

# Gapless line for the anisotropic Heisenberg spin- $\frac{1}{2}$ chain in a magnetic field and the quantum axial next-nearest-neighbor Ising chain

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We study the anisotropic Heisenberg ( $XYZ$ ) 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 nontrivial 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 corresponds to a spin-flip transition; it separates two gapped phases in one of which the  $Z_2$  symmetry of the Hamiltonian is broken. Our study has a bearing on one of the transitions of the axial next-nearest neighbor Ising chain in a transverse magnetic field. We also discuss the properties of the model when the magnetic field is increased further, in particular, the disorder line on which the ground state is a direct product of single spin states.

## I. INTRODUCTION

One-dimensional quantum spin systems have been studied extensively ever since the problem of the isotropic Heisenberg spin- $1/2$  chain was solved exactly by Bethe. Baxter later used the Bethe ansatz to solve the anisotropic Heisenberg ( $XYZ$ ) spin- $1/2$  chain in the *absence* of a magnetic field<sup>1</sup>; 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.<sup>2,3</sup> 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.<sup>4</sup>

Among the powerful analytical methods now available for studying quantum spin- $1/2$  chains is the technique of bosonization.<sup>2,5</sup> Recently, the  $XXZ$  chain in a transverse magnetic field<sup>6</sup> and the quantum ANNNI model<sup>7</sup> have been studied using bosonization. In this paper, we will study the 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 in Sec. II 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. In Sec. III, one of the transitions of the ANNNI model will be shown to be a special case of our results in which the  $zz$  coupling is equal to zero. Our results are complementary to earlier studies of the ANNNI model, which indicated a gapless phase of finite width. We will present the complete zero temperature phase diagram of the ANNNI model which has both a gapless phase of finite width as well as a gapless line.

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. In Sec. IV, we will provide a physical understanding of the gapless line by going to the classical (large  $S$ ) limit of the model; this helps us to identify it as a spin-flip transition line. In Sec. V, we will discuss a disorder line which lies at a larger value of the magnetic field. In Sec. VI, we will briefly comment on the Ising transition which occurs at an even larger value of the magnetic field.

## II. BOSONIZATION AND RENORMALIZATION GROUP ANALYSIS

We consider the anisotropic Hamiltonian defined on a chain of sites,

$$H = \sum_n [(1+a)S_n^x S_{n+1}^x + (1-a)S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z - h S_n^x], \quad (1)$$

where the  $S_n^\alpha$  are spin- $1/2$  operators. 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 magnitude of the  $zz$  coupling is smaller than the  $yy$  coupling (i.e.,  $|\Delta| < 1 - a$ ), and that the magnetic field strength  $h \geq 0$ . The Hamiltonian in Eq. (1) is invariant under the global  $Z_2$  transformation  $S_n^x \rightarrow S_n^x, S_n^y \rightarrow -S_n^y, S_n^z \rightarrow -S_n^z$ .

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 then described by the bosonic Hamiltonian<sup>2,5</sup>

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

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<sup>2,5</sup>

$$K = \frac{\pi}{\pi + 2 \sin^{-1}(\Delta)}. \quad (3)$$

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

In terms of the fields  $\phi$  and  $\theta$  introduced in Eq. (2), the spin operators can be written as<sup>6</sup>

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

$$S_n^x = [c_2 \cos(2\sqrt{\pi K} \phi) + (-1)^n c_3] \cos\left(\sqrt{\frac{\pi}{K}} \theta\right), \quad (4)$$

where the  $c_i$  are constants given in Ref. 8. The  $XY$  anisotropy term is given by

$$S_n^x S_{n+1}^x - S_n^y S_{n+1}^y = c_4 \cos\left(2\sqrt{\frac{\pi}{K}} \theta\right), \quad (5)$$

where  $c_4$  is another constant.

