Quantum phase transitions in a spin-1/2 alternating Heisenberg antiferromagnetic chain under a staggered transverse magnetic field

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The magnetic behaviors of a spin-1/2 alternating Heisenberg antiferromagnetic chain in a staggered transverse magnetic field is studied by means of the density-matrix renormalization group method and Jordan-Wigner transformation. Quantum phase transitions of different types are observed in the $S=1$ Néel and XY-like gapless phases, which result from the competitions between the staggered transverse field and magnetic orders induced by anisotropy and alternating interactions. The results are compared with the mean-field and some exactly resolved results.

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One-dimensional quantum magnets have been at the center of theoretical and experimental attention due to the exotic magnetic properties in condensed matter physics. In particular, the magnetic behaviors of low dimensional quantum magnets in an external magnetic field exhibit many novel characteristics [1]. The gapped Haldane chain [2] compound Ni(C$_2$H$_4$N$_2$)$_2$NO$_2$(ClO$_4$) in a uniform magnetic field has been widely studied both experimentally [3,4] and theoretically [5], which shows a commensurate-incommensurate transition as the gap is closed by the field [6]. A closed Haldane chain compound R$_2$BaNiO$_5$ (R=magnetic rare earth) [7,8] with an effective staggered magnetic field has been explored theoretically [9,10] and numerically [11], revealing that the effective staggered magnetic field has been explored theoretically [9,10] and numerically [11], revealing that the magnetic behavior in a staggered field is totally different from that in a uniform field. Recently, the magnetic properties of a $S=1/2$ antiferromagnetic (AF)-ferromagnetic (FM) spin chain are extensively studied [12,13,14]. This spin chain with nearly the same AF and FM interaction strength has been realized in experiment by the compound (CH$_3$)$_2$NH$_2$CuCl$_3$ [15]. Hida [16] pointed out that this chain can map onto the $S=1$ Haldane chain when the FM couplings dominate. Yamanaka et al. [17] suggested a phase diagram for the system with an AF anisotropy. The system has the Haldane, $S=1$ Néel, and XY-like gapless phases for different anisotropies and alternations. In the $S=1$ Néel and XY-like phases, the gap vanishes and some magnetic orders emerge. In this paper, we shall concentrate primarily on the magnetic properties of the system under a staggered transverse field in various phases. It is expected that the competitions between different factors would yield rich results.

Let us consider a spin-1/2 alternating Heisenberg chain with anisotropy in a transverse staggered magnetic field, as depicted in the inset of Fig. 1. The Hamiltonian reads

$$H = \sum_{j=1}^{N} (S_{j}^{x}S_{j+1}^{x} + S_{j}^{y}S_{j+1}^{y} + \lambda S_{j}^{z}S_{j+1}^{z}) + \beta \sum_{j=1}^{N} \vec{S}_{j} \cdot \vec{S}_{j+1} - h_x \sum_{j=1}^{2N} (-1)^{j} S_{j}^{z},$$

where $\lambda$ stands for the AF anisotropy, $\beta < 0$ ($> 0$) is the FM (AF) coupling, $N$ is the number of unit cells, and the last term of Eq. (1) introduces the staggered transverse magnetic field. We take the AF coupling as the energy scale and $\mu_B=1$. The transverse staggered magnetization and susceptibility are defined, respectively, as

$$m_{stag} = \frac{1}{2N} \sum_{j=1}^{2N} (-1)^{j} \langle S_{j}^{z} \rangle, \quad \chi_{stag} = \frac{\partial m_{stag}}{\partial h_s}.$$

The density-matrix renormalization group (DMRG) method [18,19] is invoked to study this system. In our calculations, the length of the chain is taken as 60, and the number of the optimal states is kept as 60. We adopt open boundary conditions. The truncation error is less than $10^{-3}$ in all calculations. The system has an $U(1)$ symmetry in absence of magnetic field, however, the staggered transverse field breaks this symmetry. Thus, there is no good quantum number that can be used to reduce the Hilbert space dimensions in our calculations.

