Critical and off-critical properties of an anisotropic Heisenberg spin- $\frac{1}{2}$ chain under a transverse magnetic field

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We present a study of *XYZ* Heisenberg spin- $\frac{1}{2}$ chain, along with its variant (*XY* Heisenberg spin- $\frac{1}{2}$ Hamiltonian), under a transverse magnetic field. It reveals from our study that two competitive massive phases are separated by a gapless line (critical line). We find in our analysis that the critical points (trivial and nontrivial) are non-Gaussian in nature. There is no phase crossover owing to the change of the critical point from the trivial to the nontrivial one. There is no evidence of magnetization plateau, however the system is in the Ising criticality. The positive and negative values of umklapp-like scattering favor a short range antiferromagnetic order because of the *XY* anisotropy and the transverse field, respectively. Higher value of Luttinger liquid parameter (*K*) also favors the short range antiferromagnetic order due to the in-plane exchange anisotropy.

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I. INTRODUCTION

Low dimensional quantum spin systems have been studied extensively for last few decades, in view of many unusual and interesting findings from both experimental and theoretical studies^{1–3}. It was observed experimentally that the physical properties of low dimensional anisotropic antiferromagnets have strong dependence on the magnetic field orientation⁴. One can also find that spin nonconserving processes introduce anisotropy in the XY plane^{3,5}. The first approach to solve the anisotropic XXZ, Heisenberg chain under a uniform magnetic field along the z direction was by Yang and Yang⁶. Here we present a study of the XYZ Heisenberg chain with its variant (XY Heisenberg spin- $\frac{1}{2}$ Hamiltonian) under a transverse magnetic field. We think that this problem is more interesting than the XXZ Heisenberg spin- $\frac{1}{2}$ chain under a uniform magnetic field along z direction. A longitudinal field commutes with XXZ Hamiltonian. This is not the case when the symmetry breaking transverse magnetic field is applied and the exact integrability is lost. Much less attention has been paid to this problem because of analytical complexities. Here we solve this problem through Abelian bosonization and renormalization group techniques.

In the present study we observe the failure of naive expectation when the perturbation of two relevant fields are present. In this situation, naive expectation is that low energy behavior of the theory would be governed by the most relevant operators and at any rate the theory would remain fully massive. But we see in our study that the two massive phases are separated by a gapless (critical) line.

Sections of this paper are the following: In Sec. II, we present the theoretical formulations of our problem with the phase diagram. A discussion about the fix points and stability analysis around the fix points are also given there. Section III is devoted to discussions and conclusions.

II. MODEL HAMILTONIANS, THEORETICAL FORMULATIONS, AND PHYSICAL ANALYSIS

We consider the anisotropic Heisenberg spin- $\frac{1}{2}$ Hamiltonian on a one dimensional lattice. The *XYZ* Heisenberg Hamiltonian is defined as

$$H_{XYZ} = \sum_{n} \left[(1+a) S_n^x S_{n+1}^x + (1-a) S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z - h S_n^x \right],$$
(1)

where S_n^{α} are the spin- $\frac{1}{2}$ operators. We assume that the *XY* anisotropy *a* and the *zz* coupling Δ satisfy $-1 \le a, \Delta \le 1$, and magnetic field strength $h \ge 0$. The Hamiltonian H_{XYZ} is invariant under the transformation $S_n^x \to S_n^x$, $S_n^y \to -S_n^y$, $S_n^z \to -S_n^z$, actually it is a Z_2 symmetry. For finite *h*, Z_2 symmetry is absent when $S_n^x \to -S_n^x$.

Spin operators can be recasted in terms of spinless fermions through Jordan-Wigner transformation and then finally one can express the spinless fermions in terms of bosonic fields³. ϕ (bare) and θ (dual) fields are related with left and right moving fields by this relation, $\phi = \phi_L + \phi_R$, $\theta = \phi_L - \phi_R$. The analytical form of the spin operators in terms of the bosonic fields are

$$S_n^x = [c_2 \cos(2\sqrt{\pi K}\phi) + (-1)^n c_3] \cos\left(\sqrt{\frac{\pi}{K}}\theta\right),$$

$$S_n^y = -[c_2 \cos(2\sqrt{\pi K}\phi) + (-1)^n c_3] \sin\left(\sqrt{\frac{\pi}{K}}\theta\right),$$

$$S_n^z = \sqrt{\frac{\pi}{K}}\partial_x \phi + (-1)^n c_1 \cos\left(2\sqrt{\pi K}\phi\right),$$
 (2)

where c_i 's are constants as given in Ref. 7. Hamiltonian H_0 is the noninteracting part of H_{XYZ} ,

$$H_0 = \frac{v}{2} \int dx [(\partial_x \theta)^2 + (\partial_x \phi)^2], \qquad (3)$$

where v is the velocity of the low-energy excitations. It is one of the Luttinger liquid parameters and the other is K, which is related to Δ by^{2,8}

$$K = \frac{\pi}{\pi + 2\sin^{-1}(\Delta)}.$$
 (4)

