Bose condensation in quasi-one-dimensional antiferromagnets in strong fields

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Recent experiments show that axially symmetric integer-spin antiferromagnetic chains undergo a phase transition at a critical applied magnetic field. It was argued, using Landau-Ginzburg theory, that this is one-dimensional Bose condensation. The theory is further analyzed at the mean-field and Gaussian level. Then some exact results concerning the critical behavior are determined using known results on one-dimensional Bose fluids. These are shown to be consistent with recent numerical simulations on spin chains. Breaking of axial symmetry produces crossover to a two-dimensional Ising transition.

I. INTRODUCTION

One-dimensional antiferromagnetic of integer spin have an excitation gap,[1] Δ. The lowest excited state is a triplet of massive bosons. As observed in recent experiments[2,3] on NENP the application of a magnetic field causes a Zeeman splitting of the triplet with one member crossing the ground state at a critical field, $h_c=\Delta$. As was argued recently,[4] using a Landau-Ginsburg theory, the ground state above h_c may be regarded as a Bose condensate of the low-energy boson. Varying the magnetic field is equivalent to varying the chemical potential for this boson and the (uniform) magnetization corresponds to the boson number.

The microscopic Hamiltonian under consideration is the integer spin antiferromagnetic chain in an applied field with crystal field anisotropy:

$$H=\sum_i \{\mathbf{S}_i\cdot\mathbf{S}_{i+1}+D(S_i^z)^2+E[(S_i^x)^2-(S_i^y)^2]-\mathbf{h}\cdot\mathbf{S}_i\} \ . \tag{1}$$

(Exchange anisotropy can also be included and does not change any of the basic conclusions. We adsorb the Bohr magneton and the g factors into the definition of the magnetic field, $\mathbf{h}$ and set $\hbar=1$.) As discussed in Ref. 4, a Landau-Ginsburg formulation of the model, based on the large-s continuum limit, gives a Hamiltonian density:

$$\mathcal{H}=\frac{v}{2}\mathbf{\Pi}^2+\frac{v}{2}\left[\frac{\partial\boldsymbol{\phi}}{\partial x}\right]^2+\sum_{i=1}^{3}\frac{\Delta_i^2}{2v}\phi_i^2+\lambda\boldsymbol{\phi}^4-\mathbf{h}\cdot(\boldsymbol{\phi}\times\mathbf{\Pi}) \ . \tag{2}$$

Here $\boldsymbol{\phi}$ is the staggered magnetization density and $\mathbf{\Pi}$ is the momentum canonically conjugate to $\boldsymbol{\phi}$; v, Δ_i are phenomenological parameters representing the spin-wave velocity, and the gaps for staggered magnetization fluctuations with polarization i. The $\boldsymbol{\phi}^4$ term is included for stability. In Ref. 4 only a partial mean-field and Gaussian analysis of the Landau-Ginsburg model was reported, referring primarily to the region $h<h_c$. Since then, a different approximate theory, based on a fermionic rather than bosonic representation was presented.[5] Furthermore some numerical results were reported.[6,7] The purpose of this paper is twofold. A more complete mean field and Gaussian analysis of the Landau-Ginsburg theory will be presented for both phases. Furthermore, some exact results concerning the critical behavior of this theory will be derived.

The critical behavior is deduced from the following observation. Since two elements of the triplet of excited states have an excitation gap at h_c, they are irrelevant and may be integrated out. Furthermore, near h_c, we may approximate the dispersion relation for the low-energy magnon by $E(k)=\Delta+v^2k^2/2\Delta$. The effective low-energy Landau-Ginsburg Lagrangian then becomes precisely the standard one used to study Bose condensation in a nonrelativistic Bose fluid with δ-function repulsion. This model has been studied extensively in one dimension.[8,9] Although true off-diagonal long-range order does not occur quasi-long-range phase coherence *does*. This corresponds to power-law decay of the staggered magnetization orthogonal to the applied field, with a continuously varying exponent η. In the limit of zero density ($h\rightarrow h_c$) the Bose system becomes equivalent to a system of free fermions and[9] $\eta\rightarrow\frac{1}{2}$, in agreement with calculations on finite spin-1 chains.[7] The known result for the ground-state energy as a function of density in the Bose fluid[8] determines the magnetization near h_c:

$$M=\frac{\sqrt{(h-h_c)2\Delta}}{\pi v} \ . \tag{3}$$

Note that this is different than the mean-field Landau-Ginsburg result $M\propto(h-h_c)$ given in Ref. 4. It agrees with the free fermion result suggested by a different type of approximate theory in Ref. 5, but disagrees with the form suggested in Ref. 6.

These results should be exact in the limit of axial symmetry. This symmetry can be broken either by crystal field anisotropy [the E term of Eq. (1)] or by the application of the external field along a direction other than the symmetry axis. Such anisotropy can be studied using the

Haldane formalism[9] for the one-dimensional Bose fluid. It is a relevant perturbation, producing long-range Ising order above h_c (it also leads to nontrivial renormalization of the *value* of h_c). The correlation length thus becomes finite above h_c; it scales as a power ν of the inverse anisotropy with a density dependent exponent, which approaches 1 as the density goes to zero. The Ising transition itself is in the *two*-dimensional universality class (since time plays the role of a second dimension here). As was pointed out in Ref. 7 three-dimensional couplings tend to produce true long-range off-diagonal order (i.e., Bose condensation) even without anisotropy.

