Onset of incommensurability at the valence-bond-solid point in the $S=1$ quantum spin chain

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Most of the present understanding of the $S=1$ quantum spin chains displaying the Haldane gap is coming from the so-called valence-bond-solid (VBS) Hamiltonian which has an exactly known ground state. We show that this point is characterized by the onset of short-range incommensurate spin correlations in the one-parameter family of Hamiltonians $H_\theta = \cos\theta \Sigma_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \sin\theta \Sigma_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$. This gives a physical meaning to this special point. We establish precise values for the gaps, correlations, the string order parameter, and identify the VBS point as a disorder point in the sense of classical statistical mechanics. It is a quantum remnant of the classical transition between a ground state with long-range Néel order and a ground state with incommensurate long-range order.

I. INTRODUCTION

It has been conjectured by Haldane[1] that antiferromagnetic quantum spin chains have a disordered ground state with a gap to spin excitation when the spins are integer. This phenomenon has been studied extensively over the years, and a simple physical picture has emerged through the consideration of the so-called valence-bond-solid (VBS) Hamiltonian.[2] This peculiar Hamiltonian contains, in addition to the simplest isotropic bilinear nearest-neighbor exchange, a biquadratic term in the case of the spin $S=1$ chain. This modification transforms the Hamiltonian in a sum of projection operators, and, as a consequence, the ground state is known exactly and has a simple structure. This is different from the exactly integrable models: Here nothing is exactly known about the excited states. It is believed that this model is smoothly connected to the usual nearest-neighbor antiferromagnetic: they share the same physics. More precisely, there is a hidden topological long-range order[3] that is common to both Hamiltonians[4,5] and that is revealed clearly in the VBS Hamiltonian. It is interesting to note that a similar situation also happens in the fractional quantum Hall effect:[6] Here the Laughlin wave function, which is the exact ground state of an approximate Hamiltonian, does possess the hidden order, which is revealed in the anyonic gauge. The VBS nature of the ground state of the $S=1$ spin chain has led to the curious consequence of effective spins $S=\frac{1}{2}$ at the end of open chains: This has been observed theoretically[7] by numerical means and experimentally.[8,9]

If we concentrate on the VBS model in the $S=1$ case, it can be written as the sum of a bilinear and a biquadratic spin-spin interaction between nearest neighbors. It is thus natural to study it as a special case of the general bilinear-biquadratic isotropic quantum $S=1$ chain:

$$H_\theta = \cos\theta \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \sin\theta \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2, \qquad (1.1)$$

with θ varying between 0 and 2π. All energies are measured in units of the global exchange coupling, which is omitted everywhere in this paper. The VBS Hamiltonian corresponds to the value θ_{VBS} with $\tan\theta_{\mathrm{VBS}} = \frac{1}{3}$. In this case, each term in the sum in Eq. (1.1) $\mathbf{S}_i \cdot \mathbf{S}_{i+1} + (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2/3$ is the projector on the spin $S=2$ state of the two neighboring spins $i, i+1$. This fact leads to a simple ground-state wave function.[2] The behavior of this model as a function of θ has been studied by numerous authors.[10–30] If one increases θ starting from the bilinear Hamiltonian $\theta=0$, which is known to possess a Haldane gap, there is no phase transition till $\theta=\pi/4$, and thus the VBS Hamiltonian ($\theta_{\mathrm{VBS}} = atan(1/3) < \pi/4$) is smoothly connected to the usual bilinear Heisenberg model. However, its precise physical meaning has remained so far unexplained.

In this paper, we clarify the physical meaning of the VBS point in the phase diagram of the family (1.1) of models. Consider first the classical limit $S \to \infty$ of Eq. (1.1). For $\theta=0$ the ground state is antiferromagnetically long-range ordered with ordering wave vector $q=\pi$ (Néel state). When θ is increased, the order becomes incommensurate when $\theta > \theta_c$ with $\tan\theta_c = \frac{1}{2}$: the wave vector shifts from $q=\pi$. As a consequence, the static structure factor $S(q)$ has a δ peak at $q=\pi$ when $\theta < \theta_c$ and a δ peak at $q<\pi$ when $\theta > \theta_c$. Now, in the quantum case $S<\infty$ with S *integer*, fluctuations wash out long-range order and we are left with short-range order below a characteristic correlation length ξ, according to Haldane's conjecture. The δ peak of $S(q)$ is thus smeared and acquires a finite width given by ξ^{-1}.

It is important to note that, because of this finite width, the incommensurate behavior cannot be seen immediately in the quantity $S(q)$ when q shifts away from the commensurate position. This is best understood by considering the analytic structure of $S(q)$ in the complex q plane. Short-range order means that singularities (poles or branch points) are away from the real axis at a distance $\approx \xi^{-1}$. In the commensurate phase, the real part of the nearest singularity is π, and the peak of $S(q)$ for q real is also at $q=\pi$. If we increase the parameter θ, at some value the real part of the leading singularity will move away from $q=\pi$: this means that real-space correlations oscillate with a new period. However, because of the width of the peak in the structure factor, the maximum of $S(q)$ remains at $q=\pi$ till the shift Δq of the real part reaches a value $O(\xi^{-1})$. Then for larger values of θ, the structure factor will exhibit an incommensurate peak.

