases, the effect of  $p$  is small. At zero temperature and with  $p$  neglected, the self-consistent equations can be simplified as

$$2(2 - t^2) = I_1(y) + I_2(y),$$

$$\frac{1}{Z} y \mu = I_2(y) - I_1(y) \quad (9)$$

with

$$y = \frac{2Zt^2}{-\mu + D + \frac{1}{2} R Z (1 - t^2)},$$

$$I_1(y) = \frac{1}{\pi^l} \int \frac{d^l k}{\sqrt{1 + y \gamma_k}}, \quad I_2(y) = \frac{1}{\pi^l} \int \sqrt{1 + y \gamma_k} d^l k, \quad (10)$$

where the integral region is  $[0, \pi]$ .

An equation about  $y$  can then be obtained:  $D - (4/y + \frac{1}{2} R) Z + \frac{1}{4} R Z I_2(y) + (2/y + \frac{1}{4} R) Z I_1(y) = 0$ . When  $y \rightarrow 1$ , the energy gap goes to 0, indicating a transition from the large- $D$  phase to the Néel phase.  $I_1(y)$  and  $I_2(y)$  are finite at  $y = 1$  and a concise formula for the critical point can be obtained:

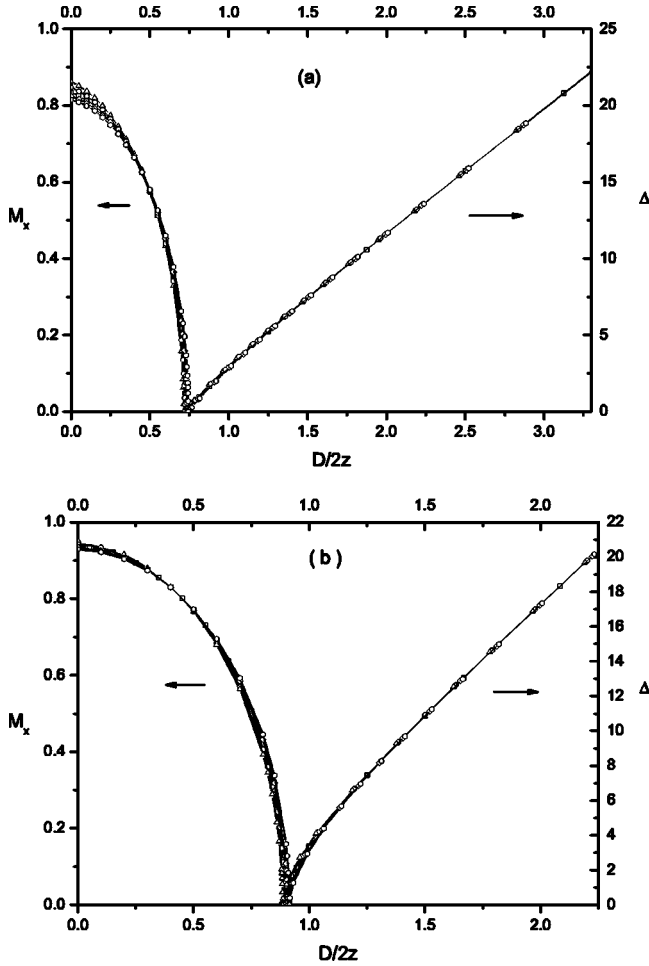


FIG. 1. Changes of the energy gap  $\Delta$  (right axis) and the staggered magnetization  $M_x$  (left axis) with  $D$  in two dimensions (a) and three dimensions (b) with  $R=0$  (triangles),  $0.5$  (circles),  $1$  (squares),  $1.5$  (diamonds),  $2$  (hexagons).

$$D_c = \left(4 + \frac{1}{2}R\right)Z - \frac{1}{4}RZI_2(1) - \left(2 + \frac{1}{4}R\right)ZI_1(1). \quad (11)$$

