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 ≤ Δ < 1) is not relevant to change the universality class. The phase diagram consists of two antiferromagnetic ordering and a paramagnetic phases. 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 on the application of our findings to the recent experiments on Cs$_2$CoCl$_4$.

PACS numbers: 75.10.Jm, 75.10.Pq, 75.40.Cx

Systems near criticality are usually characterised 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. 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 wave lengths where other methods fail to work accurately.

The spin-(s = 1/2) Hamiltonian of this model on a periodic chain of N-sites is

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

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

When $h = 0$, the XXZ model ($J_x = J_y$) is known to be solvable and critical (gapless) while $-1 \leq \Delta \leq 1$. The Ising regime is $\Delta > 1$ and $\Delta \leq -1$ 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. [8] 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 ≤ Δ < 1). However due to non-zero projection of order parameter on field axis it is a spin-flop Néel state. In fact at a special field ($h_N = 2\sqrt{2}J_x(J_z + \Delta)$) the ground state is known exactly to be of classical Néel type. Phase diagram, scaling of gap and some of the low excited states at $h_N$ has been studied in Ref. [9]. 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 which is exact as $s \to \infty$. However the study of critical region needs quantum fluctuations to be taken into account. Exact diagonalization and Density Matrix Renormalization Group (DMRG) gives us the properties of stable phases. A bosonization approach to this model in certain limits leads to a nontrivial fixed point and a gapless line which separates two gapped phases, moreover the connection to the axial next-nearest neighbor Ising model (ANNNI) has been addressed. The applicability of mean-field approximation has been studied by comparing with the DMRG results of magnetization and structure factor. Recently the effect of longitudinal magnetic field on both Ising model in Transverse Field (TF) and XXZ model in TF has been discussed. 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$_2$CoCl$_4$ in the presence of transverse magnetic field can be explained by XYZ model with $\Delta = 0.25$. 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 supports 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 to the renormalized space. We have considered a two sites block and kept the ground (|ψ⟩) and first (|φ1⟩) excited states of each block to construct the embedding operator (T = |φ1⟩⟩ |φ⟩ + |ψ⟩〉 |ψ⟩). Energy eigenvalues are 0 = -Jx - Jy - Δ and ϵ1 = Jx - √4h2 + (Jy - Δ)2. The |↑⟩ and |↓⟩ are renamed basis in the renormalized Hilbert space. The interaction between blocks define the effective interaction of renormalized chain where each block is considered as a single site. A remark is in order when projecting the Hamiltonian to the effective (renormalized) Hilbert space. The effective Hamiltonian is not exactly similar to the initial one, i.e. the sign of \(σ^y_iσ^y_{i+1}\) and \(σ^x_iσ^x_{i+1}\) terms is changed. To avoid this and producing a self similar Hamiltonian we first implement a π rotation around x-axis for even sites and leaves odd sites unchanged. Therefore the Hamiltonian is transformed to the following form,

\[
H = \sum_{n=1}^{N/2} \left[ J_x σ^x_iσ^x_{i+1} + J_y σ^y_iσ^y_{i+1} - Δσ^z_iσ^z_{i+1} - hσ^x_i \right].
\]

We note to interpret our final results in terms of this transformation. The renormalized Hamiltonian (\(H_r\)) is similar to Eq. (2) with renormalized coupling defined below.

\[
\begin{align*}
J'_x &= J_x \frac{(J_y - Δ - 2h^2)}{2(J_y - Δ)^2 + Δ^2} \\
J'_y &= J_y \frac{(J_y - Δ + 2h^2)}{2(J_y - Δ)^2 + Δ^2} \\
h' &= \frac{e0 - e1}{4} - J_x \frac{(J_y - Δ)^2 - 2h^2}{2(J_y - Δ)^2 + Δ^2} \\
Δ' &= \frac{Δ}{2} \frac{(J_y - Δ)^2 - 2h^2}{2(J_y - Δ)^2 + Δ^2}
\end{align*}
\]

