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# Critical properties of the transition between the Haldane phase and the large- $D$ phase of the spin- $\frac{1}{2}$ ferromagnetic–antiferromagnetic Heisenberg chain with on-site anisotropy

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**Abstract.** We analytically study the ground-state quantum phase transition between the Haldane phase and the large- $D$  (LD) phase of the  $S = \frac{1}{2}$  ferromagnetic–antiferromagnetic alternating Heisenberg chain with on-site anisotropy. We transform this model into a generalized version of the alternating antiferromagnetic Heisenberg model with anisotropy. In the transformed model, the competition between the transverse and longitudinal bond alternations yields the Haldane–LD transition. Using the bosonization method, we show that the critical exponents vary continuously on the Haldane–LD boundary. Our scaling relations between critical exponents explains very well the numerical results of Hida.

## 1. Introduction

Since Haldane’s prediction [1, 2], the integer spin chains have been attracting much attention. Hida [3, 4] tried to elucidate the properties of the spin-1 Heisenberg chain from the standpoint of the spin- $\frac{1}{2}$  ferromagnetic–antiferromagnetic alternating chain. He considered the Hamiltonian [4]

$$\mathcal{H}_D = 2J \sum_{j=1}^N \mathbf{S}_{2j} \cdot \mathbf{S}_{2j+1} + 2J' \sum_{j=1}^N \mathbf{S}_{2j-1} \cdot \mathbf{S}_{2j} + D \sum_{j=1}^N (S_{2j-1}^z + S_{2j}^z)^2 \quad (1.1)$$

where  $\mathbf{S}_j$  is the spin- $\frac{1}{2}$  operator. We assume that  $J > 0$  (antiferromagnetic) and  $J' < 0$  (ferromagnetic) and we are only interested in the ground state. Hereafter we call the model (1.1) the ‘ $D$ -model’ following Hida [5].

In the case of  $J' \rightarrow -\infty$ , where the spins  $\mathbf{S}_{2j-1}$  and  $\mathbf{S}_{2j}$  form a triplet, the model (1.1) reduces to a spin-1 antiferromagnetic Heisenberg chain with on-site anisotropy

$$\hat{\mathcal{H}}_D^{S=1} = \frac{J}{2} \sum_{j=1}^N \hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_{j+1} + D \sum_{j=1}^N (\hat{S}_j^z)^2 \quad (1.2)$$

where  $\hat{\mathbf{S}}_j = \mathbf{S}_{2j-1} + \mathbf{S}_{2j}$  is the spin-1 operator. When  $J' = D = 0$ , on the other hand, Hamiltonian (1.1) reduces to the two-spin problem. Its ground state is the complete dimer state in which the spins  $\mathbf{S}_{2j}$  and  $\mathbf{S}_{2j+1}$  form a singlet pair  $(1/\sqrt{2})(\uparrow_{2j}\downarrow_{2j+1} - \downarrow_{2j}\uparrow_{2j+1})$ .

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When  $D = 0$ , therefore, the Hamiltonian (1.1) smoothly connects the dimer state of the spin- $\frac{1}{2}$  chain and the Haldane state of the spin-1 chain.

Hida [3] numerically diagonalized the finite system of Hamiltonian (1.1) in the  $D = 0$  case to find that there is no evidence for the phase transition of the ground state between  $J' = 0$  and  $J' = -\infty$ . Therefore he concluded that the Haldane phase of the spin-1 chain can be interpreted as the special case of the dimer phase of the spin- $\frac{1}{2}$  chain. This picture was supported by the work of Kohmoto and Tasaki [6], and Takada [7] who used the non-local unitary transformation. Hida performed the numerical diagonalization for the  $D \neq 0$  case to draw the phase diagram of the  $D$ -model on the  $J'$ - $D$  plane [4] and also to estimate the critical exponents of the Haldane-LD transition [8].

Yamanaka *et al* [9] investigated the model

$$\mathcal{H}_\lambda = 2J \sum_{j=1}^N (S_{2j}^x S_{2j+1}^x + S_{2j}^y S_{2j+1}^y + \lambda S_{2j}^z S_{2j+1}^z) + 2J' \sum_{j=1}^N \mathbf{S}_{2j-1} \cdot \mathbf{S}_{2j} \quad (1.3)$$

where the parameter  $\lambda$  represents the interaction anisotropy of the antiferromagnetic bonds. We call this model the ' $\lambda$ -model'. This model is equivalent to the spin-1 XXZ model

$$\hat{\mathcal{H}}_\lambda^{S=1} = \frac{J}{2} \sum_{j=1}^N (\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y + \lambda \hat{S}_j^z \hat{S}_{j+1}^z) \quad (1.4)$$