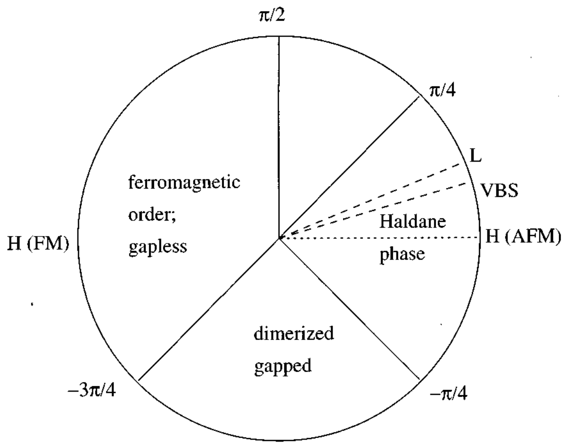

FIG. 1. Phase diagram of the bilinear-biquadratic $S=1$ isotropic quantum spin chain as a function of θ. Solid lines: transition points; dashed lines: other special points. H (antiferromagnetic): isotropic antiferromagnet; VBS: the valence-bond-solid model; L: the crossover point studied in Ref. 29; H (ferromagnetic): isotropic ferromagnet.

We have obtained evidence that, right at the VBS point, the correlations become incommensurate in real space: it is a "disorder" point in the language of classical statistical mechanics.[31] For a *larger* value of θ, the function $S(q)$ exhibits the signature of incommensurability:[29] This point is properly called a Lifshitz point. This splitting of the classical phenomenon at θ_c is typical of systems with only short-range order.

We proceed by first recalling briefly in Sec. II the state of knowledge on the bilinear-biquadratic $S=1$ quantum spin chain. In Sec. III we import the concepts of so-called disorder points from classical statistical mechanics. They are discussed by use of simple classical spin models. In Sec. IV, using the density matrix renormalization-group (DMRG) algorithm,[32] we calculate energy gaps, correlation functions, and correlation lengths, as well as the $S=1$ string order parameter in the neighborhood of the VBS point. We demonstrate that the spin correlations exhibit a change of behavior in real space right at the VBS point and that this point is a quantum example of a disorder point. Section V contains our conclusions.

II. PHASE DIAGRAM OF THE BILINEAR-BIQUADRATIC SPIN CHAIN

Let us represent the phase diagram of models H_θ as in Fig. 1. For $\theta=0$ and $\theta=\pi$, one find the isotropic (anti)ferromagnetic quantum Heisenberg model. Antiferromagnetic (ferromagnetic) models corresponds to $-\pi/2<\theta<+\pi/2$ $(+\pi/2<\theta<3\pi/2)$. Some points in the phase diagram have been studied in detail, and we summarize below the current knowledge.

$\theta=0$. Isotropic antiferromagnetic quantum Heisenberg model: This well-studied model has a nondegenerate disordered ground state with exponentially decaying antiferromagnetic correlations obeying a law $\langle \mathbf{S}_0\cdot\mathbf{S}_n\rangle \approx(-)^n \exp(-n/\xi)/\sqrt{n}$ and a gapped spectrum (Haldane gap ≈ 0.41). The static structure factor $S(q)$ is a square-root Lorentzian peaked at $q=\pi$.

$\theta=0.1024\pi$ $(\tan\theta=1/3)$. This is the VBS model with exact valence-bond-solid ground state. The spin correlations are *purely* exponential with a correlation length $\xi=(\ln 3)^{-1}\approx 0.91$. There is a gap in the spectrum $(\Delta=0.664)$.

$\theta=0.25\pi$. This is the Lai-Sutherland model, the Hamiltonian is a sum of permutation operators and exactly integrable by the Bethe ansatz.[10,11] The ground state is unique, and the model is critical. The corresponding conformal theory is $\mathrm{SU}(3)_{k=1}$. There are zero-energy modes for $q=0,\pm 2\pi/3$.

$\theta=-0.25\pi$. This model is solvable exactly by the nested Bethe ansatz.[12,13] One finds a critical system with a unique ground state. The conformal theory is $\mathrm{SU}(2)_{k=2}$. There are zero-energy modes at $q=0,\pi$.

$\theta=-0.50\pi$. The physics is that of a dimerized state; the order parameter is given by the coefficient c_2 in the singlet-singlet correlation:

$$\langle(\mathbf{S}_i\mathbf{S}_{i+1})(\mathbf{S}_j\mathbf{S}_{j+1})\rangle\rightarrow c_1+(-1)^{i-j}c_2, \tag{2.1}$$

for $|i-j|\rightarrow\infty$. The ground state is twice degenerate in the thermodynamic limit, and the spectrum is gapped $(\Delta=0.17)$. The correlation length is given as $\xi=42.2$: these are exact results.[18–21]

$\theta=-0.75\pi$. Possible location of a continuous phase transition from a ferromagnetic to a dimerized phase.[23,25,26]

$\theta=\pi$. This is the isotropic ferromagnetic Heisenberg model. There is ferromagnetic order with gapless excitations. The ground state is the ferromagnetic state for $\pi/2<\theta<5\pi/4$.

With these points, one constructs the following phase diagram:[14,17] Starting at $\theta=\pi$, one finds an ordered ferromagnetic state without gap. The ferromagnetic phase terminates at $\theta=-0.75\pi$. A continuous phase transition leads to a dimerized state. A prediction by Chubukov[22] of a nondimerized nematic phase seems refuted by Fáth and Sólyom.[25,26] In the dimerized phase, the ground state is a singlet with a double degeneracy because of a Z_2 symmetry breaking. The order parameter is given by c_2 in the correlation function (2.1). A continuous phase transition at $\theta=-0.25\pi$ leads to a Haldane phase, with a unique disordered ground state, exponentially decaying correlations, and a gapped spectrum. This gapped phase ends at the Lai-Sutherland point $\theta=+0.25\pi$, where a continuous transition leads to a phase that is possibly trimerized (see Refs. 25 and 26 for a detailed discussion). One is back to ferromagnetic phase for $\theta=+0.5\pi$. This phase diagram is displayed in Fig. 1. Up to now, the VBS point appears to be generic in the Haldane phase.

