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# Phase diagram of three-leg spin ladder

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**Abstract.** The spin- $\frac{1}{2}$  spin ladder with single-ion anisotropy and bond alternation is analysed using the bosonization technique and other methods. Our argument is mainly devoted to the case of three legs. Combining the renormalization group analysis with the results of the strong-coupling limits, we predict that the translationally invariant model is gapless regardless of the single-ion anisotropy and described by the c = 1 conformal field theory (CFT). It is also argued that the response to the bond alternation is quite different according to the sign of the interchain coupling.

#### 1. Introduction

The problem of coupled chains (of spins or electrons) has been a subject of study for years. Recently, it has found renewed interest; the Heisenberg spin ladders are considered to be the model for singlet superconductivity [1] (see also [2] and references cited therein) and the coupled electronic chains are interesting in view of extending the Luttinger liquid concepts to two dimensions [3]. One of the most striking features of this problem would be that there exist ladder-like materials such as  $Sr_{n-1}Cu_{n+1}O_{2n}$  [4, 5].

On the other hand, these models provide a good starting point for the weak-coupling approach to Haldane gap systems [6–9] and heavy-fermion systems [10, 11]. In the present paper, we investigate the  $S = \frac{1}{2}$  Heisenberg spin ladder with three legs (i.e. three coupled chains, see figure 1)

$$\mathcal{H} = \sum_{i=1}^{n_{\text{leg}}} \sum_{\alpha=1}^{S_{2i-1}} \cdot S_{2i}^{\alpha} + J' \sum_{j=1}^{n_{\text{leg}}} \sum_{\alpha=1}^{N_{\text{leg}}} S_{2j}^{\alpha} \cdot S_{2j+1}^{\alpha} + J_{\text{K}} \sum_{i=1}^{n_{\text{leg}}-1} \sum_{\alpha=1}^{n_{\text{leg}}-1} S_{i}^{\alpha} \cdot S_{i}^{\alpha+1} + D \sum_{k=1}^{n_{\text{leg}}} \left(\sum_{\alpha=1}^{n_{\text{leg}}} S_{k}^{\alpha,z}\right)^{2} \qquad (n_{\text{leg}} = 3)$$
(1)

where  $n_{\text{leg}}$  chains (labelled by  $\alpha$ ) are coupled to the neighbouring ones through the  $J_{\text{K}}$ interaction. We have introduced bond alternation J' in order to consider the difference
in the response against the alternation between the cases of S = (integer) and S =(half-odd integer). As usual, the fourth term (*D*-term, hereafter) introduces the effect of the
single-ion anisotropy.

Quite recently, the behaviour of the model (1) with  $n_{\text{leg}} = 2$  has become clear [9–13]; the transition to the 'Haldane phase' occurs at  $(J_{\text{K}} = 0, J' = 0)$  and the gap  $\Delta$  opens as  $\Delta \sim |J_{\text{K}}|(\ln |J_{\text{K}}|)^{1/2}$ .

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Figure 1. Three-leg ladders; (a) planer ladder and (b) cylindrical ladder. The choice of the topology affects the strong-coupling limit.

However, not much is known about the case  $n_{\text{leg}} = 3$  [14]. There is a (strictly speaking, *not* complete but very plausible) proof [15] stating that the homogeneous  $S = \frac{1}{2}$  Heisenberg ladder with an odd number of legs has gapless excitations<sup>†</sup>. This does not depend on the strength of the interchain coupling  $J_{\text{K}}$ . Thus we may expect that the system is gapless all along the line J' = 1. Nevertheless, the universality class of this system is not known. In particular, the universality class on the ferromagnetic side  $J_{\text{K}} < 0$  is interesting in relation to the Haldane conjecture [16, 17]. That is, the system reduces to the  $S = \frac{3}{2}$  Heisenberg chain in the limit  $-J_{\text{K}} \rightarrow \infty$ . In this sense, our model may be used as a weak-coupling approach to the problem of higher-spin chains.

The model (1) is also interesting in the context of the dimerization transition. Affleck and Haldane [18] and later Guo *et al* [19] conjectured that the features of the dimerization transition are different for S = integer and S = half-odd integer. The main purpose of the present paper is to obtain a qualitative phase diagram of the model and to clarify the difference between the case  $n_{\text{leg}} = 2$  and  $n_{\text{leg}} = 3$ .

The Abelian bosonization technique [20] is usually used in the analysis of such coupled chains. However, if we use the Abelian bosonization starting from the Jordan–Wigner fermionization, we have to deal with two types of interactions; one comes from the (intrachain) exchange interaction along the *z*-axis and the other from the *interchain* coupling. Furthermore, for special choices of the interactions, novel criticalities appear [21] which cannot be described by a naive assembly of bosons.

Instead, we develop a different type of bosonization, which manifestly preserve the SU(2) symmetry and takes into account that only the total spin is well defined in the strong-coupling  $(|J_K| \gg 1)$  limit.

We construct the present paper as follows. In section 2, we investigate the strongcoupling limits ( $|J_K| \gg 1$  or  $D \gg 1$ ), where the problem is much easier to tackle, and we derive the effective Hamiltonian to show that the system reduces to the  $S = \frac{1}{2}$  chain in many cases.

The bosonization analysis is developed in section 3. In the first part, we perform a naive perturbative renormalization after applying non-Abelian bosonization for the individual

<sup>†</sup> This 'theorem' is readily extended to include the case of the spin-S XXZ-ladder with 2S = odd,  $n_{\text{leg}} = \text{odd}$ .

chains, and extract several facts from the results. Then, we further rewrite the model in terms of the effective action of the spin sector, which is considered to be suitable for the investigation of the strong-coupling region, and the residual degrees of freedom. This is carried out by exploiting the coset construction  $\widehat{SU}(2)_1 \times \widehat{SU}(2)_1 \times \widehat{SU}(2)_1/\widehat{SU}(2)_3$ . The resulting model is given by the higher-level Wess–Zumino–Witten (WZW) conformal field theory (CFT) together with several interactions and, what is important, it is written only by the total spin.

The renormalization group analysis for this model is given in section 4. Combining it with the semiclassical argument, we discuss the nature of the phases. Several quantities such as correlation functions and susceptibility are calculated as well. Although sections 3 and 4 are the main part of the present paper, readers who are unfamiliar with the field-theoretical argument will skip section 3 and the first half of section 4.

A simple variational argument of the phase diagram is presented in section 5, where the existence of the dimerization transition is discussed.

Our main results are summarized in the last section. The difference between the cases with  $J_{\rm K} > 0$  and  $J_{\rm K} < 0$  is discussed in conjunction with the Berry phase. In the appendix, we give 'minimal' information about the coset construction used in the text.

#### 2. Strong-coupling limits

The model (1) reduces to more familiar models in the strong-coupling limits  $|J_K| \gg 1$  or  $D \gg 1$ . This will help us to obtain a global outlook for the phase diagram.

To begin with, we consider the case  $J_{\rm K} > 0$  (we call it the AF *case* or AF-*side* hereafter). For clarity, we first investigate the case of a planar ladder, i.e. a ladder with open ends in the vertical direction (see figure 1(*a*)). The cylindrical case (figure 1(*b*)) is convenient to the application of the bosonization method and is treated afterwards. In the limit  $J_{\rm K} \to \infty$ , the system reduces to the assembly of the decoupled rungs (composed of three sites) which is easily diagonalized. The ground state is given by a tensor product of the doublet ( $S = \frac{1}{2}$ ), i.e.

$$|s_1^3\rangle \otimes |s_2^3\rangle \otimes \cdots \otimes |s_L^3\rangle \tag{2}$$

where the state of the *i*th rung  $|s_i^3\rangle$  is either

$$\begin{vmatrix} \frac{1}{2} \end{pmatrix} = \frac{1}{\sqrt{6}} (2|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle)$$
  
or 
$$\begin{vmatrix} -\frac{1}{2} \end{pmatrix} = \frac{1}{\sqrt{6}} (-2|\downarrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle)$$

Therefore, the ground state for  $J_{\rm K} \to \infty$  is  $2^L$ -fold degenerate (where L is a length of the ladder).

For a large but finite value of  $J_{\rm K}$ , we can include the effect of the *intrachain* interaction by the first order degenerate perturbation [22]. The result is summarized by the following effective Hamiltonian:

$$\mathcal{H}_{\rm eff}^{\rm AF} = \sum_{i=1} s_{2i-1} \cdot s_{2i} + J' \sum_{j=1} s_{2j} \cdot s_{2j+1}$$
(3)

where  $\{s_i\}$  act as spin- $\frac{1}{2}$  representations on each rung. Note that the *D*-term reduces to a trivial constant and can be dropped in this case. The range of validity for this effective Hamiltonian is restricted to the region  $J_K \gg 1$ , J'. This is nothing but the alternating  $S = \frac{1}{2}$  Heisenberg chain, whose phase diagram is fairly well studied [23, 24]; there is a gapless

phase only on the point J' = 1 and the ground state is dimerized for  $J' \neq 1$ . According to Reigrotzki *et al* [22], an extra overall prefactor  $J_{\text{eff}} \approx 0.68$  is necessary for  $\mathcal{H}_{\text{eff}}$  around  $J_{\text{K}} \simeq 1$ . Of course this result is consistent with Affleck's theorem [15] stating the existence of gapless excitations on the J' = 1 line.

The situation is slightly more complicated in the case of a cylindrical ladder. Because the sublattices cannot be defined consistently for the AF case, the Marshall–Lieb–Mattis theorem [25] does not hold and the uniqueness of the (finite) ground state is no longer guaranteed. In fact, the ground state of a three-site ring is  $2 \times 2$ -fold degenerate—one comes from the eigenvalues  $\sum_{i=1}^{3} S_r^{i,z} = \pm \frac{1}{2}$  and the other from those of the vertical momenta  $P_r^{\perp} = \pm 2\pi/3$ . This degeneracy is resolved after switching on the first-order perturbation. Correspondingly, we obtain, after some algebra, the following Hamiltonian (cf equation (3)):

$$\mathcal{H}_{\rm eff}^{\rm AF'} = \sum_{i=1}^{N} h_{2i-1,2i}(s_{2i-1}, s_{2i}) + J' \sum_{j=1}^{N} h_{2j,2j+1}(s_{2j}, s_{2j+1})$$
(4)

where the local Hamiltonian  $h_{i,i+1}$  takes the following factorized form:

$$h_{i,i+1}(s_i, s_{i+1}) = \frac{1}{3}s_i \cdot s_{i+1} \otimes \left[1 + 2(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y)\right].$$

The Pauli matrices  $\{\sigma_i^a\}$  act on the two-dimensional module consisting of  $P_r^{\perp} = \pm 2\pi/3$ , i.e.  $P_r^{\perp} = (2\pi/3)\sigma_r^z(r=1,\ldots,L)$ . This is still a complicated problem of two coupled spin- $\frac{1}{2}$  chains; one is concerning the spin (*SU*(2)) degrees of freedom and the other originates from the 2<sup>L</sup>-fold degeneracy with respect to  $P_r^{\perp}$ . In spite of this complexity, we adopt the cylindrical ladder for technical reasons in sections 3 and 4.

