Commensurate and incommensurate correlations in Haldane-gap antiferromagnets

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We analyze the onset of incommensurabilities around the VBS point of the $S=1$ bilinear-biquadratic model. We propose a simple effective field theory which is capable of reproducing all known properties of the commensurate-incommensurate transition at the disorder point $\theta_{\rm VBS}$. Moreover, the theory predicts another special point $\theta_{\rm disp}$, distinct from the VBS point, where the Haldane gap behaves singularly. The ground state energy density is an analytic function of the model parameters everywhere, thus we do not have phase transitions in the conventional sense.

I. INTRODUCTION

The $S=1$ bilinear-biquadratic chain

$$H=\sum_i \left[\cos\theta \mathbf{S}_i\mathbf{S}_{i+1}+\sin\theta(\mathbf{S}_i\mathbf{S}_{i+1})^2\right] \tag{1}$$

is one of the prototype models for the physics of Haldane gap[1] antiferromagnets. Its zero temperature phase diagram has been the subject of intensive studies in recent years.[2–7] By now it is well established that the energy gap (Haldane gap) persists in a wide range $-\pi/4<\theta<\pi/4$ around the conventional Heisenberg point $\theta=0$. The model is gapless at the special points[8] $\theta=\pm\pi/4$ beyond which other phases with qualitatively different physical properties appear. Although the gap and the hidden (string) order[9] characterizing the Haldane-gap systems persist for the whole Haldane phase $-\pi/4<\theta<\pi/4$, one can divide this interval into (at least) two, somewhat different subphases.[4,5] These subphases are separated by the so called valence-bond-solid (VBS) point[10] $\theta_{\rm VBS}=\tan^{-1}1/3\approx 0.1024\pi$ where the ground state properties can be obtained exactly. The two subphases differ in the form of the long distance asymptotics of the two-point correlation function $\langle S_i^zS_{i+n}^z\rangle$. In the ''commensurate'' Haldane phase (C phase) for $-\pi/4<\theta<\theta_{\rm VBS}$ the leading behavior is expected to be

$$\langle S_i^zS_{i+n}^z\rangle\sim(-1)^n\frac{e^{-n/\xi}}{n^{1/2}} \quad \text{for } n\to\infty, \tag{2}$$

while in the ''incommensurate'' Haldane phase (IC phase) for $\theta_{\rm VBS}<\theta<\pi/4$ this was predicted to take the form

$$\langle S_i^zS_{i+n}^z\rangle\sim\frac{e^{-n/\xi}}{n^{1/2}}\cos(qn+\phi) \quad \text{for } n\to\infty, \tag{3}$$

where $q=q(\theta)\in(\pi,2\pi/3)$ is a θ-dependent incommensurate wave number, ϕ is a phase shift, and $\xi=\xi(\theta)$ is the correlation length. At the ''C-IC transition point'' (also called the ''disorder point'') $\theta_{\rm CIC}=\theta_{\rm VBS}$ the correlation function is known rigorously and it is purely exponential without any algebraic prefactor

$$\langle S_i^zS_{i+n}^z\rangle=\frac{4}{3}(-)^ne^{-n/\xi}-\frac{2}{3}\delta_{n0}, \tag{4}$$

with $\xi(\theta_{\rm VBS})=1/\ln 3\approx 0.9102$. Correlation functions of some other operators can also be studied rigorously at the VBS point.[7] In particular, $\langle(S^z)_i^2(S^z)_{i+n}^2\rangle$ has a similar purely exponential decay with $\xi=1/\ln 3$ at $\theta=\theta_{\rm VBS}$.

The commensurate-incommensurate (C-IC) transition of the spin-1 chain bears much similarity to C-IC transitions found in other models, e.g., in the anisotropic 2D Ising model on the triangular lattice at finite temperature, where it can be analyzed rigorously using the exact solution.[11] Other, higher dimensional, not exactly solvable models with disorder points were investigated using an RPA approach to the susceptibility in Ref. 12. In general, C-IC transitions can be divided into two categories (two kinds). In this classification scheme the transition at the VBS point of the $S=1$ chain is a C-IC transition of the *first* kind, with the property that the incommensurate wavenumber q in the IC regime is parameter dependent. For C-IC transitions of the first kind the correlation length is predicted to behave on the C and IC sides of the disorder point $\theta_{\rm CIC}$ as

$$\left.\frac{d\xi}{d\theta}\right|_{\rm C}=-\infty, \quad \left.\frac{d\xi}{d\theta}\right|_{\rm IC}=\text{finite} \tag{5}$$

with $\xi(\theta_{\rm CIC})\neq 0$ at the transition point. The characteristic wave number is expected to vary on the IC side as

$$q(\theta)-q(\theta_{\rm CIC})\sim|\theta-\theta_{\rm CIC}|^{1/2}. \tag{6}$$

Moreover, the RPA theory[12] also predicts the change of the asymptotic form of the correlation functions at the disorder point: the algebraic prefactor is $n^{-(D-1)/2}$ in D dimensions except at the disorder point where $D\to D'$, $D'<D$ should be taken, reflecting a ''dimensional reduction.'' In our case $D=1+1=2$, $D'=1$ as is seen in Eqs. (2)–(4). These general features of the C-IC transitions of the first kind have been tested numerically for the spin-1 chain, and except for some observed deviation from the predicted form in Eq. (3) slightly above $\theta_{\rm VBS}$, all were justified.[5] Note that around the VBS point finite size corrections are very small, thus the numerical results (exact diagonalization and DMRG) are extremely precise.

