Quantum Liquid in Antiferromagnetic Chains: A Stochastic Geometric Approach to the Haldane Gap

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The $S=1$ quantum antiferromagnetic chain with the Hamiltonian $H=\sum_i S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z + D(S_i^z)^2$ is studied. By developing a (path-integral-type) stochastic geometric representation and using the ideas of percolation, we find that the Haldane phase with a unique disordered ground state and a gap can be regarded as "liquid." The large-D phase and the Néel ordered phase are identified as "gas" and "solid," respectively. We introduce a new order parameter that distinguishes the Haldane phase from other disordered phases such as the large-D phase or the dimer phase.

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Haldane[1] made a fascinating conjecture that the spin S quantum Heisenberg antiferromagnetic chain with the Hamiltonian

$$H=\sum_i S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z + D(S_i^z)^2 \qquad (1)$$

has a unique disordered ground state and a finite excitation gap when S is an integer, while it has a critically ordered unique ground state and no excitation gap when S is a half odd integer. The conjecture has been tested by numerical calculations,[2] experiments in quasi-one-dimensional systems,[3,4] and rigorous studies,[5-7] *but the problem for the Heisenberg model with small integral S (such as 1) still remains to be understood theoretically.* In the present Letter we study the model (1) with $S=1$, and develop a new picture of the Haldane gap.[8]

The Haldane conjecture[1] implies that the model (1) with $S=1$ has a unique disordered ground state and an excitation gap in a finite region of parameter space containing the isotropic point $D=0$, $\lambda=1$. Further numerical studies[2] indicate that the model has at least two more distinct phases in the region $\lambda \geq 0$, namely, the Néel ordered phase with two ordered ground states, and the large-D phase with a unique disordered ground state and a gap[9] (Fig. 1). The existence of the large-D phase was first suggested by Botet, Jullien, and Kolb[2] from a numerical observation that there is a phase boundary of massless theories. But the distinction between the large-D phase and the Haldane phase was not clear since they are both characterized by a unique disordered ground state and a gap.

Here we will characterize the large-D, the Néel, and the Haldane phases as "gas," "solid," and "liquid" phases, respectively, of a stochastic geometric representation of the model. This picture naturally leads us to a definition of a new order parameter that distinguishes the Haldane phase from other disordered phases including the large-D phase and the dimer phase. Recently, den Nijs and Rommelse[10] have reached a somewhat similar conclusion from an analogy with the preroughening transition in crystal surfaces.

Let H be the Hamiltonian for a finite periodic chain of length L. The ground-state expectation value of an operator A can be expressed as

$$\omega(A) = \lim_{\beta\to\infty} [\mathrm{Tr}(Ae^{-\beta H})/\mathrm{Tr}(e^{-\beta H})] .$$

We now follow the standard procedure to develop path-integral representation of the system. By using the Lie product formula (or Trotter-Suzuki formula),[11] we write $\mathrm{Tr}(e^{-\beta H}) = \lim_{n\to\infty} \mathrm{Tr}(T^{n\beta})$, where T is defined by

$$T = \bigotimes_i \left[1 - \frac{1}{2n}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)\right] \times \exp\left[-\frac{\lambda}{n} S_i^z S_{i+1}^z - \frac{D}{n}(S_i^z)^2\right] . \qquad (2)$$

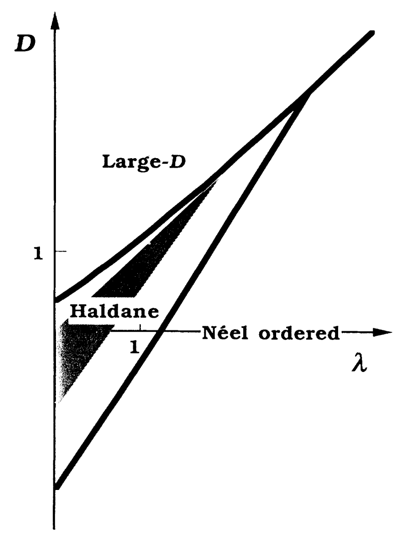

FIG. 1. Numerically obtained phase diagram for the ground state of the $S=1$ Heisenberg antiferromagnet with uniaxial anisotropy. In the shaded region, we have proof that the Haldane phase exists in the approximate model with a restricted Hilbert space.