A rough picture of the various phases is as follows. In the axially symmetric case, for $h < h_c$, there is no magnetic moment (uniform or alternating) on length scales long compared to the correlation length (about seven lattice sites for the isotropic spin-1 case). Above h_c, there is a uniform magnetic moment in the direction of the applied field (taken to be the 3-axis), corresponding to the canted spin structure shown in Fig. 1(a). However, the spins undergo long wavelength precession about the 3-axis, so that there is only quasi-long-range order (i.e., power-law decay) of the alternating transverse spin components, i.e.,

$$\begin{aligned} &\langle S_i^3 \rangle = \text{const} \\ &\langle S_i^a S_j^b \rangle \propto (-1)^{i-j} \frac{\delta^{ab}}{|i-j|^{\eta}} \quad (a,b=1,2) \ . \end{aligned} \tag{4}$$

Weak three-dimensional couplings will make this into true long-range order. Axial symmetry breaking terms in the Hamiltonian pick out two preferred orientations of canted spins (for example, lying in the 1-3 plane) as shown in Fig. 1(b). Below h_c, fluctuations produce a finite correlation length for alternating order of three transverse spin components, but allow a finite uniform magnetization in the field direction. Above h_c, both the uniform 3-component and the staggered transverse component have long-range order, i.e.,

$$\begin{aligned} &\langle S_i^3 \rangle = \text{const} \\ &\langle S_i^1 \rangle = \text{const} \times (-1)^{i-j} \ . \end{aligned} \tag{5}$$

In Sec. II we analyze the Landau-Ginsburg model in the mean-field and Gaussian approximations, with and without axial symmetry. Section III then takes into account the one-dimensional fluctuation effects using Haldane's method,[9] deriving various exact results. Section IV contains conclusions and a comparison of these predictions with numerical simulations and experiment. Some of the details of the Gaussian approximation calculations of Sec. II are relegated to the Appendix.

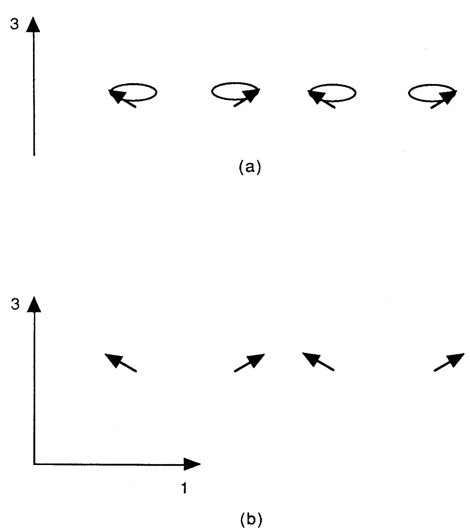

FIG. 1. (a) Spin configuration in axially symmetric case: there is a static uniform component in the 3 direction and a precessing alternating component in the 1-2 plane. (b) Spin configuration with axial symmetry breaking: there is a static uniform component in the 3 direction and a static alternating component in the 1 direction.

II. MEAN-FIELD AND GAUSSIAN APPROXIMATIONS

A simple way of performing a mean-field analysis of the Landau-Ginsburg model, is to first make a canonical transformation to the Lagrangian density:

$$\frac{\partial \boldsymbol{\phi}}{\partial t} = v\boldsymbol{\Pi} + \boldsymbol{\phi} \times \mathbf{h} \ , \tag{6}$$

$$\mathcal{L} = \frac{1}{2v}\left[\frac{\partial \boldsymbol{\phi}}{\partial t} + \mathbf{h} \times \boldsymbol{\phi}\right]^2 - \frac{v}{2}\left[\frac{\partial \boldsymbol{\phi}}{\partial x}\right]^2 - \sum_{i=1}^{3} \frac{\Delta_i^2}{2v}\phi_i^2 - \lambda \boldsymbol{\phi}^4 \ . \tag{7}$$

We see that the magnetic field adds a quadratic term to the effective potential:

$$V = \sum_{i=1}^{3} \frac{\Delta_i^2}{2v}\phi_i^2 - \frac{1}{2v}(\mathbf{h} \times \boldsymbol{\phi})^2 + \lambda \boldsymbol{\phi}^4 \ . \tag{8}$$

For small fields the minimum of V is at $\boldsymbol{\phi}=0$ but above a critical field the minimum occurs at nonzero $\boldsymbol{\phi}$.