For convenience, let us define the three operators

$$\mathcal{O}_1 = \cos(2\sqrt{\pi K} \phi) \cos\left(\sqrt{\frac{\pi}{K}} \theta\right),$$

$$\mathcal{O}_2 = \cos\left(2\sqrt{\frac{\pi}{K}} \theta\right), \quad \text{and} \quad \mathcal{O}_3 = \cos(4\sqrt{\pi K} \phi). \quad (6)$$

Their scaling dimensions are given by  $K+1/4K$ ,  $1/K$ , and  $4K$ , respectively. Using Eqs. (4) and (5), the terms corresponding to  $a$  and  $h$  in Eq. (1) can be written as

$$H_a + H_h = \int dx [ac_4 \mathcal{O}_2 - hc_2 \mathcal{O}_1], \quad (7)$$

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 the 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.<sup>9</sup> 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  $|k| < \Lambda e^{-dl}$ ) and fast fields (with wave numbers  $\Lambda e^{-dl} < |k| < \Lambda$ ), where  $\Lambda$  is the momentum cutoff 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

$$A_1 A_2 \sim e^{-(\alpha_1 \alpha_2 + \beta_1 \beta_2) dl / 2\pi} A_3. \quad (8)$$

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 Eqs. (6) have coefficients  $h$ ,  $a$ , and  $b$ , respectively, then the RG equations are

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

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

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

$$\frac{dK}{dl} = \frac{a^2}{4} - K^2 b^2, \quad (9)$$

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. Equations (9) appeared earlier in the context of some other problems.<sup>10,11</sup> However, the last two terms in the expression for  $dh/dl$  were not presented in Ref. 10; 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 nontrivial 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 nontrivial FP is given by

$$h^* = \frac{\sqrt{2K^*(2 - K^* - 1/4K^*)}}{2K^* + 1},$$

$$a^* = \left(K^* + \frac{1}{2}\right) h^{*2} \quad \text{and} \quad b^* = \frac{a^*}{2K^*}. \quad (10)$$

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  $K^* \rightarrow 1 + \sqrt{3}/2 \approx 1.866$ ; from Eq. (3), this corresponds to the  $zz$  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 Eq. (1) does not contain the operator  $\mathcal{O}_3$ , we set  $b=0$  initially. We take  $a$  and  $h$  to be very small initially, and see which set of values flows to a nontrivial FP. For

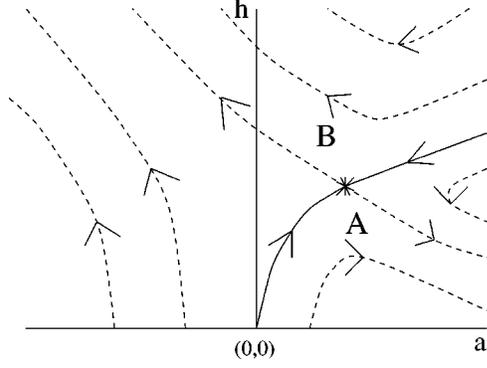


FIG. 1. RG flow diagram in the  $(a, h)$  plane. The solid line shows the set of points which flow to the FP at  $a^*=0.246$ ,  $h^*=0.404$  marked by an asterisk. The dotted lines show the RG flows in the gapped phases A and B (see the text).

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 projected on to 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 nontrivial 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 nontrivial 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  $a$  and  $h$  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  $h \ll a^{1/2}$ , 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

$$h \sim a^{(2 - K - 1/4K)/(2 - 1/K)}, \quad (11)$$

as we have numerically verified for  $K=1$ . However, Eq. (11) is only true if  $(2 - K - 1/4K)/(2 - 1/K) > 1/2$ , 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 ( $a$  and  $h$ ), one stable direction ( $b$ ), and one marginal direction ( $K$ ). The nontrivial 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. (10)]. 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 with  $(K^*, a^*, b^*, h^*) = (1, 1/4, 1/8, 1/\sqrt{6})$ , 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  $\xi \sim v/\Delta E \sim |\delta a|^{-0.786}$ .