We let L and $n\beta$ be even integers, and take the limits $L,n,\beta \to \infty$ later. We realize the trace as $\mathrm{Tr}(T^{n\beta}) = \sum_C \langle C|T^{n\beta}|C\rangle$, and interpret T as the "time-evolution operator" for the unit time interval of $1/n$. $|C\rangle$ is summed over all the basis states specified by the eigenvalues of S_i^z $(=\pm 1, 0)$.

In our first stochastic geometric representation, we regard an arbitrary basis state $|C\rangle$ as consisting of $+$ and $-$ "particles" located in the background "sea" of 0 states. Then the action of the operator T can be interpreted as *pair creation* of $+$ and $-$ states "00"$\to$"$+-$", *pair annihilation* "$+-$"$\to$"00", or *propagation* "0+"$\to$"+0". This means that the present model can be interpreted as a system of charged particles (+ states) and their antiparticles ($-$ states) propagating and being created or annihilated in pairs in the one-dimensional space.

Then we get a stochastic geometric representation $\mathrm{Tr}(T^{n\beta}) = \sum_\Gamma W(\Gamma)$, where Γ is summed over all the possible "histories" of $+$ and $-$ particles in the two-dimensional space-time. Each history is a collection of "world loops" (which we call $+-$ loops hereafter) formed by tracing the trajectories of the (anti)particles as in Fig. 2. The statistical weight $W(\Gamma)$ is a product of the following terms. For each vertical segment (of a loop) there is a factor $\exp(-D/n)$, and for each horizontal segment a factor $-1/n$. For each pair of neighboring $+$ or $-$ states, there is a factor $\exp[-(\lambda/n) \times S_i^z S_{i+1}^z]$. It is extremely important for us that we get a positive quantity after multiplying all these factors. This fact allows us to interpret the quantity $W(\Gamma)/\mathrm{Tr}(T^{n\beta})$ as the *probability* that a configuration Γ appears. There are similar representations for the expectation values of operators.

We first consider the case where the crystal-field anisotropy D is large. Since each $+$ or $-$ state gets a weight of $\exp(-D/n)$, one expects that the $+-$ loops are hard to exist. Then the whole stochastic geometric system should look like gas or the "confinement" phase of the $+-$ loops. The property of the gas phase is summarized in the following theorem.

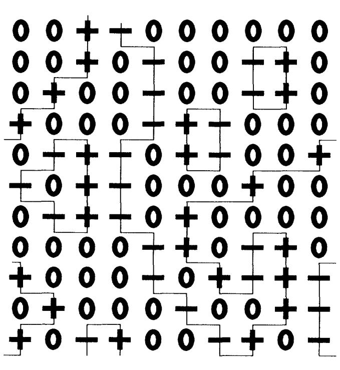

FIG. 2. A typical space- (horizontal) time (vertical) configuration of the $+-$ loops.

Theorem 1 (characterization of the large-D phase).—When $D-2\lambda$ is sufficiently large (say, ≥ 28), the ground state of the Hamiltonian (1) is unique, all the truncated correlation functions in the ground state decay exponentially, and there is a finite excitation gap immediately above the ground-state energy. In the stochastic geometric representation, the probability to find $a+-$ loop (containing a given space-time point) which has the width ω (in space) and the length τ (in time where the unit lattice spacing is $1/n$) is bounded from above by $\exp(-\omega/\xi - m\tau)$. Here ξ and m are finite constants which are independent of the system sizes L, β, and the decomposition number n.