The case  $J_K < 0$  (*the ferromagnetic case*) is less trivial. A similar argument leads to the following effective Hamiltonian:

$$\mathcal{H}_{\text{eff}}^{\text{F}} = \frac{1}{3} \sum_{i=1} \widetilde{\boldsymbol{S}}_{2i-1} \cdot \widetilde{\boldsymbol{S}}_{2i} + \frac{1}{3} J' \sum_{j=1} \widetilde{\boldsymbol{S}}_{2j} \cdot \widetilde{\boldsymbol{S}}_{2j+1} + D \sum_{k=1} \left( \widetilde{\boldsymbol{S}}_{k}^{z} \right)^{2} .$$
(5)

The operators  $\{\widetilde{S}_i\}$  are defined in the space of the spin- $\frac{3}{2}$  representations on each rung. Note that the topology of the ladder (planer or cylindrical) is irrelevant in this case. Hence we can safely use the cylindrical ladder instead of the planer one for  $J_{\rm K} < 0$ .

To study the system (5) is less trivial because of the lack of exact results. We have to keep in mind the difference between the AF ( $J_K \gg 1$ ) case and the ferromagnetic ( $-J_K \gg 1$ ) case; the former is analogous to the Kondo screening, while the latter is related to the problem of the higher-*S* model—Haldane's conjecture [16, 17].

Finally, we consider the case where the single-ion anisotropy D is large. For infinitely large D, the system reduces again to a decoupled one; states with  $\sum_{i=1}^{3} S_r^{i,z} = \pm \frac{1}{2}$ (r = 1, ..., L) are the ground states. We introduce the leg and rung interactions as perturbations to these degenerate ground states. For simplicity, it is convenient to consider the case  $|J_K| \gg 1$  and to take simultaneous eigenstates of  $D(S_i^{1,z} + S_i^{2,z} + S_i^{3,z})^2$  and  $J_K(S_i^1 \cdot S_i^2 + S_i^2 \cdot S_i^3 + S_i^3 \cdot S_i^1)$  (in fact, the effect of the *D*-term can be absorbed into the anisotropy of the interchain coupling for a cylindrical three-leg ladder. (Note that this is not the case for  $n_{\text{leg}} \ge 4$ .)

When  $J_{\rm K} < 0$ , the  $S^1, S^2, S^3$  spins are coupled ferromagnetically to form a spin- $\frac{3}{2}$  representation. For large enough D, only two states  $\tilde{S}^z = S^{1,z} + S^{2,z} + S^{3,z} = \pm \frac{1}{2}$  are allowed among the quartet. Since these two states are symmetric in  $S^1, S^2, S^3$ , we readily see that the effective Hamiltonian for the large-D case is given by the following  $S = \frac{1}{2}$  Heisenberg chain

$$\mathcal{H}_{\text{eff}}^{\text{large}-D}(J_{\text{K}}<0) = \frac{4}{3} \sum_{i=1} \left( \tilde{s}_{2i-1}^{x} \tilde{s}_{2i}^{x} + \tilde{s}_{2i-1}^{y} \tilde{s}_{2i}^{y} + \frac{1}{4} \tilde{s}_{2i-1}^{z} \tilde{s}_{2i}^{z} \right)$$

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$$+\frac{4}{3}J'\sum_{j=1}\left(\tilde{s}_{2j}^{x}\tilde{s}_{2j+1}^{y}+\tilde{s}_{2j}^{y}\tilde{s}_{2j+1}^{y}+\frac{1}{4}\tilde{s}_{2j}^{z}\tilde{s}_{2j+1}^{z}\right).$$
(6)

The spin operators  $\{\tilde{s}_i\}$  act on the effective  $S = \frac{1}{2}$  representation. For  $J_K > 0$ , a similar argument leads to the conclusion

$$\mathcal{H}_{\rm eff}^{\rm large-D}(J_{\rm K}>0) = \mathcal{H}_{\rm eff}^{\rm AF'}.$$
(7)

It is a great contrast to the case of the two-leg ladder that the large-D region for the ladder with three legs (an odd number of legs, in general) is also described by a massless model.

We can generalize the well known argument [26, 27, 15] to show the following statement: if 2S = odd and  $n_{\text{leg}} = \text{odd}$ , the  $n_{\text{leg}}$ -leg spin-S XXZ ladder  $(-1 < J^z/J^{xy} \le 1, D = \text{arbitrary})$  has either (i) a unique ground state with gapless excitations, or (ii) degenerate ground states. The proof is analogous to the one given in [27] and we do not repeat it here. The above rigorous statement makes it plausible that the model (1) is critical (gapless) all over the J' = 1 plane.

#### 3. Non-Abelian bosonization for three-leg ladder

In this section, we perform the non-Abelian bosonization [28]. The Abelian bosonization is a standard technique in the study of the one-dimensional quantum systems and it was used in analysing the coupled spin chains by several authors [6, 29]. In this method, the Jordan–Wigner fermions, which are obtained by transforming the original spin-chain problem, are approximated by the continuum Dirac fermions and then bosonized to the interacting bosons. It is important to note that the interactions come both from the exchange interaction along the *z*-axis and from the interchain coupling. Hence the situation is much more complicated than in a single spin chain.

On the other hand, the non-Abelian version of the bosonization starts from a completely different point; we bosonize fermions which transform as a multiplet under the action of a group *G* preserving the *G*-symmetry manifestly. For example, a single  $S = \frac{1}{2}$  Heisenberg chain is expressed by the level-1 *SU*(2) Wess–Zumino–Witten (WZW) model describing the spin sector of two copies of the Dirac fermion, while, in the Abelian bosonization, the same thing is realized in terms of a single free boson with a non-trivial compactification radius (or, the Luttinger liquid parameter). In mathematical language, the latter corresponds to the Frenkel–Kac construction [30] of the former. Therefore, we are free to choose these two methods of description in the case of a *single* chain.

For coupled chains, however, the situation is different. In the Abelian-bosonization treatment of ladder-type models [6, 8], we take an appropriate linear combination of the (interacting) bosons ( $n_{\text{leg}}$  bosons for the  $n_{\text{leg}}$ -leg case) to obtain an effective bosonized action of the spin sector. In spite of the simplicity of this method, it has a disadvantage that the SU(2)-symmetry of the problem is not manifest. Furthermore, it is known [21] that the coupled-chain model with special interactions is described by the higher level WZW model which cannot be realized by a single free boson. Therefore, it is important to look for the method of bosonizing the ladder model without spoiling the original SU(2) symmetry.

In the first part of this section, we calculate the renormalization group  $\beta$ -function naively starting from  $n_{\text{leg}}$  decoupled  $S = \frac{1}{2}$  Heisenberg chains.

It is fairly well known that the single  $S = \frac{1}{2}$  Heisenberg model is expressed by the bosonic level-1 SU(2) wzw model in the low-energy limit [18, 31]. It is supported by the finite-size spectrum derived from the exact solution [32] and the coincidence of the exact S-matrices [33, 34]. Similarly to the case of the Abelian bosonization, the low-energy

effective Hamiltonian is expressed in terms of bilinears of the SU(2) currents [35] (the non-Abelian analogue of the Tomonaga Hamiltonian)

$$\mathcal{H}_{\alpha} = 2\pi v_{\mathrm{F}} \int_{0}^{L} \mathrm{d}x \frac{1}{k+2} \left[ \left[ J_{\mathrm{L}}^{\alpha} \cdot J_{\mathrm{L}}^{\alpha} \right] + \left[ J_{\mathrm{R}}^{\alpha} \cdot J_{\mathrm{R}}^{\alpha} \right] \right] \qquad (\alpha = 1, 2, 3)$$
(8)

where the parameter k is called the *level* of the Kac–Moody algebras and  $v_{\rm F} = \pi/2$ . We have defined the currents so that the spatial integration yields the total spin  $S_{\rm tot} = J_0^{\rm L} + J_0^{\rm R}$ :

$$\boldsymbol{J}_{\mathrm{L/R}}(\boldsymbol{x}^{\pm}) = \frac{1}{L} \sum_{n \in \mathbf{Z}} J_n^{\mathrm{L/R}} \, \mathrm{e}^{-\mathrm{i}(2\pi/L)n\boldsymbol{x}^{\pm}}$$

In the following, we consider the case k = 1 and k = 3.