Within the IC subphase some other special points can be defined. The first one is $\theta_{\rm disp}\approx 0.1210\pi$, where the second derivative of the magnon dispersion at $k=\pi$ vanishes, and the dispersion becomes quartic. When the chain is subject to a uniform magnetic field the magnetization-vs-field curve

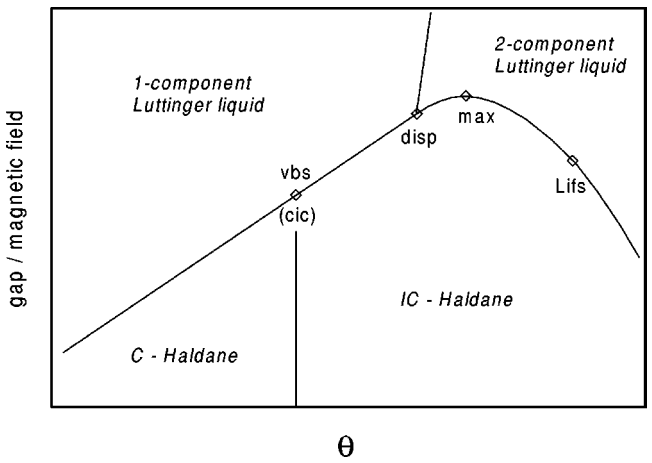

FIG. 1. Schematic phase diagram showing the neighborhood of the C-IC transition with the special points. The critical magnetic field, where the Haldane gap collapses, equals the value of the energy gap.

has an anomalous, non-square-root-like singularity at this point.[13] For $\theta > \theta_{\rm disp}$, the second derivative at $k=\pi$ is negative and the gap takes its minimum value for a momentum different from $k=\pi$.[6] In this region a strong enough field causes the Haldane gap to collapse into a *two*-component Luttinger liquid (LL) phase instead of a conventional one-component LL phase.[14] The next special point is $\theta_{\rm max} \approx 0.123\pi$ where the Haldane gap takes its maximum value. Note that this point has less physical relevance, since it strongly depends on the actual definition of the Hamiltonian; a θ-dependent rescaling of the model can easily change its location. Finally one can define the Lifsitz point $\theta_{\rm Lifs} \approx 0.1314\pi$, where the incommensurability manifests itself in the structure factor. This is different from the disordered point in massive models due to the finite linewidth of the peaks.[5] Figure 1 shows these special points.

In both the C and IC Haldane phases the energy spectrum consists of a discrete triplet branch of ''magnons'' separated by finite gaps from the singlet ground state, and also from a continuum of higher lying ''multimagnon'' excitations in a wide momentum range. This one-magnon branch is clearly discernible around the edges of the Brillouin zone $k=\pm\pi$. However, it merges into the continuum and vanishes due to magnon scattering processes in an extended range around $k=0$. The energy spectrum, especially in the Heisenberg point and the VBS point was studied numerically by many authors.[7,15–17] All concluded that the magnon-magnon interactions are rather weak, and bound states do not play a role at low energies. Many properties of the system, from ground-state correlation functions[15,18] to the onset of magnetization in uniform fields[13,19,20] can be extremely well approximated using a massive relativistic free boson theory. Such an approximate theory can be derived directly from the nonlinear σ model (NLσM) description of the spin chain at the Heisenberg point,[21] or from the Majorana fermion representation of the integrable Takhtajan-Babujian model in the vicinity of $\theta=-\pi/4$.[22] However, all these microscopic theories utilize the *a priori* assumption that the important low-energy fluctuations are at momenta $k=0$ and π, and thus they cannot account for the C-IC transition, nor can they give any reliable description of the IC regime.

Although we do not have a rigorous microscopic justification all results we possess are consistent with the assumption that the elementary excitations are essentially free bosons in the IC regime, too. Thus the aim of the present paper is to extend the free boson description to the whole Haldane phase, and give a general theory which is capable of accounting for the C-IC transition in simple terms. In the lack of a detailed microscopic formulation, however, this theory, at present, is only phenomenological.

II. EFFECTIVE THEORY—CONTINUUM VERSION

A continuum field theory to describe Heisenberg antiferromagnetic chains ($\theta=0$) with integer S was developed by Haldane.[1] This is the nonlinear σ model (NLσM)—without topological terms—which can be derived in the large S limit, but whose implications are believed to hold for $S=1$ too. The NLσM is defined by the Lagrangian[21]

$$\mathcal{L}=\frac{1}{2g}\left[\frac{1}{v}(\partial_t\vec{\phi})^2-v(\partial_x\vec{\phi})^2\right], \tag{7}$$

where $\vec{\phi}(x,t)$ is a vector field with unit length $\vec{\phi}^2=1$, v is a nonuniversal constant (velocity) setting the energy scale, and $g=2/S$ is the coupling constant. The associated Hamiltonian is

$$\mathcal{H}=\frac{v}{2}\left[g\vec{l}^2+\frac{1}{g}(\partial_x\vec{\phi})^2\right], \tag{8}$$

where the momentum canonically conjugate to $\vec{\phi}$ turns out to be

$$\vec{l}(x,t)\equiv\frac{1}{gv}\left[\vec{\phi}\times\frac{\partial\vec{\phi}}{\partial t}\right](x,t). \tag{9}$$