where \(θ = √4h^2 + (J_y - Δ)^2 - 2h\). This RG-flow is not valid when \(h \to 0\) where the U(1) symmetry at \(J_x = J_y\) can not 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 \(g_x ≤ (1 + √1 + 4g^2_0)/2\) and \(g_y ≤ g_x ≤ 1\). This covers XYZ model (\(J_x ≤ J_y\)) in transverse field when \(0 ≤ Δ < 1\). The new parameters \(g_x = \frac{J_x}{J_y}\), \(g_Δ = \frac{Δ}{J_y}\) and \(g_θ = \frac{θ}{J_y}\) 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 ≤ Δ < 1). So we have only plotted the \(Δ = 0\) 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 Ising model in TF (ITF model). So the interplay of \(J_yσ^y_iσ^y_{i+1}\) and \(h(σ^x_i + σ^x_{i+1})\) defines either ordering in y or paramagnetic in x direction. Solving the RG equation for fixed points, we found the non-trivial fixed point \(g_0^*\) (\(g_x = 0, g_θ \approx 1.26, g_Δ = 0\)) apart from the other which is at \(g_x = 0, g_θ = ∞, g_Δ = 0\) and represents saturated ferromagnet. We have linearised the RG-flow at \(g_0^*\) and found one relevant direction (whose eigenvalue is larger than one). The eigenvalues and corresponding eigenvectors of linearised RG at \(g_0^*\) in \((g_x, g_θ, g_Δ)\) space are: \(|λ_1| = 1.59\) = (0, 1, 0); \(|λ_2| = 0.31\) = (1, 1.64, 0); \(|λ_3| = 0.46\) = (0, 0.62, 1). The relevant direction (\(|λ_1|\)) is the horizontal line passing through \(g_0^*\) and \(|λ_2|\) is the tick line ending at \(g_0^*\). The critical exponents at this fixed point are \(β = 0.41, ν = 1.48\) and \(z = 0.55\). The discrepancies of exponents from exact values \((β = 0.125, ν = 1, z = 1)\) are the result of 2-sites blocking, however these are exactly equal to the exponents of ITF chain which is calculated by QRG. As far as \(g_x ≤ 1\), the control parameter is \(g_x\). When \(g_x < g_0^*\) (phase (I)), the staggered magnetization in y-direction (SM) is non-zero which is the order parameter to represents the phase transition at \(g_0^*\) (the line which ends at \(g_0^*\)). However magnetization in x-direction (M_x) is also non-zero 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 \( g_h^0 \) 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 \( g_h > g_h^0 \) 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 \( g_h^0 \). This also happens in ITF model. We have plotted both \( SM_y \) and \( M_x \) in Fig. 2(a). The comparison with Lanczos results show 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 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 3 sites blocking, the RG flow is: \( g_x' = g_x^*, \) which has 2 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 \( g_h \).

\[
g_h' = \left( \frac{2g_x\sqrt{1 + g_x^2 - g_x^2}}{1 + g_x^2} \right) g_h ; \quad g_h \to 0 \quad (4)
\]

The perturbation approach is justified since \( g_h \to 0 \). 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 \( g_x \approx 1 \). The boundary of this phase transition is shown by dashed line in Fig. 1 which is the gapless line reported in Ref. [1]. This line represents the phase transition between phases (I) and (III), AF Ising in y- and x-direction, respectively. As \( g_x \to \infty (J_y \to 0) \) the model behaves as an AF Ising in a longitudinal magnetic field. In this limit a first order phase transition at \( \frac{h}{J_x} = 1 \) divides the AF \( \frac{h}{J_x} < 1 \) from paramagnetic \( \frac{h}{J_x} > 1 \) phases. A line of fixed points comes out of a 3-sites block QRG for \( \frac{h}{J_x} < 1 \) which has been shown as a tick line at the top of phase diagram (Fig. 1). Thus a line with slope \( \frac{2g_x}{g_h} = 1 \) (as \( J_y \to 0 \)) constructs the boundary of phase transition between (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 tri-critical point (open circle in Fig. 1) which is the coexistence point of three phases. Still we do not have an 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 \( N \to \infty \). 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 \( h \) because \( h < h_c \) is the result of level crossing between ground and first excited states of this model. The last level crossing happens at \( h_1 \). 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 leads to \( SM_y = 0 \) for any value of \( h \), 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

\[
S^{aa}(q) = \sum_r <\sigma^a_r\sigma^a_0> e^{iqr} ; \quad a = x, y \quad (5)
\]

In Fig. 3(a), \( S^{yy}(q = \pi) \) is plotted versus \( N \) for different transverse field. As far as \( h > 3.1 \), \( S^{yy}(q = \pi) \) grows slowly and shows saturation at a finite value when \( N \to \infty \). In the other hand a super linear behavior versus \( N \)
compared with Lanczos ones, surprising we just mention the value of critical field for $0$. To get an impression that the QRG results are very 

$N$ shows a divergence of structure factor for $h < h_c \approx 3.1$ (in the ordered phase). All plots for $S^{xy}(q=0)$ show divergence in thermodynamic limit ($N \to \infty$). However super linear behavior for $h < h_c \approx 3.1$ and almost linear behavior for $h > h_c$ is the sign of two different phases.

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 $h_c = 3.1 \pm 0.05$. A similar computation results to $h_c = 2.9 \pm 0.05$ 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 behavior for $h < h_c = 3.1$ and $h > h_c$. The former is super linear 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 ($0 \leq \Delta < 1$) is the ITF model. Thus there exists 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 very good agreement in the sense of universal behavior with the experimental results on $Cs_2CoCl_4$. We have obtained the corresponding critical magnetic field $H_c = 1.3T$ comparing with the reported $H_c = 2.1T$. The difference should come from two doublets 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. 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 1/2 model this does not happen. At $J_y = J_y$, 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 (II).

Acknowledgments

The author would like to thank D. V. Dmitriev, V. Ya. Krivnov, A. A. Ovchinnikov, M. Peyravy, T. Vojta, K. Yang and A. P. Young for fruitful discussions and useful comments.

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