Gap generation in the XXZ model in a transverse magnetic field

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(Received 27 February 2002; published 18 April 2002)

The ground-state phase diagram of the one-dimensional XXZ model in a transverse magnetic field is obtained. It consists of the gapped phases with different types of long-range order (LRO) and critical lines at which the gap and the LRO vanish. Using scaling estimations and a mean-field approach as well as numerical results we found critical indices of the gap and the LRO in the vicinity of critical lines.

DOI: 10.1103/PhysRevB.65.172409 PACS number(s): 75.10.Jm

The study of the one-dimensional (1D) spin-1/2 XXZ model in a transverse magnetic field has been drawn much attention last years. The Hamiltonian of this model is

$$H=\sum (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z) - h\sum S_n^x. \quad (1)$$

The spectrum of the XXZ model for $-1<\Delta\leqslant 1$ is gapless. When the transverse magnetic field is applied, a gap in the excitation spectrum seems to open up. It is supposed[1] that this effect can explain the peculiarity of low temperature specific heat in Yb_4As_3.[2] The magnetic properties of this compound is described by the XXZ Hamiltonian with $\Delta \approx 0.98$ and it was shown[1] that the magnetic field in an easy plain induces a gap in the spectrum leading to a dramatic decrease of the linear term in the specific heat.

At $h=0$ the model (1) is the well-known XXZ model. In the Ising-like region $\Delta>1$ the ground state of the XXZ model has the Neel long-range order (LRO) along the Z axis and there is a gap in excitation spectrum. In the region $-1<\Delta\leqslant 1$ system is in the so-called spin-liquid phase with a power-low decay of correlations. Finally, for $\Delta<-1$ the ground state is the classical ferromagnet with the gap above the ferromagnetic state.

At $h\neq 0$ the total S^z is not conserving and the model (1) is not integrable, except some special cases: $\Delta=1$ and $\Delta\to\pm\infty$. In addition, there is a ''classical'' line $h_{\rm cl}(\Delta)=\sqrt{2(1+\Delta)}$, where the quantum fluctuations of the XXZ model are compensated by the transverse field and the exact ground state of Eq. (1) is a classical one.[3] The excited states on the classical line are generally unknown (except some of them[4]), though it is assumed that the spectrum is gapped.

In the limits $\Delta\to\pm\infty$ the model (1) reduces to the 1D Ising model in the transverse field (ITF), for which the phase transition occurs at $h_c=|\Delta|/2$. At this field the gap is closed and the LRO in the Z direction vanishes.

It was shown[5] that the phase transition of this type takes place for any $\Delta>0$. One can expect also that such a transition exists for any finite Δ at some critical value $h=h_c(\Delta)$ and there is the transition line connecting two limiting points $\Delta\to\pm\infty$. Besides, there are other transition lines charactered by vanishing both the gap and the LRO. These lines are $h=0$, $|\Delta|<1$; $\Delta=1$, $h<2$; $\Delta=-1$, $h<h_c(-1)$. However, the critical properties in the vicinity of these transition lines are not known yet.

Thus, we expect that the phase diagram of the model (1) [on the (Δ, h) plane] has a form shown on Fig. 1. It contains four regions corresponding to different phases and separated by the transition lines at which the gap vanishes. Each phase is characterized by its own type of the LRO: the Néel order along the Z axis in the region (1); the ferromagnetic order along the Z axis in the region (2); the Neel order along the Y axis in the region (3); and in the region (4) there is no LRO except magnetization along the field direction X (which, certainly, exists in all above regions).

In this paper we investigate the behavior of the gap and the LRO near the transition (critical) lines. We are interested in the critical exponents along these lines.

The line $h=0$, $|\Delta|<1$

Low-energy properties of the XXZ model are described by a free boson field theory. Therefore, to study the behavior of the system near the line $h=0$, $|\Delta|<1$, we use conformal estimations of small perturbation $h\ll 1$.