The spin operator $\vec{S}_n$ can be expressed in terms of $\vec{\phi}$ and $\vec{l}$ as

$$\vec{S}_n(t)=(-1)^n S\vec{\phi}(x_n,t)+\delta x\vec{l}(x_n,t), \tag{10}$$

where $x_n=n\delta x$, δx being the lattice constant (usually set to unity), and $S=1$ in the present case. At the mean field level the NLσM can be well approximated by a massive, essentially free vector-boson theory

$$\mathcal{L}=\frac{1}{v}(\partial_t\vec{\phi})^2-v(\partial_x\vec{\phi})^2-m^2\vec{\phi}^2, \tag{11}$$

now without any constraint on the $\vec{\phi}$ field. The boson field $\vec{\phi}$ varies smoothly on the scale of the lattice constant in the commensurate regime (the pure Heisenberg model, which the theory applies for, is in the C phase) and thus higher derivatives, neglected in Eq. (11), are indeed small. The Lagrangian gives rise to a relativistic dispersion $\omega(k)=\sqrt{m^2+v^2k^2/2m}$ which takes its minimum at $k=0$. [Note the factor $(-1)^n$ introduced in Eq. (10) shifting all momenta by π.]

The NLσM summarized above gives a good description of the low-energy behavior of the $S=1$ Heisenberg chain, but is unable to describe the C-IC transition in the bilinear-biquadratic chain. The key feature missing is that in the vicinity of our special points the shape of the magnon disper-

sion changes drastically, and the minimum at $k=\pi$ ($k=0$ in the momentum-shifted boson language) splits. Obviously, such an effect can never be obtained from a relativistic field theory such as Eq. (11) and we need to consider a nonrelativistic model. The simplest continuum Lagrangian with this property is

$$\mathcal{L}=(\partial_t\vec{\phi})^2-a(\partial_x\vec{\phi})^2-b(\partial_x^2\vec{\phi})^2-m^2\vec{\phi}^2. \tag{12}$$

At this level a, b, and m are θ-dependent phenomenological parameters. For stability b is supposed to be positive, and a is assumed to change sign at the special point $\theta_{\rm disp}$. [Note that in the relativistic case $b=0$, and a is in fact v^2, where v is the ''speed of light.'' Formally taking $a<0$, which we will consider in the sequel, implies an imaginary v. This only means, however, that one should redefine the physical (quasi)particles to live around the two new minima of the dispersion. In fact, one should introduce two new particles, now with $v=$ real, for the two minima. This immediately leads to a two-particle (two-band) description which was analyzed in detail in Ref. 14 for the massless case (above the critical magnetic field) and was shown to result a two-component (two-band) Luttinger liquid there. Here we shortcut these complications by simply assuming that the two particles are two chiral components ($k<0$ and $k>0$) of the same boson with $a<0$.]

Since our phenomenological model is not derived directly from the microscopic Hamiltonian in Eq. (1) the connection between the boson field and the original spin variables is not known rigorously. In principle $\vec{S}_n$ can be expanded in powers of the field $\vec{\phi}$ and its derivatives, and any term permitted by the symmetries of the model can appear. Being guided by the NLσM description at the Heisenberg point, in the following we will assume that the first two terms (linear and quadratic in $\vec{\phi}$) are

$$\vec{S}_n(t)=g_\phi(-1)^n\vec{\phi}(x_n,t)+g_l\vec{l}(x_n,t)+\mathcal{O}(|\vec{\phi}|^3), \tag{13}$$

where g_ϕ and g_l are unknown constants. Note that the $\vec{l}$ term, defined by Eq. (9), is the most relevant two-boson term which is even under parity and odd under time reversal as it should be. Although, we cannot exclude the possibility that up to $\mathcal{O}(\vec{\phi}^2)$ some other terms with higher derivatives also appear, such extra derivatives, due to the finite mass gap, would not modify the long distance asymptotics of $\langle\vec{S}_0\vec{S}_n\rangle$. Equation (13) shows that in the C phase where spin-spin correlations are antiferromagnetic ϕ varies smoothly, and higher order derivatives in the Langrangian have minor role. Around the C-CI transition point, and in the IC-phase, however, this is no longer the case: as $\vec{S}_n$ picks up incommensuration, $\vec{\phi}(x)$ must do so, as well. It no longer varies smoothly, and higher derivatives in the Lagrangian cannot be neglected. This is the effect which we try to take into consideration by the b term in Eq. (12).

The asymptotic behavior of the correlation function $\langle S_i^zS_{i+n}^z\rangle$ is determined by the one-boson term; the two-boson term and in general any multiboson terms only constitute minute corrections which decay at least twice as rapidly. Thus, up to the two-boson term in Eq. (13) the spin-spin correlation function has the behavior

$$\langle S_n^z(t)S_0^z(0)\rangle=g_\phi^2(-)^nG_\phi(x_n,t)+g_l^2G_l(x_n,t), \tag{14}$$

with

$$G_\phi(x,t)\equiv\langle\phi^z(x,t)\phi^z(0,0)\rangle, \tag{15}$$

$$G_l(x,t)\equiv\langle l^z(x,t)l^z(0,0)\rangle. \tag{16}$$

These are the quantities we will now calculate.