Recently, Bursill, Xiang, and Gehring[29] considered, using the DMRG, the Fourier transform of the spin-spin correlations, i.e., the static structure factor:

$$S(q)=\sum_n e^{iqn}\langle \mathbf{S}_n\cdot\mathbf{S}_0\rangle, \tag{2.2}$$

In the Haldane phase, at the isotropic point $\theta=0$, $S(q)$ is a square-root Lorentzian with a peak at $q=\pi$. Since parity is unbroken in the phases we discuss, we restrict the momenta to the interval $(0,\pi)$. It was found that the peak of the Fourier transform $S(q)$ starts to move away from $q=\pi$ towards $q=\pm 2\pi/3$. This happens at $\tan\tilde{\theta}=0.438\,06(4)$ or $\tilde{\theta}=0.1314\pi$. They found also that when $\theta\rightarrow 0.25\pi$, the peak reaches $2\pi/3$, in agreement with the period-3 zero modes that are seen at the Lai-Sutherland point. Their conclusion is then that there are three regions between $\theta=0$ and $\theta=0.50\pi$: $0<\theta<\tilde{\theta}$ with short-ranged antiferromagnetic correlations, $\tilde{\theta}<\theta<0.25\pi$ with short-ranged *spiral* order (the peak of the Fourier transform shifts from $q=\pi$ to $q=2\pi/3$; the spectrum is still gapped), and $0.25\pi\leqslant\theta,0.50\pi$ with a possible trimerized phase beyond the Lai-Sutherland phase transition.

If one considers the classical limit of model (1.1), there is a related phenomenon. For θ smaller than $\theta_c=\arctan(\frac{1}{2})=0.148\pi$, the ground state is the usual commensurate Néel order with wave vector $q=\pi$, while beyond this value of θ the ground state becomes an incommensurate spiral characterized by wave vector q such that $\cos q=-\frac{1}{2}\cot\!\operatorname{an}\theta$. Of course the classical ground states have long-range ordering, and, when going to finite spin values, this order becomes short ranged. We will show in Sec. IV that this short-range order naturally splits the commensurate-incommensurate transition in *two* distinct phenomena: one happens at θ_{VBS}, where the spin oscillations become incommensurate in real space, and one happens at $\tilde{\theta}$, where incommensurability becomes obvious in the structure factor. Before discussing our results, we now recall the corresponding concepts of classical statistical physics, first developed by Stephenson.[31]

III. SHORT-RANGE ORDER AND DISORDER POINTS

If one starts from a classical model and considers finite integer spins, then, according to Haldane's conjecture, there is only short-range order and a finite correlation length. This is, roughly speaking, an example of "quantum paramagnetism." Finite spin is, in a sense, equivalent to a finite temperature. In Haldane's mapping[1] onto a nonlinear σ model, the coupling constant is equal to the inverse of the spin, while in the nonlinear σ model describing classical two-dimensional systems the coupling is the temperature itself. This means that an integer spin chain has a physics that is related to that of a two-dimensional spin system at nonzero temperature. Since there is no long-range ordering in such a two-dimensional system according to the Mermin-Wagner theorem, the ground state of the spin chain is short-range ordered. We consider, thus, classical systems in their paramagnetic phase to understand the physics of finite-spin chains. Strictly speaking, one should consider classical two-dimensional systems, but, in fact, for our purposes, the physics is absolutely similar to that of three-dimensional systems above the critical temperature.

Let us consider a magnetic Hamiltonian that exhibits two ordered low-temperature phases, one with commensurate correlations and the other with incommensurate correlations. One may think, for example, of a square lattice of classical spins with nearest-neighbor exchange J_1 and third-nearest-neighbor J_3: When $J_3/J_1>1/8$, one destabilizes the Néel order and obtains an incommensurate spiral whose pitch

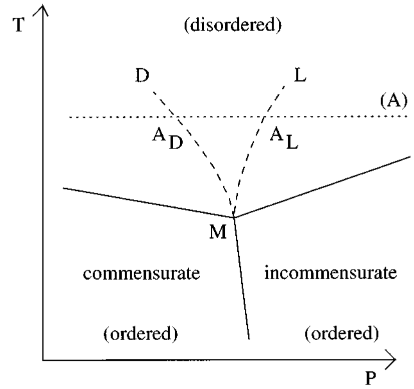

FIG. 2. Schematic phase diagram: a disordered high-T phase is linked by two continuous transitions to two ordered low-T phases. P is a parameter that controls the nature of the ground state. The dashed line represent the disorder (D) and Lifshitz (L) lines, where the behavior of the correlations changes in real and in Fourier space respectively.

evolves continuously. We note P any parameter that controls the zero-temperature phase transition (e.g., anisotropy, pressure, ratio of exchange couplings, etc.). A generic phase diagram is given in Fig. 2. We consider the case where these low-temperature phases are separated from the disordered paramagnetic high-temperature phase by *continuous* transitions [if the classical system is two dimensional (2D), then the T_c is zero and the reasoning is unchanged]. It is clear that the short-ranged correlations in the disordered phase will be of variable nature: "Close" to the commensurate phase, they will be commensurate; "close" to the incommensurate phase, they will be incommensurate. One can guess that there will be a line in this phase diagram, where the correlations change their behavior; this change will be linked to correlations of very short range, thus to a state with a minimum of short-range order. Hence, the name of the disorder line. If one moves along path A in the paramagnetic phase in Fig. 2, there should be a change in the correlations.