in the limit of  $J' \rightarrow -\infty$ . We note that the ferromagnetic bonds should be isotropic so that  $\mathbf{S}_{2j}$  and  $\mathbf{S}_{2j+1}$  form a triplet pair when  $J' \rightarrow -\infty$ . They mapped this model onto the highly anisotropic version of the two-dimensional Ashkin-Teller model and performed the 'high temperature expansion' to obtain the ground-state phase diagram. Their phase diagram consists of several phases, including the Haldane phase, the Néel phase and the XY phase. Hida [5] also drew the phase diagram of the  $\lambda$ -model by mapping the  $\lambda$ -model onto the  $D$ -model. His conclusion was consistent with that of Yamanaka *et al* [9].

Okamoto *et al* [10] have shown that the Haldane-LD boundary of Hida's phase diagram (obtained by numerical calculations) for the  $D$ -model can be semi-quantitatively reproduced by an analytical method. In this paper, we continue their work to investigate the critical properties of the Haldane-LD transition. We show that the Haldane-LD transition is of the Gaussian universality class and the critical exponents vary continuously on the boundary. In section 2, we explain the nature of the Haldane-LD transition. In section 3 the bosonization approach to the Haldane-LD transition is given and the critical properties are discussed. The last section (section 4) is devoted to a discussion.

## 2. Nature of the Haldane-LD transition

In the following we investigate Hamiltonian (1.1) assuming  $J' < 0$ . Performing the spin rotation around the  $z$ -axis,

$$\begin{aligned} \tilde{S}_j^x &= -S_j^x & \tilde{S}_j^y &= -S_j^y & \tilde{S}_j^z &= S_j^z & \text{for } j = 4l, 4l + 1 \\ \tilde{S}_j^x &= S_j^x & \tilde{S}_j^y &= S_j^y & \tilde{S}_j^z &= S_j^z & \text{otherwise} \end{aligned} \quad (2.1)$$

we can transform Hamiltonian (1.1) into an antiferromagnetic form [4]

$$\tilde{\mathcal{H}} = 2J_0 \sum_{j=1}^{2N} \{ (\tilde{S}_j^x \tilde{S}_{j+1}^x + \tilde{S}_j^y \tilde{S}_{j+1}^y + \Delta \tilde{S}_j^z \tilde{S}_{j+1}^z) + (-1)^j [\delta_\perp (\tilde{S}_j^x \tilde{S}_{j+1}^x + \tilde{S}_j^y \tilde{S}_{j+1}^y) + \delta_z \tilde{S}_j^z \tilde{S}_{j+1}^z] \} \quad (2.2)$$

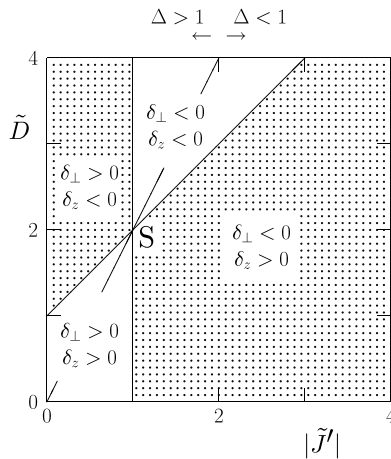
where

$$\begin{aligned}
 J_0 &= \frac{J(1 + |\tilde{J}'|)}{2} & \Delta &= 1 + \frac{\tilde{D} - 2|\tilde{J}'|}{1 + |\tilde{J}'|} \\
 \delta_{\perp} &= \frac{1 - |\tilde{J}'|}{1 + |\tilde{J}'|} & \delta_z &= \frac{1 - |\tilde{J}'| - (\tilde{D} - 2|\tilde{J}'|)}{1 + |\tilde{J}'|}
 \end{aligned}
 \tag{2.3}$$

and

$$\tilde{J}' \equiv J'/J \quad \tilde{D} \equiv D/J.
 \tag{2.4}$$

The Hamiltonian (2.2) can be interpreted as a generalized version of the alternating antiferromagnetic Heisenberg chain with anisotropy (see figure 1). The point  $(|\tilde{J}'|, \tilde{D}) = (1, 2)$  (called the S point) is the solvable point where Hamiltonian (2.2) represents the uniform and isotropic antiferromagnetic chain. The S point is the tricritical point of the Haldane phase, the LD phase and the Néel phase in Hida's phase diagram [4].