The Euler-Lagrange equation associated with our Lagrangian gives a generalized Klein-Gordon equation for each component $\alpha=x,y,z$ of $\vec{\phi}$

$$\partial_t^2\phi^\alpha-a\partial_x^2\phi^\alpha+b\partial_x^4\phi^\alpha+m^2\phi^\alpha=0, \tag{17}$$

whose Green's function is

$$G_\phi(\omega,k)=\frac{1}{\omega^2-ak^2-bk^4-m^2+i\varepsilon}. \tag{18}$$

This defines the nonrelativistic dispersion

$$\omega(k)=\sqrt{m^2+ak^2+bk^4}, \tag{19}$$

which reduces to the relativistic dispersion of Ref. 18 when $b=0$.

The generalized theory can be quantized identically to the relativistic Klein-Gordon theory.[23] The field ϕ^α, $\alpha=x,y,z$, has the following mode expansion

$$\phi^\alpha(x,t)=\int\frac{dk}{\sqrt{4\pi\omega(k)}}[d_k^\alpha e^{i\mathbf{K}\cdot\mathbf{X}}+d_k^{\alpha\dagger}e^{-i\mathbf{K}\cdot\mathbf{X}}], \tag{20}$$

where $\mathbf{K}\cdot\mathbf{X}=\omega t-kx$, and the normalization is $[d_k^\beta,d_{k'}^{\alpha\dagger}]=\delta_{\beta\alpha}\delta(k-k')$. Using the mode expansion the equal time expressions $G_\phi(x)$ and $G_l(x)$ can be easily reduced to Fourier transforms[18]

$$G_\phi(x)=\int\frac{dk}{4\pi}\frac{e^{ikx}}{\omega(k)},$$

$$G_l(x)=\frac{1}{2}\int\frac{dk'}{4\pi}\omega(k')e^{ik'x}\int\frac{dk}{4\pi}\frac{e^{ikx}}{\omega(k)}-\frac{1}{2}\delta^2(x). \tag{21}$$

Note that the integral determining G_ϕ also appears as a multiplicative factor in G_l.

Since the asymptotic behavior is determined by G_ϕ, we start our analysis with this. The evaluation of the Fourier transform starts with locating the zeros of $\omega(k)$ in the complex plane. The four zeros are given by

$$k=\pm\left[\frac{1}{2b}(-a\pm\sqrt{a^2-4m^2b})\right]^{1/2} \tag{22}$$

and depend on the single parameter θ, via a, b, and m. Since our phenomenological model is not derived directly from the microscopic one, we have to make several assumptions about the θ dependence of a, b, and m. We will assume that this dependence is smooth (analytical), $m(\theta)$ and $b(\theta)$ are nonnegative whereas a decreases with increasing θ and changes sign at $\theta_{\rm disp}$. We introduce the discriminant

$$D(\theta)=a^2-4m^2b, \tag{23}$$

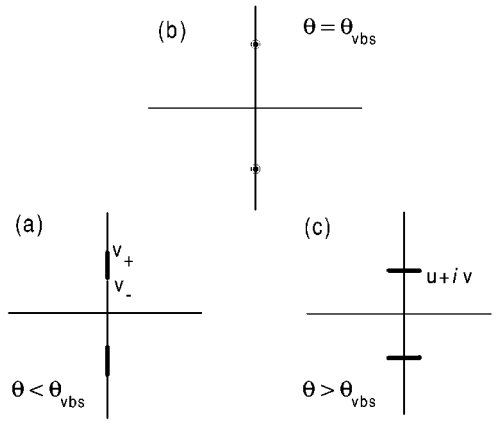

FIG. 2. Roots of $\omega(k)$ in the complex k plain. (a) $\theta<\theta_{\rm VBS}$, (b) $\theta=\theta_{\rm VBS}$, (c) $\theta>\theta_{\rm VBS}$. Branch cuts are chosen according to the conventions described in the text.

which is hence an analytic function of θ, and we suppose that it is positive for $\theta<\theta_{\rm VBS}$, vanishes at the VBS point, and it is negative from $\theta_{\rm VBS}$ to $\theta=\pi/4$ where it vanishes again. As we show below, under the above hypotheses the phenomenological model provides the expected asymptotic behavior of the correlation function in all parts of the Haldane phase.

$\theta=\theta_{\rm VBS}$: At this point $a>0$ and $D=0$. The expression under the square-root in $\omega(k)$ is a complete square, thus ω becomes quadratic in k and has two purely imaginary zeros, $\pm i\sqrt{2m^2/a}=\pm i\sqrt{a/2b}$ [see Fig. 2(b)]. The contour of integration can be closed in the upper half plane and the result is

$$G_\phi(x)=\frac{1}{2\sqrt{2a}}e^{-\sqrt{a/2b}|x|}. \tag{24}$$

Because of the purely exponential decay, this indeed corresponds to $\theta=\theta_{\rm VBS}$.