A. Axially symmetric case

Let us first consider the simplest case where the field is applied along a symmetry axis, corresponding approximately to a field applied along the b axis in NENP. We assume that $\Delta_1 = \Delta_2 \equiv \Delta$ and that the field points along the 3-axis. We see from V that the phase transition occurs at $h_c = \Delta$. Beyond the critical field the symmetry of rotation about the z axis is spontaneously broken (in mean-field theory) and $\boldsymbol{\phi}$ has a nonzero (constant) expectation value lying in the xy plane of magnitude:

$$\phi_0^2 = \frac{(h^2 - \Delta^2)}{4v\lambda} \ . \tag{9}$$

We may immediately calculate the magnetization, $\mathbf{M}$, from Eq. (6):

$$\mathbf{M} = \int \boldsymbol{\phi} \times \boldsymbol{\Pi} = L\mathbf{h}\frac{\phi_0^2}{v} = L\mathbf{h}\frac{(h^2 - \Delta^2)}{4v\lambda} \ , \tag{10}$$

where L is the length of the system. Note that, in mean-field theory, $\mathbf{M}$ is linear in $h-h_c$, as announced in Ref. 4.

We may calculate the excitation spectrum in the standard harmonic approximation by expanding $\mathcal{L}$ to quadratic order in the small fluctuations around the classical ground state. Fluctuations of $\boldsymbol{\phi}$ in the 3-direction are completely unaffected by the applied field. On the other hand planar fluctuations consist of a Goldstone phase mode together with a finite-gap longitudinal mode. We introduce amplitude and phase fluctuations, ϕ' and θ, respectively, writing ϕ as

$$\boldsymbol{\phi}=[(\phi_0+\phi')\cos\theta,(\phi_0+\phi')\sin\theta,\phi_3] \ . \tag{11}$$

The terms in $\mathcal{L}$ of quadratic order in θ, ϕ' are

$$\mathcal{L}=\frac{\phi_0^2}{2v}\left[\frac{\partial\theta}{\partial t}\right]^2-\frac{v\phi_0^2}{2}\left[\frac{\partial\theta}{\partial x}\right]^2+\frac{1}{2v}\left[\frac{\partial\phi'}{\partial t}\right]^2 -\frac{v}{2}\left[\frac{\partial\phi'}{\partial x}\right]^2-\frac{(h^2-\Delta^2)}{v}\phi'^2-\frac{2h\phi_0}{v}\frac{\partial\theta}{\partial t}\phi' \ . \tag{12}$$

Solving the resulting classical equations of motion gives frequencies

$$\omega_\pm^2=(3h^2-\Delta^2)+v^2k^2\pm\sqrt{(3h^2-\Delta^2)^2+4v^2h^2k^2} \ . \tag{13}$$

The lower frequency solution is the sound or Goldstone mode. At $k\to 0$, this frequency approaches

$$\omega_-^2\to\frac{v^2k^2(h^2-\Delta^2)}{3h^2-\Delta^2} \ . \tag{14}$$

Thus the speed of sound is $v_s=v\sqrt{(h^2-\Delta^2)/(3h^2-\Delta^2)}$, which goes to zero as $h\to h_c$.

B. Axial symmetry breaking

We now wish to discuss the effects of breaking of axial symmetry. We begin again with the Lagrangian of Eq. (7) with the field in the 3-direction, but we now consider the case $\Delta_1<\Delta_2$.

At the classical level, the transition looks essentially the same as in the axially symmetric case. The potential of Eq. (8) develops a minimum at nonzero ϕ_1 for $h>\Delta_1$. For $h>h_c$, $\langle\phi_1\rangle$ is again given by Eq. (9) with $\Delta\to\Delta_1$. A difference appears, however, in the spectrum for $h>h_c$. All modes now have a gap. We now parametrize the small fluctuations away from the ground state by

$$\boldsymbol{\phi}=(\phi_0+\phi_1,\phi_2,\phi_3) \ . \tag{15}$$

As before ϕ_3 is unaffected by the magnetic field at tree level. The terms in the Lagrangian quadratic in ϕ_1,ϕ_2 are

$$\mathcal{L}=\frac{1}{2v}\left[\frac{\partial\phi_1}{\partial t}\right]^2-\frac{v}{2}\left[\frac{\partial\phi_1}{\partial x}\right]^2-\frac{(h^2-\Delta_1^2)}{v}\phi_1^2 +\frac{1}{2v}\left[\frac{\partial\phi_2}{\partial t}\right]^2-\frac{v}{2}\left[\frac{\partial\phi_2}{\partial x}\right]^2-\frac{(\Delta_2^2-\Delta_1^2)}{2v}\phi_2^2 -\frac{h}{v}\left[\frac{\partial\phi_1}{\partial t}\phi_2-\frac{\partial\phi_2}{\partial t}\phi_1\right] \ . \tag{16}$$

Solving for the dispersion relations we find that the lower energy mode has a gap near h_c of

$$\omega_-^2(0)=\frac{(h^2-\Delta_1^2)(\Delta_2^2-\Delta_1^2)}{2h^2+(\Delta_2^2-\Delta_1^2)/2} \ . \tag{17}$$

We see that the gap rises as the square root of $h-h_c$ times the square root of the anisotropy, in, the mean-field theory.