The time-dependent correlation functions of the XXZ chain show the power-law decay at $|\Delta|<1$ and have the asymptotic form[6]

$$\langle S^x(x,t)S^x(0,0)\rangle \sim \frac{(-1)^x A_1}{(x^2-v^2t^2)^{\theta/2}} - \frac{A_2}{(x^2-v^2t^2)^{\theta/2+1/2\theta}} \quad (2)$$

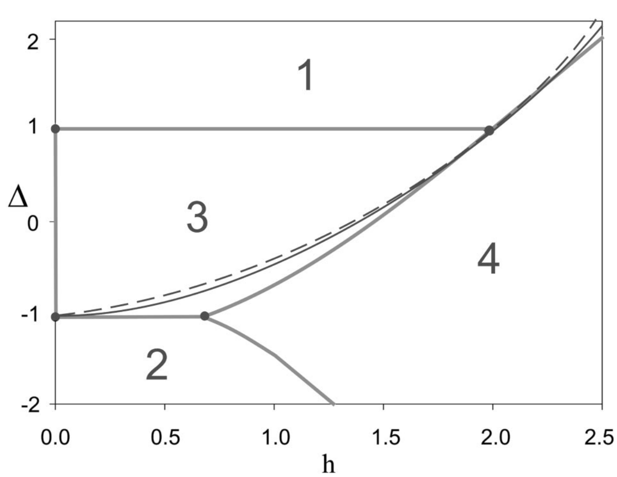

FIG. 1. Phase diagram of the model (1). The thick solid lines denote the critical lines, thin solid line is the ''classical'' line, and dashed line denotes the line $h_1(\Delta)$ (see text).

with $\theta=1-\arccos(\Delta)/\pi$, v is the spin-wave velocity, and A_1, A_2 are constants.[7]

The nonoscillating term in Eq. (2) gives scaling dimension for operator S^x–$d=\theta/2+1/2\theta$ and from the common formula[8] for mass gap m one has:

$$m \sim h^{\nu}, \quad \nu=\frac{1}{2-d}=\frac{2}{4-\theta-1/\theta}. \tag{3}$$

From Eq. (3) one could conclude that the magnetic field becomes irrelevant for $\Delta<-\cos[\pi\sqrt{3}]\simeq-0.67$ and the gap disappears for $\Delta<-0.67$. This does not look physically reasonable, since the magnetic field destroys continuous symmetry of the XXZ model and must produce the gap. In fact, due to nonzero conformal spin $S=1$ of the non-oscillating part of the operator S^x it is necessary to consider higher-order effects in h.[9] The analysis shows that in the perturbation series another critical exponent appears, giving for the mass gap

$$m \sim h^{\gamma}, \quad \gamma=\frac{1}{1-\theta}. \tag{4}$$

It turns out that the oscillating part of the operator S^x gives another, more relevant index for the gap at $\Delta<0$. Let us reproduce the usual conformal line of arguments for this oscillating part.

The perturbed action for the model is

$$S=S_0+h\int dt\, dx\, S^x(x,t), \tag{5}$$

where S_0 is the Gaussian action of the XXZ model. Let us perform an infinitesimal renorm-group step with a scale factor $\lambda=1-\delta L/L$, so that $x=\lambda x'$, $t=\lambda t'$. The correlation length changes as $\xi=\lambda\xi'$. Then, the action becomes

$$S'=S_0+h\int d(\lambda t')d(\lambda x')S^x(\lambda x',\lambda t).$$

Now let us estimate the large-distance contribution to the action of the oscillating part of the operator $S^x(x,t)$:

$$\begin{aligned} h\int dt\, dx\, S^x(x,t) &\sim h\int dt \sum_n \frac{(-1)^n}{(n^2-v^2t^2)^{\theta/4}} \\ &\sim h\int dt \sum_{n=2m} \frac{\theta n}{(n^2-v^2t^2)^{\theta/4+1}} \\ &\sim h\int dt\, dx \frac{\theta x}{(x^2-v^2t^2)^{(\theta/4)+1}}. \end{aligned}$$

So, after rescaling we get

$$h\int dt\, dx\, S^x(x,t) \to h\lambda^{1-\theta/2}\int dt'\, dx'\, S^x(x',t')$$

and, therefore, the magnetic field scales as $h'=h\lambda^{1-\theta/2}$.

Expressing λ as

$$\lambda=\frac{\xi}{\xi'}=\frac{m'}{m}=\left(\frac{h'}{h}\right)^{1/(1-\theta/2)}$$

we find that the mass gap is proportional to

$$m \sim h^{\tau}, \quad \tau=\frac{1}{1-\theta/2}. \tag{6}$$

Actually, the oscillating factor $(-1)^n$ in the correlator in some sense eliminates one singular integration over x, and into common conformal formula $m \sim h^{1/(D-d)}$, where D is the dimension of space and d is the scaling dimension of perturbation operator, one should use $D=1$ instead of conventional $D=2$.