If one considers the real-space spin-spin correlations along path A, they will develop incommensurate oscillations at some point A_D. If one considers now the correlations in Fourier space $S(q)$, one finds that the peaks of the Fourier transform still stays at the value for commensurate correlations, even though the real-space correlations are already incommensurate, because of the finite correlation length: The peak width is linked to ξ^{-1}. It is only "closer" to the incommensurate phase that the peak will start to shift. This will happen at a second point A_L on path A in Fig. 2. This is easy to understand by taking a simplified form for $S(q)$:

$$S(q)=\frac{1}{\alpha(q-q_x)^2+(q-q_x)^4+\xi^{-2}}. \tag{3.1}$$

For convenience, we shift the momenta to set $q_x=0$. It is only for $\alpha<0$ that $S(q)$ has a double-peak structure. When $\alpha>0$ is large enough, $\alpha^2>4\xi^{-2}$, all the poles of (3.1) are on the imaginary axis in complex-q space, and the real-space correlations do not oscillate, but when $\alpha^2<4\xi^{-2}$, the poles have a real part, and thus there are real-space oscillations. It

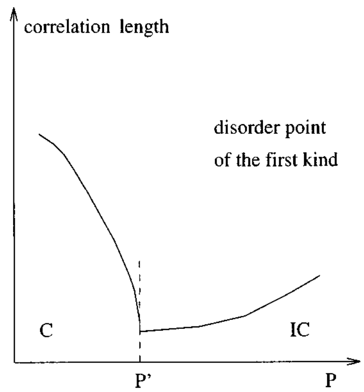

FIG. 3. Correlation length at a disorder point of the first kind (schematical from RPA): the commensurate phase is to the left.

is only when the real part of the poles is large enough that the structure factor itself displays a two-peak shape. This effect is entirely caused by the finite correlation length ξ, i.e., short-range ordering and finite width of the peak in $S(q)$. It is clear from the simple example above that it is only the analytic structure of $S(q)$ that matters and not our peculiar Eq. (3.1). As such, this is a general behavior.

The starting point of real-space oscillations is the disorder point. It extends in the plane of Fig. 2 in a disorder line D. The starting point for the double-peak structure in $S(q)$ is the Lifshitz point, extending in a line L in Fig. 2. In experiments, one normally measures the structure factor in reciprocal space and will thus observe this line. It is also clear that the two lines must end in the multicritical point, where the three phases meet, which is thus necessary for their existence.

To avoid unnecessary generalizations, we take the results from an example treated by a random-phase-approximation (RPA) method in Ref. 33. It is an Ising spin chain with a ferromagnetic J_1 interaction between nearest neighbors and an antiferromagnetic J_2 between next-to-nearest neighbors. The RPA treatment shows that there are three regimes. The disorder temperature is

$$T_D = J_1^2/4|J_2| + 2|J_2|. \tag{3.2}$$

One derives the following expressions for x large:

$$T<T_D: \quad \langle S(0)S(x)\rangle \simeq e^{-x/\xi_-(T)},$$

$$T=T_D: \quad \langle S(0)S(x)\rangle \simeq x e^{-k_0 x} \quad \text{with} \ \cosh k_0 a = J_1/4|J_2|,$$

$$T>T_D: \quad \langle S(0)S(x)\rangle \simeq e^{-x/\xi_+(T)} \cos[q(T)x]$$

$$\text{with} \ \ q(T) \sim (T-T_D)^{1/2}.$$

For $\xi_{\pm}(T)$ one finds that, on the commensurate side, the correlation length exhibits an infinite derivative at T_D; it will typically be very small, but not necessarily a minimum or zero. The derivative on the incommensurate side is finite (see Fig. 3). This characterizes a disorder line of the first kind. There are two more special properties: (i) The susceptibility shows a particularly simple form at the disorder line. (ii) If one considers the correlation functions and compares them to an Ornstein-Zernicke correlation function (for x large) for a d-dimensional system:

$$\langle S(0)S(x)\rangle \simeq e^{-x/\xi(T)}/r^{(d-1)/2}, \tag{3.3}$$

one sees that the correlation functions are those for $d=1$, as expected for a chain, except at the disorder point: formally, they correspond to $d=-1$. Let us add that the incommensurate correlations are given by a wave vector q, which shifts continuously from the commensurate value $q=0$; the exponent $\frac{1}{2}$ is, however, nonuniversal.

In the spin chain problem with $S=1$, we are always in the paramagnetic phase, i.e., we are following a path like A in Fig. 2 when varying the parameter θ in the model (1.1). We thus expect to cross the disorder point and the Lifshitz point, which are the quantum remnants of the classical transition at θ_c.