Other effects of anisotropy immerge at the level of one-loop corrections to mean-field theory (i.e., the Gaussian approximation). These results are derived in the Appendix. In the axially symmetric case the magnetization is strictly zero for $h<h_c$. Above h_c it rises linearly in the mean-field approximation but has a finite jump at the one-loop level (see Appendix). In the presence of anisotropy there is a nonzero magnetization for all nonzero h. In particular, as shown in Ref. 4 as $h\to 0$, $M\propto h$. The slope of M at $h=0$ (i.e., the susceptibility) is proportional to the square of the anisotropy.[4] M diverges logarithmically as $h\to h_c$ from below or above. Furthermore, in the presence of anisotropy there is field-dependent renormalization of the gap parameters, so that higher-loop corrections can shift h_c, away from Δ_1. Another striking effect of anisotropy is on the static correlation function. In the axially symmetric case the ground state is completely unaffected by the field below h_c so the correlation length remains unchanged (and equals v/Δ). Above h_c it is infinite. On the other hand, with anisotropy, the correlation length diverges as h_c is approached from below or above: $\xi\propto 1/\sqrt{h_c^2-h^2}$, the standard mean-field result. (See Appendix.)

III. FLUCTUATION EFFECTS AND EXACT RESULTS

A. Axially symmetric case

In order to go beyond the mean-field approximation, it will be useful to discuss two different low-energy approximations to the Lagrangian of Eq. (7). The first approximation is valid only near h_c. It consists of simply dropping the massive field, ϕ^z, which is unaffected by the external field, as well as dropping the terms quadratic in time derivatives in the Lagrangian of Eq. (7). If we combine ϕ^x and ϕ^y into a complex field

$$\phi\equiv\frac{\phi^x+i\phi^y}{\sqrt{2}} \ , \tag{18}$$

then the Lagrangian becomes

$$\mathcal{L}\to\frac{ih}{v}\left[\phi^\dagger\frac{\partial\phi}{\partial t}-\frac{\partial\phi^\dagger}{\partial t}\phi\right]-v\left|\frac{\partial\phi}{\partial x}\right|^2 -\frac{\Delta^2-h^2}{v}|\phi|^2-4\lambda|\phi|^4 \ . \tag{19}$$

This is precisely the standard nonrelativistic Lagrangian for bosons with δ-function repulsion. The upper mode of frequency, ω_+, has disappeared and we are left with only the lower mode with a frequency which is now

$$\omega=\frac{\sqrt{v^2k^2[2(h^2-\Delta^2)+v^2k^2]}}{2h} . \tag{20}$$

This is the standard Bogliubov result; it reduces to $v^2k^2/2\Delta$ at $h\to h_c$. It can be checked that this agrees with Eq. (13) up to $O(k^4)$ for h close to h_c. The second approximation is valid for all $h>h_c$, at low energies. It consists of integrating out the amplitude oscillation ϕ' in Eq. (12) obtaining an effective Lagrangian containing θ only

$$-\frac{(h^2-\Delta^2)}{v}\phi'^2-\frac{2h\phi_0\phi'}{u}\frac{\partial\theta}{\partial t}\to\frac{h^2}{4v^2\lambda}\left[\frac{\partial\theta}{\partial t}\right]^2 , \tag{21}$$

$$\mathcal{L}\to\frac{3h^2-\Delta^2}{8v^2\lambda}\left[\frac{\partial\theta}{\partial t}\right]^2-\frac{h^2-\Delta^2}{8\lambda}\left[\frac{\partial\theta}{\partial x}\right]^2 . \tag{22}$$

The frequency obtained from the Lagrangian agrees with ω_- to $O(k^2)$, the result of Eq. (14). Note that the first approximation, the Lagrangian of Eq. (19), was only valid close to h_c but was correct to $O(k^4)$ and described both sides of the critical point while the second approximation, Eq. (22) is valid for all $h>h_c$ but only to $O(k^2)$.

We now wish to go beyond the mean-field approximation. In particular we will be able to state some exact results in the limit of zero magnetization (i.e., density). It can be seen that the mean-field theory is certainly not valid there since the dimensionless parameter which controls perturbation theory is $\lambda v/(h^2-\Delta^2)$. In this limit, as discussed in Ref. 8, the Bose fluid with a δ-function interaction, or for that matter, any short-range interaction becomes equivalent to a Bose fluid with a hard-core repulsion, which in turn is equivalent to a free fermion gas in one dimension. In this low-density limit the ground state is obtained simply by arranging that the wave function vanishes when any two particles are close to each other. Such a wave function is equal to a free fermion wave function times a sign function (i.e., a function which is ±1 everywhere) in one dimension. Such a wave function has zero potential energy but has a kinetic energy of order $Nv^2\rho^2/2\Delta$, where ρ is the density and N the number of particles since the momenta of the bosons must be of $O(\rho)$. [A simple argument like this was constructed in Ref. 6 but concluded that the ground-state energy was proportional to $Ne^{-1/\rho\xi}$ where ξ is the range of the interaction. The problem with that argument is that it ignores the quantum mechanical nature of the particles and assumes they can be localized on a length scale of $O(\xi)$ without any cost in kinetic energy resulting from the uncertainty principle.] Explicitly, the kinetic energy of a nonrelativistic free fermion gas of mass Δ, expressed in terms of its density, ρ, is $\pi^2Nv^2\rho^2/6\Delta$. Including the rest energy and the chemical potential, the energy as a function of density is