The comparison of the expressions Eqs. (3), (4), and (6) shows that for $0<\Delta<1$ the leading term is given by Eq. (3), while for $-1<\Delta<0$ by Eq. (6). Thus, one has

$$\begin{aligned} &m \sim h^{\nu}, \quad 0<\Delta<1 \\ &m \sim h^{\tau}, \quad -1<\Delta<0. \end{aligned} \tag{7}$$

For example, $m \sim h$, when $\Delta \to \pm 1$ and $m \sim h^{4/3}$ for $\Delta=0$. In this respect the model (1) is different from the XXZ model in the staggered transverse field for which $m \sim h^{2/(4-\theta)}$ for all $|\Delta|<1$.[10]

The staggered magnetization (LRO) along the Y axis behaves as

$$\langle S_n^y \rangle \sim (-1)^n/\xi^{\theta/2} \sim (-1)^n m^{\theta/2}. \tag{8}$$

Therefore, the LRO has also two different critical indices:

$$\begin{aligned} &\langle |S^y| \rangle \sim h^{\theta/(4-\theta-1/\theta)} \quad 0<\Delta<1 \\ &\langle |S^y| \rangle \sim h^{\theta/(2-\theta)} \quad -1<\Delta<0. \end{aligned} \tag{9}$$

The critical indices ν and τ can be also found from the analysis of divergences of terms of perturbation series in h at $N \to \infty$ (N is the system size). As shown[4] at $N \to \infty$ the ground-state energy has a form

$$\frac{\delta E}{N}=-\frac{\chi}{2}h^2+ah^{2\nu}+bh^{2\tau}, \tag{10}$$

where ν and τ are given by Eqs. (3) and (6) and a,b are some constants.

One can see from Eqs. (3) and (6) that $\nu \to 1$ at $\Delta \to 1$ and $\tau \to 1$ at $\Delta \to -1$. Hence, in both limits one of the singular terms becomes proportional to h^2, and, therefore, gives a contribution to the susceptibility. It implies that in the symmetric points $\Delta=\pm 1$ the susceptibility has a jump. For example, $\chi=1/4$ at $\Delta=-1$ and $\chi=1/8$ at $\Delta \to -1$.[4]

The line $\Delta=1$

In the vicinity of the line $\Delta=1$ it is convenient to rewrite the Hamiltonian (1) in the form

$$H=H_0+V,$$

$$H_0=\sum \mathbf{S}_n\cdot\mathbf{S}_{n+1}-h\sum S_n^x, \tag{11}$$

$$V=-g\sum S_n^zS_{n+1}^z,$$

where the parameter $g=(1-\Delta)\ll 1$ is small. On the isotropic line $\Delta=1$ the model (1) is exactly solvable by Bethe ansatz. The ground state of H_0 remains a spin-liquid one up to the transition point $h_c=2$, where the phase transition of the Pokrovsky-Talapov type takes place and the ground state becomes completely ordered ferromagnetic state. Therefore, for $h<2$ and for small perturbation V we can use conformal estimations.

The large distance asymptotic of the correlation function on this line is

$$\langle S_i^zS_{i+n}^z\rangle\sim\frac{(-1)^n}{n^{\alpha(h)}}, \tag{12}$$

where $\alpha(h)$ is the known function obtained from the Bethe ansatz[11] and having the following limits:

$$\alpha(h)\sim 1-\frac{1}{2\ln(1/h)},\quad h\to 0 \tag{13}$$

and $\alpha(2)=1/2$.

So, the scaling dimension of operator S^z is $d_z=\alpha(h)/2$, and the scaling dimension of operator $S_i^zS_{i+1}^z$ is $d_{zz}=4d_z=2\alpha(h)$. Since $\alpha(h)<1$, then the perturbation V is relevant and leads to the mass gap and the staggered magnetization along the Y axis

$$m\sim g^{1/(2-d_{zz})}=g^{1/(2-2\alpha)}, \tag{14}$$

$$\langle|S^y|\rangle\sim 1/\xi^{d_z}\sim g^{\alpha/(4-4\alpha)}. \tag{15}$$

The above consideration is valid also for the case $\Delta>1$ (region 1) with the same exponents for the gap and the LRO. The only difference is that the staggered magnetization appears in this case along the Z axis.