The theorem is proved[8] by examining the $+-$ loop representation for the various expectation values (which we do not make explicit in the present Letter), and by making use of the cluster expansion technique based on the powerful convergence criterion obtained by Kotecký and Preiss.[12]

We conjecture that the whole large-D phase in the phase diagram of Fig. 1 is indeed the gas phase of the corresponding stochastic geometric system. As the parameter D becomes smaller, the average size of the $+-$ loops should become larger. We can prove[8] that, for each fixed values of λ (>0), there exists a finite critical value $D_c(\lambda)$, and for $D<D_c(\lambda)$, $+-$ loops percolate in the sense that there exists (with probability 1) an infinitely large $\pm$ loop (after taking the limits $L,\beta \to \infty$). We expect that the line in Fig. 1 separating the large-D phase from the other two is $D_c(\lambda)$. The following theorem states that the isotropic Heisenberg point $\lambda=1$, $D=0$ is *not* in the gas phase. Thus it establishes that the mechanisms leading to a disordered ground state and a gap in the Haldane phase and the large-D phase are indeed different.[13]

Theorem 2 (no-gas theorem).—At the SO(3)-invariant point $\lambda=1$, $D=0$, there exists (with probability 1) an infinitely larger $+-$ loop or an infinite cluster of neighboring $+-$ loops[14] (in the limits $L,\beta\to\infty$ and for sufficiently large n).

Now let us focus on the region $D<D_c(\lambda)$, in which an infinitely large $+-$loop appears. According to the phase diagram of Fig. 1, this region should include both the Néel ordered phase and the Haldane phase. An essential step in understanding of the Haldane-gap phenomena is to realize that the existence of the infinitely large $+-$ loop induces a kind of order in the stochastic geometric system. To make this point explicit, we define the *internal order parameter* μ as follows. Given a configuration Γ, we look only at its "time slice" (at a fixed time, say, $\tau=0$) to get a string of 0, +, and $-$. We then throw away all the 0's from the string, and define new spin variables $\sigma_K = \pm 1$ as the value of the kth nonzero element (counted from the left).[15] The internal

order parameter is defined as

$$\mu = \lim_{|k-k'|\to\infty} (-1)^{k-k'}\langle \sigma_k \sigma_{k'} \rangle , \qquad (3)$$

where the average $\langle \cdots \rangle$ is with respect to the probabilities associated with the $+-$ loop configurations (i.e., the equal-time average in the ground state).[16]

It is clear (from Fig. 2, for example) that the infinitely large $+-$ loop enforces a strong (antiferromagneticlike) long-range order in the variables σ_k, thus generating a nonvanishing μ.[17] Finite $+-$ loops also contribute to μ because the loops interact through the factor $\exp[-(\lambda/n)S_i^z S_{i+1}^z]$. It is expected that μ is fairly close to 1 when $\lambda - D$ is sufficiently large.

We conjecture that, in the phase diagram of Fig. 1, the large-D phase is characterized by $\mu = 0$, and the other two phases by $\mu \neq 0$. It should be stressed that the nonvanishing internal order parameter μ does not necessarily imply the existence of an observable long-range order such as Néel ordered. The definition of μ involves an expansion in a specific basis, and nonlocal procedure to pick up only the nonzero states. In the valence-bond-solid (VBS) state studied by Affleck, Kennedy, Lieb, and Tasaki,[6] which is a rigorous example of the Haldane-type disordered ground state, we strictly have $(-1)^{k-k'} \times \sigma_k \sigma_{k'} = 1$, a perfect internal order without Néel order.