Figure 1 shows that the set of points which do not flow to the nontrivial FP belong to either region A or region B. These regions can be reached from the nontrivial 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 in which the  $xx$  coupling is larger than the  $yy$  and  $zz$  couplings. In region B, both  $a$  and  $h$  flow to  $-\infty$ ; this is a gapped phase in which the  $yy$  coupling is larger than the  $xx$  and  $zz$  couplings. We will now see that the difference between these two phases lies in the way in which the  $Z_2$  symmetry of the Hamiltonian is realized. An order parameter which distinguishes between the two phases is the staggered magnetization in the  $y$  direction, defined in terms of a ground state expectation value as

$$m_y = [\lim_{n \rightarrow \infty} (-1)^n \langle S_0^y S_n^y \rangle]^{1/2}. \quad (12)$$

This is zero in phase A; hence the  $Z_2$  symmetry is unbroken. In phase B,  $m_y$  is nonzero, and the  $Z_2$  symmetry is broken. The scaling of  $m_y$  with the perturbation  $\delta a$  can be found as follows.<sup>6</sup> At  $a=h=0$ , the leading term in the long-distance equal-time correlation function of  $S^y$  is given by

$$\langle S_0^y S_n^y \rangle \sim \frac{(-1)^n}{|n|^{1/2K}}. \quad (13)$$

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  $m_y \sim (\Delta E)^{1/4K}$ . If we assume that the scaling dimension of  $S_n^y$  at the nontrivial 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.

The nature of the transition on the gapless line will be discussed in Sec. IV. We will argue there that this is a spin-flip transition line. (Spin-flip transitions in one-dimensional spin-1/2 chains have been studied earlier.<sup>12-14</sup>)

### III. QUANTUM ANNNI MODEL

We will now apply our results to the one-dimensional spin-1/2 quantum ANNNI model,<sup>4,7</sup> with nearest neighbor ferromagnetic and next-nearest neighbor antiferromagnetic Ising interactions and a transverse magnetic field. The Hamiltonian is given by

$$H_A = \sum_n \left[ -2J_1 T_n^x T_{n+1}^x + J_2 T_n^x T_{n+2}^x + \frac{\Gamma}{2} T_n^y \right], \quad (14)$$

where  $J_1, J_2 > 0$ , and the  $T_n^\alpha$  are spin-1/2 operators; we can assume without loss of generality that  $\Gamma \geq 0$ . The quantum Hamiltonian in Eq. (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 Eq. (14), with the temperature  $T$  being related to the magnetic field  $\Gamma$ .

Some earlier studies showed that the model has a floating phase of finite width which is gapless.<sup>4</sup> A recent bosonization study reached the same conclusions.<sup>7</sup> (Recent numerical studies of the two-dimensional classical ANNNI model at finite temperature have led to contradictory results for the width of the floating phase.<sup>15</sup>) All these studies (both analytical and numerical) indicate that the phase transition is of the Kosterlitz-Thouless type (with  $\xi$  diverging exponentially) from the high-temperature side (i.e., from region *B* in Fig. 1 for the quantum ANNNI model), and is of the Pokrovsky-Talapov type<sup>16</sup> (with  $\xi$  diverging as a power-law) from the low-temperature side (i.e., from region *A* in Fig. 1).

We will now apply our results to the quantum ANNNI model. Consider a Hamiltonian which is dual to Eq. (14) for spin-1/2; this will turn out to be a special case of our earlier model. The dual Hamiltonian is given by<sup>4,17</sup>

$$H_D = \sum_n [J_2 S_n^x S_{n+1}^x + \Gamma S_n^y S_{n+1}^y - J_1 S_n^x], \quad (15)$$

where  $S_n^\alpha$  are the spin-1/2 operators dual to  $T_n^\alpha$  (for instance,  $S_n^x = 2T_n^x T_{n+1}^x$  and  $T_n^y = 2S_{n-1}^y S_n^y$ ). After scaling this Hamiltonian by an appropriate factor, we see that it has the same form as in Eq. (1), with

$$\begin{aligned} a &= \frac{J_2 - \Gamma}{J_2 + \Gamma}, \\ h &= \frac{2J_1}{J_2 + \Gamma}, \\ \Delta &= 0. \end{aligned} \quad (16)$$

Hence it follows that the quantum ANNNI model has a line of points in the  $(J_2/J_1, \Gamma/J_1)$  plane on which the system is gapless. From Eq. (11), we see that the shape of this line is given by  $J_1 \sim (J_2 - \Gamma)^{3/4}$  as  $J_1 \rightarrow 0$ .

