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Quantum renormalization group of XYZ model in a transverse magnetic field

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We have studied the zero-temperature phase diagram of XYZ model in the presence of transverse magnetic field. We show that small anisotropy $(0 \leqslant \Delta < 1)$ is not relevant to change the universality class. The phase diagram consists of two antiferromagnetic ordering and a paramagnetic phase. We have obtained the critical exponents, fixed points, and running of coupling constants by implementing the standard quantum renormalization group. The continuous phase transition from antiferromagnetic (spin-flop) phase to a paramagnetic one is in the universality class of Ising model in transverse field. Numerical exact diagonalization has been done to justify our results. We have also addressed the application of our findings to the recent experiments on Cs_2CoCl_4.

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Systems near criticality are usually characterized by fluctuations over many length scales. At the critical point itself, fluctuations exist over all scales. At moderate temperatures quantum fluctuations are usually suppressed compared with the thermal ones. However if temperature is near zero, quantum fluctuations especially in the low-lying states dominate thermal ones and strongly influence the critical behavior of system. Zero-temperature (quantum) phase transition may occur in the area of spin systems by applying noncommuting magnetic field which introduces quantum fluctuations. Such a situation has been studied in the three-dimensional Ising ferromagnet $LiHoF_4$ in a transverse magnetic field.[1] However due to its high dimensionality, the system behaves in a mean-field-like manner. In this paper we are going to consider the one-dimensional XYZ model in the presence of a transverse field where quantum fluctuations of symmetry-breaking field play an essential role. Generally renormalization group (RG) is the proper method to give us the universal behavior at long wavelengths where other methods fail to work accurately.

The spin-$(s=)\frac{1}{2}$ Hamiltonian of this model on a periodic chain of N sites is

$$H=\sum_{i=1}^{N}\left[J_x\sigma_i^x\sigma_{i+1}^x+J_y\sigma_i^y\sigma_{i+1}^y+\Delta\sigma_i^z\sigma_{i+1}^z-h\sigma_i^x\right], \quad (1)$$

where $J_x>0$ and $J_y>0$ are exchange couplings in the XY easy plane, $0\leqslant\Delta<1$ is the anisotropy in Z direction which is in J_y units, and h is proportional to the transverse field. σ^α, $\alpha=x,y,z$, are Pauli matrices.

When $h=0$, the XXZ model $(J_x=J_y)$ is known to be solvable and critical (gapless) while $-1\leqslant\Delta\leqslant1$.[2] The Ising regime is $\Delta>1$ and $\Delta\leqslant-1$ is the ferromagnetic case. Magnetic field in the anisotropy direction commutes with the Hamiltonian $(h=0)$ and extends the gapless region (quasi-long-range order) to a border where a transition to paramagnetic phase takes place. The model is still integrable and can be explained by a conformal field theory with central charge $c=1$ (Ref. 3 and references therein).

In the case of XXZ model a transverse field breaks the U(1) symmetry of the Hamiltonian to a lower, Ising-like, which develops a gap. The ground state then has long-range anti-ferromagnetic order $(0\leqslant\Delta<1)$. However due to nonzero projection of order parameter on field axis it is a spin-flop Néel state. In fact at a special field $[h_N=2\sqrt{2J_x(J_x+\Delta)}]$ the ground state is known exactly to be of classical Néel type.[4,5] Phase diagram, scaling of gap and some of the low excited states at h_N, has been studied in Ref. 6. The gap vanishes at a critical field h_c, where a transition to paramagnetic phase occurs. Classical approach to this model reveals the mean-field results[7] which is exact as $s\to\infty$. However the study of critical region needs quantum fluctuations to be taken into account. Exact diagonalization[8] and density-matrix renormalization group[9] give us the properties of stable phases. Here we are going to present the phase diagram of XYZ model, Eq. (1), by means of RG flow of coupling constants to show explicitly its universality class.

Apart from theoretical point of view, recent experiments on Cs_2CoCl_4 in the presence of transverse magnetic field can be explained by XYZ model with $\Delta=0.25$.[10] Using quantum renormalization group (QRG) we will show explicitly that the anisotropy is not relevant and the universality class is governed by Ising model in transverse field (ITF). In addition QRG results rule out the existence of spin liquid phase between spin-flop and paramagnetic phases which are separated at the critical field h_c. Exact diagonalization data support our QRG results by calculating the structure factor and magnetization of finite chain sizes. Our results are in good agreement with the experimental data. We will also discuss on the reasons why magnetization does not saturate just above critical point.