There is an approximate model which captures the essential features of this region, and can be studied rigorously. The model[18] has the same Hamiltonian as (1), but its Hilbert space $\mathcal{H}_0$ is smaller than the original one. The space $\mathcal{H}_0$ consists of all the linear combinations of the basis states of the form

$$\cdots 0 \cdots 0{+}0 \cdots 0{-}0 \cdots 0{+}0 \cdots 0{-}0 \cdots 0{+}0 \cdots 0 \cdots ,$$

where $0 \cdots 0$ represents an arbitrary number (including none) of 0 states. Note that the perfect internal order is built into this space. We expect that the model approximates the original model fairly well when the internal order parameter is close to 1.

When working within the space $\mathcal{H}_0$, one can represent an arbitrary state by specifying the locations of 0 "particles" in the background of order $+-$ "sea." Let us derive our second stochastic geometric representation of $\mathrm{Tr}(T^{n\beta})$ based on this new interpretation. The action of the time-evolution operator T on an arbitrary state $|C\rangle$ can be now interpreted as *pair creation* of two 0 states "$+-$"$\to$"00", *pair annihilation* "00"$\to$"$+-$", or *propagation* "0+"$\to$"+0". Now our model can be interpreted as a system of (chargeless) particles propagating and being created or annihilated in pair in the one-dimensional space. Note that the internal order of the background $+$ and $-$ states is essential for this interpretation. The similar interpretation should be possible in the original model provided that there is a sufficiently strong internal order.

Again we get a representation $\mathrm{Tr}(T^{n\beta}) = \sum_\Lambda W(\Lambda)$, where the summation is over all the configurations Λ of the "world loops" (which we call 0 loops) formed by tracing the trajectories of the 0 particles. The statistical weight $W(\Lambda)$ is a product of a factor $\exp[(D-2\lambda)/n]$ for each vertical segment (of a loop), and a factor $-1/n$ for each horizontal segment (where we have shifted the Hamiltonian by a constant). Again $W(\Lambda)$ is positive, so we can make use of the probalistic concepts.

When $2\lambda - D$ is sufficiently large, we should have a gas phase where the density of the 0 loops is low. From the viewpoint of $+-$ loop system, this looks like a solid phase because the configurations are mainly dominated by the background ordered $+-$ sea. The internal order now manifests itself as an observable long-range Néel order since the 0 loops modify the classical Néel state locally. We conjecture that the whole Néel phase is the solid phase of the stochastic geometric system of the $+-$ loops (and/or the gas phase of the 0 loop system).

As $2\lambda - D$ becomes smaller, the average size of the 0 loops becomes larger and there can be a percolation transition of the 0 loops. When this happens, the infinitely large 0 loop modifies the classical Néel state in a global way, so the long-range Néel order immediately vanishes. *We end up with an exotic phase characterized by strong fluctuation, an unobservable internal order, and no long-range Néel order, and in which infinitely large* $+-$ *loop and 0 loop coexist.* We call this phase liquid, and conjecture that the whole Haldane phase is the liquid phase. Note that such a phase can exist only in the models with integral spins since there is no "charge-neutral" object like 0 particles in a model with a half-odd-integer spin. The following theorem and its proof[7,8] justify our picture.

Theorem 3 (Haldane gap in the approximate model).— Within the space $\mathcal{H}_0$, the ground state of the Hamiltonian is Néel ordered[19] when $\lambda - D > 2$, and is disordered when $3\lambda - 2D < 2$ and $\lambda \geq D$. In the latter case, the ground state is unique, arbitrary truncated correlation functions (in the ground state) decay exponentially, and there is an excitation gap immediately above the ground-state energy.

Our new approach recovers[8] most of the predictions made by the field-theoretic methods.[1] One of the new consequences of our approach is that we can now conclude the large-D phase and the Haldane phase are distinct.[20] The picture suggests some criterions to distinguish between the two phases, the simplest one being the measurement[16] of the internal order parameter μ. The peculiar nature of the liquid phase indicates that the energy gap in a chain of length L with *free boundary conditions* behaves as $\Delta E(L) \approx \exp(-L/\xi)$ in the Haldane phase, but not in the large-D phase. This behavior has already been observed numerically by Kennedy.[21] In

Ref. 8 we also show that the autocorrelation function of the z component of the spin variable $\omega(S_i^z e^{-\tau H} S_i^z e^{\tau H})$ [where $\omega()$ being the ground-state expectation value in the $L \to \infty$ limit] should have the asymptotic decay $\tau^{-1/2}\exp(-m\tau)$ in the Haldane phase, and $\tau^{-1} \times \exp(-m\tau)$ in the large-D phase.