The analysis in Sec. II indicates that as the transition line is approached,  $\xi$  should diverge as a power law from both sides. We now have to reconcile this with some of the earlier analytical<sup>4,7</sup> and numerical<sup>15</sup> studies which showed that as one approaches the floating phase,  $\xi$  diverges as a power-law from phase *B* but exponentially from phase *A*. The important point is that these earlier studies were carried out at values of  $J_2/J_1$  which are close to 1, while our RG results are expected to be valid only if  $a, h$  are small, i.e., if  $J_2/J_1$  is large. If  $J_2/J_1$  is close to 1, the situation is quite different for the following reason. Exactly at  $J_2/J_1 = 1$  and  $\Gamma = 0$ , the Hamiltonian in Eq. (15) can be written in the form

$$H_{MC} = J_2 \sum_n \left( S_n^x - \frac{1}{2} \right) \left( S_{n+1}^x - \frac{1}{2} \right). \quad (17)$$

This is a multicritical point with a ground state degeneracy growing exponentially with the system size, since any state in which every pair of neighboring sites  $(n, n+1)$  has at least one site with  $S^x = 1/2$  is a ground state. We can now study what happens when we go slightly away from this multicritical point. To lowest order, this involves doing perturbation theory within the large space of degenerate states.

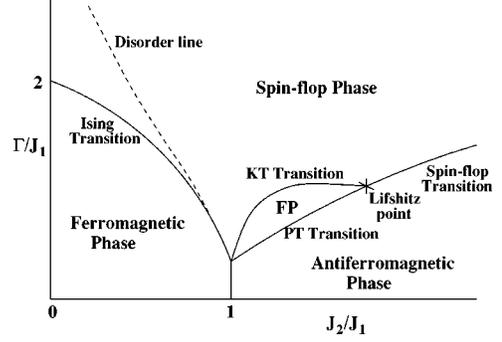


FIG. 2. Schematic phase diagram of the model described in Eq. (15). The various phases and transition lines are explained in the text. The initials FP, KT, and PT stand for floating phase, Kosterlitz-Thouless, and Pokrovsky-Talapov respectively.

An argument of Villain and Bak<sup>4</sup> showed that if  $J_2 - J_1$  and  $\Gamma$  are nonzero but small, then the low-energy properties of Eq. (15) do not change if  $\Gamma S_n^y S_{n+1}^y$  is replaced by  $(\Gamma/2)(S_n^y S_{n+1}^y + S_n^z S_{n+1}^z)$ . (This is because the difference between the two kinds of terms is given by operators which, acting on one of the degenerate ground states, take it out of the degenerate space to a higher excited state in which a pair of neighboring sites have  $S^x = -1/2$ .) Thus the fully anisotropic model becomes equivalent to a different model which is invariant under the U(1) symmetry of rotations in the  $y$ - $z$  plane. The U(1) symmetric model has been studied earlier using bosonization;<sup>2,11,18</sup> it has a gapless phase of finite width which lies between two gapped phases. Thus the difference between our study (in which  $J_2 - \Gamma$  and  $J_1$  are small) and the earlier studies (in which  $J_2 - J_1$  and  $\Gamma$  are small) is that they have different symmetries away from the transition line, namely,  $Z_2$  and U(1) respectively. Our study and the earlier studies are therefore complimentary to each other; a combination of the two leads to a complete understanding of the model over the entire parameter range.

To summarize, the transition from phase *A* to phase *B* can occur either through a gapless line (if  $a, h$  are small), or through a gapless phase of finite width (if  $a, h$  are large). The complete phase diagram of the ground state of Eq. (15) is shown in Fig. 2.<sup>4</sup> The three major phases shown are distinguished by the following properties of the expectation values of the different components of the spins. In the antiferromagnetic phase, the spins point alternately along the  $\hat{x}$  and  $-\hat{x}$  directions. In the spin-flip phase, they point alternately along the  $\hat{y}$  and  $-\hat{y}$  directions, with a uniform tilt towards the  $\hat{x}$  direction. In the ferromagnetic phase, all the spins point predominantly in the  $\hat{x}$  direction. The antiferromagnetic and spin-flip phases are separated by a floating phase of finite width for  $J_2/J_1$  close to 1/2, and by a spin-flip transition line for large values of  $J_2/J_1$ . We conjecture that the floating phase and the spin-flip transition line are separated by a Lifshitz point as indicated in Fig. 2. The disorder line and the Ising transition are discussed in Secs. V and VI, respectively.