When  $R=1$ , we get  $D_c \approx 5.471$  and  $D_c/2Z \approx 0.684$  for the two-dimensional square lattice, and  $D_c \approx 10.481$  and  $D_c/2Z \approx 0.873$  for the three-dimensional simple cubic lattice. These values agree quite well with the results 0.798 and 0.884 obtained by Wong *et al.*<sup>18</sup> with the coupled-cluster expansions. With  $p$  included, the two values become 0.728 in two dimensions and 0.889 in three dimensions, respectively. In Figs. 1(a) and 1(b) (right axis), we present the changes of the energy gap with  $D$  for various  $R=0, 0.5, 1.0, 1.5, 2.0$  in two and three dimensions. In two dimensions, the energy gap decreases linearly with decreasing  $D$  until  $D_c$ ; while in three dimensions, the energy gap decreases linearly for large  $D$  and near  $D_c$ ,  $\Delta \propto (D - D_c)^\beta$  with  $\beta \sim 0.5$ . The anisotropy  $R$  does not have large effects.

When  $D < D_c$ , the system entered into the Néel state. We assume part of the excitations are condensed at  $k=\pi$ .<sup>21</sup> Keeping  $\omega_\pi=0$ , we solve the self-consistent equations (8) with a BEC amount  $n_0(T)$  extracted:

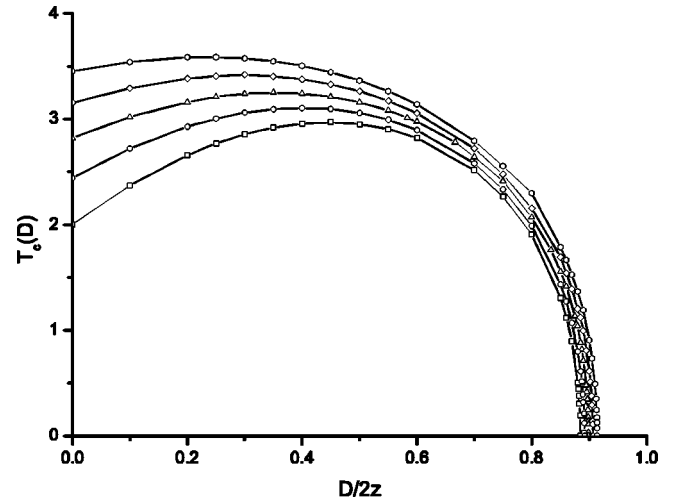


FIG. 2. Critical temperature  $T_c(D)$  for various  $D$  with  $R=0$  (squares),  $0.5$  (circles),  $1$  (triangles),  $1.5$  (diamonds),  $2$  (hexagons) in three dimensions.

$$2 - t^2 = n_0(T) + \frac{1}{N} \sum_k \frac{\Lambda_k}{\omega_k} [1 + n(\omega_k^{(1)}) + n(\omega_k^{(2)})],$$

$$p = \frac{1}{2} \frac{\Delta_\pi}{\Lambda_\pi} n_0(T) - \frac{1}{2N} \sum_k \frac{\Delta_k}{\omega_k} \gamma_k [1 + n(\omega_k^{(1)}) + n(\omega_k^{(2)})],$$

$$\mu = -\frac{Z}{N} \left(1 - \frac{\Delta_\pi}{\Lambda_\pi}\right) n_0(T) + \frac{Z}{N} \sum_k \frac{\Lambda_k - \Delta_k}{\omega_k} \gamma_k$$

$$\times [1 + n(\omega_k^{(1)}) + n(\omega_k^{(2)})]. \quad (12)$$

By calculating the correlation function  $\langle S_0^x S_r^x \rangle$ , we can get the staggered magnetization in the  $x$  direction  $m_x = 2t\sqrt{n_0(T)}$ . At  $T=0$  and neglecting  $p$ , we have  $n_0(0) = [4/(8+R)][(D_c - D)/2Z]$  and