**Figure 1.** Important parameters in the Hamiltonian (2.2) on the  $|\tilde{J}'|$ - $\tilde{D}$  plane. The transverse and longitudinal alternations are mutually competing in the shaded areas. The point S ( $|\tilde{J}'| = 1, \tilde{D} = 2$ ) corresponds to the uniform isotropic antiferromagnetic Heisenberg model.

In the bosonization theory of the bond alternation problem, it has long been considered that the  $\delta_z$  term plays an irrelevant role. However, we have recently pointed out that the ground state of the Hamiltonian (2.2) in the case of  $\delta_{\perp} = 0$  and  $\delta_z > 0$  is the dimer state [11, 12]. This shows the importance of the  $\delta_z$  term, because the ground state would be the spin-fluid state if the  $\delta_z$  term played an irrelevant role. When  $\Delta = 1$  and  $\delta_{\perp} = \delta_z = 1$ , the ground state of Hamiltonian (2.3) is the complete dimer state (an array of local singlet dimers), and both the  $\delta_z$  term and the  $\delta_{\perp}$  term give the same contribution to the excitation gap apart from a factor 2. Then, in the  $\Delta = 1$  and  $\delta_{\perp} = \delta_z > 0$  case where the ground state is the dimer state, we expect that the excitation gap should behave as

$$\varepsilon_{\text{gap}} \sim (2\delta_{\perp} + \delta_z)^{\nu}
 \tag{2.5}$$

due to the  $SU(2)$  symmetry. Here  $\nu$  is the exponent of the correlation length and we do not enter into the logarithmic correction problem [13]. Thus we can consider that the  $\delta_{\perp}$  term and the  $\delta_z$  term are mutually cooperative when  $\delta_{\perp}\delta_z > 0$ , and competing when  $\delta_{\perp}\delta_z < 0$ . Of course, when  $\Delta \neq 1$ , equation (2.5) itself may no longer be valid.

Let us consider the  $\Delta < 1$  case, where we can exclude the possibility of the Néel state. When  $\delta_{\perp} > 0$  and  $\delta_z > 0$ , an effective singlet dimer is formed by spins  $\tilde{S}_{2j}$  and  $\tilde{S}_{2j+1}$ . Their coupling is antiferromagnetic in the original spin ( $S$ ) representation before the transformation (2.1). Since this singlet dimer is still a singlet dimer in the  $S$  representation, this state is the Haldane state. On the other hand, when  $\delta_{\perp} < 0$  and  $\delta_z < 0$ , spins  $\tilde{S}_{2j-1}$  and  $\tilde{S}_{2j}$  (their coupling is ferromagnetic in the  $S$  representation) form an effective singlet pair. By the transformation (2.1), this singlet dimer is transformed into the triplet dimer (like the  $(1/\sqrt{2})(\uparrow_{2j-1}\downarrow_{2j} + \downarrow_{2j-1}\uparrow_{2j})$  state) in the  $S$  representation. This is the  $\hat{S}^z = 0$  state of the spin with  $\hat{S} = 1$ . Therefore this state is nothing more than the LD state. We note that, in the  $\tilde{S}$  representation, both the Haldane state and the LD state are the singlet dimer state, but the dimer configuration is different by one spin site between these two states.

What happens in the region where  $\delta_{\perp} < 0$  and  $\delta_z > 0$ ? If the effect of  $\delta_z$  ( $\delta_{\perp}$ ) is predominant, the ground state may be the Haldane (LD) state. Therefore the ground-state phase transition between the Haldane state and the LD state can be observed in this region. The Haldane–LD phase boundary may be determined by the line on which the effects of  $\delta_{\perp}$  and  $\delta_z$  cancel each other out. From equation (2.5), the simplest estimate for the Haldane–LD boundary may be

$$2\delta_{\perp} + \delta_z = 0 \quad (2.6)$$

which results in

$$\tilde{D} = 2|\tilde{J}'|. \quad (2.7)$$

Although this estimate is too rough because equation (2.5) may be valid only when  $\Delta = 1$ , the nature of the Haldane–LD transition is well explained by the above-mentioned picture. A more elaborate estimation will be given in the next section.