We should point out here that in terms of the original Hamiltonian in Eq. (14), some of the phases shown in Fig. 2 have somewhat different names.<sup>4</sup> The spin-flip phase is

called the paramagnetic phase; this is further divided into two phases by the disorder line, namely, a commensurate phase to the left and an incommensurate phase on the right of the disorder line. The antiferromagnetic phase is called the antiphase.

#### IV. CLASSICAL LIMIT

In this section, 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

$$H_{S1} = \sum_n [(1+a)S_n^x S_{n+1}^x + (1-a)S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z - 2ShS_n^x], \quad (18)$$

where the spins satisfy  $S_n^2 = S(S+1)$ , and we are interested in the classical limit  $S \rightarrow \infty$ .<sup>17</sup> [We have multiplied the magnetic field by a factor of  $2S$  in Eq. (18) so that we recover Eq. (1) for spin-1/2.] We assume as before that the  $zz$  coupling is smaller in magnitude than the  $yy$  coupling. Then the classical ground state of Eq. (18) 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  $-\alpha_2$  with respect to the  $x$  axis. The ground state energy per site is

$$e(\alpha_1, \alpha_2) = S^2 [-h(\cos \alpha_1 + \cos \alpha_2) + \cos(\alpha_1 + \alpha_2) + a \cos(\alpha_1 - \alpha_2)]. \quad (19)$$

Minimizing this with respect to  $\alpha_1$  and  $\alpha_2$ , we discover that there is a special line given by  $h^2 = 4a$  on which *all* solutions of the equation

$$h \cos\left(\frac{\alpha_1 - \alpha_2}{2}\right) = 2 \cos\left(\frac{\alpha_1 + \alpha_2}{2}\right) \quad (20)$$

give the same ground state energy per site,  $e_0 = -(1+a)S^2$ . The solutions of Eq. (20) range from  $\alpha_1 = \alpha_2 = \cos^{-1}(h/2)$  to  $\alpha_1 = \pi, \alpha_2 = 0$  (or vice versa); in the ground state phase diagram of the ANNNI model, these two configurations correspond respectively to an antiferromagnetic alignment of the spins with respect to the  $y$  axis (with a small tilt toward the  $x$  axis if  $h$  is small), and an antiferromagnetic alignment of the spins with respect to the  $x$  axis. The curve  $h^2 = 4a$  is therefore a phase transition line, and the form of the ground states on the two sides shows that there is a spin-flip transition across that line. Further, we see that for  $h^2 = 4a$ , there is a one-parameter set of classical ground states [characterized by, say, the value of  $\alpha_1$  which can go all the way from 0 to  $2\pi$  in the solutions of Eq. (20)] which are all degenerate. Hence the symmetry is enhanced from a  $Z_2$  symmetry away from the line to a  $U(1)$  symmetry (of rotations in the  $x$ - $y$  plane) on the line. We therefore expect a gapless mode in the excitation spectrum corresponding to the Goldstone mode of the broken continuous symmetry. We can find this gapless mode explicitly by going to the next order in a  $1/S$  expansion.<sup>17</sup>

The above arguments provide some understanding of why one may also expect such a gapless line in the spin-1/2 model. Note however that the bosonization analysis gives the scaling form in Eq. (11) for  $h$  versus  $a$ ; this agrees with the classical form only if  $\Delta \leq -0.266$ . Further, in the classical limit, the transition across the gapless line is of first order, whereas it is of second order in the spin-1/2 case. There is probably a critical value of the spin  $S$  above which the transition is of first order. [For the  $U(1)$  symmetric model described by Eq. (21) below, it is known that the transition is of first order if  $S \geq 1$ .<sup>14</sup>]

The classical limit also makes it clear why our model has a different behavior from the  $U(1)$  symmetric model governed by the Hamiltonian

$$H_{S2} = \sum_n [(1+a)S_n^x S_{n+1}^x + (1-a)S_n^y S_{n+1}^y + (1-a)S_n^z S_{n+1}^z - 2ShS_n^x]. \quad (21)$$