$$m_x = 2\sqrt{2 - \frac{1}{2}[I_1(1) + I_2(1)] - [4/(8+R)][(D_c - D)/2Z]}$$

$$\times \sqrt{[4/(8+R)][(D_c - D)/2Z]}.$$

It is pointed out that BEC only occurs at  $T=0$  in two-dimensional case, which is consistent with Mermin-Wagner theorem.<sup>22</sup> In three dimensions, a critical  $T_c(D)$  exists, above which, BEC disappears and there is no Néel long-range order. In Figs. 1(a) and 1(b), we show the changes of the staggered magnetization with  $D$  in two and three dimensions for  $R=0, 0.5, 1.0, 1.5, 2.0$  (left axis). The results agree well with those obtained by Wong *et al.* with the coupled cluster expansions.<sup>18</sup> In Fig. 2, we show the changes of the critical temperature  $T_c(D)$  for various  $R$  in three dimensions.

#### IV. LONG-RANGE ORDER INDUCED BY THE EXTERNAL MAGNETIC FIELD

Now we study the effects of the external magnetic field. The excitations split in the external magnetic field and one component decreases with the increasing magnetic field. At a critical magnetic field  $h_{c1} = \Delta_0$ , the energy gap goes to zero.

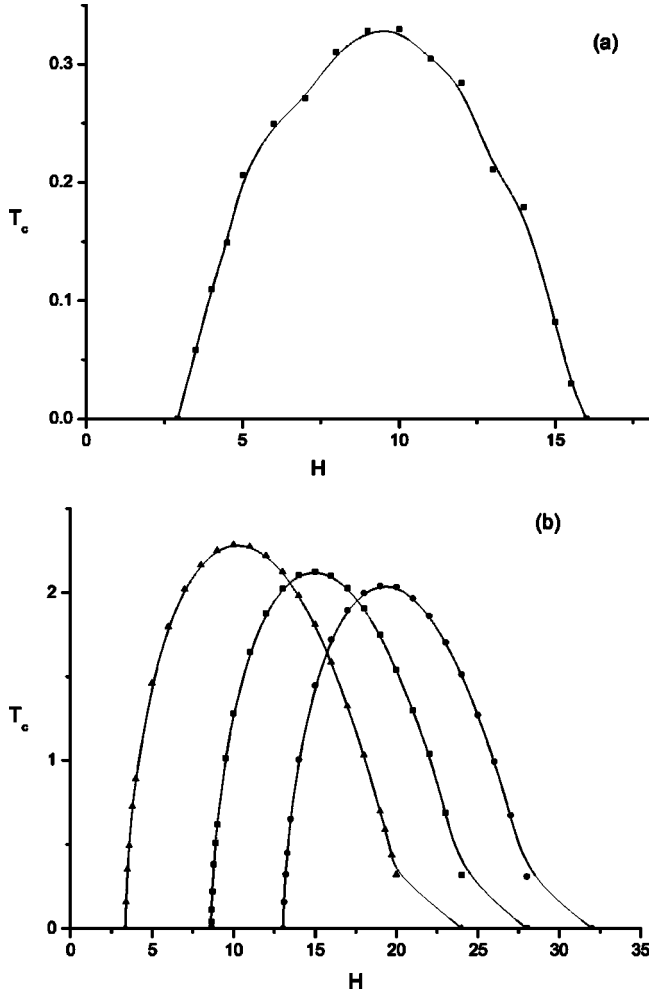


FIG. 3. Critical temperature  $T_c(h)$  with  $D=8$ ,  $R=1$  in two dimensions (a), and with  $D=12$  (triangles), 16 (squares), 20 (circles) and  $R=1$  in three dimensions (b).

When the magnetic field further increases, we assume the energy gap keeps zero and part of the excitations condense. Different from the  $h=0$  case, now only those bosons denoted by  $\alpha$  are condensed. Consequently, a magnetization parallel to the external magnetic field appears and at the same time, a staggered magnetization in the  $x$  direction occurs. At a second critical magnetic field  $h_{c2}$ , the magnetization saturates and the staggered magnetization disappears. For a given magnetic field  $h > h_{c1}$ , there exists a critical temperature  $T_c(h)$ , below which, the energy gap keeps zero, and part of the excitations are condensed. With a BEC amount  $n_h(T)$  extracted, we solve the self-consistent Eqs. (8) with  $\omega_\pi - h + \frac{1}{2}RZm = 0$ . The staggered magnetization in the  $x$  direction is  $m_x = \sqrt{2t} \sqrt{n_h(T)} \sqrt{1 - \Delta_\pi / \Lambda_\pi}$ . At  $T=0$  and neglecting  $p$ , we have  $n_h(0) = [-D/Z + 4/y + 1/2R - (2/y + \frac{1}{4}R)I_1(y) - \frac{1}{4}RI_2(y)] / [2/(2-y) + 2/y + \frac{1}{2}R]$ .