### 3. Critical properties of the Haldane–LD transition

Through a careful bosonization procedure, we can map Hamiltonian (2.2) onto a generalized version of the sine–Gordon Hamiltonian

$$\tilde{\mathcal{H}}_b = 2J_0 \int dx \{A(\nabla\theta)^2 + CP^2 + B_1 \cos 2\theta - B_{\perp} \cos \theta - B_z(\nabla\theta)^2 \cos \theta\} \quad (3.1)$$

where the commutation relation

$$[\theta(x), P(x')] = i\delta(x - x') \quad (3.2)$$

holds. The coefficients  $B_{\perp}$ ,  $B_z$  and  $B_1$  are obtained directly from the bosonization procedure as

$$B_{\perp} = \frac{\delta_{\perp}}{a} \quad B_z = \frac{\delta_z a}{\pi} \quad B_1 = \frac{\Delta}{2a} \quad (3.3)$$

where  $a$  is the spin spacing. These expressions are considered to be valid when  $\delta_{\perp} \ll 1$ ,  $\delta_z \ll 1$ ,  $\Delta \ll 1$ . Similar expressions were already obtained by Nakano and Fukuyama [14], but there was an error in the sign in their expressions. In their expressions, the  $B_{\perp}$  term

and the  $B_z$  term are mutually competing when  $\delta_\perp \delta_z > 0$ . From the discussion of section 2, these terms should be mutually cooperative when  $\delta_\perp \delta_z < 0$ , as is realized in (3.1).

Since the term  $B_I \cos 2\theta$  is irrelevant for the  $\Delta < 1$  case with which we are concerned, we may neglect this term by setting

$$B_I = 0. \tag{3.4}$$

For the coefficients  $A$  and  $C$ , the bosonization procedure leads to

$$A = \frac{a}{8\pi} \left( 1 + \frac{3\Delta}{\pi} \right) \quad C = 2\pi a \left( 1 - \frac{\Delta}{\pi} \right). \tag{3.5}$$

Of course, these expressions may be valid for  $\Delta \ll 1$ . Therefore we cannot use such expressions, because we require expressions valid near  $\Delta = 1$  to discuss the Haldane–LD transition near the S point ( $\Delta = 1$ ,  $\delta_\perp = \delta_z = 0$ ). When  $\delta_\perp = \delta_z = 0$ , the Hamiltonian (2.2) represents the uniform  $XXZ$  chain for which the exact results are available. In this case, the spin wave velocity  $v$  [15], and the power decay exponent  $\eta$  [16], defined by  $(-1)^r \langle S_0^z S_r^z \rangle \sim r^{-\eta}$ , are

$$\frac{v}{2J_0} = \frac{\pi a \sqrt{1 - \Delta^2}}{2 \cos^{-1} \Delta} \tag{3.6}$$

$$\eta = \frac{2}{1 + (\pi/2) \sin^{-1} \Delta} \tag{3.7}$$

respectively. If we use the bosonized Hamiltonian (3.1) with  $B_I = B_\perp = B_z = 0$ , we obtain

$$\frac{v}{2J_0} = 2\sqrt{AC} \quad \eta = \frac{1}{2\pi} \sqrt{\frac{C}{A}}. \tag{3.8}$$

From equations (3.6)–(3.8) we can immediately write down the expressions for  $A$  and  $C$ . This procedure for the adjustment of the coefficients was first proposed by Cross and Fisher [17] and applied by Nakano and Fukuyama [14, 18]. If we expand  $A$  and  $C$  with respect to  $\varepsilon \equiv 1 - \Delta$ , we obtain

$$\frac{v}{2J_0} = \frac{\pi a}{2} + O(\varepsilon) \quad \eta = 1 + \frac{\sqrt{2\varepsilon}}{\pi} \tag{3.9}$$

$$A = \frac{a}{8} \left( 1 - \frac{\sqrt{2\varepsilon}}{\pi} \right) \quad C = \frac{\pi^2 a}{2} \left( 1 + \frac{\sqrt{2\varepsilon}}{\pi} \right). \tag{3.10}$$

up to the lowest order of  $\varepsilon$ . Expressions (3.9) and (3.10) were also obtained by Inagaki and Fukuyama [19]. Thus our bosonized expression for the spin Hamiltonian (2.2) is equation (3.1) with equations (3.3) and (3.10). We note that this is valid for  $|\delta_\perp| \ll 1$ ,  $|\delta_z| \ll 1$  and  $\varepsilon \ll 1$ .

To discuss the critical properties of the Haldane–LD transition, we apply the self-consistent harmonic approximation (SCHA), which is essentially the variational method, to the bosonized Hamiltonian (3.1) when  $\delta_\perp < 0$  and  $\delta_z > 0$ . In the Haldane state, as is discussed in section 2, the effect of  $\delta_z$  is predominant and the average value of  $\theta$  with respect to the ground state,  $\langle \theta \rangle$ , is

$$\langle \theta \rangle = 0 \quad (\text{Haldane state}) \tag{3.11}$$

so that the  $B_z$  term gains the energy. In the LD state, on the other hand, the effect of  $\delta_z$  is predominant and

$$\langle \theta \rangle = \pi \quad (\text{LD state}). \quad (3.12)$$

Then we set the SCHA Hamiltonian

$$\tilde{\mathcal{H}}_S = 2J_0 \int dx \{A(\nabla\phi)^2 + CP^2 + \tilde{B}\phi^2\} \quad (3.13)$$

with

$$\phi \equiv \begin{cases} \theta & (\text{Haldane state}) \\ \theta - \pi & (\text{LD state}) \end{cases} \quad (3.14)$$

where  $\tilde{B}$  is the variational parameter. The parameter  $\tilde{B}$  should be determined so that  $\langle \tilde{\mathcal{H}}_b \rangle_S$  is minimized, i.e.