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[8]The details of our argument and the proofs of theorems will appear elsewhere.

[9]The phase structure near $\lambda=0$ can be much more complicated because of the possible existence of XY phases.

[10]M. den Nijs and K. Rommelse, Phys. Rev. B **40**, 4709 (1989).

[11]The product formula is a standard tool in quantum Monte Carlo simulations. See M. Suzuki, J. Stat. Phys. **43**, 883 (1986), and references therein. The early use of the product formula in quantum spin systems can be traced back to D. Robinson, Commun. Math. Phys. **14**, 195 (1969); J. Ginibre, Commun. Math. Phys. **14**, 205 (1969); T. Asano, J. Phys. Soc. Jpn. **29**, 350 (1970), Phys. Rev. Lett. **24**, 1409 (1970); M. Suzuki and M. E. Fisher, J. Math. Phys. **12**, 235 (1971).

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[13]The latter possibility occurs in the dimer phase, and is not expected in the models considered here.

[14]The theorem and the discussion apply to all rotationally invariant models including the VBS model studied in Ref. 6. Roughly speaking, the proof of the theorem goes as follows. We suppose that the isotropic model is in the gas phase, and thus the set of 0's *do* percolate in the two-dimensional lattice. We apply the $\pi/2$ rotation around the x axis: $|\pm\rangle \to (i/\sqrt{2})|0\rangle \pm (|+\rangle - |-\rangle)/2$, $|0\rangle \to (i/\sqrt{2})(|+\rangle + |-\rangle)$. After the rotation, we see that now + and − should percolate, but this is a contradiction because the system is rotationally invariant.

[15]In an infinite chain, we shall call the nonzero element closest to the origin $k=0$, and name the other elements preserving their relative order.

[16]den Nijs and Rommelse (Ref. 10) defined the order parameter $\rho_s = -\lim_{k\to\infty}[\omega(S_0^z \exp(i\pi\sum_{j=1}^{k-1} S_j^z) S_k^z)]$ where $\omega()$ is the ground-state expectation value. This order parameter also measures the internal order. A numerical calculation of the order parameter ρ_s can be found in S. M. Girvin and D. P. Arovas, Phys. Scrip. **T27**, 156 (1989). A detailed (and rigorous) study of the order parameter ρ_s will appear in a paper by T. Kennedy and H. Tasaki (to be published).

[17]The possibility of a translation-invariant internally ordered phase *without* infinite +− loops is quite interesting. Such a phase breaks parity, but preserves all the other symmetries.

[18]The model is discussed in G. Gómez-Santos, Phys. Rev. Lett. **63**, 790 (1989), by using a kind of mean-field approximation. A rigorous treatment appears in Ref. 7 in the context of quasi-one-dimensional system.

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[20]Our stochastic geometric picture turns out to be also useful (Ref. 8) in the problem of the transition between the Haldane phase and the dimer phase: I. Affleck and F. D. M. Haldane, Phys. Rev. B **36**, 5291 (1987); R. R. P. Singh and M. P. Gelfand, Phys. Rev. Lett. **61**, 2133 (1988); I. Affleck, Phys. Rev. Lett. **62**, 839 (1989); D. Guo, T. Kennedy, and S. Mazumdar, Phys. Rev. B **41**, 9592 (1990). The internal order parameter μ can be used to distinguish the Haldane phase from the dimer phase since we have $\mu=0$ in the latter [see Kennedy and Tasaki (Ref. 16)].

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