$$E=\frac{\pi^2Nv^2\rho^2}{6\Delta}+(\Delta-h)N . \tag{23}$$

Thus the magnetization per unit length is

$$M/L=\rho=\frac{\sqrt{(h-\Delta)2\Delta}}{\pi v} . \tag{24}$$

A somewhat different free fermion approximation was discussed in Ref. 5. The two models do not in general agree in detail, but they do at the critical field, both giving Eq. (24) near h_c. The above argument shows that this result should be universal and exact, and not merely a consequence of the approximations. Other critical properties of the one-dimensional Bose superfluid have been calculated using a scaling theory.[9] The low-energy Lagrangian for the phase field, θ, of Eq. (22) is qualitatively correct. However, long-range order does not occur due to the logarithmic behavior of the propagator in two dimensions. In general, with the complex field ϕ parametrized as

$$\phi\sim\phi_0e^{i\theta} \tag{25}$$

and the low-energy effective Lagrangian written

$$\mathcal{L}=\frac{1}{2\pi}\left[\frac{1}{v_N}\left[\frac{\partial\theta}{\partial t}\right]^2-v_J\left[\frac{\partial\theta}{\partial x^2}\right]\right] . \tag{26}$$

The correlation function behaves as

$$\langle\phi(x)^\dagger\phi(0)\rangle\sim e^{-\langle\theta(x)\theta(0)\rangle/2}\sim e^{-\eta/n|x|}=\frac{1}{|x|^\eta} , \tag{27}$$

where

$$\eta=\frac{1}{2}\sqrt{v_N/v_J} . \tag{28}$$

The second term in this Lagrangian just comes from the kinetic energy and is unaffected by the interactions (at least in the nonrelativistic limit), hence

$$v_J=2\pi v\phi_0^2=\frac{2\pi v^2\rho}{h} . \tag{29}$$

However, the first term, which arises from the interactions, in general has a coefficient, which is much different from the mean-field value of Eq. (22):

$$v_N=\frac{4v^2\lambda}{\pi(3h^2-\Delta^2)} . \tag{30}$$

In particular, Haldane argues[9] using a Jordan-Wigner transformation, that, at the critical point, $\eta=\frac{1}{2}$ and hence $v_N=v_J\to0$. Near h_c the original spin correlation functions have the behavior

$$\langle S^3(x)S^3(0)\rangle=\rho^2+\frac{1}{\eta(2\pi x)^2}+\frac{\text{const}}{|x|^{1/\eta}}\cos(2\pi\rho x) , \tag{31}$$

$$\langle S^a(x)S^b(0)\rangle\sim\frac{(-1)^x\delta^{ab}}{x^\eta}\quad(a,b=1,2) , \tag{32}$$

where $\rho=M/L$, the magnetization per unit length. The exponent η is given by

$$\eta=\tfrac{1}{2}-O(\rho) . \tag{33}$$

B. Axial symmetry breaking

Finally we wish to consider fluctuation effects in the presence of anisotropy. Since a Z_2 symmetry is being broken in a (1+1)-dimensional quantum field theory, we expect the transition to be in the two-dimensional Ising universality class. The external field plays the role of the effective temperature, and the uniform magnetization is hence the effective energy operator. The Ising order parameter is the staggered magnetization (in the x direction). We may now invoke various known results about the two-dimensional Ising model. At the critical point the staggered magnetization has a correlation exponent $\eta=\frac{1}{4}$ and the uniform magnetization has $\eta=2$. Since the Ising model energy operator, corresponding to the uniform magnetization, has scaling dimension 1, the singular part of the magnetization near h_c, is linear in $h-h_c$; i.e., the slope should be finite as h_c is approached from below or above, but should be discontinuous at this point. The correlation length diverges as $\xi \propto |h-h_c|^{-1}$ as h_c is approached from below or above.

We may also specify a crossover exponent governing the flow from the unstable axially symmetric critical line to the Ising ordered phase in the presence of anisotropy. For small anisotropy the critical behavior can be studied using the nonrelativistic model discussed above [see Eq. (19)]. The axial symmetry breaking modifies the Lagrangian to

$$\mathcal{L}=\frac{ih}{v}\left[\phi^\dagger\frac{\partial\phi}{\partial t}-\frac{\partial\phi^\dagger}{\partial t}\phi\right]-v\left|\frac{\partial\phi}{\partial x}\right|^2 -\frac{1}{v}\left[\frac{\Delta_1^2+\Delta_2^2}{2}-h^2\right]|\phi|^2 +\frac{\Delta_2^2-\Delta_1^2}{4v}(\phi^2+\phi^{\dagger 2})-4\lambda|\phi|^4 . \quad (34)$$

