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Haldane gap antiferromagnets in a transverse magnetic field

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Abstract. We study the $S = 1$ antiferromagnetic Heisenberg chain with uniaxial anisotropy, which exhibits the Haldane gap phenomenon. We argue that, when a magnetic field in a direction transverse to the anisotropy axis is applied, a sharp phase transition takes place at a critical value of the field. The transition is characterized by vanishing of the hidden antiferromagnetic order which can be measured by the string order parameter of den Nijs and Rommelse. The existence of such a transition distinguishes a Haldane gap system from other disordered quantum spin systems.

1. Introduction

Haldane [1] argued that the Heisenberg antiferromagnetic chain with an integer spin has a unique disordered ground state with a finite excitation gap, while the same model with a half-odd-integer spin has no excitation gap. The conclusion for the integer spin models was rather surprising since it was against common sense that a quantum system with a rotation-invariant ground state has no gap in the infinite volume limit. However, numerous experimental, numerical and theoretical studies have confirmed Haldane's prediction [2].

Recent theoretical investigations have also revealed highly non-trivial structures underlying the mechanism of the gap generation in the integer spin models. den Nijs and Rommelse [3] and Tasaki [4] argued that the existence of a hidden antiferromagnetic order is a common and essential feature in the Haldane gap systems. Kennedy [5] showed numerically that the ground states of a Haldane gap antiferromagnet in a finite open chain are nearly fourfold degenerate even though the ground state is unique in the infinite-volume limit. These structures had already been observed in the exact ground state of an $S = 1$ biquadratic Hamiltonian obtained in [6] which was shown to possess almost all the properties that Haldane predicted. Recently Kennedy and Tasaki [7] introduced a non-local unitary transformation and showed that these features of the Haldane gap system can be regarded as consequences of the breaking of a $Z_2 \times Z_2$ symmetry in the transformed system.

Of course, the Haldane mechanism is not the only way to get a gap in the spectrum of a quantum spin system. Consider, for example, an $S = 1$ system whose Hamiltonian is dominated by the crystal-field anisotropy term $\Sigma_i D(S_i^z)^2$ with positive D. It is intuitively clear (and can be proved rigorously [4, 8]) that the ground state is essentially the product of the states with $S_i^z = 0$ and there is a gap approximately equal to D.

Although the disordered nature of this ground state resembles the Haldane-type ground state, it lacks the hidden antiferromagnetic order [8]. We must realize that the nature of the gap in this case is distinct from the Haldane gap.

Thus it is desirable to have definite criteria that enable us to distinguish between the disordered ground states generated by the subtle (and interesting) Haldane mechanism and trivial mechanisms such as the above large-D mechanism. From a theoretical (and a numerical experimental) point of view, the direct measurement of the hidden antiferromagnetic order or the $Z_2 \times Z_2$ symmetry breaking would be among the best criteria, but the hidden order can never be observed directly by experiment. Hagiwara *et al* [9] reported an experimental observation of the fourfold near-degeneracy.

In the present paper, we consider the $S = 1$ Heisenberg antiferromagnetic chain with a crystal-field anisotropy. We study the behaviour of the magnetization when a magnetic field transverse to the anisotropy axis is applied. We argue that the behaviour of the magnetization curve provides a sharp criterion for distinguishing a Haldane gap system. Our conclusion is that the magnetization curve shows a singularity at a critical value of the field if the gap is due to the Haldane mechanism, while the curve is analytic if the gap is due to the trivial large-D mechanism. Note that, when a magnetic field is applied in the same direction as the anisotropy, the magnetization shows a singularity in both the cases. The measurements [10] of the high-field magnetization process of NENP are consistent with our conclusion and give a strong indication that the gap observed in NENP is indeed a Haldane gap.

Affleck [11] obtained conclusions similar to ours. See [11, 12] for theoretical work on the other aspects of the field effect in the Haldane gap antiferromagnets.

2. The model

We consider an $S = 1$ chain with the Hamiltonian

$$\mathcal{H} = \sum_i J\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + D[(S_i^x)^2 - 1] - HS_i^z \tag{1}$$

where we assume that $D > 0$ for the crystal-field anisotropy parameter. Note that we have used (for a technical reason) a non-standard convention where the x axis is the anisotropy axis, and the uniform transverse field is applied in the z direction.

We are interested in the H-dependence (for a fixed value of D) of the magnetization in the direction of the field:

$$M(H) = \lim_{L\to\infty}\left(\frac{1}{L}\sum_{i=1}^{L}\langle S_i^z\rangle\right) \tag{2}$$

where L is the number of the sites, and $\langle\ldots\rangle$ denotes the ground-state expectation value.