We take  $n_{\text{leg}}(=3)$  copies of the WZW model, and then introduce both the interchain coupling and the bond alternation to these continuum models. The spin operator on each chain is bosonized to be given by [18]

$$S_n^{\alpha} \approx \left[ J_{\rm L}^{\alpha} + J_{\rm R}^{\alpha} \right] + \text{constant} \times (-1)^n \text{Tr}(g_{\alpha} \sigma) \,.$$
(9)

The  $2 \times 2$  matrix  $g_{\alpha}$  is the fundamental field of the level-1 SU(2) WZW model for the  $\alpha$ th chain and  $\sigma$  denotes the Pauli matrices. The trace is taken over the matrix indices. Because of the hermiticity of  $S_n^{\alpha}$ , the constant appearing in (9) is purely imaginary. The continuum interactions corresponding to the interchain coupling are obtained as follows: first we rewrite the interchain coupling  $\sum_{\alpha=1}^{3} S_n^{\alpha} \cdot S_n^{\alpha+1}$  using (9), and then drop rapidly varying terms. The bond alternation is rewritten by calculating the operator-product expansion  $S(x) \cdot S(x')$ . As a result, similarly to the two-leg case [13], we are left with the following ten interactions:

$$\lambda_{1}(J_{L}^{1}\cdot J_{R}^{1} + J_{L}^{2}\cdot J_{R}^{2} + J_{L}^{3}\cdot J_{R}^{3}) \quad \text{intrachain}$$

$$\lambda_{2}(J_{L}^{1}\cdot J_{R}^{2} + J_{L}^{2}\cdot J_{R}^{1} + J_{L}^{2}\cdot J_{R}^{3} + J_{L}^{3}\cdot J_{R}^{2} + J_{L}^{3}\cdot J_{R}^{1} + J_{L}^{1}\cdot J_{R}^{3}) \quad \text{interchain-1}$$

$$\lambda_{3} \left[ \text{Tr}(g_{1}\sigma)\cdot\text{Tr}(g_{2}\sigma) + \text{Tr}(g_{2}\sigma)\cdot\text{Tr}(g_{3}\sigma) + \text{Tr}(g_{3}\sigma)\cdot\text{Tr}(g_{1}\sigma) \right] \quad \text{interchain-2}$$

$$\lambda_{4}(\text{Tr}g_{1} + \text{Tr}g_{2} + \text{Tr}g_{3}) \quad \text{bond alternation}$$

$$\lambda_{5}(\text{Tr}g_{1}\cdot\text{Tr}g_{2} + \text{Tr}g_{2}\cdot\text{Tr}g_{3} + \text{Tr}g_{3}\cdot\text{Tr}g_{1}) \quad (10)$$

$$\lambda_{6}(J_{L}^{1,z}J_{R}^{2,z} + J_{L}^{2,z}J_{L}^{1,z} + J_{L}^{2,z}J_{R}^{3,z} + J_{L}^{3,z}J_{L}^{2,z} + J_{L}^{3,z}J_{R}^{1,z} + J_{L}^{1,z}J_{L}^{3,z})$$

$$\lambda_{7} \left[ \text{Tr}(g_{1}\sigma^{z})\text{Tr}(g_{2}\sigma^{z}) + \text{Tr}(g_{2}\sigma^{z})\text{Tr}(g_{3}\sigma^{z}) + \text{Tr}(g_{3}\sigma)\cdot\text{Tr}(g_{1}\sigma^{z}) \right]$$

$$\lambda_{8} \left[ \text{Tr}(g_{1}\sigma)\cdot\text{Tr}(g_{2}\sigma^{z})\text{Tr}g_{3} + \text{Tr}(g_{2}\sigma^{z})\text{Tr}(g_{3}\sigma^{z})\text{Tr}g_{1} + \text{Tr}(g_{3}\sigma^{z})\text{Tr}(g_{1}\sigma^{z})\text{Tr}g_{2} \right]$$

$$\lambda_{10} \left[ \text{Tr}(g_{1}\sigma^{z})\text{Tr}(g_{2}\sigma^{z})\text{Tr}g_{3} + \text{Tr}(g_{2}\sigma^{z})\text{Tr}(g_{3}\sigma^{z})\text{Tr}g_{1} + \text{Tr}(g_{3}\sigma^{z})\text{Tr}(g_{1}\sigma^{z})\text{Tr}g_{2} \right].$$

Since we use a cylindrical ladder in sections 3 and 4, interactions are always invariant under  $g_i \mapsto g_{i+1}$ . The interactions  $\lambda_5$ ,  $\lambda_8$ ,  $\lambda_9$  and  $\lambda_{10}$  have been introduced in order to guarantee the renormalizability. We have also introduced the last two terms corresponding to the anisotropic (*XXZ*-like) interchain interaction. They are important in considering the *D*-term perturbation (recall that it can be absorbed in the anisotropy of the interchain interaction). The initial values are given by

$$\lambda_1^{(0)} < 0 \qquad \lambda_2^{(0)} = \frac{J_{\rm K}}{(2\pi)^2} \qquad \lambda_3^{(0)} \sim -J_{\rm K} \qquad \lambda_4^{(0)} = J' - 1 \qquad \lambda_5^{(0)} = 0$$

$$\lambda_6^{(0)} = \frac{2D}{(2\pi)^2} \qquad \lambda_7^{(0)} \sim -D \qquad \lambda_8^{(0)} = \lambda_9^{(0)} = \lambda_{10}^{(0)} = 0.$$
(11)

There are several methods to calculate the RG beta-function. Among them, the most convenient one may be to use the procedure developed by Kosterlitz (see [36] for a detailed

account). With this method, the calculation of the 1-loop beta-function reduces to the evaluation of the operator algebra. The operator algebras for the WZW model worked out in [37] would be helpful in the calculation.

Since similar calculations can be found in the literature [11, 13], we show only the final results

$$\frac{\mathrm{d}\lambda_1}{\mathrm{d}\ln L} = 2\pi\lambda_1^2\tag{12}$$

$$\frac{\mathrm{d}\lambda_2}{\mathrm{d}\ln L} = 2\pi\lambda_2^2 + 2\pi\lambda_2\lambda_6 \tag{13}$$

$$\frac{\mathrm{d}\lambda_3}{\mathrm{d}\ln L} = \lambda_3 + 4\pi\lambda_3^2 - \pi\lambda_1\lambda_3 + 2\pi\lambda_2\lambda_3 + \pi\lambda_2\lambda_5 + \pi\lambda_2\lambda_7 + \pi\lambda_3\lambda_6 - 4\pi\lambda_4\lambda_8 \tag{14}$$

$$\frac{\mathrm{d}\lambda_4}{\mathrm{d}\ln L} = \frac{3}{2}\lambda_4 + \frac{3}{2}\pi\lambda_1\lambda_4 - 8\pi\lambda_4\lambda_5 - 24\pi\lambda_3\lambda_8 - 8\pi\lambda_5\lambda_9 - 8\pi\lambda_7\lambda_8 - 8\pi\lambda_3\lambda_{10} - 8\pi\lambda_7\lambda_{10}$$
(15)

$$\frac{\mathrm{d}\lambda_5}{\mathrm{d}\ln L} = \lambda_5 + 3\pi\lambda_1\lambda_5 + 3\pi\lambda_2\lambda_3 - 2\pi\lambda_4^2 - 4\pi\lambda_5^2 + \pi\lambda_3\lambda_6 + \pi\lambda_2\lambda_7 + \pi\lambda_6\lambda_7 - 4\pi\lambda_4\lambda_9$$
(16)

$$\frac{\mathrm{d}\lambda_6}{\mathrm{d}\ln L} = -2\pi\lambda_2\lambda_6\tag{17}$$

$$\frac{\mathrm{d}\lambda_7}{\mathrm{d}\ln L} = \lambda_7 + 4\pi\lambda_7^2 - \pi\lambda_1\lambda_7 - \pi\lambda_2\lambda_7 - \pi\lambda_3\lambda_6 + 8\pi\lambda_3\lambda_7 + \pi\lambda_5\lambda_6 - 4\pi\lambda_4\lambda_{10}$$
(18)

$$\frac{\mathrm{d}\lambda_8}{\mathrm{d}\ln L} = \frac{1}{2}\lambda_8 - 2\pi\lambda_3\lambda_4 + \frac{1}{2}\pi\lambda_1\lambda_8 + 4\pi\lambda_2\lambda_8 + \pi\lambda_2\lambda_9 + \pi\lambda_6\lambda_8 + \pi\lambda_2\lambda_{10}$$
(19)

$$\frac{\mathrm{d}\lambda_9}{\mathrm{d}\ln L} = \frac{1}{2}\lambda_9 - 6\pi\lambda_4\lambda_5 + 9\pi\lambda_2\lambda_8 + \frac{9}{2}\pi\lambda_1\lambda_9 + 3\pi\lambda_6\lambda_8 + 3\pi\lambda_6\lambda_9 + 3\pi\lambda_2\lambda_{10} + 3\pi\lambda_6\lambda_{10}$$
(20)

$$\frac{\mathrm{d}\lambda_{10}}{\mathrm{d}\ln L} = \frac{1}{2}\lambda_{10} + \pi\lambda_6\lambda_8 + \frac{1}{2}\pi\lambda_1\lambda_{10} + \pi\lambda_2\lambda_{10} + 2\pi\lambda_6\lambda_{10}$$
(21)

where L stands for a certain length scale. Although the equations (12)–(21) are rather complicated to handle, some important facts can be read off from them.

First the solution  $\lambda_4(L) = \lambda_8(L) = \lambda_9(L) = \lambda_{10}(L) = 0$  is one of the stable solutions to the above equations, which implies that the bond alternation is not generated under the renormalization. The initial values  $\lambda_6^{(0)} = 0$  and  $\lambda_7^{(0)} = 0$ ) are also stable, i.e. the SU(2) symmetry is not distorted under the renormalization. The beta-functions suggest that the decoupling point  $(J_K, J') = (0, 1)$  is an unstable fixed point, i.e. any small deviation from it drives the system to other fixed points.

Another important observation is that the beta-functions for  $\lambda_2$  and  $\lambda_6$  are decoupled from others and of the Kosterlitz–Thouless type [38]. The behaviour of the couplings is well known; a stable fixed line appears for  $\lambda_2^{(0)} + \lambda_6^{(0)} < 0$  and  $-|\lambda_2^{(0)} + \lambda_6^{(0)}| < \lambda_2^{(0)} < |\lambda_2^{(0)} + \lambda_6^{(0)}|$ . In terms of the original coupling constants, this condition becomes  $J_K > 0$ ,  $D < -J_K < 0$  or  $J_K < 0$ , D < 0; we expect the strong-coupling flow for D > 0.

If we take into account the strong-coupling results (6) and (7), we expect that the *D*-term does not destroy the effective SU(2) symmetry for low energies and that the system is essentially described by the isotropic  $S = \frac{1}{2}$  Heisenberg chain both on the AF-side and on the ferromagnetic side.

A remark is in order here about the validity of the above calculation. In the  $(WZW)^3$  description, the SU(2) currents  $J_L^i$ ,  $J_R^i$  of each chain are conserved separately and, hence, so is their spatial integral  $S_{tot}^i = S_L^i + S_R^i$  (i = 1, 2, 3). In other words, the system has a large

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symmetry  $SU(2)_{S^1} \times SU(2)_{S^2} \times SU(2)_{S^3}$  at the decoupling point  $J_{\rm K} = 0$ . However, when the interchain interaction  $J_{\rm K}$  is not small, this is no longer true; the sum  $S_{\rm tot}^1 + S_{\rm tot}^2 + S_{\rm tot}^3$ is conserved. The RG analysis presented above actually indicates the strong-coupling flow. Therefore, a naive weak-coupling expansion starting from three decoupled wZW models would be inappropriate and such a description that only the total spin is a good quantum number is preferable in investigating the strong-coupling region. In the second half of this section, we look for another way of bosonizing the three-leg ladder.