The axial symmetry breaking adds an additional term to the phase-field Lagrangian of Eq. (26):

$$\mathcal{L}=\frac{1}{2\pi}\left[\frac{1}{v_N}\left[\frac{\partial\theta}{\partial t}\right]^2-v_J\left[\frac{\partial\theta}{\partial x}\right]^2\right]+\frac{\Delta_2^2-\Delta_1^2}{2v}\rho\cos2\theta . \quad (35)$$

The Ising symmetry breaking corresponds to the classical ground states with $\theta=0,\pi$. The anisotropy term has a scaling dimension of $2\eta\equiv\sqrt{v_N/v_J}$, where η is the staggered magnetization exponent in the absence of anisotropy. In the zero-density limit, this scaling dimension goes to 1. Thus the anisotropy is indeed relevant along the critical line.

IV. CONCLUSIONS

Here we briefly summarize the expected results based on a combination of the mean-field/Gaussian analysis and exact results in the critical region, and compare with numerical simulations and experiments.

In the axially symmetric case, the magnetization is rigorously zero below $h_c=\Delta$ and then rises as

$$M=\frac{\sqrt{(h-h_c)2\Delta}}{\pi v} \quad (36)$$

near h_c [Fig. 2(a)]. With broken axial symmetry, the magnetization is nonzero at all h. It vanishes linearly as $h\to 0$ with a coefficient proportional to the square of the anisotropy. It has a finite slope as $h\to h_c$ from below or above, but the two slopes are not the same [Fig. 2(b)]. In the axially symmetric case, the correlation length for the alternating, transverse spin components is rigorously field independent below h_c and then is strictly infinite above h_c [Fig. 3(a)] where power-law decay occurs with an exponent η which is exactly $\frac{1}{2}$ at h_c and initially decreases above h_c. With axial symmetry breaking, the transverse alternating spin correlation length is finite everywhere except right at h_c. It diverges linearly in $1/|h-h_c|$ as h_c is approached from below or above [Fig. 3(b)]. It also diverges linearly in the inverse anisotropy, just above h_c. At h_c, $\eta=\frac{1}{4}$ for the alternating transverse spin components and $\eta=2$ for the uniform spin component parallel to the applied field.

Finite-temperature effects should round off the discontinuous derivative of M, produce a finite-correlation length in the axially invariant superfluid phase ($\xi\propto 1/T$), and destroy the Ising order with axial symmetry breaking. In the strictly one-dimensional system this occurs at $T=0$. Three-dimensional coupling will produce a finite T_c.

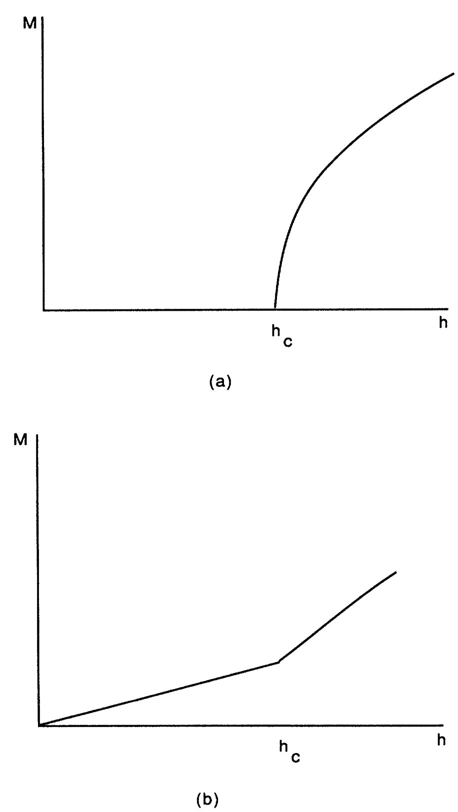

FIG. 2. (a) Qualitative sketch of the zero-temperature magnetization in the axially symmetric case. (b) Qualitative sketch of the zero-temperature magnetization with axial symmetry breaking.

Numerical results on the magnetization were presented in Ref. 6 for chains of length, L, up to 16, based on which it was argued that the energy had an exponential dependence on magnetization:

$$E(M)-M\Delta \propto Me^{-\rho\xi} . \quad (37)$$

This disagrees with the cubic dependence of Eq. (23). We believe that the results of Ref. 6 are dominated by finite-size effects and do not reflect the true asymptotic behavior. While the $(M=1)$ energy gap can be determined to about 10% accuracy from a chain of length 16 (and a few percent for length 32) much longer chains will be necessary to accurately determine the asymptotic form of the magnetization. The reason for this is that the finite-density corrections to Eq. (23) have the form of Eq. (37). This follows, essentially from the argument of Ref. 6; the typical distance between bosons is $1/\rho$ and the interaction between the particles drops off with exponent ξ. Until these finite-density corrections become small the asymptotic behavior cannot be deduced. This occurs when $\rho \ll 1/\xi$, i.e., $L/M \gg \xi$. For spin 1 this means $L \gg 7M$. Since a reliable result for $M=1$ required $L=16-32$, we might estimate that chains of length $16M-32M$ will be necessary. Of course the number of states decreases with increasing M for fixed L so this may not be hopeless. Numerical results on the transverse correlation function are completely consistent with the behavior derived here, and, in fact, the value $\eta=\frac{1}{2}$ at h_c was guessed from extrapolation of finite-size results in Ref. 7.