Figure 3(a) exhibits the critical  $T_c(h)$  as a function of  $h$  with  $D=8$ ,  $R=1$  in the two-dimensional case. Fitting the data with  $h_{c1}(T) - h_{c1}(0) \propto T^\alpha$ , we find  $\alpha \sim 1$ . In three dimensions, we connect our calculations to the experimental data of  $\text{NiCl}_2 \cdot 4\text{SC}(\text{NH}_2)_2$ .<sup>5</sup> It is reported that  $2zJ/k_B = 5.1$  K and  $D/k_B = 8.3$  K by fitting the data with the molecular theory<sup>23</sup>

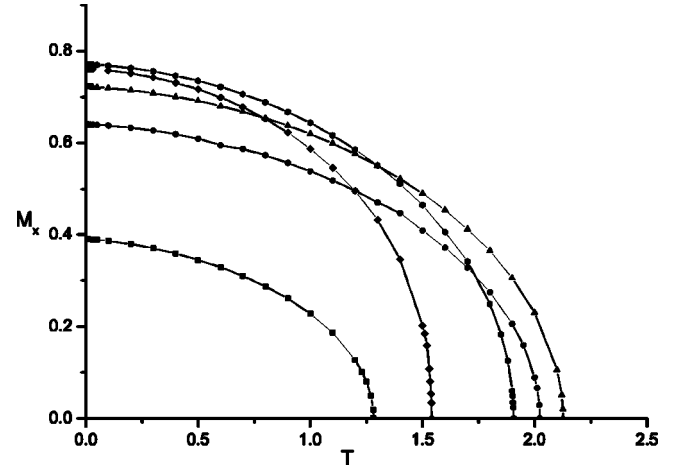


FIG. 4. Changes of the field-induced staggered magnetization  $M_x$  with temperature in three dimensions, with  $D=16$  and  $R=1$ . The corresponding applied field is  $h=10$  (squares), 13 (circles), 15 (triangles), 18 (hexagons), and 20 (diamonds).

and  $2zJ/k_B = 4.5$  K and  $D/k_B = 7.6$  K from the zero-field susceptibility, which generates  $D/J \sim 20$ . At  $D/J=20$ , we get a gap of 13.14, much larger than the reported critical magnetic field  $h_{c1}$  or the excitation gap  $\Delta_0(\sim 8J)$ . Instead,  $D/J=16$  produces a gap of  $8.62J$ , close to the experimental value. In Fig. 3(b), we show the variations of  $T_c(h)$  with  $h$  at  $D=12$ , 16, and 20 and  $R=1$ . The results agree qualitatively with the experimental results. Near  $h_{c1}$ , fitting the data with  $h_{c1}(T) - h_{c1}(0) \propto T^\alpha$ , we get  $\alpha \sim 1.5$ , consistent with that of the Bose-Einstein Hartree-Fock theory<sup>9</sup> and that of the cubic coupled dimer models obtained from the quantum Monte Carlo simulations.<sup>11</sup> The experimentally reported value is 2.6, larger than our value. Discrete values were reported in other materials, i.e.,  $\alpha \approx 2.2$  in  $\text{TiCuCl}_3$  and  $\alpha \approx 2.3$  in  $\text{KCuCl}_3$ ,<sup>2</sup>  $\alpha \approx 1.5$  in  $\text{Cu}_2(\text{C}_5\text{H}_{12}\text{N}_2)_2\text{Cl}_4$ ,<sup>3</sup> and  $\alpha \approx 1.95$  when  $H \parallel c$  axis and 3.07 when  $H \perp c$  axis in  $\text{Ni}(\text{C}_5\text{H}_{14}\text{N}_2)_2\text{N}_3(\text{ClO}_4)$  NDMAZ,<sup>1</sup> which deserves more detailed studies. In Fig. 4, we show the change of the field-induced staggered magnetization  $M_x$  with the external magnetic field. We determine the critical magnetic field  $h_{c2}$  at zero temperature. It is found that  $h_{c2} = -\mu + D + RZ$  with  $p=0$ ,  $t=0$ ,  $\mu=-Z$ ,  $\rho=1$ , and  $m=1$ . The staggered magnetization is zero since  $t=0$ . Near  $h_{c2}$ , the critical temperature  $T_c(h)$  is difficult to obtain. The reason may be that  $t$  is too small and the assumption of  $t_z$  condensation is not a good starting point. However, more profound physics may exist here. When  $t$  is small and comparable with the small amount  $p$ , the minimum energy gap may deviate from  $\tilde{\pi}$ , the condensed bosons may have some other momentum, and then incommensurate phase will appear. A spin-polarized Luttinger liquid is observed near  $h_{c2}$  at low temperatures.<sup>11</sup>