$$\frac{\partial \langle \tilde{\mathcal{H}}_b \rangle_S}{\partial \tilde{B}} = 0 \quad (3.15)$$

where  $\langle \dots \rangle_S$  denotes the average with respect to the ground state of  $\tilde{\mathcal{H}}_S$ .

The excitation spectrum of  $\tilde{\mathcal{H}}_S$  is

$$\omega_S(q) = v\sqrt{q^2 + q_c^2} \quad (3.16)$$

where

$$q_c^2 \equiv \tilde{B}/A \quad (3.17)$$

and  $vq_c$  is the excitation gap. Since  $\tilde{\mathcal{H}}_S$  is harmonic, the relations

$$\langle \exp(iu\phi) \rangle_S = \exp\left(-\frac{u^2}{2} \langle \phi^2 \rangle_S\right) \quad (3.18)$$

$$\langle (\nabla\phi)^2 \cos\phi \rangle_S = \langle (\nabla\phi)^2 \rangle_S \langle \cos\phi \rangle_S \quad (3.19)$$

hold with  $u$  being a real number. The average  $\langle (\nabla\theta)^2 \rangle_S$  is

$$\langle (\nabla\theta)^2 \rangle_S = \frac{C}{L} \sum_q \frac{q^2}{\omega_S(q)} = \frac{\eta}{2} Q \quad (3.20)$$

$$Q \equiv \int_0^{\alpha_0^{-1}} \frac{q^2 dq}{\sqrt{q^2 + q_c^2}} \simeq \frac{1}{\alpha_0^2} \quad (\alpha_0 q_c \ll 1) \quad (3.21)$$

where  $L$  is the system length, and the upper cut-off of the  $q$ -summation is denoted by  $\alpha_0^{-1}$  which may be proportional to  $a^{-1}$ . Luther and Peschel [20] suggested  $\pi\alpha_0 = a$ . However, care must be taken to estimate  $Q$ , because equation (3.20) is strongly dependent on  $Q$ . Let us consider the  $\Delta = 1$  (i.e.  $\eta = 1$ ) case. As discussed in section 2, for  $\Delta = 1$ , the effect

of  $\delta_\perp$  and  $\delta_z$  cancel out each other when equation (2.6) holds. Here we estimate that the equation

$$\langle B_\perp \cos \theta + B_z (\nabla \theta)^2 \cos \theta \rangle_S = 0 \quad (3.22)$$

reproduces equation (2.6) when  $\Delta = 1$ , which yields

$$Q = \pi/a^2. \quad (3.23)$$

After some calculations, for the Haldane state, we obtain

$$\begin{aligned} \frac{\partial \langle \tilde{\mathcal{T}}_{\text{b}} \rangle_S}{\partial \tilde{B}} = L \left\{ \frac{B_\perp}{2} \exp\left(-\frac{\langle \phi^2 \rangle_S}{2}\right) + \frac{B_z}{2} \exp\left(-\frac{\langle \phi^2 \rangle_S}{2}\right) \langle (\nabla \phi)^2 \rangle_S - \tilde{B} \right\} \frac{\partial \langle \phi^2 \rangle_S}{\partial \tilde{B}} \\ - L B_z \exp\left(-\frac{\langle \phi^2 \rangle_S}{2}\right) \frac{\partial \langle (\nabla \phi)^2 \rangle_S}{\partial \tilde{B}}. \end{aligned} \quad (3.24)$$

The second term of the RHS of equation (3.24) can be dropped, because  $\langle (\nabla \phi)^2 \rangle_S$  is almost independent of  $\tilde{B}$ , as can be seen from equations (3.20) and (3.21). Then, equation (3.15) with equation (3.24) is reduced to

$$\tilde{B} = \frac{1}{2} \exp\left(-\frac{\langle \phi^2 \rangle_S}{2}\right) \left(B_\perp + \frac{\pi \eta}{2a^2} B_z\right). \quad (3.25)$$

