Gapless Phase in the XYZ Spin-1/2 Chain in a Magnetic Field and the Quantum ANNNI Chain

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We study the XYZ spin-1/2 chain placed in a magnetic field pointing along the x-axis. We use bosonization and a renormalization group analysis to show that the model has a non-trivial fixed point at a certain value of the XY anisotropy $a$ and the magnetic field $h$. Hence, there is a line of critical points in the $(a,h)$ plane on which the system is gapless, even though the Hamiltonian has no continuous symmetry. The quantum critical line separates a gapped commensurate phase from a gapped incommensurate phase. Our study explains why the floating phase of the axial next-nearest neighbor Ising (ANNNI) chain in a transverse magnetic field is only a line, as shown by recent numerical studies.

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One-dimensional quantum spin systems have been studied extensively ever since the isotropic spin-1/2 chain was solved exactly by Bethe. Baxter later used the Bethe ansatz to solve the fully anisotropic (XYZ) spin-1/2 chain in the absence of a magnetic field [1], the problem has not been analytically solved in the presence of a magnetic field. Experimentally, quantum spin chains and ladders are known to exhibit a wide range of unusual properties, including both gapless phases with a power-law decay of the two-spin correlations and gapped phases with an exponential decay [2,3]. There are also two-dimensional classical statistical mechanics systems (such as the axial next-nearest neighbor Ising (ANNNI) model) whose finite temperature properties can be understood by studying an equivalent quantum spin-1/2 chain in a magnetic field. The ANNNI model has been studied by several techniques, and it was believed for a long time to have a floating phase of finite width in which the system is gapless [1]. However, a recent large-scale numerical study has shown that the width of this phase seems to be zero within numerical errors [1].

Amongst the powerful analytical methods now available for studying quantum spin-1/2 chains is the technique of bosonization [2]. Recently, the XXZ chain in a magnetic field [4] and the quantum ANNNI model [5,6] have been studied using bosonization. In this work, we will study the fully anisotropic XYZ model in a magnetic field pointing along the x-axis. For small values of the XY anisotropy $a$ and the magnetic field $h$, we will show that there is a non-trivial fixed point (FP) of the renormalization group (RG) in the $(a,h)$ plane: the system is gapless on a quantum critical line of points which flow to this FP. The floating phase of the ANNNI model will be shown to be a special case of our results corresponding to $\Delta = 0$. The gapless line is somewhat unusual because the XY anisotropy and the magnetic field both break the continuous symmetry of rotations in the $x - y$ plane. We will provide a physical understanding of this line by going to the classical (large $S$) limit of the model.

We consider the Hamiltonian defined on a chain of sites

$$H = \sum_n \left[ (1 + a) S_n^x S_{n+1}^z + (1 - a) S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z - hS_n^z \right].$$

(1)

We will assume that the XY anisotropy $a$ and the $zz$ coupling $\Delta$ satisfy $-1 \leq a, \Delta \leq 1$. We can assume without loss of generality that the magnetic field strength $h \geq 0$. For $a = h = 0$, the model is symmetric under rotations in the $x - y$ plane and is gapless. The low-energy and long-wavelength modes of the system are described by the bosonic Hamiltonian

$$H_0 = \frac{v}{2} \int dx \left[ (e^\phi)^2 + (\partial_x \phi)^2 \right],$$

(2)

where $v$ is the velocity of the low-energy excitations (which have the dispersion $\omega = v|k|$); $v$ is a function of $\Delta$. (The continuous space variable $x$ and the site label $n$ are related through $x = nd$, where $d$ is the lattice spacing). The bosonic theory contains another parameter called $K$ which is related to $\Delta$ by

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

(3)

$K$ takes the values 1 and 1/2 for $\Delta = 0$ (which describes noninteracting spinless fermions) and 1 (the isotropic antiferromagnet) respectively; as $\Delta \to -1$, $K \to \infty$. We thus have $1/2 \leq K < \infty$.