$\theta<\theta_{\rm VBS}$: In this region $a>0$ and $D>0$. We may suppose $b>0$; the case when $b=0$ can be obtained by continuity. We get four purely imaginary zeros $\pm iv_\pm$,where

$$v_\pm=\left[\frac{1}{2b}(a\pm\sqrt{D})\right]^{1/2}. \tag{25}$$

Now

$$\omega(k)=\sqrt{b}(k^2+v_+^2)^{1/2}(k^2+v_-^2)^{1/2} \tag{26}$$

is single-valued in the complex plane with two cuts, one between $-iv_+$ and $-iv_-$ and another one between iv_- and iv_+ [see Fig. 2(a)]. (We use the convention that $z^{1/2}$ has a cut along the negative real axis.) The contour of integration can be closed in the upper half-plane and drawn onto the upper cut, giving

$$G_\phi(x)=\frac{1}{2\pi\sqrt{b}}\int_{v_-}^{v_+}\frac{e^{-t|x|}}{[(t^2-v_-^2)(v_+^2-t^2)]^{1/2}}dt. \tag{27}$$

This function is positive for all x, so with the factor $(-1)^n$ introduced in Eq. (13) we obtain the expected antiferromagnetic modulation. As $|x|$ goes to infinity, the main contribution to the integral is coming from the vicinity of the end point v_-, and it is legitimate[24] to expand the integrand around this point. For $|x|>|D|^{-1/2}$ this yields

$$G_\phi(x)=\frac{e^{-v_-|x|}}{2[2\pi v_-\sqrt{D}]^{1/2}}[|x|^{-1/2}+O(|x|^{-3/2})]. \tag{28}$$

Together with Eq. (13), we find the expected asymptotic form Eq. (2) of the spin-spin correlation function with a correlation length $\xi=1/v_-$ which is continuous at $\theta=\theta_{\rm VBS}$.

$\theta>\theta_{\rm VBS}$: Here D becomes negative and ω has four complex zeros $k_j=\pm u\pm iv$ $(j=1,\ldots,4)$ with

$$u=\left[\frac{m}{2\sqrt{b}}-\frac{a}{4b}\right]^{1/2},\quad v=\left[\frac{m}{2\sqrt{b}}+\frac{a}{4b}\right]^{1/2}. \tag{29}$$

If we write ω in the form

$$\omega(k)=\sqrt{b}\prod_{j=1}^{4}(k-k_j)^{1/2} \tag{30}$$

we see that it is single-valued on the complex plane with a cut between $-u-iv$ and $u-iv$ and another cut between $-u+iv$ and $u+iv$ [see Fig. 2(c)]. For k real we get back the original positive function. The integration can be carried out along a contour which starts at $-u+i\infty$, goes vertically down to $-u+iv$, passes below the upper cut and goes vertically to $u+i\infty$. Next, we replace the integral below the cut by an integral going above the cut and in the opposite sense, and this latter by the sum of the two integrals along the vertical half lines. These are complex conjugate to each other, so finally we obtain

$$G_\phi(x)=\frac{1}{\pi\sqrt{b}}\times\int_v^\infty\frac{e^{-|x|t}\cos[u|x|-\varphi(t)]dt}{\sqrt{t^2-v^2}[4u^2+(t-v)^2]^{1/4}[4u^2+(t+v)^2]^{1/4}}, \tag{31}$$

where

$$\varphi(t)=\frac{1}{2}\left(\arctan\frac{t-v}{2u}+\arctan\frac{t+v}{2u}\right). \tag{32}$$

Now $G_\phi(x)$ changes sign periodically, and we can identify $\pi-u$ with the wave number q of the incommensurate oscillation. At the VBS point $u=0$, and as it is shown by Eq. (29), the assumed analyticity of m, a and b assures that it has a square-root-type singularity above the VBS point in accordance with Eq. (6). The large-$|x|$ asymptotics of $G_\phi(x)$ can be obtained by Watson's lemma[24] or by a direct expansion

$$G_\phi(x)=\frac{e^{-v|x|}\cos[u|x|-(1/2)\arctan(v/u)]}{(2\pi)^{1/2}\left(\dfrac{-mD}{\sqrt{b}}\right)^{1/4}}\times[|x|^{-1/2}+O(|x|^{-3/2})]. \tag{33}$$

Formulas (31) and (33) apply for any θ between $\theta_{\rm VBS}$ and $\pi/4$, including $\theta_{\rm disp}$ which is a symmetry point of the domain

of incommensurate oscillations ($u=v$). As θ approaches $\pi/4$, D goes to zero and the zeros of $\omega(k)$ tend to the real axis. Thus, v goes to zero and the correlation length diverges. This is what we expect at the boundary of the Haldane phase $\theta=\pi/4$ where the gap disappears. At this special point the ground state has a tripled periodicity,[3,8] implying $u(\theta=\pi/4)=2\pi/3$.

For *any fixed* x, $G_\phi(x)$ depends analytically on θ inside the whole Haldane phase. This can be seen from the original form Eq. (21) of $G_\phi(x)$ by inserting the original, nonfactorized expression Eq. (19) for $\omega(k)$. A proof can be found in Ref. 25. The argument makes use of the continuity of the integrand in k real, its (supposed) analyticity for any fixed k as a function of θ in suitable complex domains, and the uniform convergence of the integral for θ in any of these domains. It is interesting to examine another kind of asymptotics, valid in a close neighborhood of $\theta_{\rm VBS}$, when $|D|/a^2 \ll 1$. In this case Eq. (27) reduces to the form

$$G_\phi(x)\approx \frac{e^{-\sqrt{a/2b}|x|}}{\sqrt{8a}}\frac{1}{\pi}\int_0^\pi \cosh\left[\sqrt{\frac{D}{8ab}}|x|\sin\alpha\right]d\alpha$$
$$\equiv \frac{e^{-\sqrt{a/2b}|x|}}{\sqrt{8a}} I_0\left(\sqrt{\frac{D}{8ab}}|x|\right) \tag{34}$$

where I_0 is the zeroth order Bessel function. We can arrive at the same equation from Eq. (31), by changing the contour of integration (integrating around the upper cut). Now analyticity at the VBS point is manifest, because in the expansion of the hyperbolic cosine about zero only the even powers of $\sqrt{D}$ appear. Equation (34) shows that the crossover to the decay with the $|x|^{-1/2}$ prefactor sets in at the characteristic distance $|x|\sim D^{-1/2}$, which diverges at the VBS point. This explains the numerical difficulties[5] verifying the expected asymptotic behavior very close to the VBS point.