In order to investigate the effects of the anisotropy and FM interaction on $m_{stag}$, we first calculate exactly $m_{stag}$
of two $S=1/2$ spins coupled by XXZ AF and isotropic FM interactions, respectively. For the spins coupled by XXZ AF coupling, $m_{stag}$ behaves as

$$ m_{stag}^{AF} = \frac{2h_s}{\sqrt{16h_s^2 + (1 + \lambda)^2}}. $$

(4)

It can be seen that with increasing $\lambda$, $m_{stag}$ is suppressed by the anisotropy that destroys the transverse magnetic ordering. For the spins coupled by the FM interaction, $m_{stag}$ behaves as

$$ m_{stag}^{FM} = \frac{h_s}{\sqrt{4h_s^2 + \beta^2}}. $$

(5)

Clearly, the FM interaction makes the spins align in the same direction, which competes with the staggered magnetic field. Thus, $m_{stag}$ is suppressed with increasing $\beta$. It seems that the anisotropy and FM interaction have similar effects on $m_{stag}$. However, when the FM coupling and the staggered magnetic field are considered simultaneously, $m_{stag}$ shows more complex behaviors. In the following, the transverse staggered magnetic properties will be studied by means of the DMRG method for the parameters indicated by the arrows of Fig. 1.

Figure 2 shows the evolution of the magnetic properties from the Haldane phase to the $S=1$ Néel phase with changing $\beta$ from $\beta=1$ to $\beta=-4$ for $\lambda=4.0$. In Fig. 2(a), $m_{stag}$ increases with $h_s$ and approaches 0.5 when $h_s\rightarrow\infty$. With increasing FM interactions, $m_{stag}$ declines for any field, which agrees with the depressing effect of the FM coupling. In the Haldane phase, $\chi_{stag}$ continuously declines with $h_s$ in a simple way

$$ \chi_{stag} \sim \frac{1}{(h_s^2 + A)^{1/2}}, $$

(6)

where $A$ is a constant determined by the couplings. At $h_s=0$, the zero-field susceptibility $\chi_{stag}(0)$ is finite, which is analogous to the $S=1$ Haldane chain due to the existence of a gap. For the $S=1$ Haldane chain, $\chi_{stag}(0)=Zv/\Delta^2$ (where $\Delta$ is the spin gap) [6]. In the present case, the spin gap $\Delta$ and $\chi_{stag}(0)$ decrease simultaneously with increasing FM coupling. Therefore, it is expected that the product of the renormalization parameter $Z$ and the spin-wave velocity $v$ decrease more rapidly than the gap. With further increasing the FM coupling, $\chi_{stag}$ becomes flat at low fields when approaching the phase boundary. In the $S=1$ Néel phase, a broad peak emerges in $\chi_{stag}$ [Fig. 2(b)], indicating the distinct magnetic properties below the transition field from those in the Haldane phase. The peaks, which move to higher fields with increasing $-\beta$, are attributed to the competition between the field and magnetic interactions. In the absence of magnetic field, the longitudinal spin-spin correlation function $\langle S^z_i S^z_j \rangle$ has a long-range order (LRO) and behaves as $\langle S^z_i S^z_{j-1} \rangle\sim0(2)^{\Delta z}$ due to the FM coupling [Fig. 2(c)]. The Néel order in the $z$ axis prevents the magnetization in the $x$ direction and is destructed by the transverse staggered field. As shown in Fig. 2(c), with increasing $h_s$, $\langle S^z_i S^z_j \rangle$ decays with a power law, and when $h_s$ exceeds a critical magnetic field, $h_{sc}$, it decays exponentially. Below $h_{sc}$, the suppressed Néel order facilitates the magnetization in the transverse axis, yielding the increase of $\chi_{stag}$. Above $h_{sc}$, the Néel order is fully broken and thus $\chi_{stag}$ declines similar to that in the Haldane phase. In the Haldane phase, the gap enlarges with increasing $h_s$. In the Néel phase, a gap is opened when $h_s$ exceeds $h_{sc}$ and increases with the field, as shown in Fig. 2(d). In the transition field $h_{sc}$, a quantum phase transition (QPT) [22] which is from the $S=1$ Néel phase to a gapped staggered magnetic ordered phase happens. In the vicinity of $h_{sc}$, the ground-state energy $e$ and its derivatives with respect to the field are studied to characterize this transition. It is found that both $\partial e/\partial h_s$ and $\partial^2 e/\partial h_s^2$ are continuous and nonsingular in the field $h_s$, but $\partial^2 e/\partial h_s^2$ has a minimum at $h_{sc}$, as shown in the inset of Fig. 2(d). Below $h_{sc}$, the phase is gapless with a power law decaying $\langle S^z_i S^z_j \rangle$. Above $h_{sc}$, a gap emerges and $\langle S^z_i S^z_j \rangle$ decays exponentially. This is analogous to the transition from the XY-like phase to the Haldane phase in the absence of the field [21], which is of the Kosterlitz-Thouless (KT) [22] type. By considering the nonsingularity of the derivatives of $e$, we argue that this QPT may be also of the KT type. The critical behavior of $\Delta$ near $h_{sc}$ is fitted by the KT type with the lines in Fig. 2(d)

$$ \Delta = De^{-c/\sqrt{h_s-h_{sc}}}. $$

(7)