Quantum RG scheme in real space is started by decomposing lattice into isolated blocks. The Hamiltonian of each block is diagonalized exactly and some of the low-lying states are kept to construct the basis for renormalized Hilbert space. Finally the Hamiltonian is projected onto the renormalized space.[11] We have considered a two-site block and kept the ground $(|\epsilon0\rangle)$ and first $(|\epsilon1\rangle)$ excited states of each block to construct the embedding operator $(T$

$=|\epsilon 1\rangle\langle\uparrow|+|\epsilon 0\rangle\langle\downarrow|)$.[12] Energy eigenvalues are $\epsilon 0=-J_x-J_y-\Delta$ and $\epsilon 1=J_x-\sqrt{4h^2+(J_y-\Delta)^2}$. The $|\uparrow\rangle$ and $|\downarrow\rangle$ are renamed basis in the renormalized Hilbert space. The interaction between blocks defines the effective interaction of renormalized chain where each block is considered as a single site. A remark is in order when projecting the Hamiltonian onto the effective (renormalized) Hilbert space. The effective Hamiltonian is not exactly similar to the initial one, i.e., the signs of $\sigma_i^y\sigma_{i+1}^y$ and $\sigma_i^z\sigma_{i+1}^z$ terms are changed. To avoid this and producing a self-similar Hamiltonian we first implement a π rotation around x axis for even sites and leave odd sites unchanged. Therefore the Hamiltonian is transformed to the following form:

$$H=\sum_{i=1}^{N/2}\left[J_x\sigma_i^x\sigma_{i+1}^x-J_y\sigma_i^y\sigma_{i+1}^y-\Delta\sigma_i^z\sigma_{i+1}^z-h\sigma_i^x\right]. \quad (2)$$

We note to interpret our final results in terms of this transformation. The renormalized Hamiltonian $[H^{ren}=T^{\dagger}H(transformed)T]$ is similar to Eq. (2) with renormalized coupling defined below.

$$J_x'=\frac{J_x}{4}\left(\frac{(J_y-\Delta)^2-\vartheta^2}{(J_y-\Delta)^2+\vartheta^2}\right)^2,$$

$$J_y'=\frac{J_y}{2}\,\frac{(J_y-\Delta+\vartheta)^2}{(J_y-\Delta)^2+\vartheta^2},$$

$$h'=\frac{\epsilon 0-\epsilon 1}{2}-\frac{J_x}{2}\left(\frac{(J_y-\Delta)^2-\vartheta^2}{(J_y-\Delta)^2+\vartheta^2}\right)^2,$$

$$\Delta'=\frac{\Delta}{2}\,\frac{(J_y-\Delta-\vartheta)^2}{(J_y-\Delta)^2+\vartheta^2}, \quad (3)$$

where $\vartheta=\sqrt{4h^2+(J_y-\Delta)^2}-2h$. This RG flow is not valid when $h\to 0$ where the U(1) symmetry at $J_x=J_y$ cannot be recovered by Eq. (3). It will be discussed later. However due to level crossing which happens for the eigenstates of block Hamiltonian, Eq. (3) is valid when $g_x\leqslant(1+\sqrt{1+2g_h^2})/2$ and $g_\Delta\leqslant g_x\leqslant 1$. This covers XYZ model ($J_x\leqslant J_y$) in transverse field when $0\leqslant\Delta<1$. The new parameters $g_x=J_x/J_y$, $g_\Delta=\Delta/J_y$, and $g_h=h/J_y$ are defined because these ratios actually define competing phases.