At the VBS point there is an infinite jump in the derivative of the correlation length, as predicted by Eq. (5). Indeed, Eq. (25) yields

$$\left.\frac{d\xi}{d\theta}\right|_{\theta_{\rm VBS}-0} \approx \left.\frac{D'}{4\sqrt{2am}}\right|_{\theta_{\rm VBS}} D^{-1/2}\sim -(\theta_{\rm VBS}-\theta)^{-1/2} \tag{35}$$

because $D'(\theta_{\rm VBS})<0$. On the other hand, from Eq. (29)

$$\left.\frac{d\xi}{d\theta}\right|_{\theta_{\rm VBS}+0} = -\frac{1}{2\sqrt{a}}\left(\frac{m'}{2m}+\frac{a'}{2a}+\frac{m^2}{a^2}\right)\Bigg|_{\theta_{\rm VBS}}, \tag{36}$$

which is finite. The singularity of the correlation length at $\theta_{\rm VBS}$ is in no contradiction with the analyticity of $G_\phi(x)$ at a *fixed* x. Indeed, the divergence of the derivative of ξ was extracted from the single-exponential asymptotic form Eq. (28) which, again, is valid only for $|x|>(v_+-v_-)^{-1}\sim D^{-1/2}$.

To see the role of the two-boson term G_l in the correlation functions, we can use the identity (after proper regularization)

$$\int \frac{dk}{4\pi}\omega(k)e^{-ikx} = \omega^2\left(i\frac{\partial}{\partial x}\right)\int\frac{dk}{4\pi}\frac{e^{-ikx}}{\omega(k)}, \tag{37}$$

where $\omega^2(i\partial/\partial x)$ is a shorthand for $m^2-a\partial^2/\partial x^2+b\partial^4/\partial x^4$ in the present case. With this

$$G_l(x)=G_\phi(x)\omega^2\left(i\frac{\partial}{\partial x}\right)G_\phi(x), \tag{38}$$

where we have neglected the singular, delta-function term of Eq. (21). This term can be evaluated directly for large x, knowing the asymptotic form of G_ϕ in the different regimes. Using Eqs. (24), (28), and (33) we obtain

$$G_l(x)\sim\begin{cases}\dfrac{e^{-2v_-x}}{x^2} & \text{if } \theta<\theta_{\rm VBS},\\ 0 \quad \text{if } \theta=\theta_{\rm VBS},\\ \dfrac{e^{-2vx}}{x^2}[c_1+c_2\cos(2ux+\alpha)] & \text{if } \theta>\theta_{\rm VBS},\end{cases} \tag{39}$$

where the constants c_1, c_2, and α can be expressed straightforwardly with a, b, and m. It is interesting to remark that G_l is exactly zero for any $x>0$ at the disorder point, i.e., the two-boson processes do not contribute to the equal time correlation function there. This can be easily verified by calculating $\omega^2(i\partial/\partial x)G_\phi(x)$ using Eq. (24) and the fact that $D=0$ at the VBS point. Here $\langle S^z_n S^z_0\rangle$ only contains the G_ϕ term in full accordance with the exact solution. For other values of θ, G_l decays twice as rapidly as G_ϕ.

It is also of interest to see what predictions our simple field theory gives for the analytic properties of the ground state energy density and the gap. Using the mode expansion in Eq. (20), the Hamiltonian can be written as

$$H=\int_{-\Lambda}^{\Lambda} dk\,\omega(k)\left[d_k^\dagger d_k+\frac{1}{2}\right], \tag{40}$$

where Λ is an appropriate UV momentum cutoff, proportional to the inverse of the lattice constant. From this the ground state energy is

$$E=\frac{1}{2}\int_{-\Lambda}^{\Lambda} dk\,\omega(k). \tag{41}$$

The ground state energy depends analytically on a, b, and m whenever the zeros of $\omega(k)$ are not on the real axis. Together with the supposed analyticity of $a(\theta)$, etc., this means that $E(\theta)$ is also analytic inside the whole Haldane phase.[25] A straightforward expansion around $\theta_{\rm VBS}$ yields

$$\lim_{\Lambda\to\infty}[E(\theta)-E(\theta_{\rm VBS})]$$
$$=-\frac{8\pi a^{3/2}}{\sqrt{2}b}\sum_{n=1}^{\infty}\frac{2^{-6n}(4n-4)!}{(2n-2)!n!(n-1)!}\left(\frac{D}{a^2}\right)^n, \tag{42}$$

which is convergent if $|D|/a^2<1$. We notice that in general $E(\theta)$ can be expressed in a closed form in terms of elliptic integrals of the first and second kind.