For $\beta=-3(-4)$, $D=2.7(3.4)$, $C=2.0(2.0)$, $h_{sc}=0.7(1.27)$. The behavior of $\Delta$ near $h_{sc}$ can be fitted well by Eq. (7).

Figure 3 shows the changes of magnetic properties from the Haldane phase to the XY-like gapless phase with changing $\beta$ from $\beta=1$ to $\beta=-5$ for $\lambda=-0.5$. In the XY-like gapless phase, $m_{stag}$ has an inflexion with increasing $h_s$, which is explicitly characterized by the sharp peak of $\chi_{stag}$ and indicates a transition of magnetic properties. Like the Néel phase, the peak moves to higher fields with increasing $-\beta$ [Fig. 3(b)]. This transition is due to the competition between the magnetic field and transverse magnetic order. In the absence of magnetic field, $\langle S^z_i S^z_j \rangle$ has a quasi-LRO, and due to the FM interaction, $\langle S^z_i S^z_{j-1} \rangle$ has a translation symmetry with a period of 4 [Fig. 3(c)]. As the staggered field competes with the FM interaction, this transverse quasi-LRO prevents the staggered magnetization, and meanwhile, is destructed by increasing the field. With increasing $h_s$, $\langle S^z_i S^z_j \rangle$ becomes disordered in short range but builds an order with a 2-period translation symmetry in long range, as shown in Fig. 3(c) for $h_s=0.5$. When $h_s$ exceeds the transition field, the short-range disorder is replaced by the staggered magnetic ordering, as in the case of $h_s=1.4$ in Fig. 3(c). These variations are also visible in
spin static structure factor $S(q)$, which are not presented here for concise. In the absence of magnetic field, $S(q)$ has two peaks at $q=\pi/2$ and $3\pi/2$. With increasing $h_z$, the old peaks decline rapidly and a new peak emerges at $q=\pi$, indicating the changing periodicity of $\langle S_0^x S_q^x \rangle$. Below $h_{stag}$, the destructive quasi-LRO facilitates the staggered magnetization and thus $\chi_{stag}$ increases. Above $h_{stag}$, the quasi-LRO is fully broken and $\chi_{stag}$ declines as in the Haldane phase. Similar to the $S=1$ Néel phase, this transition is also accompanied by the opening of a gap, which, however, behaves in a different manner above $h_{stag}$.

$$\Delta \sim (h_z - h_{stag})^\alpha.$$  

The critical behaviors of $\Delta$ are fitted by Eq. (8) in Fig. 2(d) with $\alpha=1.15$ and 1.1 for $\beta=-3$ and $-5$, respectively. These observations indicate that a QPT happens in $h_{stag}$.

To characterize this QPT, the ground-state energy and its derivatives with the field are studied. It is found that both $e$ and $\partial e/\partial h_z$ are nonsingular, but $\partial^2 e/\partial h_z^2$ is singular at $h_{stag}$, indicating that this transition is of the second-order, as shown in the inset of Fig. 2(d).

As discussed above, the staggered transverse magnetic properties have different behaviors in three phases. Although the QPT is observed in the $S=1$ Néel and XY-like phases, the physical quantities have different behaviors in these phases. The QPT in the Néel phase is argued to be of the KT type, while that in the XY-like phase is confirmed to be of the second-order. For further discussions, the staggered magnetization is studied in terms of the Jordan-Wigner (JW) transformation. As the field is applied transversely, the transformation is introduced as

$$S_i^z = \frac{1}{2} \langle c_i^\dagger e^{-i\pi \sum_{j\neq i} c_j^\dagger c_j} + h.c. \rangle,$$

$$S_i^y = \frac{1}{2} \langle e^{-i\pi \sum_{j\neq i} c_j^\dagger c_j} + h.c. \rangle,$$

$$S_i^x = c_i^\dagger c_i - \frac{1}{2}.$$  

(9)