When D is sufficiently large, the exchange interaction (the J-term) can be regarded as a perturbation. The ground state is essentially that of the single-spin Hamiltonian obtained by setting $J = 0$ in (1). Thus† the magnetization (2) is an analytic function of H. We expect that the analyticity holds in the whole large-D phase which is characterized by vanishing hidden antiferromagnetic order.

† It is possible to prove this rigorously by developing a convergent cluster expansion. See [8] for examples of such expansions.

When D is sufficiently small, it is believed that the ground state for $H = 0$ has a non-vanishing den Nijs Rommelse [3] string order parameter

$$O^z_{\text{string}} = -\lim_{L\to\infty}\left[\frac{1}{L}\sum_{j=1}^{L}\langle S_0^z \exp\left(\mathrm{i}\pi\sum_{k=1}^{j-1} S_k^z\right)S_j^z\rangle\right]. \tag{3}$$

In the next section, we show that the string order parameter should remain non-vanishing when a sufficiently small magnetic field H is added. On the other hand, it is not hard to prove that the string order parameter (3) is vanishing when H is sufficiently large. Then we should have a sharp phase transition from the phase with non-vanishing O^z_{string} to the phase with vanishing O^z_{string}, when D is fixed to a sufficiently small value and H is increased. Since the hidden antiferromagnetic order is incompatible with the uniform magnetization, we expect a small (but finite) susceptibility in the region with $O^z_{\text{string}} \neq 0$. When the magnetic field exceeds its critical value, we expect a sudden jump in the susceptibility. Our geometric picture also suggests that the transition resembles that in the antiferromagnetic Ising model at a fixed temperature under varying uniform magnetic field.

Affleck [11] studied a phenomenological field theory with built-in mass gap and obtained similar conclusions about the nature of the phase transition, but no information about the string order parameter. For a numerical experimentalist, it would be an interesting problem to make a direct measurement of the string order parameter in the present situation.

3. Geometric picture

In the present section, we show that the ground state of (1) with sufficiently small D and H has non-vanishing hidden antiferromagnetic order. Our argument is based on the standard path integral technique which represents a quantum spin system as a classical statistical mechanical system. By using the Lie–Trotter–Suzuki product formula [13], the ground-state expectation value of a local observable A can be expressed as

$$\langle A\rangle = \lim_{\beta\to\infty}\left(\frac{\mathrm{Tr}[A\exp(-\beta\mathcal{H})]}{\mathrm{Tr}[\exp(-\beta\mathcal{H})]}\right) = \lim_{\beta,n\to\infty}\left(\frac{\mathrm{Tr}(AT^{n\beta})}{\mathrm{Tr}(T^{n\beta})}\right) \tag{4}$$

where the 'time evolution operator' $T = T_{xy}T_z$ is defined by

$$\begin{aligned} T_{xy} &= \bigotimes_i\left(1 - \frac{J}{2n}(S_i^+S_{i+1}^- + S_i^-S_{i+1}^+) - \frac{D}{4n}\{(S_i^+)^2 + (S_i^-)^2\}\right) \\ T_z &= \exp\left(\sum_i -\frac{J}{n}S_i^zS_{i+1}^z + \frac{H}{n}S_i^z\right). \end{aligned} \tag{5}$$

We insert a complete system into the product as

$$\mathrm{Tr}(T^{n\beta}) = \sum_{\{\sigma_m\}_{m=0,1,\ldots,n\beta-1}} \langle\sigma_0|T|\sigma_1\rangle\langle\sigma_1|T|\sigma_2\rangle\ldots\langle\sigma_{n\beta-1}|T|\sigma_0\rangle \tag{6}$$

where $|\sigma_m\rangle = \otimes_i|\sigma_{m,i}\rangle_i$ with $\sigma_{m,i} = \pm1, 0$ is summed over all the basis states. ($|\pm1\rangle_i$ and $|0\rangle_i$ denotes the normalized eigenstate of S_i^z with the eigenvalues ±1 and 0, respectively.) The right-hand-side of (6) can be regarded as a classical spin system defined on a two-dimensional 'space–time' lattice where the chain site i denotes the space coordinate and

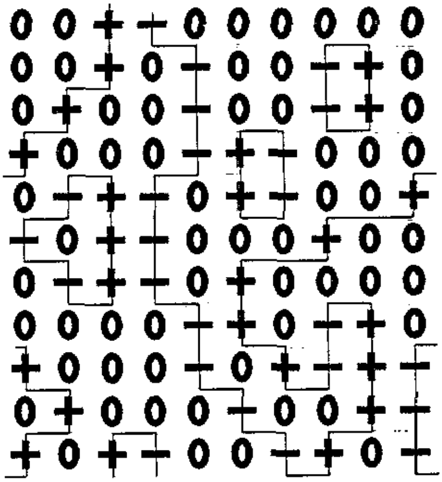

Figure 1. A typical loop configuration at the Heisenberg point $D = H = 0$. There is a strong hidden antiferromagnetic order.