The energy gap of the model is by definition

$$\Delta=\min_k\omega(k). \tag{43}$$

This is obviously analytic at $\theta_{\rm CIC}=\theta_{\rm VBS}$ but has a singularity at $\theta_{\rm disp}$, where the minima of $\omega(k)$ move away from $k=0$ as the parameter $a=0$ changes sign. While for $\theta\leqslant\theta_{\rm disp}$ the minimum is taken at $k=0$, for $\theta>\theta_{\rm disp}$ it is taken at $k=\pm\sqrt{-a/2b}$. The gap Δ and its derivatives with respect to θ on the two sides of $\theta_{\rm disp}$ turn out to be, respectively,

$$\Delta(\theta_{\rm disp}-0)=m,\quad \Delta(\theta_{\rm disp}+0)=m,$$

$$\Delta'(\theta_{\rm disp}-0)=m',\quad \Delta'(\theta_{\rm disp}+0)=m', \tag{44}$$

$$\Delta''(\theta_{\rm disp}-0)=m'',\quad \Delta''(\theta_{\rm disp}+0)=m''-\left.\frac{a'^2}{4bm}\right|_{\theta_{\rm disp}}.$$

We see that there is a discontinuity in the second derivative. This behavior of the effective theory seems consistent with the numerical results shown in Fig. 9 of Ref. 5.

III. EFFECTIVE THEORY—LATTICE VERSION

The effective theory presented above is capable of providing a complete qualitative description of the C-IC transition of the spin-1 bilinear-biquadratic model in accordance with the available numerical data. However, in order to give quantitative predictions, too, the theory needs some refinement. We have seen earlier that our simple theory identifies the disorder point $\theta_{\rm CIC}$ with the point where the discriminant D defined by Eq. (23) vanishes. It is easy to verify that the second and fourth derivatives of $\omega(k)$ at $k=0$ are, respectively,

$$\frac{\partial^2\omega}{\partial k^2}(k=0)=\frac{a}{m},\quad \frac{\partial^4\omega}{\partial k^4}(k=0)=-\frac{3D}{m^3}, \tag{45}$$

thus in the above theory the fourth derivative vanishes at the disorder point. In contrast with this, Golinelli *et al.*[6] measured numerically the second and fourth derivatives at the known disorder point $\theta_{\rm VBS}$ and found

$$\frac{\partial^2\omega}{\partial k^2}(k=0)=0.9778(1),\quad \frac{\partial^4\omega}{\partial k^4}(k=0)=-1.202(1). \tag{46}$$

Note that the fourth derivative is only zero far inside the IC regime, which seems inconsistent with the above theory.

One step to improve the theory is to realize that the model is defined on a lattice, and thus the dispersion $\omega(k)$ must be a 2π-periodic function of k (from now on the lattice constant is set $\delta x=1$). This can be incorporated into the Lagrangian in Eq. (12) by the standard replacement $\partial_x\phi\to[\phi(n+\delta x)-\phi(n)]/\delta x$, leading to the substitution $k^2\to 2[1-\cos(k)]$ in the dispersion

$$\omega(k)=\sqrt{m^2+2a+6b-(2a+8b)\cos(k)+2b\cos(2k)}. \tag{47}$$

The Green's function now reads

$$G_\phi(n)=\int_{-\pi}^{\pi}\frac{dk}{4\pi}\frac{1}{\omega(k)}e^{ikn}. \tag{48}$$

The condition that the expression under the square root in $\omega(k)$ is a complete square is again $D(\theta)=0$ with D defined in Eq. (23). When this is satisfied the dispersion simplifies to

$$\omega_{\rm VBS}(k)=m_{\rm VBS}+\frac{a_{\rm VBS}}{m_{\rm VBS}}[1-\cos(k)], \tag{49}$$

and $1/\omega_{\rm VBS}(k)$ has poles instead of branch cuts. [One pole within the Brillouin zone $-\pi<{\rm Re}(k)\leqslant\pi$ with $0<{\rm Im}(k)$.] Now the second and fourth derivatives at $k=0$ are [see Eq. (45)]

$$\frac{\partial^2\omega}{\partial k^2}(k=0)=\frac{a}{m},\quad \frac{\partial^4\omega}{\partial k^4}(k=0)=-\frac{3D}{m^3}-\frac{a}{m}. \tag{50}$$

At the disorder point we find

$$\frac{\partial^4\omega}{\partial k^4}(k=0)=-\frac{a_{\rm VBS}}{m_{\rm VBS}}, \tag{51}$$

which is nonzero. The correlation length $\xi=1/{\rm Im}(k)$ at the disordered point is determined by the position of the pole, i.e., by the solution of the transcendental equation

$$1+\frac{a_{\rm VBS}}{m_{\rm VBS}^2}[1-\cos(k)]=0. \tag{52}$$

Working the other way around, knowing that at the VBS (C-IC) point $\xi_{\rm VBS}=1/\ln 3$, Eq. (52) gives $a_{\rm VBS}=3m_{\rm VBS}^2/2$ and thus the dispersion

$$\omega_{\rm VBS}=m_{\rm VBS}\left[\frac{5}{2}-\frac{3}{2}\cos(k)\right]. \tag{53}$$

With this expression the lattice Green's function defined in Eq. (48) reads

$$G_\phi(n)=\frac{1}{4m_{\rm VBS}}e^{-|n|\ln 3}, \tag{54}$$

which should be conferred to Eq. (4). The functional form of the dispersion relation in Eq. (53) is exactly the same as the one appearing in the *single mode approximation* of the VBS model.[16,17] There, one derives an upper bound for the gap $\Delta_{\rm VBS}=m_{\rm VBS}=\sqrt{40}/9$, whereas here we should use the phenomenological (numerical) value $\Delta_{\rm VBS}=0.664314$ in Eq. (53). This, together with Eq. (51) yields the value $\partial^4\omega/\partial k^4=-3m_{\rm VBS}/2\approx-1.0$, which is rather close to the numerical estimate in Eq. (46).