In the limit  $S \rightarrow \infty$ , there is now a *two-parameter* set of degenerate ground states on the line  $h^2 = 4a$ ; these are obtained by taking the one-parameter family of configurations given in Eq. (19) and rotating them by an arbitrary angle about the  $x$  axis. Hence, the symmetry of this model is enhanced from  $U(1)$  to  $SU(2)$  on the line  $h^2 = 4a$ , and there are now two Goldstone modes instead of one. Considering this difference in symmetry for large  $S$ , it is not surprising that even the spin-1/2 models with  $U(1)$  symmetry and  $Z_2$  symmetry respectively exhibit very different behaviors at the spin-flip transition line.

#### V. DISORDER LINE

We have seen that as the magnetic field  $h$  is increased from zero for the spin-1/2 model described by Eq. (1), there is a spin-flip transition at a critical field  $h_c$  whose value depends on  $a$  and  $\Delta$ . One might wonder what happens if the field is increased well beyond  $h_c$ .

It turns out that above  $h_c$ , there is an interesting value of the field  $h = h_d$  where the ground state of the model is exactly solvable.<sup>19,20</sup> This field is given by

$$h_d = \sqrt{2(1+a+\Delta)}. \quad (22)$$

At this point, the ground state has a very simple direct product form in which all the spins lie in the  $x$ - $y$  plane, with the spins on even and odd sublattices pointing at the angles  $\alpha$  and  $-\alpha$ , respectively, with respect to the  $x$ -axis, where

$$\alpha = \cos^{-1}\left(\frac{h_d}{2}\right). \quad (23)$$

To show that this configuration is the ground state of the Hamiltonian, we observe that the Hamiltonian can be written, up to a constant, as the sum

$$H = \sum_n [H_{2n,2n+1} + H_{2n,2n-1}],$$

$$\begin{aligned}
H_{2n,2n\pm 1} = & \left( \cos \alpha S_{2n}^x + \sin \alpha S_{2n}^y - \frac{1}{2} \right) \\
& \times \left( \cos \alpha S_{2n\pm 1}^x + \sin \alpha S_{2n\pm 1}^y - \frac{1}{2} \right) \\
& + \left( \cos \alpha S_{2n}^x - \sin \alpha S_{2n}^y - \frac{1}{2} \right) \\
& \times \left( \cos \alpha S_{2n\pm 1}^x - \sin \alpha S_{2n\pm 1}^y - \frac{1}{2} \right) \\
& + \Delta \left[ \frac{1}{4} - (\cos \alpha S_{2n}^x + \sin \alpha S_{2n}^y) \right. \\
& \times (\cos \alpha S_{2n\pm 1}^x - \sin \alpha S_{2n\pm 1}^y) \\
& \left. - (\sin \alpha S_{2n}^x - \cos \alpha S_{2n}^y) \right. \\
& \left. \times (\sin \alpha S_{2n\pm 1}^x + \cos \alpha S_{2n\pm 1}^y) + S_{2n}^z S_{2n\pm 1}^z \right], \quad (24)
\end{aligned}$$

where  $\alpha$  is given in Eqs. (22) and (23). We now use the theorem that the ground state energy of  $H$  is greater than or equal to the sum of the ground state energies of  $H_{2n,2n\pm 1}$ , with equality holding if and only if there is a state which is simultaneously an eigenstate of all the  $H_{2n,2n\pm 1}$ . Now, each of the Hamiltonians  $H_{2n,2n\pm 1}$  in Eq. (24) is a sum of three operators whose eigenvalues are non-negative if  $\Delta \geq 0$ .<sup>20</sup> The state described in Eq. (23), in which all the spins on the even sublattice satisfy  $\cos \alpha S_{2n}^x + \sin \alpha S_{2n}^y = 1/2$  and all the spins on the odd sublattice satisfy  $\cos \alpha S_{2n+1}^x - \sin \alpha S_{2n+1}^y = 1/2$ , is the ground state of all the Hamiltonians in Eq. (24) with zero eigenvalue. We can actually show, by looking at a two-site system governed by a single Hamiltonian  $H_{2n,2n+1}$ , that even if  $\Delta < 0$ , the state described above is its ground state provided that  $1 - a \geq -\Delta$ , i.e., as long as the magnitude of the  $zz$  coupling is smaller than the  $yy$ , which is what we have assumed already.