IV. THE NEIGHBORHOOD OF THE VBS POINT

For our calculations, we use the DMRG: See Ref. 32 for a detailed discussion of the algorithm. We apply it to chains of a length $L=96$ and keep $M=80$ states. This is sufficient to find truncation errors smaller than 10^{-12} in the considered region. It is therefore not necessary to extrapolate results in M, as they are extremely close to the exact results. For the VBS point, we recover the exact results within machine precision. Because of the very small correlation lengths (typically smaller than 3), a length $L=96$ is sufficient to obtain the results of the thermodynamic limit. From the DMRG viewpoint, this situation is ideal. There is, however, a problem with purely computational errors: The spin-spin correlations are, for a distance of 30 to 40 sites, of the order 10^{-13} or less. As they are obtained by summing small numbers below machine precision (in a double precision calculation), they must be rejected. To judge the importance of this effect, we have adopted the following strategy: As the system under study is isotropic and disordered in the region where the Haldane and the trimerized phase meet, the spin-spin correlations must obey the relation

$$\langle S_i^+ S_j^- \rangle = \langle S_i^x S_j^x + S_i^y S_j^y \rangle = 2\langle S_i^z S_j^z \rangle. \tag{4.1}$$

These two quantities are calculated independently; we reject correlations that show a deviation of more than a thousandth from this relation. As a matter of fact, we find that the correlations $\langle S_i^z S_j^z \rangle$ reach a minimum value that oscillates randomly around 10^{-14}, whereas $\langle S_i^+ S_j^- \rangle$ continues to diminish regularly. We conclude that the values for the latter correlation are more precise; analyzing the calculation, we find that for the latter all the important contributions and weights show the same sign, whereas it changes for the former.

The key to our analysis is not to analyze the Fourier transform of the correlations but to analyze them directly in real space. We will thus show that the VBS point, so far without special role in the phase diagram, is effectively a disorder point. It shows all the characteristics of a disorder point of the first kind, as described in Sec. III.

Consider the real-space correlations (Fig. 4) for some values of θ between 0.10π and 0.125π. This includes the VBS point ($\theta_{\text{VBS}}=0.1024\pi$). The correlations for $\theta<0.1024\tau$ are

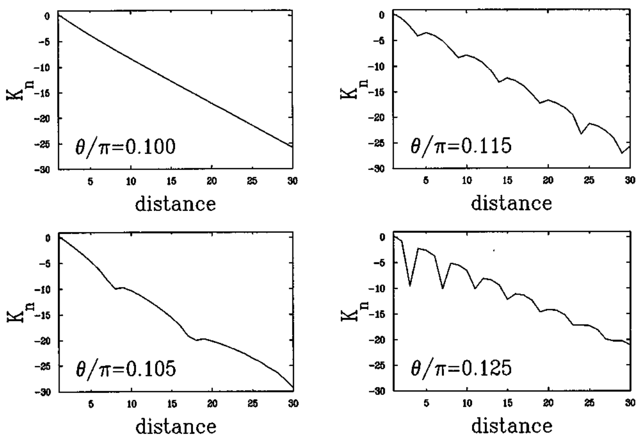

FIG. 4. Real-space spin-spin correlations as a function of the distance, for several values of θ below and above the VBS point (at $\theta_{\mathrm{VBS}}=0.1024\pi$). The modulations appear above the VBS point. Here $K_n=\ln[|(-)^n\sqrt{n}\langle \mathbf{S}_0\cdot\mathbf{S}_n\rangle|]$.

perfectly antiferromagnetic; this is most evident in a logarithmic plot of $|(-1)^n\sqrt{n}\langle \mathbf{S}_n\cdot\mathbf{S}_0\rangle|$. For antiferromagnetic correlations, the curve shows no modulations. Above $\theta_{\mathrm{VBS}}=0.1024\pi$, the logarithmic plots show oscillations with periods that become shorter for increasing θ, to end at a period of 3 for $\theta\rightarrow 0.25\pi$. Thus the VBS point is a disorder point. The correlations are no longer antiferromagnetic but already incommensurate: This point is missed if one considers only the Fourier transform, as in Ref. 29. These modulations can be understood from the classical law for an incommensurate high-temperature phase (adapted to $d=2$):

$$\langle \mathbf{S}_n\cdot\mathbf{S}_0\rangle \approx \cos[q(\theta)n]\frac{e^{-n/\xi(\theta)}}{\sqrt{n}}$$

$$=(-1)^n\cos[(\pi-q)n]\frac{e^{-n/\xi(\theta)}}{\sqrt{n}}. \qquad (4.2)$$

The modulations should thus show a period $\pi/(\pi-q)$, which is easier to see than the period originating directly from $\cos qn$. To show that the correlation functions can be well described by (4.2), we have attempted a direct fit of our results. This fit is complicated by the fact that there are effectively three parameters to be controlled, the wave vector q, the correlation length ξ and also a phase factor ϕ, from replacing $n=i-j$ by $(n-\phi)$ in the argument of the cosine. We find that the fit is extremely sensitive to the parameter values, which allows for a good fit. As an example, we take $\theta=0.115\pi$, sensibly below the point given so far for the change of the correlations. We obtain the fit shown in Fig. 5, for $\phi=0.65$, $\xi=1.08$, and $\pi-q=0.198\pi$. The wave vector q has already shifted by 20% from the antiferromagnetic value $q=\pi$.