K takes the values 1 and 1/2 for $\Delta = 0$ (free field), and $\Delta = 1$ (isotropic antiferromagnet), respectively. The relation between *K* and Δ is not preserved under the renormalization, so this relation is only correct for the initial Hamiltonian. The Hamiltonian H_{XYZ} in terms of bosonic fields is the following:

$$H_{XYZ} = H_0 + a \int \cos\left(2\sqrt{\frac{\pi}{K}}\theta(x)\right) dx$$
$$+ \Delta \int \cos[4\sqrt{\pi K}\phi(x)] dx$$
$$- h \int \cos[2\sqrt{\pi K}\phi(x)] \cos\left(\sqrt{\frac{\pi}{K}}\theta(x)\right) dx. \quad (5)$$

One can get the H_{XY} Hamiltonian by simply setting $\Delta = 0$ in the above Hamiltonian. In this derivation, different powers of coefficients c_i have been absorbed in the definition of a, hand Δ . The integration of the oscillatory terms in the Hamiltonian yield negligible small contributions, the origin of the oscillatory terms are the spin operators. So it is a resonably good approximation to keep only the nonoscillatory terms in the Hamiltonian^{3,8}. We will now study how the parameters a_{1} , h, Δ , and K flow under RG. The operators in Eq. (1) are related to each other through the operator product expansion; the RG equations for their coefficients will therefore be coupled to each other. Here we derive the RG equations by using the perturbative renormalization group approach scheme. We use operator product expansion to derive these RG equations which is independent of boundary condition⁹. RG equations themselves have been established in a perturbative expansion in coupling constant $\lceil g(l) \rceil$, they cease to be valid beyond the certain length scale, where $g(l) \sim 1^3$. The RG equations for the coefficients of Hamiltonian H_{XYZ} are

$$\frac{dh}{dl} = \left(2 - K - \frac{1}{4K}\right)h - \frac{1}{K}ah - 4KOh,$$

$$\frac{da}{dl} = \left(2 - \frac{1}{K}\right)a - \left(2K - \frac{1}{2K}\right)h^{2},$$

$$\frac{dO}{dl} = (2 - 4K)O + \left(2K - \frac{1}{2K}\right)h^{2},$$

$$\frac{dK}{dl} = \frac{a^{2}}{4} - K^{2}O^{2},$$
(6)

We consider K > 1/2 [see the analysis of Eq. (7)] in study of RG flow diagram, where the umklapp (Δ) term is irrelevant. So we drop the Δ term during the RG calculations. The RG equation for the *O* term is originating dynamically due to round up the operator product expansion of *a* and *h* term. $O = \cos[4\sqrt{\pi K}\phi(x)]$, which is similar to the Δ term. In principle *v* can renormalize but it will not effect the behavior of critical points¹⁰. In our problem there is no velocity anisotropy, i.e., the velocity is the same for all fields. The effect of velocity anisotropy is discussed briefly in Ref. 17. One can get the RG equations for the Hamiltonian H_{XY} by simply setting O=0 in Eqs. (6), for this case we get only three RG equations. We have obtained the same set of RG equations as in Ref. 10 for the Hamiltonian H_{XYZ} . Here we report some extensive and improved studies compared to that in Ref. 10. We solve the RG equations numerically, with the help of a sophisticated numerical package, MATLAB¹¹. The same RG equations appeared earlier in different contexts. However, the last two terms in the expression for dh/dl were not present in Ref. 12; these two terms have some importance to keep the duality invariant. Note that Eqs. (6) are invariant under the duality invariant for the RG equations of H_{XY} Hamiltonian.

Now we analyze the fixed points (FP). RG equations (6) have two fixed points, one is trivial and the other is non-trivial. For nontrivial FP, any value of K^* lying in the range $1/2 < K^* < 1 + \sqrt{3}/2$ is physical for our study. The nontrivial FP is given by

$$h^* = \frac{\sqrt{2K^*(2 - K^* - 1/4K^*)}}{2K^* + 1},$$
$$a^* = \left(K^* + \frac{1}{2}\right)h^{*2}, \quad \text{and} \quad O^* = \frac{a^*}{2K^*}.$$
(7)

Upperbound of $K^* \rightarrow 1 + \sqrt{3}/2 \approx 1.866$, yields the XXZ anisotropic coupling Δ [from Eq. (4)] ≈ -0.666 , which is consistent with our assumption, i.e., $|\Delta| < 1$. There is only one FP (trivial) for the RG equations of the H_{XY} Hamiltonian.

