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Spin-1 XXZ chains in a staggered magnetic field

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Phase transitions of the spin-1 XXZ chain with a single-ion anisotropy in a staggered magnetic field are studied. We obtain interesting phase diagrams consisting of ferromagnetic, partially ferromagnetic, XY, antiferromagnetic (AF) and large-D phases. By using the twist-boundary-condition method, a Gaussian critical line is found between the AF phase and the large-D phase. A multicritical point lies among the XY, AF and large-D phases. An Ashkin-Teller type of bifurcation does not appear. [S0163-1829(98)51414-2]

Haldane's conjecture[1] has renewed the interest in the one-dimensional (1D) quantum spin systems. It is now accepted that the antiferromagnetic Heisenberg chain (AFHC) with spin $S=1$ has an energy gap in the lowest excitation, in contrast to the $S=1/2$ case, by many theoretical,[2] numerical,[3,4] and experimental[5] studies.

Affleck *et al.*[6] discovered the valence-bond-solid (VBS) state which satisfies the ground-state properties of the $S=1$ AFHC. Kennedy and Tasaki[7] transformed the $S=1$ XXZ chain into the explicit form with a hidden $Z_2\times Z_2$ symmetry, and found that the Haldane gap is generated as a consequence of the complete breaking of the $Z_2\times Z_2$ symmetry. Oshikawa[8] showed the existence of the hidden $Z_2\times Z_2$ symmetry for arbitrary integer S.

In the quasi-1D systems, interchain interactions effectively make a bond-alternating coupling,[9] or give rise to a staggered magnetic field,[10] from a viewpoint of the mean field. There have been many works on the bond-alternating chains, since Affleck and Haldane[11] predicted that the ground state of the spin-S AFHC undergoes continuous dimerization transitions $2S$ times as the bond alternation varies. Oshikawa[8] suggested that the successive transitions are caused by repetition of breaking and recovering the $Z_2\times Z_2$ symmetry. For $S=1$, the transition point was estimated in Refs. 12–14, and the universality is the same class as the level-1 $SU(2)$ Wess-Zumino-Witten model.[14,15] Recently, the correct phase diagram of the XXZ type was obtained by Kitazawa *et al.*[16] They emphasized the Gaussian critical line between the Haldane phase and the dimer phase. The study of the bond-alternating systems has been advancing for $S=3/2,2,\ldots$.[17–19]

On the other hand, the effect of the staggered magnetic field has not been discussed, except by Alcaraz and Malvezzi,[20] who examined the ground-state phase transitions of the $S=1/2$ XXZ chain by numerical calculation.

In the present paper, we study the whole phase diagram of the $S=1$ XXZ chain with a single-ion anisotropy in a staggered magnetic field, whose Hamiltonian is described by

$$H=\sum_{i=1}^{L}\left(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z\right)-\lambda\sum_{i=1}^{L}(-1)^iS_i^z+D\sum_{i=1}^{L}(S_i^z)^2. \tag{1}$$

For $D=\lambda=0$, there are ferromagnetic ($\Delta<-1$), XY ($-1<\Delta<0$), Haldane ($0<\Delta<\Delta_{c2}\approx 1.17$), and Néel ($\Delta_{c2}<\Delta$) phases. The XY-Haldane transition is of the Berezinskii-Kosterlitz-Thouless (BKT) type,[16,21,22] and the Haldane-Néel transition belongs to the 2D Ising universality class.[23–25] As $\lambda=0$ and $D>D_c\approx 0.4$,[26,27] besides four phases in $D=0$, there appears the massive large-D phase, in which the unique ground state holds the $Z_2\times Z_2$ symmetry differently from the Haldane phase.[7] And these two phases are separated by the Gaussian line. When λ is added, the Haldane phase is continuously connected to the antiferromagnetic (AF) phase.[28] Note that the AF long-range order in the AF phase ($\lambda\neq 0$) is not spontaneously symmetry breaking, and that the ground state is singlet, while it is doublet in the Néel phase ($\lambda=0$). From the above fact, it is expected that a Gaussian transition occurs between the large-D phase and the AF phase.