For a given value of  $\Delta$ , the line in the  $(a, h)$  plane described by Eq. (22) is called a disorder line because the direct product form of the ground state implies that the two-spin correlation function  $\langle S_n^\alpha S_m^\beta \rangle - \langle S_n^\alpha \rangle \langle S_m^\beta \rangle$  (with  $\alpha, \beta = x, y, z$ ) is exactly zero if  $m \neq n$ . Hence the correlation length is extremely short. The disorder line exists even for values of the spin larger than 1/2. Starting with the Hamiltonian in Eq. (18), one finds a disorder line at the same value of  $h$  given in Eq. (22). The proof that it is a disorder line is similar to the proof given above for the spin-1/2 case if  $\Delta \geq 0$ . We will not study here how far the proof can be extended to negative values of  $\Delta$ ; for spin  $S$ , this requires an examination of the spectrum of a two-site problem governed by a  $(2S+1) \times (2S+1)$  dimensional Hamiltonian matrix.

## VI. ISING TRANSITION

If the magnetic field  $h$  is increased even further, the system undergoes an Ising transition.<sup>4</sup> If the  $yy$  and  $zz$  couplings are equal (i.e.,  $1 - a = \Delta$ ), this occurs at a saturation field  $h_s = 2$ , where there is transition to a state in which all

the spins point along the  $x$  axis. But if the  $yy$  and  $zz$  couplings are not equal, there is no saturation of the spins for any finite value of the field although the ground state expectation value of  $S_n^x$  approaches 1/2 [as  $(1 - a - \Delta)^2/h^2$ ] as  $h$  goes to infinity. (This can be shown by considering a two-site system and doing perturbation theory in the limit  $h \rightarrow \infty$ .) However, there is still a transition field  $h_s$  beyond which a  $Z_2$  symmetry of a different kind is broken. To see this, we consider a Hamiltonian  $\tilde{H}$  which is dual to the Hamiltonian given in Eq. (1). This is given by

$$\begin{aligned}
\tilde{H} = \sum_n \left[ (1+a) T_n^x T_{n+2}^x + \frac{1-a}{2} T_n^y - 2\Delta T_{n-1}^x T_n^y T_{n+1}^x \right. \\
\left. - 2h T_n^x T_{n+1}^x \right]. \quad (25)
\end{aligned}$$

This Hamiltonian is invariant under the global  $Z_2$  transformation  $T_n^x \rightarrow -T_n^x, T_n^y \rightarrow T_n^y, T_n^z \rightarrow -T_n^z$ . For  $\Delta = 0$ , this  $Z_2$  symmetry is known to be broken if  $h$  is larger than a critical value  $h_s$ .<sup>4</sup> We expect that this will be true even if  $\Delta \neq 0$ . The order parameter for this symmetry is

$$m_x = \left[ \lim_{n \rightarrow \infty} \langle T_0^x T_n^x \rangle \right]^{1/2}. \quad (26)$$

Note that in terms of the operators  $S_n^x, T_0^x T_n^x$  is equal to a string of operators,  $(1/4) \prod_{m=0}^{n-1} (2S_m^x)$ . Similarly, the order parameter  $(-1)^n S_0^y S_n^y$  in Eq. (12) is equal to the string of operators  $[(-1)^n/4] \prod_{m=1}^n (2T_m^y)$ .

## VII. DISCUSSION

We have shown in this paper that the  $XYZ$  spin-1/2 chain in a magnetic field exhibits a gapless phase on a particular line. It would be interesting to use numerical techniques like the density-matrix renormalization group method<sup>21</sup> to examine various ground state properties of this model, in particular, to study the behavior of the order parameter defined in Eq. (12), and to find out if there is indeed a Lifshitz point as conjectured in Fig. 2.

Finally, 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,<sup>10</sup> and one-dimensional conductors with spin-anisotropic electron interactions.<sup>11</sup> The gapless phase may therefore also appear in other systems.

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