The uniform magnetization  $m$  shows a minimum around the transition temperature  $T_c(h)$ , which has been observed in  $\text{NiCl}_2 \cdot 4\text{SC}(\text{NH}_2)_2$  and other gapped magnetic systems such as  $\text{TiCuCl}_3$ ,  $\text{KCuCl}_3$ , and  $\text{Cu}_2(\text{C}_5\text{H}_{12}\text{N}_2)_2\text{Cl}_4$ . The change from the bottom to the given highest amount is about 5%. From Eqs. (8), we get  $m = (\omega_\pi / \Lambda_\pi) n_h(T) + (1/N) \sum_k [n(\omega_k^{(1)}) - n(\omega_k^{(2)})]$ . The first part comes from the BEC of magnons,



which decreases with increasing temperature and goes to zero at  $T_c(h)$ ; the second one is from the thermal fluctuations and always increases with increasing temperature. It is expected that a minimum appears around  $T_c(h)$ . However, in our calculations, such a minimum is observed very close to zero temperature, and the dip is much narrower and shallower (the change is about 1/1000) than the experimentally reported values. It seems that the change of the BEC amount is underestimated since we neglect the fluctuation of  $t_z$ . The deviations may also partly come from the relaxed constraint. We extract  $D$  and  $J$  from our calculations in the following. The experimentally observed  $B_{c1}=2.11$  T,  $B_{c2}=12.11$  T, and  $B_{c2}/B_{c1}\approx 5.74$ . Taking the critical magnetic field  $B_{c1}$  as the energy gap  $\Delta(D)$  and the saturated magnetic field  $B_{c2}$  as  $D+2Z$ , we have  $(D+2Z)/\Delta(D)=5.74$ . Fitting this equation with numerically calculated energy gap [Fig. 1(b)], we get  $D/J=12.7$  and then  $J=0.74$  K and  $D=9.45$  K, they are not far from the experimentally reported values.

### V. SUMMARY

In summary, we studied the Heisenberg antiferromagnetic model with a single-ion anisotropy in two and three dimen-

sions and present a self-consistent, intuitive theory to show the Bose-Einstein condensation-induced long-range order in the gapped magnetic systems, when the energy gap is tuned to zero by changing the physical parameters or by applying an external field. The very recent experimental results on  $\text{NiCl}_2\cdot 4\text{SC}(\text{NH}_2)_2$  are interpreted. Many other gapped spin systems share the same physical picture, including the quasi-one-dimensional  $S=1$  chains, quantum spin dimer models, the even-leg spin ladders and alternating spin chains or frustrated magnetic systems. The present theory may also shed light on the superfluid-Mott insulator transition in the optical lattice of ultracold atoms,<sup>24</sup> a class of tunable strongly correlated many body systems.<sup>25</sup>

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