Using the g factor $g=2.2$ and experimentally determined values[10] of the velocity and gap

$$v=110\text{ K},\quad \Delta=14\text{ K} , \quad (38)$$

we obtain the behavior of the susceptibility at $T=0$ for NENP for fields applied along the b axis ignoring any breaking of axial symmetry:

$$M \to 0.041\sqrt{h-h_c}\ (\mu_B \text{ per } Ni^{2+}, h \text{ in T}) . \quad (39)$$

Only a slight bump in dM/dh was observed in the experiment of Ref. 3 and none whatever in that of Ref. 2. This is presumably due to finite-temperature effects, axial symmetry breaking, and crystal defects.

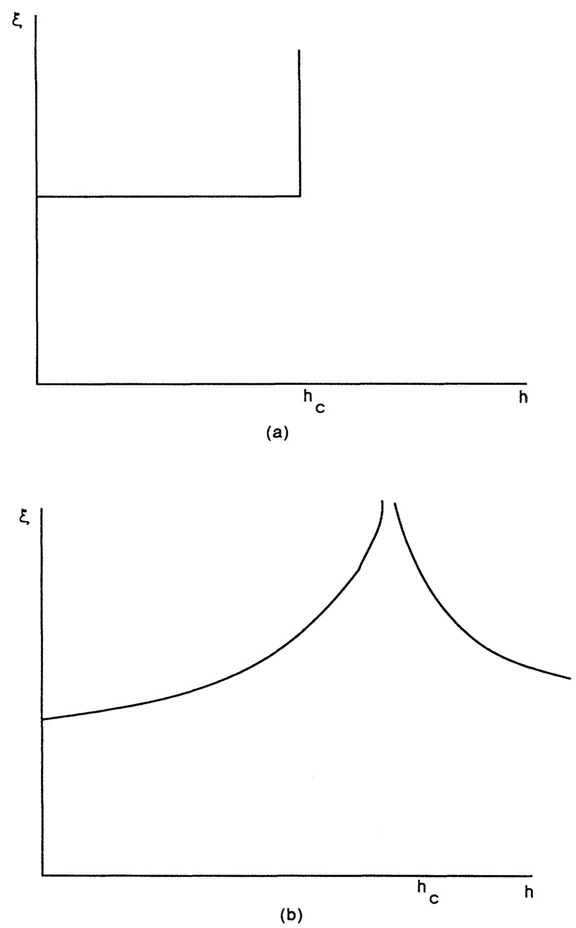

FIG. 3. (a) Correlation length in the axially symmetric case. (b) Qualitative sketch of the correlation length with axial symmetry breaking.

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APPENDIX

Here we give more details of the one-loop corrections to mean-field theory referred to in Sec. II. The one-loop correction to the ground-state energy from the field-dependent modes, $\omega_\pm$ is simply the harmonic oscillator zero point energy:

$$E_0^{(1)}=\frac{L}{2}\int\frac{dk}{(2\pi)}[\omega_-(k)+\omega_+(k)] . \quad (40)$$

The one-loop contribution to the magnetization is obtained by differentiating $E_0^{(1)}$:

$$M/L=-\frac{1}{2}\int\frac{dk}{(2\pi)}\left[\frac{d\omega_-(k)}{dh}+\frac{d\omega_+(k)}{dh}\right] . \quad (41)$$

The field-dependent energies below h_c were discussed in Ref. 4. In the isotropic limit they are simply

$$\omega_\pm=\sqrt{\Delta^2+v^2k^2}\pm h . \quad (42)$$

Note that the ω_+ and ω_- contributions to M cancel. With anisotropy, the energies are given by[4]

$$\omega_\pm^2=\frac{\omega_2^2+\omega_1^2}{2}+h^2 \pm\left[\left[\frac{\omega_2^2-\omega_1^2}{2}\right]^2+2h^2(\omega_2^2+\omega_1^2)\right]^{1/2} , \quad (43)$$

where we have defined

$$\omega_i(k)\equiv\sqrt{\Delta_i^2+v^2k^2}\quad (i=1,2) . \quad (44)$$

Now, in general, the two terms in M/L of Eq. (41) do not cancel. In particular, as $h \to 0$, we have

$$\omega_+ \to \omega_2 \ , \quad \omega_- \to \omega_1 \ ,$$

$$\frac{d\omega_+^2}{dh^2} \to \frac{3\omega_2^2+\omega_1^2}{\omega_2^2-\omega_1^2} \ , \qquad (45)$$

$$\frac{d\omega_-^2}{dh^2} \to -\frac{3\omega_1^2+\omega_2^2}{\omega_2^2-\omega_1^2} \ ,$$

and hence

$$M/L \to h \int \frac{dk}{2\pi} \frac{(\omega_2-\omega_1)^2}{2\omega_1\omega_2(\omega_1+\omega_2)} \ . \qquad (46)$$