The quantity  $\langle \phi^2 \rangle_S$  is estimated as

$$\langle \phi^2 \rangle_S = \frac{C}{L} \sum_q \frac{1}{\omega_S(q)} = \eta \log \frac{2\pi}{aq_c} \quad (aq_c \ll 1) \quad (3.26)$$

which leads to the self-consistent gap equation

$$Aq_c^2 = \frac{1}{2a} \left(\frac{aq_c}{2\pi}\right)^{\eta/2} \left(\delta_\perp + \frac{\eta}{2} \delta_z\right). \quad (3.27)$$

A similar calculation can be performed for the LD state. If we replace  $\delta_\perp + (\eta/2) \delta_z$  in equation (3.27) by  $|\delta_\perp + (\eta/2) \delta_z|$ , the gap equation becomes valid both for the Haldane state and for the LD state. Thus the excitation gap behaves as

$$\varepsilon_{\text{gap}} = vq_c \sim \left|\delta_\perp + \frac{\eta}{2} \delta_z\right|^{2/(4-\eta)}. \quad (3.28)$$

The Haldane-LD phase boundary can be obtained from  $\varepsilon_{\text{gap}} = 0$ , which leads to

$$2(1 - |\tilde{J}'|) + (1 - \tilde{D} + |\tilde{J}'|) \left(1 + \frac{1}{\pi} \sqrt{\frac{2|\tilde{J}'| - \tilde{D}}{1 + |\tilde{J}'|}}\right) = 0. \quad (3.29)$$

where equations (2.3), (3.3) and (3.9) are employed. Okamoto *et al* [10] have already obtained this phase boundary equation, compared it with Hida's numerical result [8] and discussed its validity.



If the critical value of  $D$  is denoted by  $D_c$  when  $|J'|$  is fixed, we can rewrite equation (3.28) as

$$\varepsilon_{\text{gap}} \sim |D - D_c|^\nu \tag{3.30}$$

$$\nu = \frac{2}{4 - \eta}. \tag{3.31}$$

Thus we obtain

$$\nu_H = \nu_{LD} = \nu \tag{3.32}$$

where  $\nu_H$  ( $\nu_{LD}$ ) is the critical exponent of the excitation gap when the Haldane–LD boundary is approached from the Haldane (LD) phase.

The calculation of the longitudinal spin correlation  $\langle S_j^z S_l^z \rangle$  by the use of  $\tilde{\mathcal{H}}_S$  has already been done by the author [21]. Here we only write down the final expression for  $\langle S_j^z S_l^z \rangle$ , without entering into details:

$$\langle S_j^z S_l^z \rangle \sim \frac{(-1)^{|j-l|}}{\sqrt{|j-l|}} \exp\left(-\frac{|j-l|a}{\xi}\right) \quad (|j-l| \rightarrow \infty) \tag{3.33}$$

where  $\xi$  is the correlation length defined by

$$\xi = \frac{\nu}{\varepsilon_{\text{gap}}} \sim \left| \delta_\perp + \frac{\eta}{2} \delta_z \right|^{-\nu} \sim |D - D_c|^{-\nu}. \tag{3.34}$$

Thus  $\nu$  is also the exponent of the correlation length as expected. Comparing the result of [21] with the exact result for the  $XY$  case [22], we may rely on the exponential factor in equation (3.33), although the preceding power factor is not reliable.

Hida [8] proposed string order parameters for the Haldane phase and the LD phase. In the  $\tilde{S}$  representation, these string order parameters are defined by

$$O_{\text{even}}^\alpha = \lim_{|j-l| \rightarrow \infty} O_{\text{even}}^\alpha(j-l) \quad (\text{for the Haldane phase}) \tag{3.35}$$

$$O_{\text{odd}}^\alpha = \lim_{|j-l| \rightarrow \infty} O_{\text{odd}}^\alpha(j-l) \quad (\text{for the LD phase}) \tag{3.36}$$

with

$$O_{\text{even}}^\alpha(j-l) = -4 \langle \tilde{S}_{2j}^\alpha \exp\{i\pi(\tilde{S}_{2j+1}^\alpha + \tilde{S}_{2j+2}^\alpha + \cdots + \tilde{S}_{2j-2}^\alpha)\} \tilde{S}_{2l-1}^\alpha \rangle \tag{3.37}$$

$$O_{\text{odd}}^\alpha(j-l) = -4 \langle \tilde{S}_{2j-1}^\alpha \exp\{i\pi(\tilde{S}_{2j}^\alpha + \tilde{S}_{2j+1}^\alpha + \cdots + \tilde{S}_{2l-1}^\alpha)\} \tilde{S}_{2l}^\alpha \rangle \tag{3.38}$$