In fact, the  $SU(2)_{S^1} \times SU(2)_{S^2} \times SU(2)_{S^3}$ -symmetry at the decoupling point is enlarged to a larger (infinite-dimensional) symmetry  $\widehat{SU}(2)_{k=1} \times \widehat{SU}(2)_{k=1} \times \widehat{SU}(2)_{k=1}$  in the lowenergy limit. Again, the parameter k denotes the level of the affine SU(2) symmetry. Upon turning on the interchain coupling, it reduces to the diagonal  $\widehat{SU}(2)_{k=3}$  corresponding to the SU(2) symmetry generated by the total spin:  $J_{L/R}^{diag} = J_{L/R}^1 + J_{L/R}^2 + J_{L/R}^3$ . Thus it would be preferable to rewrite the model in terms of the level-3 WZW model describing the spin sector and the remaining degrees of freedom in order to extract the effective action.

To this end, it is important to investigate how the diagonal  $\widehat{SU}(2)_{k=3}$  is embedded in the  $\widehat{SU}(2)_{k=1} \times \widehat{SU}(2)_{k=1} \times \widehat{SU}(2)_{k=1}$  symmetry. In the two-leg case [13], it was given by the well known coset construction of the Ising CFT [39]. In the present three-leg case, however, little study has been done for the above embedding. Therefore, first we have to look for the branching rules for this case.

As was already remarked in [13], the residual CFT has the central charge  $c = 1 + 1 + 1 - \frac{9}{5} = \frac{6}{5}$ . In the appendix, we show that this CFT is given by a member of the so-called  $W_3$  minimal models [40] whose central charge is given by the formula

$$c(m) = 2\left(1 - \frac{12}{(m+3)(m+4)}\right) \qquad (m = 1, 2, \ldots).$$
(22)

The case m = 2 is relevant to ours. The representation theory of this series of CFTs was studied by several authors (see [41] and references cited therein) and the character formulae are obtained [42]. Using these results, we obtain the following identities:

$$\chi_{j=1/2}^{(k=1)}(q)\chi_{j=0}^{(k=1)}(q)\chi_{j=0}^{(k=1)}(q) = \chi_{1/10}^{W_3}(q)\chi_{j=1/2}^{(k=3)}(q) + \chi_{1/2}^{W_3}(q)\chi_{j=3/2}^{(k=3)}(q)$$
(23)

$$\chi_{j=1/2}^{(k=1)}(q)\chi_{j=1/2}^{(k=1)}(q)\chi_{j=0}^{(k=1)}(q) = \chi_{1/10}^{W_3}(q)\chi_{j=1}^{(k=3)}(q) + \chi_{1/2}^{W_3}(q)\chi_{j=0}^{(k=3)}(q)$$
(24)

(see the appendix for the meaning of the notations and the remaining identities). They give a clue to how to rewrite the interactions in terms of the level-3 WZW model and the  $W_3$  CFT.

As in [13], the operator-product expansion (OPE) is used to rewrite the interactions of  $\widehat{SU}(2)_1 \times \widehat{SU}(2)_1 \times \widehat{SU}(2)_1$ —description into that of the  $\widehat{SU}(2)_3$ -description. Since detailed information about the OPEs of the  $c = \frac{6}{5} W_3$  CFT is lacked, we cannot explicitly establish the identities. However, on the basis of the symmetry argument and the requirement that the scaling dimensions should be equal on both sides, we expect that the following relations hold:

$$Trg_{1}(z,\bar{z}) + Trg_{2}(z,\bar{z}) + Trg_{3}(z,\bar{z}) = \Phi_{1/10}^{W_{3}}(z,\bar{z})Trh(z,\bar{z})$$

$$Tr[g_{1}(z,\bar{z})\sigma] + Tr[g_{2}(z,\bar{z})\sigma] + Tr[g_{3}(z,\bar{z})\sigma] = \Phi_{1/10}^{W_{3}}(z,\bar{z})Tr[h(z,\bar{z})\sigma]$$

$$Trg_{1}Trg_{2} + Trg_{2}Trg_{3} + Trg_{3}Trg_{1} = 3C_{1/10,1/10}^{1/2} \Phi_{1/2}^{W_{3}} + \frac{3K}{2\pi}C_{1/10,1/10}^{1/10}\Phi_{1/10}^{W_{3}}Tr\Phi_{j=1}^{WZW}$$

$$Tr(g_{1}\sigma) \cdot Tr(g_{2}\sigma) + Tr(g_{2}\sigma) \cdot Tr(g_{3}\sigma) + Tr(g_{3}\sigma) \cdot Tr(g_{1}\sigma)$$

$$= -9C_{1/10,1/10}^{1/2} \Phi_{1/2}^{W_{3}} + \frac{3K}{2\pi}C_{1/10,1/10}^{1/10}\Phi_{j=1}^{WZW}$$
(25)

where the constant K is given by

$$K = \pi \sqrt{\frac{\Gamma(1/5)\Gamma^3(3/5)}{\Gamma^3(2/5)\Gamma(4/5)}} \simeq 3.432$$

and the operators h,  $\Phi_{j=1}^{WZW}$ , and  $\Phi_{j=3/2}^{WZW}$  on the right-hand side denotes the spin  $\frac{1}{2}$ , 1 and  $\frac{3}{2}$  primary fields of the level-3 SU(2) WZW model, respectively. According to the observation described in the appendix, the  $W_3$  fields are expected to be of the following form:

$$\Phi_{1/10}^{W_3} = \phi_{1/10}^{(1)} + \phi_{1/10}^{(2)} + \phi_{1/10}^{(3)} \qquad \text{and} \qquad \Phi_{1/2}^{W_3} = \phi_{1/2}^{(1)} + \phi_{1/2}^{(2)} + \phi_{1/2}^{(3)} \,. \tag{26}$$

The constants  $C_{1/10,1/10}^{i}$  are the OPE coefficients for the  $W_3$ -CFT and are not calculated explicitly here.

According to (26), the  $W_3$ -CFT sector contains a relevant (energy-like) operator  $\Phi_{1/2}^{W_3}$ and it becomes gapped [43] for generic values of  $(J_K, J')$  and that it is decoupled from the spin (SU(2)) sector. As in [13], the 'fused' spin operator is given by

$$S_i^1 + S_i^2 + S_i^3 \approx J_{\rm L}^{\rm diag} + J_{\rm R}^{\rm diag} + \text{constant}(-1)^i \text{Tr} h \boldsymbol{\sigma} \,.$$
<sup>(27)</sup>

However, this is not the whole story. The resulting action for the spin sector

$$S_{\text{spin}} = S_{\text{WZW}}^{k=3} + \alpha \int d^2 x \operatorname{Tr} \Phi_{j=1}^{\text{WZW}} + \beta \int d^2 x \operatorname{Tr} h + \gamma \int d^2 x \operatorname{Tr} \Phi_{j=3/2}^{\text{WZW}}$$
(28)

still contains several (relevant) interactions. The physical meaning of  $\alpha$ ,  $\beta$  and  $\gamma$  is given as follows; the coupling constants  $\alpha$  and  $\beta$  correspond to the interchain interaction  $J_{\rm K}$  and bond alternation, respectively. The last term on right-hand side has been appended as a counter term. In the two-leg case [13], the case  $J_{\rm K} > 0$  ( $J_{\rm K} < 0$ ) corresponds to the high-(low-) temperature phase of the Ising sector and hence the (Trh)-interaction, which plays a role of the bond alternation disappears from the effective action for  $J_{\rm K} > 0$ . A similar situation may occur in the present case. Note that this kind of the effective action for generic spin chains was first conjectured by symmetry argument in [18]. Our derivation may provides a fast foundation to the treatment in [18].

#### 4. Renormalization group and semiclassical analysis

In the last section, we have derived an effective action (28) for the spin sector. In order to investigate the low-energy behaviour, we calculate the renormalization group (RG) beta-function up to the 1-loop and then discuss the qualitative nature of the phases.

The calculation is the same as in section 3 and the final result reads

$$\frac{\mathrm{d}\alpha}{\mathrm{d}\ln L} = \frac{6}{5}\alpha - K\alpha^2 - K\beta^2 - \frac{8}{3}\pi\alpha\gamma \tag{29}$$

$$\frac{\mathrm{d}\beta}{\mathrm{d}\ln L} = \frac{17}{10}\beta - 3K\alpha\beta \tag{30}$$

$$\frac{\mathrm{d}\gamma}{\mathrm{d}\ln L} = \frac{1}{2}\gamma - 2\pi\alpha\beta \tag{31}$$

where the constant K is already given in the last section. Reflecting the symmetry of the equations (12)–(21), they are invariant under  $(\alpha, \beta, \gamma) \rightarrow (\alpha, -\beta, -\gamma)$  and the line  $\beta(L) = 0$  is stable.



**Figure 2.** The renormalization group flow obtained by the 1-loop calculation for the effective action in section 4. Note that three *non-trivial* fixed points (FP-2, FP-3, FP-3') appear. They are connected with the trivial one with massless flows.

The system of equations (29)–(31) has four fixed points:

FP-1 (0, 0, 0) FP-2 
$$\left(\frac{6}{5K}, 0, 0\right)$$
  
FP-3  $\left(\frac{17}{30K}, +\beta_0, \frac{34\pi}{15K}\beta_0\right)$  FP-3'  $\left(\frac{17}{30K}, -\beta_0, \frac{34\pi}{15K}\beta_0\right)$ 
(32)

where

$$\beta_0 = \sqrt{\frac{323}{900K^2 + 5440\pi^2}} \approx 0.070\,88$$

The first one (FP-1) corresponds to the point  $(J_K, J') = (0, 0)$  and is unstable. The others are non-trivial ones. A schematic RG-flow is shown in figure 2. For  $\alpha^{(0)} < 0$   $(J_K > 0)$  and  $\beta^{(0)} = \gamma^{(0)} = 0$ , the system flows to the strong-coupling fixed point, which has the lowenergy physics in common with the  $S = \frac{1}{2}$  Heisenberg chain. The translationally invariant fixed point FP-2 implies the existence of a massless phase on a half line J' = 1,  $J_K < 0^{\dagger}$ . The fixed points FP-3 and FP-3' are non-translationally invariant and are considered to be the dimerization transition from the partially-dimerized phase to the dimerized one; exponents for the dimerization transitions are governed by the three FPs. Moreover, there seems to exist two different types of the strong-coupling behaviour:  $\alpha$ ,  $\beta = \text{finite}$ ,  $|\gamma| \nearrow \infty$  and  $|\alpha|$ ,  $|\beta|$ ,  $|\gamma| \nearrow \infty$ .