The spin-density operators can be written as

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

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

(4)
where the $c_i$ are constants given in Ref. 10. The XY anisotropy term is given by
\[ S_n^x S_{n+1}^x - S_n^y S_{n+1}^y = c_4 \cos(2\sqrt{\frac{\pi}{K}} \theta), \tag{5} \]
where $c_4$ is another constant.

For convenience, let us define the three operators
\[ \mathcal{O}_1 = \cos(2\sqrt{\frac{\pi}{K}} \phi) \cos(\sqrt{\frac{\pi}{K}} \theta), \]
\[ \mathcal{O}_2 = \cos(2\sqrt{\frac{\pi}{K}} \theta), \quad \text{and} \quad \mathcal{O}_3 = \cos(4\sqrt{\pi} K \phi). \tag{6} \]

Their scaling dimensions are given by $K + 1/4K$, $1/K$ and $4K$ respectively. Using Eqs. (4-5), the terms corresponding to $a$ and $h$ in Eq. (6) can be written as
\[ H_a + H_h = \int dx \left[ ac_2 \mathcal{O}_2 - hc_2 \mathcal{O}_1 \right], \tag{7} \]
where we have dropped rapidly varying terms proportional to $(−1)^n$ since they will average to zero in the continuum limit. (We will henceforth absorb the factors $c_4$ ($c_2$) in the definitions of $a$ ($h$)). We will now study how the parameters $a$ and $h$ flow under RG.

The operators in Eqs. (6) are related to each other through the operator product expansion; the RG equations for their coefficients will therefore be coupled to each other (11). In our model, this can be derived as follows. Given two operators $A_1 = \exp(i\alpha_1 \phi + i\beta_1 \theta)$ and $A_2 = \exp(i\alpha_2 \phi + i\beta_2 \theta)$, we write the fields $\phi$ and $\theta$ as the sum of slow fields (with wave numbers $\vert k \vert < \Lambda e^{-dl}$) and fast fields (with wave numbers $\Lambda e^{-dl} < \vert k \vert < \Lambda$), where $\Lambda$ is the momentum cut-off of the theory, and $dl$ is the change in the logarithm of the length scale. Integrating out the fast fields shows that the product of $A_1$ and $A_2$ at the same space-time point gives a third operator $A_3 = e^{i(\alpha_1 + \alpha_2) \phi + i(\beta_1 + \beta_2) \theta}$ with a prefactor which can be schematically written as
\[ A_1 A_2 \sim e^{-(\alpha_1 + \alpha_2 + \beta_1 + \beta_2) dl/2\pi} A_3. \tag{8} \]

If $\lambda_i(l)$ denote the coefficients of the operators $A_i$ in an effective Hamiltonian, then the RG expression for $d\lambda_3/dl$ will contain the term $(\alpha_1 \alpha_2 + \beta_1 \beta_2) \lambda_1 \lambda_2 / 2\pi$. Using this, we find that if the three operators in (6) have coefficients $h$, $a$ and $b$ respectively, then the RG equations are
\[ \frac{dh}{dl} = (2 - K - \frac{1}{4K})h - \frac{1}{K} ah - 4K bh, \]
\[ \frac{da}{dl} = (2 - \frac{1}{K})a - (2K - \frac{1}{2K})h^2, \]
\[ \frac{db}{dl} = (2 - 4K)b + (2K - \frac{1}{2K})h^2, \]
\[ \frac{dK}{dl} = \frac{a^2}{4} - K^2 b^2, \tag{9} \]
where we have absorbed some factors involving $v$ in the variables $a$, $b$ and $h$. (We will ignore the RG equation for $v$ here). It will turn out that $K$ renormalizes very little in the regime of RG flows that we will be concerned with. Eqs. (9) have appeared earlier in the context of some other problems (8). However, the last two terms in the expression for $dh/dl$ were not presented in Ref. 8; these two terms turn out to be crucial for what follows. Note that Eqs. (9) are invariant under the duality transformation $K \leftrightarrow 1/4K$ and $a \leftrightarrow b$.