Now we present the phase diagram from the study of Abelian bosonization. We do this analysis from the consideration that the low-energy properties of the system will be governed by the most relevant perturbation. This analysis is only valid very near to the trivial FP. Scaling dimensions for the perturbations a, Δ , and h are $\frac{1}{K}$, 4K, and $K + \frac{1}{4K}$, respectively. The system shows the short range antiferromagnetic order due to the transverse field for the values of K lying in the range, $1/2 \le K \le 1 + \frac{\sqrt{3}}{2}$. One can also find from the comparison of scaling dimension that a short range antiferromagnetic order due to the in-plane exchange anisotropy will prevail for the values of K lying in the range, $\frac{\sqrt{3}}{2} < K < 1 + \frac{\sqrt{3}}{2}$. Here the phase diagram of Hamiltonian H_{XYZ} is the same as in H_{XY} because the lower bound of K is 1/2. If $\Delta > 1$ (K < 1/2) then the umklapp term of Hamiltonian H_{XYZ} will become relevant. This phase analysis through the Abelian bosonization study near to the trivial fixed point has not been covered in Ref. 10.

In Fig. 1, we present the RG flow diagram in the a-h plane for Eqs. (6). Solid lines are the RG flow lines and the arrows indicate the directions. Two massive phases are marked by the regions A and B. We observe in our study that there is a unique line in the a-h plane for very small values of a and h for each value of K. Now we present some analytical results in a special limit: we observe that if $h \ll a^{1/2}$, then $h(l) \sim h(0)\exp(2-K-1/4K)l$ while $a(l) \sim \exp(2-1/K)l$. Hence h must initially scale with a as



FIG. 1. RG flow diagram on the a-h plane for Eqs. (6). The solid lines and arrows are indicating the flows and directions of this phase diagram. A and B are the gapped phases (see text). Initial values of the parameters are K=1 and O=0.

$$h \sim a^{(2-K-1/4K)/(2-1/K)}$$
 (8)

as we have numerically verified for K=1. However, Eq. (8) is only true, if $K < (1 + \sqrt{2})/2 = 1.207$ (i.e., $\Delta \le -0.266$), the initial scaling form is given by $h \sim a^{1/2}$. In region A, the points flow to $a=\infty$; this corresponds to a gapped phase in which the *xx* coupling is larger than the *yy* coupling. In region B, *a* flows to $-\infty$ and *h* flow to ∞ ; this is a gapped phase in which the *yy* coupling is larger than the *xx* coupling. The staggered magnetization in the *y* direction, defined in terms of a ground state expectation value as

$$m_{y} = \left[\lim_{n \to \infty} (-1)^{n} \langle S_{0}^{y} S_{n}^{y} \rangle\right]^{1/2}, \tag{9}$$

mark the difference between the two phases. This is zero in phase A. In phase B, m_y is nonzero, and the Z_2 symmetry is broken. The scaling of m_y with δE can be found as follows¹³. At a=h=0, the leading term in the long-distance equal-time correlation function of S^y is given by

$$\langle S_0^y S_n^y \rangle \sim \frac{(-1)^n}{|n|^{1/2K}}.$$
 (10)

Hence the scaling dimension of S_n^y is 1/4K. In a gapped phase in which the correlation length is much larger than the lattice spacing, m_y will therefore scale with the gap as $m_y \sim (\Delta E)^{1/4K}$.

Apart from the trivial FP, we predict one more FP, which is nontrivial. Both of them are non-Gaussian in nature and Ising type. We now examine the stability of small perturbations away from the nontrivial FP. The nontrivial FP has two stable directions, one unstable direction and one marginal direction. The presence of two stable directions implies that there is a two-dimensional surface of points which flows to this FP; the system is gapless on that surface. A perturbation in the unstable direction produces a gap in the spectrum. At the nontrivial FP with



FIG. 2. Critical lines are on the a-h plane for Eqs. (6), solid line for O=0, dashed lines are for O=0.3, 0.2, 0.05 from upper to lower one, respectively. Dotted lines are for O=-0.3, -0.2, -0.05 from lower to upper one, respectively. Fix points are marked by asterisk. Initial value of K is 1.