We have plotted the RG flow (arrows) and different phases in Fig. 1. The RG equations [Eq. (3)] show running of Δ to zero. In other words the anisotropy term is irrelevant ($0\leqslant\Delta<1$). So we have only plotted the $\Delta=0$ plane. It means that the universality class of XYZ model in transverse field (TF) is the same as XY model in TF. Moreover the exchange interaction in the x direction is also irrelevant while $J_x<J_y$. As J_x vanishes under RG, there are only two effective terms in the Hamiltonian. This is exactly the case of ITF model. So the interplay of $J_y\sigma_i^y\sigma_{i+1}^y$ and $h(\sigma_i^x+\sigma_{i+1}^x)$ defines either ordering in y or paramagnetic in x direction. Solving the RG equation for fixed points, we found the nontrivial fixed point $g_h^*\equiv(g_x=0,g_h\simeq 1.26,g_\Delta=0)$ apart from the other which is at $(g_x=0,g_h=\infty,g_\Delta=0)$ and represents saturated ferromagnet. We have linearized the RG flow at g_h^* and found one relevant direction (whose eigenvalue is larger than one). The eigenvalues and corresponding eigenvectors of linearized RG at g_h^* in (g_x,g_h,g_Δ) space are the following: $|\lambda_1=1.59\rangle=(0,1,0)$; $|\lambda_2=0.31\rangle=(1,1.64,0)$; and $|\lambda_3=0.46\rangle=(0,0.62,1)$. The relevant direction ($|\lambda_1\rangle$) is the horizontal line passing through g_h^* and $|\lambda_2\rangle$ is the tick line ending at g_h^*. The critical exponents at this fixed point are $\beta=0.41$, $\nu=1.48$, and $z=0.55$. The discrepancies of exponents from exact values ($\beta=0.125$, $\nu=1$, and $z=1$, Ref. 13) are the result of two-site blocking, however these are exactly equal to the exponents of ITF chain which is calculated by QRG.[12] As far as $g_x\leqslant 1$, the control parameter is g_h. When $g_h<g_h^c$ [phase (I)], the staggered magnetization in y direction (SM_y) is nonzero which is the order parameter to represent the phase transition at g_h^c (the line which ends at g_h^*). However magnetization in x direction (M_x) is also nonzero which causes to consider this phase as a spin-flop phase. This is an Ising-like phase which has a nonzero gap. This gap is going to be closed at g_h^c where the transition to paramagnetic phase takes place. At this point the quantum fluctuation of TF destroys the antiferromagnetic (AF) ordering completely. The paramagnetic phase (II) appears at $g_h>g_h^c$ where spins are aligned in the field direction and will be saturated in high TF. Note that the proper order parameter for this phase transition is *staggered magnetization in y direction*. So it is not necessary to gain the saturation value for M_x just after g_h^c. This also happens in ITF model. We have plotted both SM_y and M_x in Fig. 2(a). The comparison with Lanczos results shows a very good qualitative agreement. Although it is not expected that QRG gives good quantitative results we got fairly well agreement with Lanczos results.

To discuss the behavior close to $h=0$, we need to take

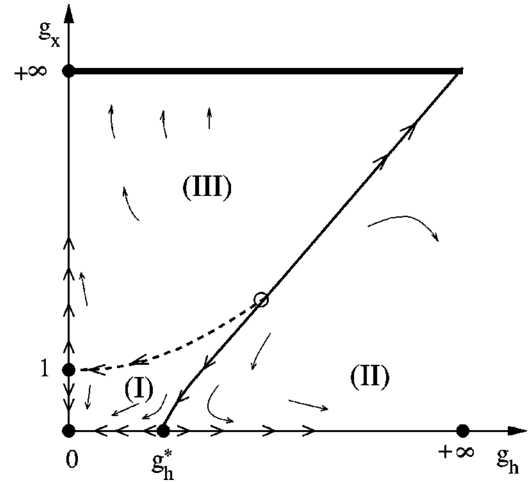

FIG. 1. Phase diagram of XY model in transverse field. Arrows show running of couplings under RG. Filled circles show fixed points and the open circle is the tricritical point where lines separating different phases merge. The tick line at the top of phase diagram ($g_x=+\infty$) is a line of fixed points (Ref. 14). Phase (I) is antiferromagnetic Ising in y direction (spin flop), (II) paramagnetic in x direction, and (III) is antiferromagnet in x direction. g_h^* is the ITF fixed point.

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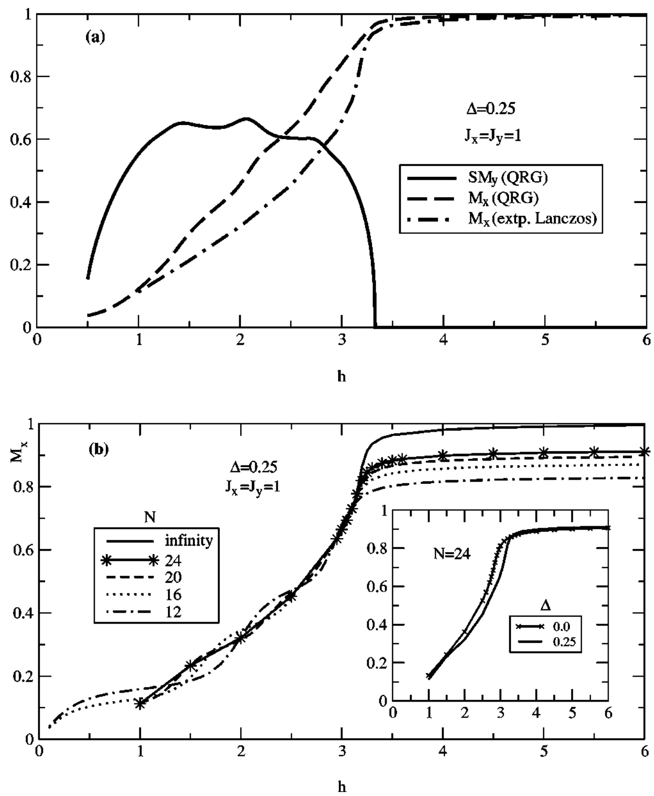