Let us now consider the fixed points of Eqs. (9). For any value of $K = K^*$, a trivial FP is $(a^*, b^*, h^*) = (0, 0, 0)$. Remarkably, it turns out that there is a non-trivial FP for any value of $K^*$ lying in the range $1/2 < K^* < 1 + \sqrt{3}/2$; we will henceforth restrict our attention to this range of values. (The upper bound on $K^*$ comes from the condition $2 - K^* - 1/4K^* > 0$). The non-trivial FP is given by
\[ h^* = \frac{\sqrt{2K^* (2 - K^* - 1/4K^*)}}{(2K^* + 1)}, \]
\[ a^* = \frac{K^* + 1}{2} h^{*2}, \quad \text{and} \quad b^* = \frac{a^*}{2K^*}. \tag{10} \]

The system is gapless at this FP as well as at all points which flow to this FP. One might object that Eqs. (9) can only be trusted if $a$, $b$ and $h$ are not too large, otherwise one should go to higher orders. We note that the FP approaches the origin as $K^* \rightarrow 1 + \sqrt{3}/2 \approx 1.866$; this corresponds to the $\phi\phi$ coupling $\Delta = -\sin[\pi(\sqrt{3} - 3/2)] \approx -0.666$. Thus the RG equations can certainly be trusted for $K^*$ close to $1.866$. For $K^* = 1$, the FP is at $(a^*, b^*, h^*) = (1/4, 1/8, 1/\sqrt{6})$.

We have numerically studied the RG flows given by Eqs. (9) for various starting values of $(K, a, b, h)$. Since the Hamiltonian in (9) does not contain the operator $O_3$, we set $b = 0$ initially. We take $a$ and $h$ to be very small initially, and see which set of values flows to a non-trivial FP. For instance, starting with $K = 1$, $b = 0$, and $a, h$ very small, we find that there is a line of points which flow to a FP at $(K^*, a^*, b^*, h^*) = (1.020, 0.246, 0.122, 0.404)$. This line in the $(a, h)$ plane is shown in Fig. 1. We see that $K$ changes very little during this flow; if we start with a larger value of $K$ initially, then it changes even less as we go to the non-trivial FP. It is therefore not a bad approximation to ignore the flow of $K$ completely.

We can characterize the set of points $(a, h)$ lying close to the origin which flow to the non-trivial FP. Numerically, we find that there is a unique flow line in the $(a, h)$ plane for each starting value of $K$ and $b = 0$, provided that $a, h$ are very small initially. This means that $a(l)$ and $h(l)$ given by Eqs. (9) must follow the same line regardless of the starting values of $a, h$. From Eqs. (9), we see that if $h << a^{1/2}$, 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
\[ h \sim a^{(2 - K - 1/4K)/(2 - 1/K)}, \tag{11} \]
as we have numerically verified for $K = 1$. However, Eq.
is only true if \((2 - K) / (2 - 1/K) > 1/2\), i.e., if \(K < (1 + \sqrt{2})/2 = 1.207\). For \(K \geq 1.207\) (i.e., \(\Delta \leq -0.266\)), the initial scaling form is given by \(h \sim a^{1/2}\).

We now examine the stability of small perturbations away from the fixed points. The trivial FP at the origin has two unstable directions \((a, h)\), one stable direction \((b)\) and one marginal direction \((K)\). The non-trivial FP has two stable directions, one unstable direction and a marginal direction (which corresponds to changing \(K^*\) and simultaneously \(a^*, b^*\) and \(h^*\) to maintain the relations in Eqs. (11)). The presence of two stable directions implies that there is a two-dimensional surface of points (in the space of parameters \((a, b, h)\)) which flows to this FP; the system is gapless on that surface. A perturbation in the unstable direction produces a gap in the spectrum. For instance, at the FP \((K^*, a^*, b^*, h^*) = (1, 1/4, 1/8, 1/\sqrt{6})\), the four RG eigenvalues are given by 1.273 (unstable), 0 (marginal), and \(-1.152 \pm 1.067i\) (both stable). The positive eigenvalue corresponds to an unstable direction given by \((\delta K, \delta a, \delta b, \delta h) = \delta a(0.113, 1, -0.092, -0.239)\). A small perturbation of size \(\delta a\) in that direction will produce a gap in the spectrum which scales as \(\Delta E \sim |\delta a|^{1/1.273} = |\delta a|^{0.786}\); the correlation length is then given by \(\xi \sim \nu/\Delta E \sim |\delta a|^{-0.786}\).