For θ close to the VBS point, the fit is made more complicated by the errors in the correlation function because of the finite precision of the computer. To estimate the behavior $q(\theta)$, we therefore consider the periodicity: For a period $p, \pi-q\approx\pi/p$. The discrete nature of the problem limits this approach. We find the behavior shown in Fig. 6. Clearly, it is compatible with $q\propto(\theta'-\theta_{\mathrm{VBS}})^{\sigma}$ with $0<\sigma<1$, the behavior

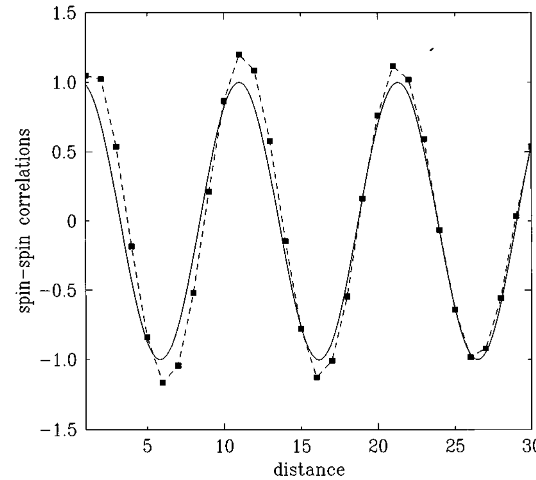

FIG. 5. Comparison between the spin-spin correlations predicted (solid line) and calculated numerically (squares+dashed line) for $\theta=0.115\pi$, above θ_{VBS} but below $\tilde{\theta}$. The dotted line is $(-)^n\sqrt{n}\exp(n/\xi)\langle S_0^zS_n^z\rangle$, and the solid line is $\cos[(n-\phi)(\pi-q)]$.

of a disorder point of the first kind. The curve would be compatible with $\sigma\approx\frac{1}{2}$, but we are in no position to give a precise estimate.

We have also calculated the Fourier transform of the correlation function and find results in agreement with those given by Bursill, Xiang, and Gehring.[29] The VBS point has no special significance for its behavior; the point $\tilde{\theta}=0.1314\pi$, where the peak starts to shift, can now be identified as a Lifshitz point: see Fig. 7. As expected in a system with short-range order, it is distinct from the disorder (VBS) point.

For the correlation lengths, we find that they show a minimum for the VBS point, with an infinite slope (numerically very large) for ξ in the commensurate regime ($\theta<0.1024\pi$), and a slow increase in the incommensurate regime with a finite slope, given in Fig. 8. The correlation lengths have been found by different methods: In the regime

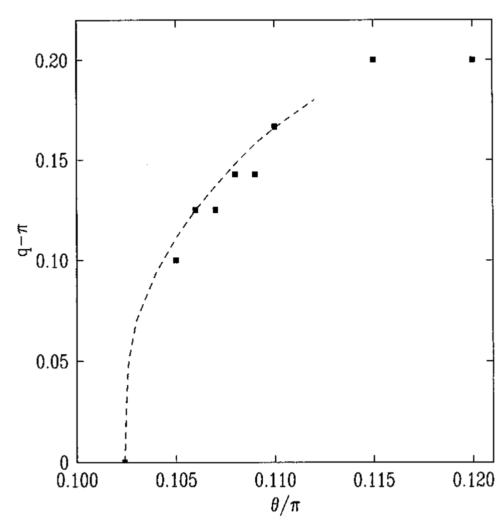

FIG. 6. Wave vector π-q characteristic of the spin correlations. There is a singularity at the VBS point consistent with the identification of a disorder point.

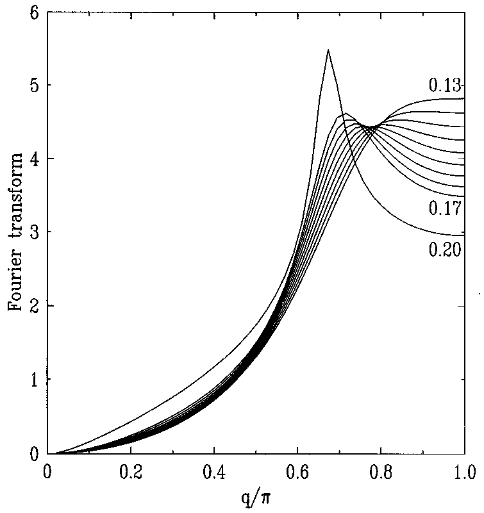

FIG. 7. The Fourier transform $S(q)$ as a function of momentum for various values of θ. The two-peak structure appears only for $\theta > \tilde{\theta} = 0.1314\pi$, while nothing is seen at θ_{VBS}.

$\theta < \theta_{\mathrm{VBS}}$, we have compared the spin-spin correlations numerically and graphically to a law $\exp(-n/\xi)/\sqrt{n}$, which were in all cases in good agreement. We estimate the precision of the results of the order of 1%: The truncation errors are of the order 10^{-13}, and a serious underestimation can therefore be excluded. For $L=96$ and $\xi \approx 1-2$, finite-size effects are of no importance. The situation is more complicated for the regime $\theta > \theta_{\mathrm{VBS}}$. As we have seen, the fit of the theoretically expected behavior to the found curve is rather complex. If one considers a plot of $|(-1)^n \sqrt{n} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle|$ (Fig. 4), one finds that a linear fit for the maxima is quite good. This is stable in the sense that a factor $\cos qx$ influences the logarithm least when it is close to 1. Very generously estimated, the error of the graphical evaluation should be below 5%. We estimate that for $\theta > 0.15\pi$ the underestimation caused by a non-negligible truncation error dominates. For $\theta_{\mathrm{VBS}} < \theta \leqslant 0.11\pi$, we could not obtain the correlation length: On the one hand, the periods caused by the incommensurability are too long to separate them well from the exponential behavior. On the other hand, neither a fit $\exp - r/\xi$ nor $\exp(-r/\xi)/\sqrt{r}$ is satisfactory. We do not know whether this observation is because of the crossover of the behavior of the correlation function or simply because of problems of the numerical method. In any case, the results indicate strongly an extrapolation to the VBS point with a finite slope.