 $(K^*, a^*, \Delta^*, h^*) = (1.522, 0.248, 0.081, 0.35)$, the four RG eigenvalues are given by 1.521 (unstable), 0(marginal), and -2.3216+0.9031i (stable) -2.3216-0.9031i (stable). A small perturbation of size δa in that direction will produce a gap in the spectrum which scales as $\Delta E \sim |\delta a|^{1/1.522} = |\delta a|^{0.657}$; the correlation length is then given by $\xi \sim v / \Delta E \sim |\delta a|^{-0.657}$.

In Fig. 2, we present the role of the O term (umklapp-like) in the RG flow diagram for the Eqs. (6). We find some importance of the O term in the RG flow diagram. The positive values of the O term favor the existence of short range antiferromagnetic order due to in-plane exchange anisotropy. As a result the critical line as well as the nontrivial FP shift in the upward direction. The negative values of the O term favor the short range antiferromagnetic order owing to the transverse field. This causes shift in both the critical line and nontrivial FP in the downward direction. This study has not covered in Ref. 10.

In Fig. 3, we present the critical lines for the RG flow diagrams of Eq. (6) and the XY limit of these RG equations for different values of the Luttinger liquid parameter (K), which are consistent with our theory. We observe that the higher values of K favor the short range antiferromagnetic order due to the in-plane exchange anisotropy. This study has not been covered in Ref. 10.

III. DISCUSSIONS AND CONCLUSIONS

We have presented the RG flow phase diagram of XYZHeisenberg spin- $\frac{1}{2}$ chain under transverse magnetic field. The basic nature of the phase diagram, viz., two massive phases separated by a gapless line, is the same for both model Hamiltonians. This gapless line is nothing but the spin-flip transition line, short range antiferromagnetic order is changing the direction of the alignment across this line. We have predicted two kinds of fixed points, one is trivial and the



FIG. 3. Critical lines are on the *a*-*h* plane for Eqs. (6) (dotted), and the dashed line is for the *XY* limit of Eqs. (6) for different values of K=3/2,1,3/4 from higher to lower, respectively. Critical points are marked by asterisks. Initial value of *O* is 0.

other is the nontrivial. Both are non-Gaussian. An Ising criticality occurs in phase B, around both fixed points. It is common in the literature, that the trivial fixed point corresponds to the Gaussian fixed points (free field) while the nontrivial fixed point corresponds to the interacting phase of the system¹⁴, there is phase crossover due to the change of fixed point from Gaussian to non-Gaussian^{14,15}. But in our study, we have not seen any phase crossover. This phase diagram has already been studied in Ref. 10. However, there are some differences between the Ref. 10 findings and our findings.

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The locus of the critical line, especially after the nontrivial FP and also the coordinate of nontrivial FP, as we have obtained, are different from Ref. 10. We have done the Abelian bosonization study to extract the phase regions near the trivial fixed point. This study has not been covered in Ref. 10. It is revealed in our study that the positive values of umklapp-like scattering terms are favoring the short range antiferromagnetic order due to in-plane exchange anisotropy, whereas the negative values of umklapp scattering are favoring the short range antiferromagnetic order due to transverse magnetic field. This study has not been covered in Ref. 10. We observe that higher values of K favor the short range antiferromagnetic due to in-plane exchange anisotropy. This study has not been covered in Ref. 10. The anisotropic Heisenberg (XXZ) spin chain in a transverse magnetic field has already been studied in Ref. 13. They found the Néel order along the Y and Z axis for $\Delta < 1$ and $\Delta > 1$, respectively. The anisotropic Heisenberg model under a longitudinal field have already been studied in Ref. 16. They have found evidence of magnetization plateaus for K < 1/2 and short range antiferromagnetic order due to in-plane exchange anisotropy for K > 1/2. In our study, there is no possibility for finding the magnetization plateau phase for two reasons. One is for the lacking of in-plane rotational symmetry and the other is that $\Delta < 1$ (*K*<1/2).

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- ¹⁷For the velocity anisotropy situation $(v_{\phi} \neq v_{\theta})$, one can write the $H_0 = \frac{\sqrt{v_{\phi}v_{\theta}}}{2} \int dx \left[K_1(\partial_x \theta)^2 + \frac{1}{K_1}(\partial_x \phi)^2 \right]$, where $K_1 = K \sqrt{\frac{v_{\theta}}{v_{\phi}}}$ and v_{ϕ} and v_{θ} are the velocity for ϕ and θ fields, respectively. So the velocity anisotropy effect can be absorbed in the renormalization of *K*. Now the system has effective velocity, $\sqrt{v_{\phi}v_{\theta}}$. For this expression of H_0 , there will be no K_1 term in the sine-Gordon couplings.