Fig. 1 shows that the set of points which do not flow to the non-trivial FP belong to either region A or region B. These regions can be reached from the non-trivial FP by moving in the unstable direction, with \(\delta a > 0\) for region A, and \(\delta a < 0\) for region B. In region A, the points flow to \(a = \infty\); this corresponds to a gapped phase which is commensurate since the magnetic field \(h\) asymptotically flows to zero. In region B, both \(a\) and \(h\) flow to \(-\infty\); this is a gapped incommensurate phase. The line separating the two regions is a commensurate-incommensurate transition line. An order parameter which distinguishes between regions A and B is the staggered magnetization in the \(y\) direction, defined as

\[
m_y = \lim_{n \to \infty} \frac{1}{n^{1/2}} \frac{(1 - (-1)^n)}{< S_n^y >}^{1/2}.
\]

This is zero in the commensurate phase A. In the incommensurate phase B, it is non-zero, and its scaling with the perturbation \(\delta a\) can be found as follows [3]. At \(a = h = 0\), the leading term in the long-distance equal-time correlation function of \(S^y\) is given by

\[
< S_n^y S_{n+m}^y > \sim \frac{(-1)^n}{|n|^{1/2}}.
\]

Hence the scaling dimension of \(S^y_n\) is 1/4K. In a gapped incommensurate phase in which the correlation length is much larger than the lattice spacing, \(m_y\) will therefore scale with the gap as \(m_y \sim (\Delta E)^{1/4K}\). If we assume that the scaling dimension of \(S^y_n\) at the non-trivial FP remains close to 1/4K, then the numerical result quoted in the previous paragraph for \(K = 1\) implies that \(m_y \sim |\delta a|^{0.196}\) for \(\delta a\) small and negative.

We will now apply our results to the one-dimensional spin-1/2 quantum ANNNI model [5], with nearest neighbor ferromagnetic and next-nearest neighbor antiferromagnetic Ising interactions and a transverse magnetic field. The Hamiltonian is given by

\[
H_A = \sum_i \left[ -2J_1S_i^T S_{i+1}^T + J_2S_i^T S_{i+2}^T + \frac{\Gamma}{2} S_i^y \right],
\]

where \(J_1, J_2 > 0\); we can assume without loss of generality that \(\Gamma \geq 0\). The quantum Hamiltonian in (14) is related to the transfer matrix of the two-dimensional classical ANNNI model; the finite temperature critical points of the latter are related to the ground state quantum critical points of (14), with the temperature \(T\) being related to the magnetic field \(\Gamma\). Earlier studies showed that the model has a floating phase of finite width which is gapless and incommensurate [6]. A recent bosonization study reached the same conclusions [7]. However, a more recent numerical study involving very large two-dimensional classical systems at finite temperature concluded that the floating phase seems to have zero width [8]. We can now understand this as follows. Consider a Hamiltonian which is dual to (14) for spin-1/2; this will turn out to be a special case of our earlier model. The dual Hamiltonian is given by

\[
H_D = \sum_n \left[ J_2T_n^x T_{n+1}^x + \Gamma T_n^y T_{n+1}^y - J_1T_n^x \right],
\]