However, since the non-trivial fixed points are not close to the trivial one (FP-1) from which we perform the perturbative renormalization group, we cannot trust our 1-loop calculation *quantitatively*. Instead of doing higher-order calculations, we give a semiclassical argument to support the existence of the above-mentioned phases.

We follow the method first used by Affleck and Haldane [18]. In the sense of the operator-product expansion, the primary fields of the k = 3 wzw model are expressed as

$$\operatorname{Tr}\Phi_{j=1} \sim (\operatorname{Tr}h)^2$$
  $\operatorname{Tr}\Phi_{j=3/2} \sim (\operatorname{Tr}h)^3 + \operatorname{constant} \times \operatorname{Tr}h$ 

† Of course, the existence of massless phases, inversely, does not always imply that there *must* be a fixed point on the α-axis. Away from FP-1, a non-trivial fixed point, which is outside the  $(\alpha, \beta, \gamma)$ -space may occur.

Therefore, it is sufficient to consider the following action:

$$S = S_{k=3WZW} + \mu \int d^2 x \, (\mathrm{Tr}h)^2 + \nu \int d^2 x \, \mathrm{Tr}h + \rho \int d^2 x \, (\mathrm{Tr}h)^3 + D \int d^2 x \, (\mathrm{Tr}h\sigma^z)^2 \,.$$
(33)

Then, we parametrize the fundamental field *h* using an angular variable  $\phi(x_1, x_2)$   $(0 \le \phi < 2\pi)$  and a vectorial one  $\widehat{\phi}(x_1, x_2)$   $(|\widehat{\phi}| = 1)$ :

$$h(x_1, x_2) = \exp\left(\frac{\mathrm{i}}{2}\phi(x_1, x_2)\boldsymbol{\sigma}\cdot\widehat{\varphi}(x_1, x_2)\right).$$
(34)

It is easy to check that the unit-vector field transforms as an O(3) vector under the diagonal SU(2):  $h \mapsto U^{-1}hU$  ( $U \in SU(2)$ ). The translational symmetry by one site is realized as the discrete  $\mathbb{Z}_2$  symmetry  $h \to -h$ . In the above parametrization, it corresponds to the operation  $\phi \to 2\pi - \phi$ ,  $\hat{\varphi} \to -\hat{\varphi}$ .

Substituting (34) into the action (33), we obtain

$$S[\phi, \widehat{\varphi}] = \frac{1}{8\pi} \int d^2 x \left[ (\partial_\sigma \phi)^2 + 2(1 - \cos \phi)(\partial_\sigma \widehat{\varphi})^2 \right] + \frac{1}{8\pi} \int d^2 x \, 3(\phi - \sin \phi) \left[ \epsilon_{\alpha\beta} \widehat{\varphi} \cdot (\partial_\alpha \widehat{\varphi} \times \partial_\beta \widehat{\varphi}) \right] + \int d^2 x \left[ 4\mu \cos^2 \left(\frac{\phi}{2}\right) + 2\nu \cos \left(\frac{\phi}{2}\right) + 8\rho \cos^3 \left(\frac{\phi}{2}\right) \right] + \mathcal{D} \int d^2 x \, \left( \widehat{\varphi}^z \right)^2 \sin^2 \left(\frac{\phi}{2}\right).$$
(35)

As in [13], we first look for the uniform solution  $\phi_{\min}$  which minimizes the potential term (the third line), and then replace the  $\phi$ -field by it. The resulting effective action (the O(3) nonlinear sigma model)

$$\mathcal{S}_{\text{eff}}[\widehat{\varphi}] = \frac{g}{4\pi} \int d^2 x \left(\partial_\sigma \widehat{\varphi}\right)^2 + \frac{1}{8\pi} \Theta_{\text{top}} \int d^2 x \,\epsilon_{\alpha\beta} \widehat{\varphi} \cdot \left(\partial_\alpha \widehat{\varphi} \times \partial_\beta \widehat{\varphi}\right) + \mathcal{D}' \int d^2 x \,\left(\widehat{\varphi}^z\right)^2 \tag{36}$$

gives qualitative information about the phase diagram. The parameters are defined as  $g = (1 - \cos \phi_{\min})$ ,  $\Theta_{top} = 3(\phi_{\min} - \sin \phi_{\min})$ , and  $\mathcal{D}' = \mathcal{D} \sin^2 (\phi_{\min}/2)$ . Using the expressions

$$J_{\rm L} = \frac{3\mathrm{i}}{2}h(\partial_+ h^{-1})$$
 and  $J_{\rm R} = \frac{3\mathrm{i}}{2}h^{-1}\partial_- h$ 

the SU(2)-current is rewritten as

$$\boldsymbol{J}_0 = \boldsymbol{J}_{\mathrm{L}} + \boldsymbol{J}_{\mathrm{R}} = -\frac{3}{2}(1 - \cos\phi_{\min})(\widehat{\boldsymbol{\varphi}} \times \partial_0\widehat{\boldsymbol{\varphi}}) \,. \tag{37}$$

Note that  $J_0$  generates the O(3)-symmetry of the above  $S_{\text{eff}}[\hat{\varphi}]$ .

In figure 3, we show the semiclassical phase diagram obtained in this way. There are three regions where the topological angle  $\Theta_{top} = \pi \pmod{2\pi}$ : a half plane  $\nu = 0$ ,  $\mu > 0$ and two planes  $\rho \pm a\mu + b\nu = 0$  ( $a \simeq 0.602$ ,  $b \simeq 0.272$ ). In these regions, the system is expected to be gapless [16, 34] and to flow towards the fixed points of the level-1 SU(2)WZW model. In a major region of the parameter space, the minimum occurs at  $\phi = 0$ or  $2\pi$  and the *D*-term drops out. The values  $\phi = 0, 2\pi$  imply that the system dimerizes (indicated by 'dimerized' and 'dimerized'' in figure 3), i.e. it breaks the above translational symmetry. It is worth mentioning that there appears *no* translationally-invariant *massive* phase (e.g. the singlet phase à la Haldane) at least within this treatment; the RG-analysis



**Figure 3.** The semiclassical phase diagram for the effective action. The system is predicted to dimerize in a large part of the  $(\alpha, \beta, \gamma)$ -space. There exist three planes on which the topological angle  $\Theta_{top} = \pi$ .

and the semiclassical treatment of [13] suggest that it does exist around the  $\alpha$ -axis for the two-leg case.

In the above derivation of (36), the model seems massive on the line  $(J' = 1, J_K > 0)$ in contradiction to the rigorous result [15]. This is a shortcoming of our description based on the level-3 wZw model. In order to show that this is not true, we derive the sigma model by a completely different method. First we assume some kind of short-range order from the beginning. For example, the short-range Néel order is assumed for  $J_K > 0$ . Then, following the standard procedure of mapping the spin-S chain onto the sigma model [44, 45] via the path integral, we obtain for D = 0

$$S_{\text{eff}}[\boldsymbol{m}] = \frac{1}{2g'} \int d^2 x \left[ \frac{1}{v} (\partial_0 \boldsymbol{m})^2 - v (\partial_1 \boldsymbol{m})^2 \right] + \frac{\Theta'_{\text{top}}}{8\pi} \int d^2 x \, \epsilon_{\mu\nu} \boldsymbol{m} \cdot (\partial_\mu \boldsymbol{m} \times \partial_\nu \boldsymbol{m})$$
$$(|\boldsymbol{m}| = 1)$$
(38)

where the coupling constant g' and the velocity of 'light' v for  $J_{\rm K} > 0$  are given by

$$v^{2} = \frac{12(aS)^{2}(2+2J'+3J_{\rm K})}{6+6J'+J_{\rm K}}$$

$$\frac{1}{2g^{2}} = \frac{\sqrt{3}S}{2(1+J')}\sqrt{\frac{6+6J'+J_{\rm K}}{2+2J'+3J_{\rm K}}}.$$
(39)

For  $J_{\rm K} < 0$ , they do not depend on  $J_{\rm K}$ . The topological angle is given by<sup>†</sup>

$$\Theta_{\text{top}}' = \begin{cases} \frac{4\pi J'S}{1+J'} & \text{for } J_{\text{K}} > 0\\ \frac{4\pi J'(3S)}{1+J'} & \text{for } J_{\text{K}} < 0 \end{cases}$$
(40)

where  $S = \frac{1}{2}$  in our case. Note that this is the same as the one obtained for a *single* spin-*S* (or 3*S*) chain [46, 47]. Again, we are interested in such values of *J'* that  $\Theta'_{top} = \pi \pmod{2\pi}$ . For  $J_K > 0$ , it takes  $\pi \pmod{2\pi}$  only on the line J' = 1, as expected. On the other hand,  $\Theta'_{top}$  takes the value  $\pi$  three times for  $J_K < 0$ . This quite different behaviour is understood as a consequence of the difference in how the Berry phases of individual spins on each rung are summed up. Thus, we have obtained from the semiclassical analysis the conclusions

† In deriving  $S_{\text{eff}}$ , it is important to take into account that the short-range *ferromagnetic* order on the individual rung is presumed for  $J_{\text{K}} < 0$ .

consistent with the RG results; the three non-trivial fixed points may be identified with  $\Theta_{top} = \pi$  planes.

From the above argument, we may expect that the low-energy effective theory for the region J' = 1, D = 0 and the dimerization lines is given by the level-1 SU(2) wZw model, which is believed to be equivalent for low energies to the O(3) nonlinear sigma model with  $\Theta_{\text{top}} = \pi \pmod{2\pi}$  [34]. Below we give another argument which supports this expectation. It is far from rigorous and should be regarded as a possible scenario.

It is well known that the level-3 SU(2) WZW model can be described by a product of  $\mathbb{Z}_3$ -parafermion CFT and c = 1 Gaussian CFT [48]; the Gaussian sector corresponds to  $S_{\text{tot}}^z$  and the  $\mathbb{Z}_3$ -sector describes the residual degrees of freedom. Using the formulae of [48], we can show that  $\text{Tr}\Phi_{j=1}$  contains the thermal operator of the three-state Potts model which drives the  $\mathbb{Z}_3$ -sector massive.