$$\alpha = x, y, z. \tag{3.39}$$

By the use of the identity  $\tilde{S}_j^z = \exp(i\pi \tilde{S}_j^z)/2i$  valid for the spin- $\frac{1}{2}$  operators, we can rewrite equations (3.37) and (3.38) as

$$O_{\text{even}}^z(j-l) = \langle \exp\{i\pi(\tilde{S}_{2j}^z + \tilde{S}_{2j+1}^z + \cdots + \tilde{S}_{2l-1}^z)\} \rangle \tag{3.40}$$

$$O_{\text{odd}}^z(j-l) = \langle \exp\{i\pi(\tilde{S}_{2j-1}^z + \tilde{S}_{2j}^z + \cdots + \tilde{S}_{2l}^z)\} \rangle \tag{3.41}$$

respectively. Since the slowly varying part of the  $z$ -component of the spin density is expressed as  $(1/2\pi)(\partial\theta/\partial x)$ , the boson representations of  $O_{\text{even}}^z(j-l)$  and  $O_{\text{odd}}^z(j-l)$  are

$$\begin{aligned} O_{\text{even}}^z(x-x') &= O_{\text{odd}}^z(x-x') \\ &= \langle \exp\{i[\theta(x) - \theta(x')]/2\} \rangle \\ &= \langle \exp\{i[\phi(x) - \phi(x')]/2\} \rangle \\ &\equiv O^z(x-x'). \end{aligned} \quad (3.42)$$

We note that the difference between the  $O_{\text{even}}^z(x-x')$  and  $O_{\text{odd}}^z(x-x')$  is lost due to the continuum approximation used in the bosonization method.

Let us calculate  $O^z$  in the framework of the SCHA. Due to the harmonic nature of  $\tilde{\mathcal{H}}_S$ , we have

$$\begin{aligned} O^z(x-x') &= \exp\left\{-\frac{1}{8}\langle [\theta(x) - \theta(x')]^2 \rangle_S\right\} \\ &= \exp\left(-\frac{1}{4}\langle \phi^2 \rangle_S\right) \exp\left\{\frac{1}{4}\langle \phi(x)\phi(x') \rangle_S\right\}. \end{aligned} \quad (3.43)$$

The average  $\langle \phi(x)\phi(x') \rangle_S$  is estimated as [21]

$$\langle \phi(x)\phi(x') \rangle_S = \frac{C}{\pi v} K_0(q_c[|x-x'| + \alpha_1]) \quad (3.44)$$

$$\alpha_1 = \frac{ae^{-\gamma}}{\pi} \quad \gamma = 0.5772\dots \quad (\text{Euler's constant}) \quad (3.45)$$

where  $K_n(y)$  is the  $n$ th order modified Bessel function of the second kind. We note that the parameter  $\alpha_1$  is determined so that equation (3.26) is reproduced when  $|x-x'| = 0$ . Using the asymptotic behaviour of  $K_0(y)$

$$K_0(y) \simeq \sqrt{\frac{\pi}{2y}} e^{-y} \quad (y \rightarrow \infty) \quad (3.46)$$

we obtain

$$\begin{aligned} O^z &= \exp\left(-\frac{1}{4}\langle \phi^2 \rangle_S\right) \\ &\sim q_c^{\eta/4} \sim |D - D_c|^{\eta/(8-2\eta)}. \end{aligned} \quad (3.47)$$

If we denote the exponents of  $O_{\text{even}}^z$  and  $O_{\text{odd}}^z$  by  $2\beta_{\text{H}}^z$  and  $2\beta_{\text{LD}}^z$  respectively (for the factor 2, we follow Hida's definition [8]), we see

$$\beta_{\text{H}} = \beta_{\text{LD}} = \frac{\eta}{16 - 4\eta} \equiv \beta. \quad (3.48)$$

We can also calculate the asymptotic behaviour of  $O^z(x-x')$  when  $|x-x'| \rightarrow \infty$  just on the Haldane-LD boundary. Using equations (3.43)–(3.45) and taking the limit  $q_c \rightarrow 0$ , we obtain

$$O^z(x-x')|_{D=D_c} \sim |x-x'|^{-\eta/4} \quad (3.49)$$

where the asymptotic form

$$K_0(y) \simeq -\log y \quad (y \rightarrow 0) \quad (3.50)$$

is employed. Hida [8] also numerically calculated the system size dependence of  $O_{\text{even}}^z$  and  $O_{\text{odd}}^z$  on the Haldane–LD boundary. He defined