We perform numerical calculations for $D=1$ and $D=3$, and obtain interesting phase diagrams (Fig. 1). The BKT transition lines ($XY\leftrightarrow$large D, $XY\leftrightarrow$AF) are determined, using the level spectroscopy[29] utilized for $D=0$ in our previous paper.[28] The Gaussian critical line (large $D\leftrightarrow$AF) is found by means of the twist-boundary-condition (TBC) method.[30] The BKT multicritical structure appears, in which one Gaussian line branches into two BKT lines, and it may reflect a hidden $Z_2\times Z_2$ symmetry. However, in the staggered magnetic field, Kennedy-Tasaki transformation is not applicable and it seems difficult to characterize the AF phase and the large-D phase, based on the Kennedy-Tasaki type $Z_2\times Z_2$ symmetry. Fortunately, for the $S=1$ bond-alternating chain, Kitazawa and Nomura[14] found that, from the VBS picture, it is possible to distinguish the Haldane phase from the dimer phase by such good quantum numbers

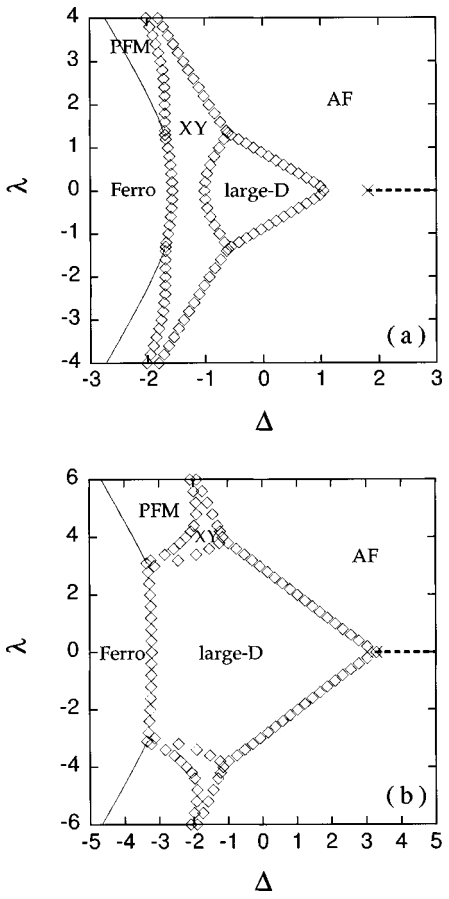

FIG. 1. Phase diagram for (a) $D=1$ and for (b) $D=3$. The BKT transitions occur on the XY–large-D boundary, and on the XY-AF boundary. The transition between the large-D phase and the AF phase is of the $c=1$ Gaussian type. The dashed line on $\lambda=0$ stands for the first-order transition.

as parity and time reversal instead of by the hidden $Z_2\times Z_2$ symmetry, using the TBC. As we see later, the ground state in the AF (Haldane) phase is characterized by $P_\pi=T_\pi=-1$ under the TBC, and in the large-D phase it is characterized by $P_\pi=T_\pi=+1$ under the TBC (Table I). Thus we can determine the Gaussian transition from the crossing point of two low levels with different parity (time reversal), as is shown in Fig. 2.

From the field theoretical viewpoint, by the bosonization,[2] the 1D quantum spin systems are effectively described by the 2D sine-Gordon model. The Lagrangian in Euclidean space is given by

$$\mathcal{L}=\frac{v}{2\pi K}[\nabla\phi(\tau,x)]^2+\frac{y_\phi}{2\pi\alpha^2}\cos\sqrt{2}\phi(\tau,x). \qquad (2)$$

Here v is the spin-wave velocity, and α is a short distance cutoff. The dual field $\theta(\tau,x)$ defined as

TABLE I. Symmetry of the ground state on the TBC.

	Haldane	AF	large D
P_π	-1	-1	$+1$
T_π	-1	-1	$+1$

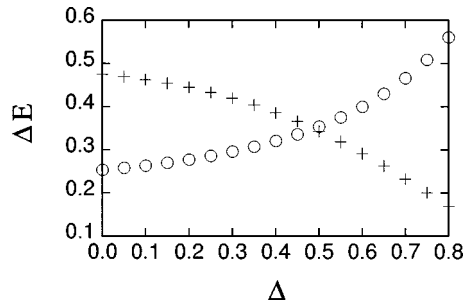

FIG. 2. Two low-lying energies in $S^z_{\rm total}=0$ subspace on the TBC. The system size is $L=14$, and $\lambda=0.5$, $D=1$. The eigenstates have $P_\pi=T_\pi=+1$ (○) and $P_\pi=T_\pi=-1$ (+), respectively. The ground state energy of the periodic system is set to be zero.

$$\frac{\partial}{\partial\tau}\phi(\tau,x)=-iK\frac{\partial}{\partial x}\theta(\tau,x), \qquad (3)$$

$$\frac{\partial}{\partial x}\phi(\tau,x)=iK\frac{\partial}{\partial\tau}\theta(\tau,x), \qquad (4)$$

has internal U(1) symmetry. The vertex operators $O_{n,m}=\exp(in\sqrt{2}\phi)\exp(im\sqrt{2}\theta)$ are the primary fields of the Gaussian model, and their scaling dimensions are $x_{n,m}=(n^2K+m^2K^{-1})/2$. By the identification $\phi\equiv\phi+2\pi/\sqrt{2}$, $\theta\equiv\theta+2\pi/\sqrt{2}$, the U(1) charges n,m are restricted to integral value. Since the scaling dimension of the operator $\cos\sqrt{2}\phi$ is $K/2$, the second term of Eq. (2) becomes a relevant perturbation for $K<4$. When $y_\phi\to+\infty$, $\langle\phi\rangle=\pi/\sqrt{2}$. On the other hand, when $y_\phi\to-\infty$, $\langle\phi\rangle=0$. The former corresponds to the Haldane phase (and the AF phase), and the latter the large-D phase. For $K>4$, the cosine term is irrelevant and y_ϕ is renormalized to 0, that is, the massless XY phase. The BKT transition takes place at $K=4$.