If the non-trivial fixed point (FP-2) possesses the SU(2) Kac–Moody symmetry, there would exist a corresponding current algebra realized by the remaining Gaussian CFT. This theory (c = 1) is the level-1 SU(2) wZw model, which corresponds to a special point of the Gaussian CFT.

Assuming the above conclusion, we can estimate the effect of the *D*-term on the correlation functions. The RG analysis of the effect of the *D*-term has been already given in the last section. Below we give yet another argument supporting the preceding conclusion. Contrary to the single-chain case, the *D*-term is *not* trivial here, as has been discussed in section 2. Up to the lowest order, its effect can be included as follows. First, we rewrite  $D(S_i^{1,z} + S_i^{2,z} + S_i^{3,z})^2$  into a normal-ordered form using (27). In the above (Gaussian  $\oplus \mathbb{Z}_3$ )-description, the contribution to the Gaussian sector comes from a marginal operator  $(J_L^{\text{diag},z} + J_R^{\text{diag},z})^2$ . It is well known [49, 50] that another marginal (usually called 'Umklapp') operator exists in addition to the above one. The RG beta-function is easily calculated in a similar manner to the one used in sections 3 and 4, and it leads to the conclusion that the system undergoes the Kosterlitz–Thouless (KT) transition [38] into the strong-coupling region for D > 0. This is consistent with the results of the bosonization study starting from the three decoupled WZW models in section 3; the long-distance physics of the ferromagnetic side is the same as that of the  $S = \frac{1}{2} XXZ$  chain and the exponents depend on *D*; only the asymptotic form  $(D, -J_K \gg 1)$  is known analytically:

$$\eta_z \to \frac{\pi - \cos^{-1}(1/4)}{\pi} \approx 0.58 \qquad \eta_{xy} = 1/\eta_z \approx 1.72.$$
 (41)

Following the standard steps (see [51] for example), we obtain the correlation functions in the intermediate-*D* region as  $(k_F = \pi/(2a))$ 

$$\langle S^{+}(x,t)S^{-}(0,0)\rangle \sim \frac{\cos 2k_{F}x}{(x+iv_{F}t)^{1/4R^{2}}(x-iv_{F}t)^{1/4R^{2}}} + \text{(higher order)}$$

$$\langle S^{z}(x,t)S^{z}(0,0)\rangle \sim \frac{\cos 2k_{F}x}{(x+iv_{F}t)^{R^{2}}(x-iv_{F}t)^{R^{2}}} + \text{(higher order)}$$
(42)

where the parameter R is a function of  $J_{\rm K}$  and D. In particular, the correlation exponents for D = 0 are constant independent of  $J_{\rm K}$  and given by  $\eta_{aa} = 1$   $(R = 1/\sqrt{2})$ .

From these results, the low-temperature asymptotics of the susceptibility is easily calculated following the CFT-method [52]. Both for D = 0 and for D > 0, the leading irrelevant operator allowed by the U(1)- and the translational symmetry would be  $\therefore \cos 2\sqrt{2}\tilde{\phi}$ , which yields a logarithmic correction term to the low-temperature asymptotics as

$$\chi_{aa}(T) \sim \frac{1}{2\pi v_{\rm F}} + \frac{1}{4\pi v_{\rm F} \ln(T_0/T)}$$
(43)

regardless of the sign of  $J_{\rm K}$ . For D > 0, the logarithmic term is expected to be replaced by a power-like one  $T^{8R^2-4}$ .

### 5. Variational calculation

In this section, we demonstrate the existence of other transitions than the usual dimerization transition<sup>†</sup> at J' = 1. The existence of these transitions for higher-S models was predicted by Affleck and Haldane on the basis of the field-theoretical argument [18, 46]. They argued that the  $\Theta_{top} = \pi$  sigma model is realized several times as the strength of the bond alternation is varied. For  $S = \frac{3}{2}$  Heisenberg model, which is a special case of ours, second-order transitions are predicted to occur three times; one is at J' = 1 and the others are at non-zero J'.

A natural trial state for the intermediate region  $J'_{\rm c} < J' < 1$  (D = 0) is given by a product

$$|\text{inhom-VBS}\rangle = \text{Tr}\left(g_1^{A} \otimes g_2^{B} \otimes g_3^{A} \otimes \ldots \otimes g_{L-1}^{A} \otimes g_L^{B}\right)$$

of the following matrices:

$$g_{i}^{A} = \begin{pmatrix} -\left\{ \begin{array}{c} |\uparrow\downarrow\downarrow\downarrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle \\ +|\downarrow\downarrow\uparrow\rangle \\ 3|\downarrow\downarrow\downarrow\rangle \\ 3|\downarrow\downarrow\downarrow\rangle \\ g_{j}^{B} = \begin{pmatrix} \left\{ \begin{array}{c} |\uparrow\uparrow\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle \\ +|\downarrow\downarrow\uparrow\uparrow\rangle \\ +|\uparrow\downarrow\downarrow\uparrow\rangle \\ +|\uparrow\downarrow\uparrow\uparrow\rangle \\ -\sqrt{2} \left\{ \begin{array}{c} |\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle \\ +|\uparrow\downarrow\uparrow\uparrow\rangle \\ +|\downarrow\downarrow\uparrow\uparrow\rangle \\ 3|\downarrow\downarrow\downarrow\rangle \\ 3|\downarrow\downarrow\downarrow\rangle \\ \end{array} \right\} \begin{pmatrix} |\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle \\ -\sqrt{2} \left\{ \begin{array}{c} |\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle \\ +|\downarrow\downarrow\uparrow\uparrow\rangle \\ +|\downarrow\downarrow\uparrow\uparrow\rangle \\ 3|\downarrow\downarrow\downarrow\rangle \\ \end{array} \right\} -\sqrt{2} \left\{ \begin{array}{c} |\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow + |\uparrow\downarrow\uparrow\uparrow\rangle \\ +|\uparrow\uparrow\downarrow\uparrow\rangle \\ +|\downarrow\uparrow\downarrow\uparrow\rangle \\ +|\downarrow\downarrow\uparrow\uparrow\rangle \\ \end{array} \right\}$$
(44)

where ket vectors  $|\cdots\rangle$  stand for the states on a given rung. This is a ladder analogue of the inhomogeneous VBS state [19,53], where the valence-bond structure alternates as  $\cdots = - = - = - \cdots$ , and expected to be suitable for the case  $J_K < 0$ .

On the other hand, we expect that the 'dimer' state, which is the *exact* ground state when J' = 0, is a good approximant of the ground state for small enough J'. Although the derivation of the state by diagonalizing the six-site cluster is straightforward, the explicit expression of it is lengthy and we do not write down it here. A variational phase-boundary is determined by comparing the two values (inhom-VBS| $\mathcal{H}$ |inhom-VBS) and (dimer| $\mathcal{H}$ |dimer). The calculation [54] is rather straightforward. The final result is given by

$$J_{\rm c}'(J_{\rm K}, D=0) = \frac{3\{48+108J_{\rm K}^2+(36J_{\rm K}+5)\sqrt{4+9J_{\rm K}^2}\}}{50\sqrt{4+9J_{\rm K}^2}}.$$
(46)

This is shown in figure 4. In the limit  $J_{\rm K} \to -\infty$ ,  $J'_{\rm c}$  approaches 0.3. According to a recent numerical calculation for the alternating  $S = \frac{3}{2}$  Heisenberg chain using the density-matrix renormalization group (DMRG) [55],  $J'_{\rm c}$  is given by  $0.41 \pm 0.02$  and our result of a simple variational calculation underestimates the true value. Another transition line is obtained using the symmetry  $(J', J_{\rm K}) \to (1/J', J_{\rm K}/J')$ .

The result is consistent with the argument of the previous sections. Just as in the  $S = \frac{1}{2}$  case, the critical phase of the homogeneous chain is located at the boundary of the two

<sup>†</sup> We mainly focus on the case D = 0 here.



**Figure 4.** Phase boundary obtained by a simple variational calculation in section 5. Above it, a partially dimerized phase would be realized. Although the shape is quite reasonable, it underestimates the true value.

non-translationally invariant phases; the above inhomogeneous VBS phase and the phase obtained by translating it by one site.

Next we briefly consider the effect of the *D*-term. As described in section 2, the effective Hamiltonian for large enough *D* and  $J_K$  is given by the  $S = \frac{1}{2} XXZ$  chain and phases with partial dimerization are not allowed to exist there. Therefore, we expect that the region of them gets smaller as *D* increases and finally squeezed out for vary large values of *D*. However, the non-existence of the partially dimerized phases for small  $J_K$ , where the strong-coupling (large-*D*) Hamiltonian takes a complicated form, is not conclusive and deserves further investigation.

#### 6. Summary and discussions

In the present paper, we have investigated the phase diagram of the three-leg ladder with the single-ion anisotropy. The resulting phase diagram is shown in figure 5. It is rather different from that of the two-leg ladder [13].

Instead of using the usual method [6] based on the Jordan–Wigner fermionization, we started from the non-Abelian bosonization of a single Heisenberg chain. In this treatment, the  $(S_i^{\alpha,z}S_{i+1}^{\alpha,z})$ -interaction is fully taken into account and the starting point itself is already non-trivial. Then the interchain interaction (and bond alternation) has been introduced as a perturbation around the above fixed point.

Naive application of the perturbative renormalization group in section 3 showed that the fixed point  $(J_K, J', D) = (0, 0, 0)$  is unstable and the system flows to the strong-coupling region. Therefore, it is preferable to use another description based on the total spin only, i.e.  $(k = 3 \text{ WZW} + W_3 \text{ CFT})$ -description. In obtaining the decomposition, we adopted the coset construction of CFT. Then, we carried out the perturbative RG for the spin sector and obtained a RG-flow suggesting that three non-trivial fixed points appear; one corresponds to a gapless line  $(J_K < 0, J' = 1)$  and others to two dimerization-transition lines. On the basis of the semiclassical analysis and another argument, we identified the universality class of the above three fixed points (D = 0) with the level-1 SU(2) WZW model. The spin-correlation exponent is given by  $\eta = 1$  along these lines. Three dimerization-transition lines correspond to outgoing flows from the three non-trivial fixed points; the gap is expected to open as  $\Delta_{\text{dimer}} \sim |J' - J'_c|^{2/3}$ . A simple variational calculation suggests that partially dimerized phases (P-Dim and P-Dim') are realized in the regions between these lines.