From the general expressions for the mass gap (3), in the limit $h\to 2$ we obtain $m\sim g$.

The LRO in the vicinity of the point $(\Delta=1, h=2)$ vanishes on both lines: at $\Delta=1$ from Eq. (14) as $g^{1/4}$; and at $h=h_c$ as $|h_c-h|^{1/8}$ [see Eq. (19)]. Combining these facts we arrive at the following formula:

$$\langle S_n^y\rangle\simeq(-1)^n g^{1/4}|h_c-h|^{1/8}, \tag{16}$$

which is in accordance with the exact expression for LRO on the classical line.[3]

The behavior of the system near the point $\Delta=1$, $h=0$ is more complicated. As it follows from Eq. (7), for very small h the mass gap is $m\sim h$, while on the other hand from Eq. (14) one obtains another scaling $m\sim g^{\ln(1/h)}$. Really,[4,12] there are two regions near this point with different behavior of the mass gap and a crossover line $\sqrt{g}\ln(1/h)\sim 1$:

$$m\sim h\quad \text{for}\quad \sqrt{g}\ln(1/h)\gg 1,$$

$$m\sim g^{\ln(1/h)}\quad \text{for}\quad \sqrt{g}\ln(1/h)\ll 1. \tag{17}$$

The transition line $h=h_c(\Delta)$

Now we consider the behavior of the model in the vicinity of the transition line $h_c(\Delta)$. For this we have used the Fermi representation of Eq. (1). At first, in Eq. (1) we perform a rotation of the spins around the Y axis by $\pi/2$ (so that the magnetic field will be directed along the Z axis) followed by the Jordan-Wigner transformation to the Fermi operators $a_n^\dagger, a_n$. As a result, we obtain the Fermi Hamiltonian in the form

$$H_{\mathrm{F}}=-\frac{hN}{2}+\frac{N}{4}+\sum\left(h-1-\frac{1+\Delta}{2}\cos k\right)a_k^\dagger a_k$$
$$+\frac{1-\Delta}{4}\sum \sin k(a_k^\dagger a_{-k}^\dagger+a_{-k}a_k)$$
$$+\sum a_n^\dagger a_n a_{n+1}^\dagger a_{n+1}. \tag{18}$$

Treating the Hamiltonian H_{F} in the mean-field approximation we find the ground-state energy E_0 and the excitation spectrum $\varepsilon(k)$.

The main results following from the mean-field consideration are

(1) The function $\varepsilon(k)$ has a minimum at $k_{\min}$, which is changed from $\pi/2$ at $h=0$ to zero at $h=h_1(\Delta)$ and $k_{\min}=0$ for $h>h_1(\Delta)$. The gap in the spectrum $\varepsilon(k)$ vanishes at $h_c(\Delta)$ $(h_c>h_1)$ and for $h>h_1$ is $m\sim|h-h_c|$. The dependencies of $h_1(\Delta)$ and $h_c(\Delta)$ are shown on Fig. 1. There is the staggered magnetization along $Y(Z)$ axis for $\Delta<1(\Delta>1)$ at $h<h_c$ and it behaves as $\sim|h-h_c|^{1/8}$ at $h\to h_c$. The magnetization $s=\langle S_n^x\rangle$ has a logarithmic singularity at $h\to h_c$. These results show that the transition at $h=h_c(\Delta)$ belongs to the universality class of the ITF model.

(2) The mean field approximation is exact on the classical line $h=h_{\mathrm{cl}}(\Delta)$.

(3) In the vicinity of the point $h=2$, $\Delta=1$ the fermion density is small and the mean field approximation gives the accuracy in the energy, at least, up to g^3 or $(2-h)^4$. For this case the gap is

$$m=|h-h_c|,\quad h>h_1$$

$$m=\frac{g}{2\sqrt{2}}\sqrt{h_c-h-\frac{g^2}{32}},\quad h<h_1 \tag{19}$$

where $h_c=2-g/2-g^2/32$, $h_1=h_c-g^2/16$.

It is interesting to compare Eqs. (19) with the conformal estimation of the gap $m\sim g$. The conformal approach determines g dependence only, while Eq. (19) gives a prefactor depending on h.