$$O_{\text{even}}^z(N)|_{D=D_c} \sim N^{-\mu_H} \tag{3.51}$$

$$O_{\text{odd}}^z(N)|_{D=D_c} \sim N^{-\mu_{LD}} \tag{3.52}$$

where  $N$  is the system size. Although Hida [8] used  $\eta^z$  for these exponents, we use  $\mu$  to avoid confusion. From equation (3.49), we can expect

$$\mu_H = \mu_{LD} = \frac{\eta}{4} \equiv \mu. \tag{3.53}$$

This result can also be obtained from the finite size scaling ansatz

$$O^z(|D - D_c|, N) \sim N^{-\mu} f(N|D - D_c|^\nu) \tag{3.54}$$

where we note that  $N/\xi \sim N|D - D_c|^\nu$ . The form of equation (3.54) is chosen so that equations (3.51) and (3.52) are reproduced at  $D = D_c$ . If we fix  $|D - D_c|$  and take the limit  $N \rightarrow \infty$ , we obtain

$$f(x) \sim x^\mu \quad (x \rightarrow \infty) \tag{3.55}$$

$$O^z(|D - D_c|, N = \infty) \sim |D - D_c|^{\mu\nu} \tag{3.56}$$

from the condition that  $O^z(|D - D_c|, N)$  should be independent of  $N$  when  $N \rightarrow \infty$ . From equations (3.47) and (3.48) it follows that

$$\mu\nu = 2\beta \tag{3.57}$$

which readily leads to equation (3.53). The relation (3.57) was also noticed by Hida [8].

#### 4. Discussion

We have calculated several critical exponents of the Haldane–LD transition. These exponents are controlled by  $\nu$ , which varies continuously on the Haldane–LD boundary. Thus the present transition is of the Gaussian universality class. This fact has already been pointed out by several groups [8–10].

**Table 1.** Critical exponents of the Haldane–LD transition. The exponents  $\nu$ ,  $\beta_H$ ,  $\beta_{LD}$ ,  $\mu_H$  and  $\mu_{LD}$  are numerical results of Hida [8, 23], and  $\beta_{\text{theor}}$  and  $\mu_{\text{theor}}$  are calculated from Hida’s  $\nu$  by the use of equations (4.2) and (4.3).

$ \vec{J}' $	$\nu$	$\beta_H$	$\beta_{LD}$	$\beta_{\text{theor}}$	$\mu_H$	$\mu_{LD}$	$\mu_{\text{theor}}$
1.5	0.801	0.165 ± 0.002	0.141 ± 0.004	0.150	0.411 ± 0.002	0.352 ± 0.004	0.375
2.0	0.879	0.200 ± 0.003	0.184 ± 0.002	0.190	0.454 ± 0.005	0.419 ± 0.003	0.431
2.5	0.975	0.238 ± 0.002	0.223 ± 0.002	0.238	0.489 ± 0.003	0.458 ± 0.003	0.487
3.0	1.031	0.255 ± 0.001	0.257 ± 0.002	0.266	0.494 ± 0.001	0.500 ± 0.003	0.515
4.0	1.120	0.297 ± 0.005	0.294 ± 0.02	0.310	0.530 ± 0.01	0.525 ± 0.04	0.553

In this paper we have used the mapping of the original spin Hamiltonian onto the generalized version of the sine–Gordon Hamiltonian. Since several approximations have been used in the course of the mapping, the values of  $D_c$  and the critical exponent themselves are unreliable. We believe, however, that the present theory well describes the qualitative feature of the Haldane–LD transition. From equations (3.31), (3.48) and (3.53), our predictions for the relations between critical exponents are

$$\nu_H = \nu_{LD} = \nu \quad (4.1)$$

$$\beta_H = \beta_{LD} = \beta = \frac{2\nu - 1}{4} \quad (4.2)$$

$$\mu_H = \mu_{LD} = \mu = 1 - \frac{1}{2\nu}. \quad (4.3)$$

The reliability of the present theory can be examined by testing whether equations (4.2) and (4.3) hold or not in Hida's numerical result [8, 23]. This test is summarized in table 1, where the exponents  $\nu$ ,  $\beta_H$ ,  $\beta_{LD}$ ,  $\mu_H$  and  $\mu_{LD}$  are numerical results of Hida and  $\beta_{\text{theor}}$  and  $\mu_{\text{theor}}$  are calculated from Hida's  $\nu$  through equations (4.2) and (4.3). As can be seen, the values of  $\beta_{\text{theor}}$  and  $\mu_{\text{theor}}$  agree very well with  $\beta_H$  and  $\beta_{LD}$ , and  $\mu_H$  and  $\mu_{LD}$ , respectively. Therefore we can say that our theory successfully describes the qualitative feature of the Haldane–LD transition.

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