**Figure 5.** Conjectured phase diagram of our Hamiltonian (1). Shown are sections by (i) D = 0, (ii) J' = 1, and (iii)  $J_{\rm K} = \text{constant} (< 0)$ . The universality class of the level-1 SU(2) wzw model is realized in the regions depicted by 'AF- $J_{\rm K}$ ' and 'L-1' ~ 'L-3'. On 'D-1' ~ 'D-3', the system is Luttinger-liquid-like. A cross-over from 'L-1' to 'D-1' occurs for D > 0. P-Dim (P-Dim') and 'Dim' ('Dim'') denote the partially dimerized and dimerized phase, respectively.

As the single-ion anisotropy increases from zero, the domain of the above intermediate phases (P-Dim and P-Dim') becomes smaller and smaller and finally disappears for very large values of D. On the boundaries of these phases (D-1 ~ D-3), the c = 1 Gaussian CFT is realized. The low-energy behaviour of the system is governed by a single parameter  $R(J_{\rm K}, D)$  and the exponents depend on D. Asymptotically  $(D, -J_{\rm K} \gg 1)$ , they are given by

$$\eta_{xy} \rightarrow \frac{\pi - \cos^{-1}(1/4)}{\pi}$$
 and  $\eta_{zz} = 1/\eta_{xy}$ .

This is consistent with the rigorous statement that the system is gapless on the J' = 1 plane. In this respect, our phase diagram is different from the one obtained by Schulz [6].

As was seen in section 2, any transition at finite non-zero D is excluded also in the large- $J_K$  ( $J_K \gg 1$ ) region, where the D-term effectively becomes trivial. Combining this with the RG-results, we expect that the D-term is irrelevant in the *whole* AF-region ( $J_K > 0$ , shown as AF- $J_K$ ); the low-energy behaviour is always described by the strong-coupling ( $J_K \gg 1$ ) limit, or, the  $S = \frac{1}{2}$  Heisenberg model. Note, however, that our argument based on the assumption that diverging flows in weak-coupling regions are smoothly connected to those in strong-coupling regimes bears the risk of overlooking some novel intermediate phases, since the region  $|J_K| \ll 1$  and  $D \gtrsim 1$  of the present model is far from trivial.

The RG-analysis and the strong-coupling argument tell us that no partially dimerized phase is realized in this region. That is, the fully-dimerized phases spread over except on the J' = 1 plane. In this sense, the phase diagram for the AF-side is somewhat trivial. Of course, the strong-coupling ( $J_{\rm K} \gg 1$ ) limit of a cylindrical ladder is slightly complicated

and hence our RG results, which are derived for the cylindrical case, may be different from what really happens for a planer ladder. However, the sigma-model mapping based on the spin path-integral in section 4 also supports the above conclusions.

Finally, we comment on generic ladders. In principle, we can repeat the same procedure for ladder models with more than three legs, although the calculation becomes harder and harder. From the knowledge of the two- and three-leg ladder, we speculate that the system is described by the strong-coupling picture even for small  $J_{\rm K}$ . The phase diagram for the AF-side is simple and essentially depends only on the parity of  $n_{\rm leg}$ ; the spin-gapped singlet phase for  $n_{\rm leg}$  = even and the two dimerized phases separated by a single massless (the c = 1Luttinger-liquid) plane for  $n_{\rm leg}$  = odd, on which the correlation exponents do not depend on D. To some extent, this can be understood by repeating the semiclassical treatment in section 4; the topological angle vanishes for integer-S, whereas it is *always* given by  $\Theta_{\rm top} = 2\pi J'/(1 + J')$  for half-odd-integer S, as first emphasized by Khveshchenko [56].

The phase diagram for the ferromagnetic case becomes more complicated and richer as  $n_{\text{leg}}$  is increased. In a sense, this can be viewed as a consequence of the addition of the Berry phases of the spins on each rung. That is, the topological angle for the spin-*S* ferromagnetic ladder explicitly depends on the number of legs,  $n_{\text{leg}}$ , and is given by  $\Theta_{\text{top}} = 4\pi J'(n_{\text{leg}}S)/(1 + J')$ . This is in contrast with the case of antiferromagnetic  $J_{\text{K}}$ , where the Berry phases tend to cancel each other. When the chain is uniform (J' = 1), it satisfies  $\Theta_{\text{top}} = \pi \pmod{2\pi}$  only for 2S = odd and  $n_{\text{leg}} = \text{odd}$ . This is consistent with a rigorous statement mentioned in section 1.

As first predicted by Affleck and Haldane on the basis of the field-theoretical argument, we expect several intermediate phases in the region 0 < J' < 1 (and also in the region J' > 1). Moreover, we may consider the possibility of the intermediate-*D* phases. To verify this, we have to wait further studies on this problem.

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## Appendix A. Branching formulae

In this appendix, we derive the branching rules for the embedding

$$\frac{\widehat{SU}(\widehat{2})_1 \times \widehat{SU}(\widehat{2})_1 \times \widehat{SU}(\widehat{2})_1}{\widehat{SU}(\widehat{2})_3} \tag{A1}$$

in section 2. This kind of embedding is called *diagonal* in the literatures since subgroup appearing in the denominator corresponds to the diagonal one of the numerator. The diagonal subgroup is generated by the diagonal current

$$J_{L/R}^{\text{diag}} = J_{L/R}^{(1)} + J_{L/R}^{(2)} + J_{L/R}^{(3)}$$
(A2)

which corresponds to the *total spin* and satisfies the level-3 SU(2) Kac–Moody algebra.

According to the general theory of the coset construction [39], the coset (G/H) CFT is governed by the  $c_{G/H} = c_G - c_H$  Virasoro algebra generated by the operators

$$K_n = L_n^G - L_n^H \qquad (n \in \mathbf{Z}) \tag{A3}$$

satisfying  $[K_n, L_m^H] = 0$ . As usual,  $L_n^G$  and  $L_n^H$  are realized by the Sugawara construction [35]. Correspondingly, we have character identities

$$\chi_{G,R}(q) = \sum_{R'} b(R, R'; q) \chi_{H,R'}(q)$$
(A4)

where  $\chi_{G,R}$  and b(R, R') denote the character for the representation R of the algebra  $\widehat{G}$  and the branching function, respectively.

In our case, the central charge of the coset CFT is given by  $c = \frac{6}{5}$  ( $c_G = 3$ ,  $c_H = \frac{9}{5}$ ). The finite-reducibility theorem [57] says that if the sum in (A4) is finite and  $c_{G/H} > 1$ , then we have to regard the branching function *b* as the characters for a larger algebra than the Virasoro algebra. Symmetry consideration suggests that this extended algebra is given by the  $W_3$  algebra [40, 58] with  $\mathbb{Z}_3$ -symmetry (for a detailed account for the *W*-symmetry, see [41] and references therein).

The  $W_3$  minimal CFT relevant for our purpose is also known to be given by the coset construction [41]

$$\frac{\widehat{SU(3)}_1 \times \widehat{SU(3)}_2}{\widehat{SU(3)}_3} \,.$$

The characters  $\chi_h^{W_3}(q) = \text{Tr}q^{L_0(W_3)}$  are given in [42] for all 20 primary fields of this CFT. Among them, the following six ones are necessary:

$$\begin{split} \chi_{0}^{W_{3}}(q) &= 1 + q^{2} + 2q^{3} + 3q^{4} + 4q^{5} + 8q^{6} + 10q^{7} + 17q^{8} + 24q^{9} + \cdots \\ \chi_{1/10}^{W_{3}}(q) &= q^{1/10} + 2q^{11/10} + 4q^{21/10} + 8q^{31/10} + 13q^{41/10} + 22q^{51/10} + 35q^{61/10} + \cdots \\ \chi_{1/2}^{W_{3}}(q) &= q^{1/2} + 2q^{3/2} + 3q^{5/2} + 6q^{7/2} + 10q^{9/2} + 16q^{11/2} + 26q^{13/2} + \cdots \\ \chi_{3/5}^{W_{3}}(q) &= \chi_{3/5^{*}}^{W_{3}}(q) = q^{3/5} + q^{8/5} + 2q^{13/5} + 3q^{18/5} + 6q^{23/5} + 9q^{28/5} + 15q^{33/5} + \cdots \\ \chi_{8/5}^{W_{3}}(q) &= q^{8/5} + 2q^{13/5} + 3q^{18/5} + 6q^{23/5} + 9q^{28/5} + 14q^{33/5} + 22q^{38/5} + \cdots \end{split}$$

and

$$\chi_2^{W_3}(q) = \chi_{2^*}^{W_3}(q) = q^2 + q^3 + 3q^4 + 4q^5 + 7q^6 + 10q^7 + 17q^8 + 23q^9 + \cdots$$

Using the above expressions and the  $\widehat{SU(2)}$  affine characters for level-1 and 3, we can show that the following identities hold for the embedding (A1)

$$\chi_{j=0}^{(1)}\chi_{j=0}^{(1)}\chi_{j=0}^{(1)} = \left(\chi_{3/5}^{W_3} + \chi_{3/5^*}^{W_3} + \chi_{8/5}^{W_3}\right)\chi_{j=1}^{(3)} + \left(\chi_0^{W_3} + \chi_2^{W_3} + \chi_{2^*}^{W_3}\right)\chi_{j=0}^{(3)}$$
(A5)

$$\chi_{j=1/2}^{(1)}\chi_{j=0}^{(1)}\chi_{j=0}^{(1)} = \chi_{1/10}^{W_3}\chi_{j=1/2}^{(3)} + \chi_{1/2}^{W_3}\chi_{j=3/2}^{(3)}$$
(A6)

$$\chi_{j=1/2}^{(1)}\chi_{j=1/2}^{(1)}\chi_{j=0}^{(1)} = \chi_{1/10}^{W_3}\chi_{j=1}^{(3)} + \chi_{1/2}^{W_3}\chi_{j=0}^{(3)}$$
(A7)

$$\chi_{j=1/2}^{(1)}\chi_{j=1/2}^{(1)}\chi_{j=1/2}^{(1)} = \left(\chi_{3/5}^{W_3} + \chi_{3/5^*}^{W_3} + \chi_{8/5}^{W_3}\right)\chi_{j=1/2}^{(3)} + \left(\chi_0^{W_3} + \chi_2^{W_3} + \chi_{2^*}^{W_3}\right)\chi_{j=3/2}^{(3)}$$
(A8)

where  $\chi_j^{(k)}$  denotes the character for the spin-*j* representation of the level- $k \ \widehat{SU}(2)$ . Two primary fields  $(\phi_{h=2}, \phi_{h=2^*})$  (and  $(\phi_{h=3/5}, \phi_{h=3/5^*})$ ) are mutually conjugate **Z**<sub>3</sub>-neutral fields. The second and third lines were already given in section 2 in order to rewrite the interactions.