The magnetic susceptibility $\chi(h)$ is

$$\chi=\frac{2}{\pi g}\ln\left(\frac{g^2}{h_c-h}\right),\quad g\gg\sqrt{h_c-h}$$

$$\chi=\frac{1}{\sqrt{2}\pi}\frac{1}{\sqrt{h_c-h}}, \quad g\ll\sqrt{h_c-h}. \tag{20}$$

As follows from Eq. (20) there is a crossover from square root to logarithmic divergence of χ.

The line $\Delta=-1$

On the line $\Delta=-1$ the model (1) reduces to the isotropic ferromagnet in a staggered magnetic field. This model is nonintegrable, but it was suggested[13] that the system is governed by a $c=1$ conformal field theory up to some critical value $h=h_0$, where the phase transition of the Kosterlitz-Thouless type takes place. In the vicinity of the line $\Delta=-1$ the Hamiltonian (1) becomes

$$H=-\sum \mathbf{S}_n\cdot\mathbf{S}_{n+1}-h\sum(-1)^n S_n^x+(1+\Delta)\sum S_n^z S_{n+1}^z, \tag{21}$$

where $(1+\Delta)\ll 1$ is a small parameter.

It can be shown[4] that at $h_{\mathrm{cl}}(\Delta)<h\ll 1$ low energy states of Eq. (21) is described by the XYZ Hamiltonian

$$H=-\sum\left[\left(1-\frac{h^2}{2}\right)S_n^xS_{n+1}^x+S_n^yS_{n+1}^y-\Delta S_n^zS_{n+1}^z\right]. \tag{22}$$

The derivation of this mapping is based on the fact that the transition operator $\Sigma(-1)^n S_n^x$ connects the low-lying states with the states with high energies ~ 2 only. The coincidence of the low-energy spectra of Eqs. (21) and (22) for $h_{\mathrm{cl}}(\Delta)<h\ll 1$ has been checked numerically. The spectrum of low-lying excitations of the XYZ model[14] as well as the initial model (1) in the vicinity of the point $\Delta=-1,h=0$ can be described asymptotically exactly by the spin-wave theory,[1] which gives

$$m=h\sqrt{(1+\Delta)/2}, \quad \Delta>-1$$

$$m=\sqrt{(1+\Delta)(1+\Delta-h^2/2)}, \quad \Delta<-1. \tag{23}$$

The validity of the spin-wave approximation is quite natural because in the vicinity of the point $\Delta=-1,h=0$ the number of magnons forming the ground state is small.

We note that the gap (23) for $\Delta\geqslant-1$ coincides with the conformal theory result (7) and provides us with preexponential factor for the gap.

On the line $\Delta=-1$ the model (22) is the XXZ model and the correlation functions have the power-law decay. The scaling dimensions of operators S_i^x and S_i^y,S_i^z on this line are $d_x=\beta(h)/2$ and $d_y=d_z=1/2\beta(h)$. The function $\beta(h)$ is generally unknown, but at $h\ll 1$, where the mapping to XYZ model is valid, $\beta(h)\sim\pi/h$.

Strictly on the line $\Delta=-1$ at some value of $h=h_0$ the gap appears. It means that the magnetic field term is irrelevant at $h<h_0$ $(\beta(h)>4)$ and becomes marginal at $h=h_0$, where $\beta(h_0)=4$. So, at the point $h=h_0$ the transition is of the Kosterlitz-Thouless type, and for $h>h_0$ the mass gap is exponentially small.

Using the conformal invariance of the model (21) at $\Delta=-1$ and $h<h_0$ we carried out finite-size calculation of the exponent $\beta(h)$. The extrapolated function $\beta(h)$ agree well with the dependence π/h at $h\ll 1$ and $\beta=4$ at $h_0\simeq 0.52$. On the other hand, the mean-field approach gives the rather crude value $h_0=h_c(-1)=0.69$.

In summary, we have studied the 1D XXZ model in the transverse magnetic field. It is shown that the spectrum of the model is gapped except critical lines on the (h,Δ) plane, where the LRO vanishes. We found the critical exponents of the gap and the LRO in the vicinity of these lines.

The authors would like to thank Professor P. Fulde and Dr. A. Langari for many useful discussions. The authors are also grateful to Max-Planck-Institut für Physik Komplexer Systeme for kind hospitality. This work was supported under RFFR Grants No. 00-03-32981 and No. 00-15-97334.

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