This agrees with the zero field susceptibility calculated in Ref. 4, Eq. (3.26). On the other hand, when $h \to \Delta_1$, M/L blows up because $\omega_- \to 0$ while $d\omega_-^2/dh^2$ remains finite:

$$\frac{d\omega_-^2}{dh^2} \to -\frac{\omega_2^2-\omega_1^2}{3\omega_1^2+\omega_2^2} \ ,$$
$$\omega_-^2 \to \frac{\Delta_2^2-\Delta_1^2}{3\Delta_1^2+\Delta_2^2}[(v^2k^2+(h_c^2-h^2)] \ . \qquad (47)$$

There is a logarithmic divergence at $k \to 0$, $h \to h_c$, giving

$$M/L \to \frac{\Delta_1}{4\pi v} \left[\frac{\Delta_2^2-\Delta_1^2}{\Delta_2^2+3\Delta_1^2} \right]^{1/2} |\ln(h-h_c)| \ . \qquad (48)$$

Above h_c, we must use Eq. (14) for the two frequencies, in the axially symmetric case. $\omega_- \to 0$ at $k \to 0$, as given by Eq. (14), however, we see from this equation that $d\omega_-/dh$ also goes to zero, so consequently M/L has a finite limiting value as h_c is approached from above. Hence at the one-loop level there is a finite jump in M/L at h_c, in the axially symmetric case. With axial asymmetry, ω_- is only zero right at h_c and $d\omega_-/dh$ is nonzero there. Hence, there is again a logarithmic divergence in M/L as h_c is approached from above.

We now consider the transverse Green's function in the Gaussian approximation. The equal time Green's function is given by

$$G_{ij}(x) = \int \frac{dk\, d\kappa}{(2\pi)^2} e^{ikx} \begin{bmatrix} \kappa^2+\omega_1^2-h^2 & 2h\kappa \\ -2h\kappa & \kappa^2+\omega_2^2-h^2 \end{bmatrix}^{-1} \quad (i,j=1,2)$$
$$= \frac{1}{(\kappa^2+\omega_+^2)(\kappa^2+\omega_-^2)} \int \frac{dk\, d\kappa}{(2\pi)^2} e^{ikx} \begin{bmatrix} \kappa^2+\omega_2^2-h^2 & -2h\kappa \\ 2h\kappa & \kappa^2+\omega_1^2-h^2 \end{bmatrix} \ . \qquad (49)$$

Here κ is the imaginary frequency. We may do the κ integral by the contour method. The encircled poles are at $\kappa = i\omega_\pm$. In the axially invariant case, we find the h-independent result:

$$G_{ij(x)} = \delta_{ij} \int \frac{dk}{2\pi} e^{ikx} \frac{1}{2\sqrt{\Delta^2+v^2k^2}} \ . \qquad (50)$$

This gives the standard two-dimensional relativistic propagator, with asymptotic behavior:

$$G(x) \to \frac{e^{-\Delta|x|/v}}{2\sqrt{2\pi\Delta|x|v}} \ . \qquad (51)$$

The correlation length is $\xi = v/\Delta$, independent of h. In this case, the residue of the pole at $\kappa = i\omega_-$ is finite as $h \to h_c$ since the ω_- factor in the denominator is cancelled by a similar factor in the numerator. Such a cancellation does not occur when the axial symmetry is broken. Consequently the correlation length diverges as h_c. Keeping only the dominant contribution as $h \to h_c$, we find

$$G_{ij} \to \frac{1}{2} \left[\frac{\Delta_2^2-\Delta_1^2}{\Delta_2^2+3\Delta_1^2} \right]^{1/2} \int \frac{dk}{2\pi} e^{ikx} \frac{1}{2\sqrt{(h_c^2-h^2)+v^2k^2}} \ . \qquad (52)$$

Thus the correlation length diverges at h_c:

$$\xi \to v/\sqrt{h_c^2-h^2} \ . \qquad (53)$$

Above h_c, we see from Eq. (16) that the propagator is again given by Eq. (49) except that now we must make the replacements

$$\Delta_1^2-h^2 \to 2(h^2-\Delta_1^2) \ , \quad \Delta_2^2-h^2 \to \Delta_2^2-\Delta_1^2 \ . \qquad (54)$$

In the axially symmetric case, $\omega_- \to 0$ as $k \to 0$ for all $h > h_c$. The residue of the pole at ω_- diverges as $k \to 0$ since no cancellation of the ω_- in the denominator occurs. Hence the correlation length is infinite, the propagator behaving as

$$G(x) \propto \int \frac{dk}{2\pi} e^{ikx} \frac{1}{|k|} \propto \text{const} + \ln|x| \ . \qquad (55)$$

With broken axial symmetry, the correlation length is finite above h_c, but diverges as $h \to h_c$,

$$\xi \to v/\sqrt{h^2-h_c^2} \ , \qquad (56)$$

due to the behavior of ω_- and the noncancellation of the ω_- factor in the denominator.

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