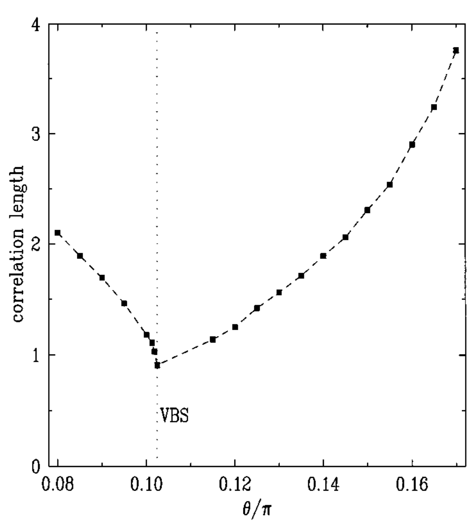

FIG. 8. Correlation lengths for various values of θ. The minimum is at the VBS point.

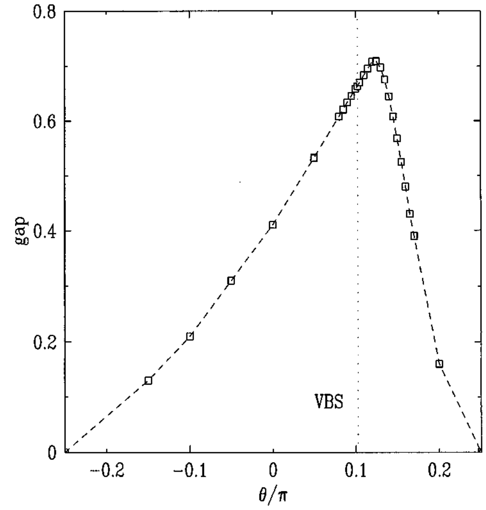

FIG. 9. Gaps in the Haldane phase as a function of θ. The maximum value is between the VBS point and the Lifshitz point.

The other important quantities are the gap and the string order parameter $O_\pi(i,j) = \langle S_i^z \exp(i\pi \Sigma_{k=i-1}^{j-1} S_k^z) S_j^z \rangle$. The gap shows a maximum for $\theta \approx 0.123\pi$, which is thus linked neither to the disorder nor the Lifshitz point: See Fig. 9. For the transition points $\theta = \pm 0.25\pi$ we have not obtained serious estimates: The critical fluctuations imply a greater M, and the vanishing gap is difficult to see. Our results are well compatible with a zero gap but not precise enough to give a serious estimate. The point $\theta = -0.20\pi$ is sufficiently close to the transition to cause the same problem. For the VBS point, we find a gap value $\Delta = 0.664$, in agreement with Ref. 25. Since the gap is smooth at θ_{VBS}, this implies that the spin-wave velocity has a singularity at this point ($c = \Delta \xi$).

The string order parameter in the thermodynamic limit $i - j \rightarrow \infty$ has its extremum for the VBS point: $|O_\pi| = 4/9$: See Fig. 10. One sees that the VBS point, though a point of minimal *spin* order, is a point of maximum hidden topological order.

To complete the identification of the VBS point as a disorder point, we note that there is the equivalent of the particularly simple form of the susceptibility of the classical model of Sec. III. The exact correlations at the VBS point obey a one-dimensional Ornstein-Zernicke form: They are purely exponential (no prefactor), whereas the nonlinear σ model yields two-dimensional correlation laws. This "dimensional reduction" is accompanied by a particularly simple form of the Hamiltonian: It can be decomposed into a sum of local projection operators. The problem loses its quantum character and turns into a classical one-dimensional problem.

V. CONCLUSION

We have shown that the VBS point[2] is a disorder point in the sense of classical statistical mechanics. It is thus identi-

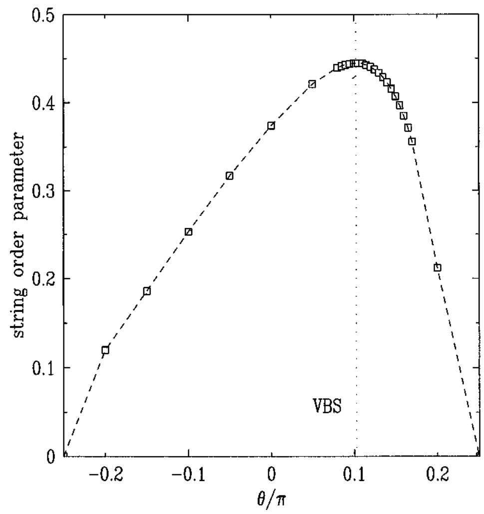

FIG. 10. String order parameter $|O_\pi|$ in the thermodynamic limit in the Haldane phase. The maximum is exactly at the VBS point.

fied as a point that is not just by chance exactly solvable but shows this property for more profound physical reasons. The results of Bursill, Xiang, and Gehring, who have considered the Fourier transform of the spin-spin correlations, fit naturally in the picture we have developed: The point they identify as the point where correlations change is simply the Lifshitz point following the definition given above. Quantum fluctuations in the integer spin chain wash out long-range order. As a consequence, the transition that happens at the classical level for θ_c is no longer a phase transition. However, the change of short-range correlations still happens in the quantum system at the VBS point in real space. Because of the finite correlation length, this is not seen immediately in $S(q)$ and, hence, we have the Lifshitz point, which is distinct. Since $\xi\to\infty$ when the spin increases, one expects that these two points should merge in the classical limit right at θ_c. This is summarized in Fig. 11.