The branching functions  $(q = e^{2\pi i \tau})$ 

$$\begin{aligned} \chi_1(\tau) &\equiv \chi_0^{W_3} + \chi_2^{W_3} + \chi_{2^*}^{W_3} \qquad \chi_2(\tau) \equiv \chi_{1/10}^{W_3} \\ \chi_3(\tau) &\equiv \chi_{1/2}^{W_3} \qquad \chi_4(\tau) \equiv \chi_{3/5}^{W_3} + \chi_{3/5^*}^{W_3} + \chi_{8/5}^{W_3} \end{aligned}$$

appearing in (A5)-(A8) transform as follows:

$$\chi_{1}(-1/\tau) = c_{1}\chi_{1}(\tau) + 3c_{2}\chi_{2}(\tau) + 3c_{1}\chi_{3}(\tau) + c_{2}\chi_{4}(\tau)$$

$$\chi_{2}(-1/\tau) = c_{2}\chi_{1}(\tau) + c_{1}\chi_{2}(\tau) - c_{2}\chi_{3}(\tau) - c_{1}\chi_{4}(\tau)$$

$$\chi_{3}(-1/\tau) = c_{1}\chi_{1}(\tau) - c_{2}\chi_{2}(\tau) - c_{1}\chi_{3}(\tau) + c_{2}\chi_{4}(\tau)$$

$$\chi_{4}(-1/\tau) = c_{2}\chi_{1}(\tau) - 3c_{1}\chi_{2}(\tau) + 3c_{2}\chi_{3}(\tau) - c_{1}\chi_{4}(\tau)$$
(A9)

where the constants  $c_1$  and  $c_2$  are given by

$$c_1 \equiv \frac{\sqrt{5}\sin(\pi/5)}{2(2+\cos(\pi/5)-\cos(2\pi/5))} \qquad c_2 \equiv \frac{\sqrt{5}\sin(2\pi/5)}{2(2+\cos(\pi/5)-\cos(2\pi/5))}$$

and satisfy  $4(c_1^2 + c_2^2) = 1$ . From these relations, it is easy to verify that the above branching functions are building blocks of the following modular-invariant partition function:

$$Z(\tau) = |\chi_0^{W_3} + \chi_2^{W_3} + \chi_{2^*}^{W_3}|^2 + 3|\chi_{1/10}^{W_3}|^2 + 3|\chi_{1/2}^{W_3}|^2 + |\chi_{3/5}^{W_3} + \chi_{3/5^*}^{W_3} + \chi_{8/5}^{W_3}|^2$$
  
=  $|\chi_1|^2 + 3|\chi_2|^2 + 3|\chi_3|^2 + |\chi_4|^2$ . (A10)

The fusion rule algebra [59] is closely related to the operator-product expansion (OPE) and gives information about which fields appear in the OPE. The fusion-rule coefficients  $N_{ij}^k$  are conveniently derived from the so-called modular *S*-matrix with the help of the Verlinde formula [60]. Using the modular *S*-matrix calculated in [42] (equation (4.2.3)), we obtain the following fusion rules for the charge-neutral fields

$$\begin{aligned} [\phi_{h=1/2}] \times [\phi_{h=1/2}] &= [\mathbf{1}] + 2[\phi_{h=1/2}] + [\phi_{h=2}] + [\phi_{h=2^*}] \\ [\phi_{h=1/10}] \times [\phi_{h=1/10}] &= [\mathbf{1}] + 2[\phi_{h=1/10}] + 2[\phi_{h=1/2}] + [\phi_{h=8/5}] \\ &+ [\phi_{h=2}] + [\phi_{h=2^*}] + [\phi_{h=3/5}] + [\phi_{h=3/5^*}] \\ [\phi_{h=1/10}] \times [\phi_{h=1/2}] &= 2[\phi_{h=1/10}] + [\phi_{h=8/5}] + [\phi_{h=3/5^*}] \\ [\phi_{h=1/2}] \times [\phi_{h=8/5}] &= [\phi_{h=1/10}] + [\phi_{h=1/2}] \\ [\phi_{h=1/10}] \times [\phi_{h=8/5}] &= [\phi_{h=1/10}] + [\phi_{h=1/2}] \\ [\phi_{h=2}] \times [\phi_{h=2,*}] &= [\mathbf{1}] + [\phi_{h=8/5}] \\ [\phi_{h=2}] \times [\phi_{h=2,*}] &= [\phi_{h=3/5^*}] \\ [\phi_{h=2}] \times [\phi_{h=3/5}] &= [\phi_{h=3/5^*}] \\ [\phi_{h=2}] \times [\phi_{h=3/5}] &= [\phi_{h=3/5}] \\ [\phi_{h=2}] \times [\phi_{h=1/10}] &= [\phi_{h=3/5}] \\ [\phi_{h=2}] \times [\phi_{h=1/2}] &= [\phi_{h=3/5^*}] \\ [\phi_{h=2}] \times [\phi_{h=3/5}] &= [\phi_{h=3/5^*}] \\ [\phi_{h=3/5}] \times [\phi_{h=3/5^*}] &= [\phi_{h=3/5^*}] \\ [\phi_{h=3/5}] \times [\phi_{h=3/5^*}] &= [\phi_{h=1/10}] \\ [\phi_{h=3/5}] \times [\phi_{h=3/5^*}] &= [\phi_{h=1/10}] \\ [\phi_{h=1/2}] \times [\phi_{h=3/5^*}] &= [\phi_{h=1/10}] \\ [\phi_{h=1/2}] \times [\phi_{h=3/5^*}] &= [\phi_{h=1/10}] \\ [\phi_{h=1/2}] \times [\phi_{h=3/5^*}] &= [\phi_{h=1/10}] \\ [\phi_{h=1/10}] \times [\phi_{3/5}] &= [\phi_{1/2}] + [\phi_{1/10}] \\ [\phi_{h=1/10}] \times [\phi_{3/5^*}] &= [\phi_{1/2}] + [\phi_{1/10}] \\ [\phi_{h=1/10}] \times [\phi_{3/5^*}] &= [\phi_{1/2}] + [\phi_{1/10}] \end{aligned}$$

Note that the above rules are (as they should be) consistent with the  $\mathbf{Z}_3$ -symmetry underlying this CFT.

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The above fusion rules and modular invariant (A10) suggest that the order 3 simple currents  $\phi_{h=2}$  and  $\phi_{h=2^*}$  act on triplets  $\phi_{h=1/10} = (\phi_{h=1/10}^{(1)}, \phi_{h=1/10}^{(2)}, \phi_{h=1/10}^{(3)})$  and  $\phi_{h=1/2} = (\phi_{h=1/2}^{(1)}, \phi_{h=1/2}^{(2)}, \phi_{h=1/2}^{(3)})$  as  $\mathbf{Z}_3$  operators. That is, the following OPEs hold:

$$\phi_{h=2}(z)\phi_h(w) = \frac{1}{(z-w)^2} \begin{pmatrix} 0 & 1 & 0\\ 0 & 0 & 1\\ 1 & 0 & 0 \end{pmatrix} \phi_h(w) + (\cdots)$$
  
$$\phi_{h=2^*}(z)\phi_h(w) = \frac{1}{(z-w)^2} \begin{pmatrix} 0 & 0 & 1\\ 1 & 0 & 0\\ 0 & 1 & 0 \end{pmatrix} \phi_h(w) + (\cdots)$$

where  $h = \frac{1}{10}$  or  $\frac{1}{2}$ . They corresponds to the following  $\mathbb{Z}_3$ -operations for the  $g_{1,2,3}$ -fields:

$$\phi_{h=2}: g_i \mapsto g_{i+1} \qquad \phi_{h=2^*}: g_i \mapsto g_{i-1}$$

On the other hand, two extended fields  $\tilde{1}$  and  $\tilde{\phi}h = \frac{3}{5}$  behave like

$$\phi_{h=2}(z)\widetilde{\mathbf{1}} \sim 0$$
  $\phi_{h=2}(z)\widetilde{\phi}_{h=3/5}(w) \sim \frac{1}{(z-w)^2}\widetilde{\phi}_{h=3/5}(w) + (\cdots)$ 

The 'extended' modular S-matrix compatible with this observation does exist; the new fusion rules are much simpler than those listed in the above:

$$\begin{split} & [\phi_{h=1/10}^{(1)}] \times [\phi_{h=1/10}^{(1)}] = [\widetilde{\mathbf{1}}] + [\widetilde{\phi}_{h=3/5}] \\ & [\phi_{h=1/10}^{(1)}] \times [\phi_{h=1/2}^{(2)}] = [\phi_{h=1/10}^{(3)}] + [\phi_{h=1/2}^{(3)}] \quad (\text{cyclic perm}) \\ & [\phi_{h=1/10}^{(1)}] \times [\phi_{h=1/2}^{(1)}] = [\widetilde{\phi}_{h=3/5}] \\ & [\phi_{h=1/10}^{(1)}] \times [\phi_{h=1/2}^{(2)}] = [\phi_{h=1/10}^{(3)}] \qquad [\phi_{h=1/10}^{(1)}] \times [\phi_{h=1/2}^{(3)}] = [\phi_{h=1/10}^{(2)}] \quad (\text{cyclic perm}) \\ & [\phi_{h=1/2}^{(1)}] \times [\phi_{h=1/2}^{(1)}] = [\widetilde{\mathbf{1}}] \\ & [\phi_{h=1/2}^{(1)}] \times [\phi_{h=3/5}^{(2)}] = [\phi_{h=1/2}^{(3)}] \\ & [\phi_{h=1/2}^{(1)}] \times [\widetilde{\phi}_{h=3/5}] = [\phi_{h=1/10}^{(1)}] \\ & [\widetilde{\phi}_{h=3/5}] \times [\widetilde{\phi}_{h=3/5}] = [\widetilde{\mathbf{1}}] . \end{split}$$

We have used symbols  $[\tilde{1}]$  and  $[\phi_{h=3/5}]$  in the extended sense.

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