To determine numerically the Gaussian critical line ($y_\phi=0$), the TBC method is more accurate than the usual phenomenological renormalization group. Kitazawa[30] paid attention to the following operators as

$$O^e_{1/2}\equiv\sqrt{2}\cos\frac{\phi}{\sqrt{2}}, \qquad (5)$$

$$O^o_{1/2}\equiv\sqrt{2}\sin\frac{\phi}{\sqrt{2}}. \qquad (6)$$

From the conformal field theory,[31] the finite-size corrections of the corresponding energies result in

$$\Delta E^e(L)=\frac{2\pi v}{L}\left[\frac{K}{8}+\frac{y_\phi}{\sqrt{2}}\left(\frac{2\pi}{L}\right)^{K/2-2}+O(y_\phi^2)\right], \qquad (7)$$

$$\Delta E^o(L)=\frac{2\pi v}{L}\left[\frac{K}{8}-\frac{y_\phi}{\sqrt{2}}\left(\frac{2\pi}{L}\right)^{K/2-2}+O(y_\phi^2)\right]. \qquad (8)$$

Thus these energies cross linearly at $y_\phi=0$. The boundary condition on θ, $\theta(\tau,L)=\theta(\tau,0)+\Phi/\sqrt{2}$, means the change of

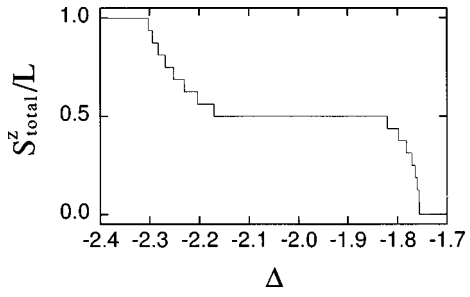

FIG. 3. Magnetization of the ground state through the PFM phase fixed $\lambda=3$, $D=1$. System size $L=16$ is used.

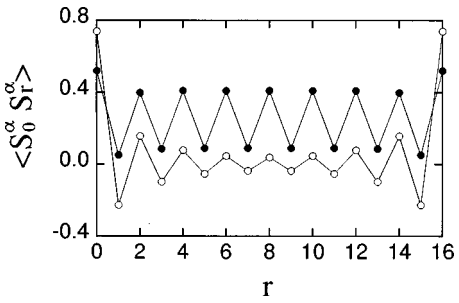

FIG. 4. Spin correlation functions at ($\Delta=-2$, $\lambda=3$, $D=1$). System length is $L=16$. Transverse correlation function ($\alpha=x$ or y) is denoted by the open circles, and longitudinal correlation ($\alpha=z$) by the closed circles.

the magnetic charge $\pm\Phi/2\pi$ at $\tau=\pm\infty$, that is, $n\to n+\Phi/2\pi$, $m\to m$.[32,33] In the spin notation, this is related to the TBC ($S^{\pm}_{L+1}=e^{\mp i\Phi}S^{\pm}_1$, $S^z_{L+1}=S^z_1$). Hence under the TBC ($\Phi=\pi$), it is possible to define such operators as Eqs. (5) and (6).

Next we discuss the symmetry of the excitations. The Hamiltonian (1) commutes with $P_\Phi\equiv V_\Phi P V_\Phi$ and $T_\Phi\equiv V_\Phi T V_\Phi$ only for $\Phi=0,\pi$. Here P, T, and V_Φ denote space inversion reflecting on a spin site ($S_i\to S_{L-i}$), time reversal with translation by one site ($S^{\pm}_i\to -S^{\mp}_{i+1}$, $S^z_i\to -S^z_{i+1}$), and the unitary operator $V_\Phi=\exp(i\Phi\Sigma_{j=1}^{L} jS^z_j/L)$, respectively. In sine-Gordon language, the symmetry operation for P_Φ is represented by

$$\phi\to-\phi,\quad \theta\to\theta,\quad x\to -x, \tag{9}$$

and for T_Φ

$$\phi\to-\phi,\quad \theta\to-\theta+\frac{\pi}{\sqrt{2}}. \tag{10}$$

The eigenstate $O^e_{1/2}|0\rangle$ with $P_\pi=T_\pi=+1$ is the ground state under the TBC in the large-D phase ($y_\phi<0$), and $O^o_{1/2}|0\rangle$ with $P_\pi=T_\pi=-1$ is that in the Haldane phase ($y_\phi>0$). The Lagrangian (2) is invariant under the transformation $y_\phi\to -y_\phi, \phi\to\phi+\pi/\sqrt{2}$. With this transformation, the roles of $O^e_{1/2}$ and $O^o_{1/2}$ are interchanged.