FIG. 2. (a) The order parameter (SM_y) and magnetization in x direction (M_x) vs transverse field. QRG and extrapolated Lanczos results are compared for (M_x). (b) Lanczos results of M_x vs transverse field for $N=12,16,20,24$ and extrapolation to $N\rightarrow\infty$, at $\Delta=0.25$ and $J_x=J_y=1$. The inset shows that M_x behaves qualitatively the same for $\Delta=0$ and 0.25.

into account the U(1) symmetry in the QRG scheme. So we will consider the XY model at $h=0$ and the effect of TF is taken into account by perturbation. In this case the only relevant parameter is g_x. Implementing a three-site blocking, the RG flow is $g_x'=g_x^3$, which has two stable $g_x^*=0,\infty$ and an unstable fixed point $g_x^*=1$. The stable fixed points define two AF Ising phases ordered in y direction ($g_x^*=0$) and x direction ($g_x^*=\infty$). The $g_x^*=1$ is the critical point where a transition occurs between two stable phases. Now the transverse field is considered perturbatively which gives the following RG flow for g_h:

$$g_h'=\left(\frac{2g_x\sqrt{1+g_x^2}-g_x^2}{1+g_x^2}\right)g_h, \quad g_h\rightarrow 0. \tag{4}$$

The perturbation approach is justified since $g_h\rightarrow 0$. For any value of g_x, Eq. (4) leads to $g_h'<g_h$, which means the direction of flow is toward the g_x axis. As a result of QRG at $g_h=0$ we expect to have a phase transition at small g_h by changing g_x close to $g_x\simeq 1$. The boundary of this phase transition is shown by dashed line in Fig. 1. This line represents the phase transition between phases (I) and (III), AF Ising in y and x directions, respectively. As $g_x\rightarrow\infty$ ($J_y\rightarrow 0$) the model behaves as an AF Ising in a longitudinal magnetic field. In this limit a first-order phase transition at $h/J_x=1$ divides the AF, $h/J_x<1$, from paramagnetic, $h/J_x>1$, phases. A line of fixed points comes out of a three-sites block QRG (Ref. 14) for $h/J_x<1$ which has been shown as a tick line at the top of phase diagram (Fig. 1). Thus a line with slope $g_x/g_h=1$ (as $J_y\rightarrow 0$) constructs the boundary of phase transition between phases (II) and (III). This phase transition is in the universality class of AF Ising in a magnetic field. To complete the structure of phase diagram we propose a tricritical point (open circle in Fig. 1) which is the coexistence point of three phases. Still we do not have a RG equation at this point.

We have implemented the Lanczos algorithm on finite sizes ($N=12,16,20,24$) using periodic boundary conditions to calculate M_x and structure factors both in x and y directions. In Fig. 2(b) we have plotted M_x for different chain sizes at $\Delta=0.25$ and an extrapolation to $N\rightarrow\infty$. The value of $\Delta=0.25$ is chosen to fit the case of Cs_2CoCl_4. The general behavior is similar to what we have obtained from QRG [Fig. 2(a)]. There is no sharp transition to the saturation value at a given h because M_x is not the proper order parameter to this phase transition. Oscillations of M_x at finite N for $h<h_c$ are the result of level crossing between ground and first excited states of this model. The last level crossing happens at h_N. We have also plotted the case of $\Delta=0$ to show the same qualitative behavior as $\Delta=0.25$ in the inset of Fig. 2(b). Lanczos results lead to $SM_y=0$ for any value of h,