where \(T_n^x\) are the spin-1/2 operators dual to \(S_n^x\). Let us scale this Hamiltonian by a factor to make \(J_2 + \Gamma = 2\).
Then this has the same form as in Eq. (1), with $J_2 = 1 + a$, $\Gamma = 1 - a$, $J_1 = h$, and $\Delta = 0$. Hence it follows that the quantum ANNNI model has a line of points in the $(J_2 - \Gamma, J_1)$ plane on which the system is gapless. (From Eq. (1), we see that the shape of this line is given by $J_1 \sim (J_2 - \Gamma)^{3/4}$ as $J_1 \to 0$.) This line can be identified with the floating phase. Our results for the width of the floating agree completely with those obtained for the two-dimensional classical ANNNI model in Ref. 5. We should point out, however, that Ref. 5 shows the phase transition to be of the Kosterlitz-Thouless type (with $\xi$ diverging exponentially) from the high-temperature side (i.e., from region B in Fig. 1), and is of the commensurate-incommensurate type (with $\xi$ diverging as a power-law) from the low-temperature side (region A in Fig. 1). Our analysis indicates that it should be of the commensurate-incommensurate type from both sides. This discrepancy remains to be resolved. One comment to be made here is that Ref. 5 has studied two values of $J_2/J_1$ (0.6 and 0.8) which are not large; our RG results may be expected to be valid if $a, h$ are small, i.e., if $J_2/J_1$ is large.

Finally, we would like to provide a physical picture of the gapless line in the $(a, h)$ plane by looking at the classical limit of Eq. (1). Consider the Hamiltonian

$$H_S = \sum_n \left[ (1 + a) S_n^x S_{n+1}^x + (1 - a) S_n^y S_{n+1}^y \right. \right.$$

$$+ \Delta S_n^z S_{n+1}^z - h S S_n^z \left. \right] \, ,$$

where the spins satisfy $S_n^2 = S(S + 1)$, and we are interested in the classical limit $S \to \infty$ [12]. Let us assume that the $zz$ coupling is smaller in magnitude than the $xx$ and $yy$ couplings. Then the classical ground state of (16) is given by a configuration in which all the spins lie in the $x - y$ plane, with the spins on odd and even numbered sites pointing respectively at an angle of $\alpha_1$ and $-\alpha_2$ to the $x$-axis. The ground state energy per site is

$$e(\alpha_1, \alpha_2) = S^2 \left[ \frac{h}{2} (\cos \alpha_1 + \cos \alpha_2) \right.$$

$$+ \cos(\alpha_1 + \alpha_2) + a \cos(\alpha_1 - \alpha_2) \left. \right] \, .$$

Minimizing this with respect to $\alpha_1$ and $\alpha_2$, we discover that there is a special line given by $h^2 = 16a$ on which all solutions of the equation

$$h \cos\left(\frac{\alpha_1 + \alpha_2}{2}\right) = 4a \cos\left(\frac{\alpha_1 - \alpha_2}{2}\right) \, ,$$

give the same ground state energy per site, $e_0 = -(1 + a)aS^2$. The solutions of Eq. (18) range from $\alpha_1 = \alpha_2 = \cos^{-1}(4a/h)$ to $\alpha_1 = \pi, \alpha_2 = 0$ (or vice versa); in the ground state phase diagram of the ANNNI model, these two configurations correspond to the paramagnetic incommensurate phase and the antiphase respectively [11]. Classically, we see that the line $h^2 = 16a$ separates these two phases; we therefore identify this line with the floating phase [12]. The fact that there is a one-parameter set of ground states (characterized by, say, the value of $\alpha_1$ in the solution of (18)) which are all degenerate for $h^2 = 16a$ means that there is a gapless mode in the excitations; we can derive this explicitly by going to the next order in a $1/S$ expansion. Hence the model is gapless on that line. This provides some understanding of why one may expect such a gapless line in the spin-1/2 model also. Note however that the bosonization analysis gives the scaling form in (11) for $h$ versus $a$; this agrees with the classical form only if $\Delta \leq -0.266$.

To summarize, we have shown that the XY$Z$ spin-1/2 chain in a magnetic field exhibits a gapless phase on a particular line. It may be interesting to use numerical techniques like the density-matrix renormalization group method [13] to study various ground state properties of this model, in particular the behavior of order parameters such as the one defined in Eq. (12). The RG equations studied in this paper appear in other strongly correlated systems, such as the problem of two spinless Tomonaga-Luttinger chains with both one- and two-particle interchain hoppings [8], and one-dimensional conductors with spin-anisotropic electron interactions [8]. The gapless phase may therefore also appear in other systems.

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