m the time coordinate. *To get a geometric representation of* (6), *we expand each* T_{xy} and represent (6) as a (huge) summation. Next we draw a vertical bond of the unit length through a space–time point (m, i) if $\sigma_{m,i} \neq 0$, and a horizontal bond $(m + \frac{1}{2}, i)$–$(m + \frac{1}{2}, i + 1)$ whenever one picks up the terms $S_i^+ S_{i+1}^-$ or $S_i^- S_{i+1}^+$ in the matrix element $\langle \sigma_m | T_{xy} | \sigma_{m+1} \rangle$. Then we can rewrite (6) as $\mathrm{Tr}(T^{n\beta}) = \Sigma_\Gamma W(\Gamma)$ where Γ is summed over all the graphs consisting of the vertical and horizontal bonds [4, 8]. It is not hard to check that the statistical weight $W(\Gamma)$ is non-negative†. *Moreover the weight is non-vanishing* only when Γ can be regarded as a collection of closed loops. These properties are extremely useful for our purpose. In particular, they enable us to rewrite the quantum mechanical system as a statistical mechanical system of random loops where the probability that a loop configuration Γ appears is given by $W(\Gamma)/\Sigma_\Gamma W(\Gamma)$.

The argument of den Nijs and Rommelse [3], a numerical calculation of Girvin and Arovas [14] and a geometric picture (together with a rigorous 'no gas theorem') in [4] suggest that, at the Heisenberg point $D = H = 0$, the random loop system is in the 'percolating phase'. Then the existence of an infinitely large loop inevitably implies that there is a strong antiferromagnetic order in the following sense. Take a space-like slice of a typical random loop configuration to get a string of +, − and 0. Next drop all the 0s from the string, to get a string of + and −. Then one should observe a (normal) long-range antiferromagnetic order in this string (figure 1). The existence of such a hidden order cannot be observed as ordinary long-range order but can be detected by the non-vanishing den Nijs–Rommelse string order parameter (3).

Next we consider the effect of positive crystal-field anisotropy D and magnetic field H. In the basis where each S_i^z is diagonal, the D-term flips spin as $+ \leftrightarrow -$. Thus it creates intervals of flipped spins on the loops. The H-term contributes from the exponential weight in (6) and increases the probability of having + spins. A crucial fact is that the existence of the hidden antiferromagnetic order is incompatible with the 'all + state' favoured by the uniform magnetic field. The situation is closely analogous to the classical

† The weight $W(\Gamma)$ is a product of $-J/2n$ for each horizontal bond, $-D/4n$ for each point where there is a spin flip between $+1$ and -1, and a positive factor that comes from T_I. Since each loop must contain even numbers of horizontal bonds and spin flips, we have the non-negativity. (We are assuming that $n\beta$ is even.)

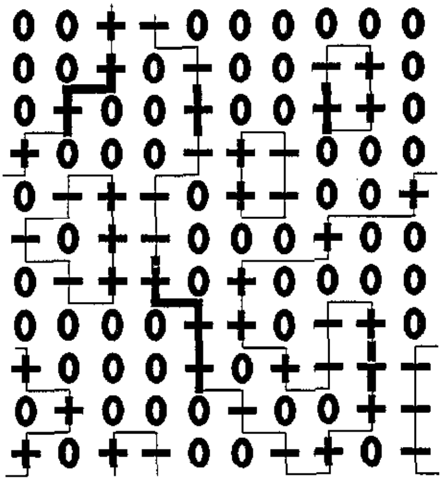

Figure 2. A typical loop configuration when D and H are finite (but small). There are intervals of flipped spins (indicated by grey lines), but the hidden antiferromagnetic order still remains.

2D antiferromagnetic Ising model under a uniform magnetic field, where it is known rigorously that the long-range antiferromagnetic order survives a sufficiently small magnetic field if the temperature is sufficiently low. In the Haldane gap antiferromagnets, D plays the role of the temperature in the Ising model. We expect that, when D is sufficiently small, the hidden order remains finite for sufficiently small values of H, and it vanishes above a critical value of H (figure 2). The behaviour of the magnetization curve is expected to be similar to that in the antiferromagnetic Ising model. The susceptibility should be small (but finite) for the values of the field lower than its critical value, and we expect a sudden jump in the susceptibility when the field exceeds its critical value. We stress that the magnetization curve is determined by a subtle cooperative phenomenon.

To make the above discussion more convincing, we evaluate the appearance probability of a flipped interval and the expected sizes of the flipped intervals. In these estimates, we let D and H be much smaller than the Haldane gap, and assume that there is a strong hidden antiferromagnetic order. The estimates show that flipped intervals are indeed rare, and thus the assumption of the strong hidden order is valid. This provides a (non-rigorous) self-consistency argument which supports our conclusion.