The above statement can be justified in another way by the VBS picture. On the TBC, the variational VBS states in the Haldane, AF ($\lambda>0$), and large-D phases are written as

$$(a^\dagger_L b^\dagger_1+b^\dagger_L a^\dagger_1)\prod_{j=1}^{L-1}(a^\dagger_j b^\dagger_{j+1}-b^\dagger_j a^\dagger_{j+1})|0\rangle, \tag{11}$$

$$\prod_{j=1}^{L/2}(a^\dagger_{2j-1}b^\dagger_{2j})^2|0\rangle, \tag{12}$$

$$\prod_{j=1}^{L} a^\dagger_j b^\dagger_j|0\rangle, \tag{13}$$

where $a^\dagger_j$ ($b^\dagger_j$) denotes the Schwinger boson which creates the spin-1/2 up (down) spin at the jth site. Using the identity $V_\pi a^\dagger_j b^\dagger_{j'} V^\dagger_\pi = a^\dagger_j b^\dagger_{j'}\exp(i\pi(j-j')/2L)$, it is easy to say that both the AF state (12) and the Haldane state (11) have the same eigenvalues $P_\pi=T_\pi=-1$. Therefore there is no transition between them. On the contrary, the large-D state (13) has $P_\pi=T_\pi=+1$. They are summarized in Table I. Although the above states (11)–(13) are variational, the discrete symmetry P_π, T_π under the TBC are good quantum numbers, thus they can be used to characterize the Haldane, AF, and large-D phases.

We consider the discrete symmetry in numerical results. Figure 2 shows two low-lying energies ($S^z_{\rm total}=m=0$) of the antiperiodic system with $L=14$, $\lambda=0.5$, $D=1$. The ground state has $P_\pi=T_\pi=+1$ on the left side, and $P_\pi=T_\pi=-1$ on the opposite side, as is expected. The level crossing indicates the transition from the large-D phase to the AF phase. At the critical point ($\lambda=0.5$, $\Delta=0.4856$, $D=1$), we also estimate the central charge, and confirm the Gaussian universality $c=1.000$. The whole phase diagrams are shown in Fig. 1. Each critical point is extrapolated from the system sizes $L=8-16$. The BKT multicritical structure strongly suggests that some hidden $Z_2\times Z_2$ symmetry exists even in $\lambda\neq 0$. Its symmetry is expected to be broken in the AF (Haldane) phase, and unbroken in the large-D phase. Unlike the bond-alternating systems, the bifurcation point of the Ashkin-Teller type is absent. Far from that, there is no 2D Ising critical line. The Néel region does not extend in the λ direction and it forms a first-order transition line, since λ is conjugate field to the Néel order. When $D=3$, the first-order transition line reaches the Gaussian line. This feature cannot be explained by the double sine-Gordon theory. What the universality class is at the multicritical point is a future problem. As D is increased, the XY region reduces and the large-D region grows. Conversely, the Gaussian line disappears for $D<D_c$.

Finally we remark the partially ferromagnetic (PFM) phase whose ground states are doubly degenerate with $S^z_{\rm total}=\pm M$, $(0<M<L)$. When the transition goes from the XY phase to the ferromagnetic (Ferro) phase by way of the PFM phase, the magnetization site increases continuously from 0 to 1 (see Fig. 3), whereas it jumps from 0 to 1 on the XY-Ferro boundary. Most of the area of the PFM phase is occupied by the place where $S^z_{\rm total}=\pm L/2$. It is instructive to consider the Ising limit $\Delta\to\infty$. Within the region $|\lambda+2\Delta|<D<\lambda$, the ground states are $(0\uparrow 0\uparrow 0\uparrow 0\uparrow\cdots)$ and $(\downarrow 0\downarrow 0\downarrow 0\downarrow 0\cdots)$. Such ordering behavior survives in the PFM

phase. We calculate the correlation functions $\langle S_0^\alpha S_r^\alpha \rangle (\alpha = x,y,z)$ at the point $(\Delta = -2,\ \lambda = 3,\ D = 1)$ in the PFM phase, using the $S^z_{\text{total}} = L/2$ ground state of the $L = 16$ system. They are shown in Fig. 4. The transverse correlation function seems to decay algebraically. The longitudinal correlations with even sites remain finite in long range, and the odd-site correlations are almost zero.

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