The split of the double root in the vicinity of the disorder point can be analyzed similarly to the continuum theory. We do not go into details here, but emphasize that the critical exponents characterizing the behavior of $\xi(\theta)$ and $q(\theta)$ at $\theta_{\rm VBS}$, and the type of the singularity of the gap at $\theta_{\rm disp}$ remain the same. Similarly, we find that the ground state energy is analytic everywhere.

One can wonder about the possible consequences of keeping higher order terms in the continuum Lagrangian Eq. (12) or in the improved lattice version. If the theory remains free the only effect is to bring about additional branch cuts or poles in $1/\omega(k)$. If the higher order terms are small the additional branching points are far in k space, and the C-IC

transition remains intact. The long distance asymptotics of the correlation functions do not change. Since at the VBS point the exact correlation function in Eq. (4) only contains a single exponential term, the free boson approximation does not allow any higher order spatial derivatives in the effective Lagrangian there.

Although the dispersion ω_{VBS} in Eq. (53) gives rise to the exponential term in Eq. (4), it misses the $\delta_{n,0}$ contribution. This is, however, another artifact of the continuum approach, which necessarily neglects some important short distance details. In fact, we should recall that in a quantum spin liquid with short-range valence bond ground state the elementary excitations (bosons) are physically triplet bonds living *between* lattice sites, rather than on the sites themselves. As was argued in Ref. 16, S_i^z acting on the VBS ground state produces the linear combination of two states, one of which containing a boson at site $i-1/2$, the other a boson at site $i+1/2$. Hence the one-boson term of $\langle S_i S_{i+n}\rangle$ is in fact

$$\langle S_n^z S_0^z\rangle = g_\phi^2(-)^n[G_\phi(n-1)+2G_\phi(n)+G_\phi(n+1)]. \tag{55}$$

Using Eq. (54) this leads directly to Eq. (4), including the δ-function piece, if $g_\phi^2 = m_{\mathrm{VBS}}$.

IV. SUMMARY AND DISCUSSION

In summary, we proposed a simple effective field theory to describe the commensurate-incommensurate transition in the Haldane phase of the spin-1 bilinear-biquadratic chain. The theory is capable of reproducing many features of this transition previously seen in the numerical studies. Moreover it also has some new predictions. The effective theory predicts that the C-IC transition at θ_{VBS} is not a phase transition in the conventional sense, since the ground state energy remains an analytic function of the control parameter θ. The only singularity occurring is in the correlation length. We should emphasize, however, that the correlation function itself remains analytic as a function of θ for any fixed distance, unlike in conventional phase transitions.

There is another point θ_{disp} close to the disorder point where another quantity becomes singular. This is the energy gap (Haldane gap) whose second derivative produces a jump. This singularity in the singlet-triplet gap becomes important when a high enough magnetic field is applied, producing a crossing between these levels, and thus leading to the collapse of the gap. At the critical field, as θ is varied a real phase transition takes place at θ_{disp}, thus this point is the endpoint of a phase transition line on the magnetic field vs θ plain separating two Luttinger liquid type phases.

In a technical sense the C-IC transition is a consequence of an accidental degeneracy of roots of the dispersion relation. We have shown in the free boson approach that this degeneracy causes the ''dimensional reduction'' of the correlation function, and makes it to be a pure exponential at the VBS point. We also found that the two-magnon contributions, and presumably any higher order, multimagnon contributions too, vanish exactly at this point. We derived a formula valid in the vicinity of the VBS point showing how the pure exponential decay emerges from the standard form with algebraic prefactors. In particular we found that there is a crossover between a pure exponential decay and a decay containing algebraic prefactors. The characteristic distance of this crossover tends to infinity as the VBS point is approached.

The spin-1 bilinear-biquadratic model studied in this paper is not the only model which produces a C-IC transition. Another example is the spin-1/2 chain with next-nearest-neighbor interaction (this can also be visualized as a two-leg zig-zag ladder).[26] By now it is well established that the Majumdar-Ghosh point of this model is a disorder point where a C-IC transition of the first kind occurs. On the same footing as described here, it seems possible to develop an effective theory which supposes that the elementary excitations (spin-1/2 solitons in that case) are essentially free particles with a nonrelativistic dispersion. Care should, however, be taken on the facts that solitons are always created in pairs and that they are spin-1/2 particles. Beside the $S=1/2$ case, the appearance of disorder points has been demonstrated in other $S\geqslant 1$ frustrated Heisenberg chains too.[27] Another interesting quasi-one-dimensional system where a commensurate-incommensurate transition has been reported in a numerical investigation is the $\mathrm{SU}(2)\times\mathrm{SU}(2)$ symmetric coupled spin-orbit model.[28] The elaboration and testing of effective theories, similar to the one described in this paper, for these models could be a possible direction of future research.

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