This implies the following description of the phase diagram: There are three regions for $0<\theta<0.25\pi$.

$0<\theta<\theta_{\rm VBS}$. There are short-range antiferromagnetic correlations, the Haldane phase with a gapped spectrum. A generic description is given by the VBS model and also the isotropic antiferromagnetic Heisenberg model.

$\theta_{\rm VBS}<\theta<\tilde{\theta}$. There are incommensurate short-range correlations with a wave vector $q<\pi$, that shifts away from π as $\pi-q\propto(\theta-\theta_{\rm VBS})^\sigma,\sigma\approx 1/2$. In the Fourier transform, the peak stays at $q=\pi$. The spectrum is gapped: We expect that the low-lying Haldane modes are now at the incommensurate wave vector. Part of the VBS physics remains valid: the gap, the hidden order, and the free spins $\frac{1}{2}$ at the ends of an open chain.

$\tilde{\theta}<\theta<0.25\pi$. The physics is similar to that of the preceding region; the peak of the Fourier transform shifts from $q=\pi$ to $q=\pm 2\pi/3$ and the incommensurate correlations become visible. The spectrum is gapped. There is, however, no profound physical difference between this region and the preceding one.

The above picture does not challenge conventional wisdom in the sense that the usual Heisenberg Hamiltonian $\theta=0$ shares the same physics with the VBS Hamiltonian and there are no additional phase transitions between the point[12,13] $\theta=-0.25\pi$ and the Lai-Sutherland point $\theta=+0.25\pi$. However, the VBS point itself means that the physics has changed beyond $\theta_{\rm VBS}$: Because of the incommensurate correlations, it is no longer possible to capture the low-lying excitations by a nonlinear σ model with a symmetry-breaking pattern $O(3)/O(2)$ as used originally by Haldane. In the incommensurate regime, the full rotation group is broken down. Appropriate nonlinear σ models have been contemplated before.[34] Since they involve a non-Abelian symmetry, they are generically massive, consistent with the gapped nature of the Haldane phase.

With the present algorithm, we cannot calculate dynamical quantities. For $\theta=0$, it is known that the dynamical structure factor is dominated by the Haldane mode whose minimum energy is at $q=\pi$. The simplest expectation is that this minimum will shift away from $q=\pi$. The simplest expectation is that this minimum will shift away from $q=\pi$ right at the VBS point (because the Lifshitz point has *a priori* no dynamical meaning) and will evolve continuously till it softens for $\theta=\pi/4$ at a wave vector $q=2\pi/3$ in agreement with the Bethe-Ansatz excitation spectrum at the Lai-Sutherland point.

There is an interesting relationship[6] with the fractional quantum Hall effect (FQHE). The present understanding[35] of the physics of the FQHE at filling $\nu=1/m$, m odd, is based on Laughlin's wave function ψ_m, which is the exact ground state of a truncated Hamiltonian. In addition, this function embodies the hidden long-range-order that is revealed in the anyonic gauge. This is similar to the situation of the VBS wave function. Expectation values computed with the Laughlin wave function correspond to a classical statistical problem, which is the two-dimensional one-component plasma (2D OCP): This is Laughlin's plasma analogy. The case of the full Landau level ψ_1 corresponds to the special point[36] $\Gamma=2$ of the 2D OCP (Γ being the ratio of the squared electric charge to the temperature) at which the density correlations begin to oscillate in real space, a precursor phenomenon of the crystallization that occurs at $\Gamma\approx 140$ when the plasma is dilute enough. This special point also has

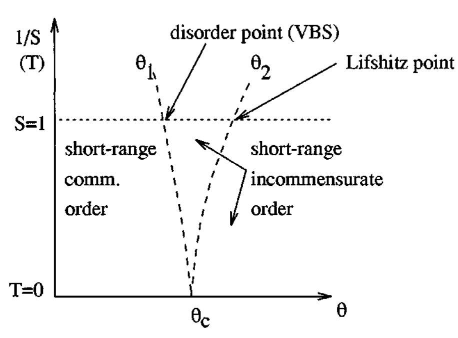

FIG. 11. Schematic phase diagram of integer spin chains with biquadratic coupling: model (1.1). Here the inverse spin plays the role of a temperature: The $S=1$ case corresponds to short-range ordered phases. Of course this picture may be altered by other types of ordering, such as dimerization.

some of the properties expected from a disorder point.[36] This is similar to what we observe at the VBS point.

We also note that a similar phenomenon happens in the spin-$\frac{1}{2}$ Heisenberg chain with next-to-nearest-neighbor interaction J_2. When J_2 is large enough, the antiferromagnetic state with algebraically decaying correlations is destroyed, and dimerization takes place. Inside the dimerized phase, there is the so-called Majumdar-Ghosh point,[37] where the correlation between dimers vanishes and the ground state is a simple wave function. In the dimerized phase, the antiferromagnetic spin order is short ranged contrary to the dimer order, and we thus expect that the Majumar-Ghosh point is a disorder point: In the classical limit the increase of J_2 leads to incommensurability (as the biquadratic term in the $S=1$ case). Because of the short-range order, the incommensurability will take place in real space right at the disorder point (Majumdar-Ghosh), and the structure factor will display the two-peak structure only for a larger value of J_2.

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