where $c_i^\dagger$ and $c_i$ are the creation and annihilation operators of spinless fermions, which satisfy the anticommutation relation $\{c_i, c_j^\dagger\} = \delta_{ij}$. We denote the fermions in odd and even sites as $a_i$ and $b_i$, respectively. The density-density interaction terms are treated with the Hartree-Fock (HF) approximation,

$$n_{a,j}n_{b,j} \approx n_{a,j} \langle n_{b,j} \rangle + \langle n_{a,j} \rangle n_{b,j} - \langle a_j^\dagger b_j \rangle \langle b_j a_j \rangle + h.c.,$$

$$+ \langle a_j^\dagger b_j a_j \rangle + h.c. - \langle n_{a,j} \rangle \langle n_{b,j} \rangle - \langle b_j a_j \rangle \langle b_j a_j \rangle.$$  

(10)

We denote $\langle a_j^\dagger a_i \rangle = n_{a,i}$, $\langle b_j^\dagger b_i \rangle = n_{b,i}$, $\langle b_j a_i \rangle = p_{1}$, $\langle b_j^\dagger a_i \rangle = p_{2}$, $\langle a_{i+1} b_i \rangle = p_{3}$, and $\langle a_{i+1} a_i \rangle = p_{4}$. After making Fourier transform, the Hamiltonian is transformed into

$$H_{HF} = \sum_k (\omega_k a_k^\dagger a_k + \omega_k^* b_k^\dagger b_k) + \sum_k (\omega_k a_k^\dagger b_k + \omega_k^* b_k^\dagger a_k^\dagger) + h.c. + const.,$$  

(11)

where $\omega_k = (n_{b} - 1/2)(\beta + 1) - h_z$, $\omega_k^* = (n_{a} - 1/2)(\beta + 1) + h_z$, $\omega_k = [(\lambda + 1)/4 - p_1] e^{ik/2} + (1/2 - p_3) \beta e^{-ik/2}$, and $\omega_k^* = [(\lambda - 1)/4 + p_1] e^{ik/2} + p_3 \beta e^{-ik/2}$. Then, we introduce the Bogoliubov transformation

$$a_k = u_{11} a_k + u_{12} b_k + u_{13} \gamma_k + u_{14} \lambda_k,$$

$$b_k = u_{21} a_k^\dagger + u_{22} b_k^\dagger + u_{23} \gamma_k^\dagger + u_{24} \lambda_k,$$
The singular couplings also shows QPT and may be compared with that has a competition between the field and magnetic in the Néel phase. However, some exactly soluble case which are not presented here. The gap above $h_s$ reproduces the QPT in other phases. Figure 4(a) shows describe the behavior in the Haldane phase, but fails to following, we find that this mean-field theory is able to numerical calculations. The staggered magnetic properties of the spin-1/2 AF-FM Heisenberg chain with AF anisotropy in a transverse staggered magnetic field by means of the DMRG method. The physical quantities are explored in the Haldane, $S=1$ Néel, and XY-like gapless phases. In the Haldane phase, $m_{stag}$ and $\chi_{stag}$ behave as those of the $S=1$ Haldane chain, and do not have transition behaviors. In the Néel phase and the XY-like gapless phase, due to the competitions between the field and different magnetic couplings, most quantities have a transition at a field $h_{s_c}$, indicating a QPT induced by the field happens in the system. $m_{stag}$ has an inflexion in $h_{s_c}$, which corresponds to a maximum in $\chi_{stag}$. The transition is also accompanied by the open of a gap. In the Néel phase, $\partial^2 e / \partial h_{s_c}^2$ is nonsingular, but it still describes the transition with a minimum at the critical field. The QPT is argued to be of the KT type. The critical behavior of $\Delta$ is well fitted by that in the KT transition near $h_{s_c}$. In the XY-like gapless phase, $\partial^2 e / \partial h_{s_c}^2$ is singular in $h_{s_c}$, indicating that the transition is of the second order. The gap near $h_{s_c}$ behaves as $\Delta \sim (h_{s_c} - h_{s_c})^{a}$. Due to the distinct magnetic orders, the transitions behave differently in the two phases. Using the Jordan-Wigner transformation, the magnetic properties are also investigated analytically. In the present HF approximation, the features in the Haldane phase are reproduced, but it fails to describe the transitions in other two phases. The Ising case of the Hamiltonian (1) is exactly resolved, which has a second-order QPT that behaves like the one in the XY-like phase. The differences between the Ising case and the Néel phase show the important role of the quantum fluctuations.

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