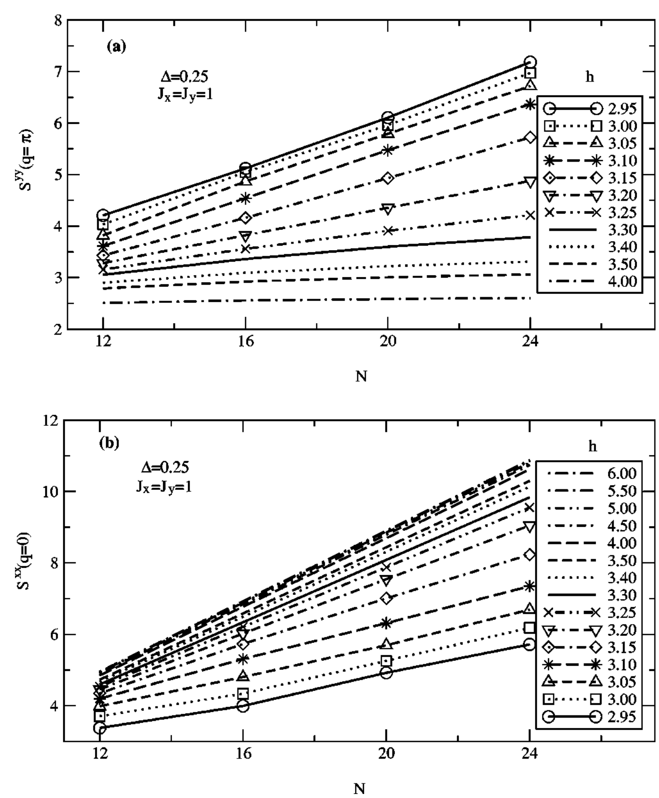

FIG. 3. Structure factor (a) $S^{yy}(q=\pi)$, (b) $S^{xx}(q=0)$ vs N for different transverse fields. $S^{yy}(q=\pi)$ shows divergence as $N\rightarrow\infty$ while $h<h_c\simeq 3.1$ (in the ordered phase). All plots for $S^{xx}(q=0)$ show divergence in thermodynamic limit ($N\rightarrow\infty$). However superlinear behavior for $h<h_c\simeq 3.1$ and almost linear behavior for $h>h_c$ is the sign of two different phases.

since in a finite system no symmetry breaking happens. However the structure factor $[S^{yy}(q=\pi)]$ diverges in the ordered phase as $N\to\infty$. The structure factor at momentum q is defined as

$$S^{\alpha\alpha}(q)=\sum_{r}\langle\sigma_0^{\alpha}\sigma_r^{\alpha}\rangle e^{iqr},\quad \alpha=x,y. \tag{5}$$

In Fig. 3(a), $S^{yy}(q=\pi)$ is plotted versus N for different transverse fields. As far as $h>3.1$, $S^{yy}(q=\pi)$ grows slowly and shows saturation at a finite value when $N\to\infty$. On the other hand a superlinear behavior versus N shows a divergence of structure factor for $h<3.1$. It corresponds to ordered phase which is AF in y direction. Thus the critical field at $\Delta=0.25$ is $h_c=3.1\pm0.05$. A similar computation results to $h_c=2.9\pm0.05$ for $\Delta=0$. To get an impression that the QRG results are very surprising we just mention the value of critical field for comparison with Lanczos ones, $h_c(\Delta=0.25)=3.32$ and $h_c(\Delta=0)=3.12$.

We have also plotted the structure factor $S^{xx}(q=0)$ versus N in Fig. 3(b). This shows divergence for any value of h as $N\to\infty$ which verifies ordering in x direction. The spin-flop phase (I) has nonzero M_x which increases by h to the saturation value in paramagnetic phase (II). However we observe different qualitative behaviors for $h<h_c=3.1$ and $h>h_c$. The former is superlinear and the latter is almost linear. As mentioned before, M_x is not the proper order parameter and is not expected to be saturated at a specific h. The saturation happens for enough large value of TF.

Summing up the QRG and numerical results, we claim that the universality class of XYZ model in TF $(0\leqslant\Delta<1)$ is the ITF model. Thus there exist only two stable phases, namely, (I) and (II), which are distinguished by a critical field at h_c. In this respect there is no spin liquid phase just after transition point. We found a very good agreement in the sense of universal behavior with the experimental results[10] on Cs_2CoCl_4. We have obtained the corresponding critical magnetic field $H_c=1.3^T$ comparing with the reported $H_c=2.1^T$. The difference should come from two-doublet nature $(s=3/2)$ of actual material and the effective Hamiltonian of $s=1/2$ in our calculation which is responsible for low fields. The other mismatching is the observed crossover behavior in M_x. As proposed in Ref. 10 the crossover behavior is related to the saturation of the lower doublet of Co^{2+} and the inset of higher doublet effects. However for the XYZ chain as a spin-$\frac{1}{2}$ model this does not happen. At $J_x=J_y$, applying small noncommuting fields break the U(1) rotational symmetry and develops a gap which has the consequence of promoting long-range order in a spin-flop phase (I). Increasing field stabilizes the perpendicular AF order which can be observed by the maximum in SM_y. Higher TF reduces ordering up to a critical field h_c where gap vanishes. Just after this transition point a gapped paramagnetic phase appears, phase (II).

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