Suppose that a fixed space–time point is contained in such an interval of flipped spins whose length in the temporal direction is L. From (5) we see that the statistical weight associated with the interval is $(D^2/4n^2)\exp[(-2\Delta/n \pm 2H/n)L]$ when the spins inside the interval are ± 1, respectively. We have assumed that the spins surrounding the interval have perfect antiferromagnetic order, and the interaction between the spins is effectively reduced (from J) to Δ, the magnitude of the Haldane gap.

Let

$$Z_{\pm} = \frac{D^2}{4n^2}\sum_{L=1}^{\infty} L\exp\left(\frac{2(-\Delta \pm H)}{n}L\right) \simeq \left(\frac{D}{2(\Delta \mp H)}\right)^2 \tag{7}$$

and

$$Y_{\pm} = \frac{D^2}{4n^2}\sum_{L=1}^{\infty} \frac{L^2}{n}\exp\left(\frac{2(-\Delta \pm H)}{n}L\right) \simeq \frac{D^2}{16(\Delta \mp H)^3}. \tag{8}$$

Then the probability that a fixed space-time point is contained in a flipped interval can be estimated as $P_\pm \simeq Z_\pm(1 + Z_\pm)^{-1}$. This probability is approximately $(D/4\Delta)^2$ when $H \ll \Delta$ and is thus very small when $D \ll \Delta$. The expectation value of the length (in the temporal direction measured in the physical unit) of the flipped interval of spins ± 1 is approximately $\langle L_\pm/n \rangle = Z_\pm/Y_\pm = (\Delta \mp H)^{-1}$, which is finite when $H \ll \Delta$.

The above calculations also give an order-of-magnitude estimate of $M(H)$. We can write $M(H) = \sigma(P_+ - P_-)/2$ where σ is the 'density' of the random loops†. Therefore we get $M(H) \simeq (\sigma D/8\Delta^3)H$ when $D, H \ll \Delta$. This behaviour is in contrast with that in the region $D \gg \Delta$, where we have $M(H) \simeq D^{-1}H$.

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References

[1] Haldane F D M 1983a *Phys. Lett.* **93A** 464; 1983b *Phys. Rev. Lett.* **50** 1153
[2] Affleck I 1989 *J. Phys.: Condens. Matter* **1** 3047
[3] den Nijs M and Rommelse K 1989 *Phys. Rev.* B **40** 4709
[4] Tasaki H 1991 *Phys. Rev. Lett.* **66** 798
[5] Kennedy T 1990 *J. Phys.: Condens. Matter* **2** 5737
[6] Affleck I, Kennedy T, Lieb E H and Tasaki H 1987 *Phys. Rev. Lett.* **59** 799; 1988 *Commun. Math. Phys.* **115** 477
Kennedy T, Lieb E H and Tasaki H 1988 *J. Stat. Phys.* **53** 383
[7] Kennedy T and Tasaki H 1991 Hidden $Z_2 \times Z_2$ symmetry breaking in Haldane gap antiferromagnets *Preprint* (University of Arizona)
[8] Kennedy T and Tasaki H 1991 unpublished
[9] Hagiwara M, Katsumata K, Affleck I, Halperin B I and Renard J P 1990 *Phys. Rev. Lett.* **65** 3181
[10] Katsumata K, Hori H, Takeuchi T, Date M, Yamagishi A and Renard J P 1989 *Phys. Rev. Lett.* **63** 86
Ajiro Y, Goto T, Kikuchi H, Sakakibara T and Inami T 1989 *Phys. Rev. Lett.* **63** 1424
[11] Affleck I 1991 *Phys. Rev.* B at press
[12] Affleck I 1990 *Phys. Rev.* B **41** 6697
Takahashi M and Sakai T 1991 *J. Phys. Soc. Japan* at press
Nomura K and Sakai T 1991 *Preprint* (ISSP, Tokyo)
Sakai T and Takahashi M 1991 *Preprint* (ISSP, Tokyo)
[13] The use of the product formula in quantum spin systems can be traced back to the following references
Robinson D 1969 *Commun. Math. Phys.* **14** 195
Ginibre J 1969 *Commun. Math. Phys.* **14** 205
Asano T 1970a *J. Phys. Soc. Japan* **29** 350; 1970b *Phys. Rev. Lett.* **24** 1409
Suzuki M and Fisher M E 1971 *J. Math. Phys.* **12** 235
For recent applications, see Suzuki M 1986 *J. Stat. Phys.* **43** 883 and references therein
[14] Girvin S M and Arovas D P 1989 *Phys. Scr.* T **27** 156

† A rough estimate of σ can be obtained by noting that σ^2 is approximately equal to the expectation value of the string order parameter (3). From the numerical estimate of Girvin and Arovas [14] we see that $\sigma \simeq 0.6$.