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# Correlation functions of the 2D sine–Gordon model

Kiyohide Nomura†

Laboratoire de Physique des Solides, Université Paris-Sud, 91405, Orsay, France

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**Abstract.** A number of two-dimensional (2D) critical phenomena can be described in terms of the 2D sine–Gordon model. With bosonization, several 1D quantum systems can be transformed to the same model. However, the transition of the 2D sine–Gordon model, the Berezinskii–Kosterlitz–Thouless (BKT) transition, is essentially different from a second-order transition. The divergence of the correlation length is more rapid than any power law, and there are logarithmic corrections. These pathological features make it difficult to determine the BKT transition point and critical indices from finite-size calculations. In this paper we calculate correlation functions of this model using a real-space renormalization technique. It is found that several correlation functions, or eigenvalues of the corresponding transfer matrix for a finite system, become degenerate on the BKT line, including the logarithmic corrections. By the use of this degeneracy, which reflects the hidden  $SU(2)$  symmetry on the BKT line, it is possible to determine the BKT critical line with high precision from a small amount of data and to identify the universality class. In addition, new universal relations are found. These results shed light on the relation between Abelian and non-Abelian bosonization.

## 1. Introduction

The two-dimensional (2D) sine–Gordon model, which is a natural extension of the Gaussian or free-boson model, plays an important role in 2D classical and one-dimensional (1D) quantum systems, such as the 2D XY model, 2D helium films, 1D quantum spin models and 1D fermion models.

The peculiarity of the phase transition of the 2D XY model (helium films) was first noticed with the spin-wave approximation or free-boson model [1, 2]. In these theories there is no continuous symmetry breaking as required by the Mermin–Wagner–Coleman theorem [3–5], but the correlation length  $\xi$  is infinite at all temperatures and the correlation functions decay as power laws with continuously varying exponents. Although this picture is qualitatively correct at low temperatures, it is clearly wrong at high temperatures where one expects a finite  $\xi$  and the associated exponential decay of correlations.

Berezinskii [6] and Kosterlitz and Thouless [7] pointed out the importance of vortex excitations which essentially modify the spin-wave theories. The vortex structure reflects the periodic nature of the spin variable  $\phi \equiv \phi + 2n\pi$ . The vortices carry integer vorticity and interact among themselves via a logarithmic 2D Coulomb interaction. At low temperatures all of the particles are bound into neutral ‘quasi-molecules’ with zero vorticity and so the couplings of the spin-wave model are changed. At higher temperatures the binding of the quasi-molecules decreases and eventually this causes a phase transition.

Kosterlitz [8] subsequently performed a renormalization group calculation, following the method of Anderson *et al* [9, 10]. In fact, the renormalization equations are the same

† On leave from: Department of Physics, Tokyo Institute of Technology, Tokyo 152, Japan.

for both cases. He found that close to the Berezinskii–Kosterlitz–Thouless (BKT) transition point, the correlation length diverges as  $\xi \propto \exp(b\sqrt{t})$ , which is faster than any power of  $t$ . Also, logarithmic corrections to various quantities, such as correlation functions and susceptibilities, appear at the BKT critical point. These features are entirely different from those of the conventional second-order transition.

The 2D XY model has been treated in the more general framework of the 2D Coulomb gas, having two kinds of quantum number: one for ‘charges’ and one for ‘magnetic monopoles’ [11, 12]. In this representation, the meaning of the duality transformation, which exchanges the roles of electrons and magnetic monopoles, becomes apparent. Several models, such as  $p$ -clock models, the Ising model, three- and four-state Potts models and the Ashkin–Teller model are mapped in a unified way to the 2D Coulomb gas [13].

Kadanoff [14] and Kadanoff and Brown [15] identified correlation functions of the Gaussian, eight-vertex and Ashkin–Teller models, whose critical dimensions vary continuously on the critical line. In the latter two models, only a few correlation functions are known, except at the decoupling point. They first made a comparison of the correlation functions of the three models at a special point on each critical line. and then used the marginal operator and the operator product expansion to extend these connections to the whole critical line.

The equivalence of the sine–Gordon model with the 2D Coulomb gas model has been shown by several authors [16, 17]. Coleman [18] showed the equivalence of the massive one-component Thirring model and the sine–Gordon model, order by order in a perturbation expansion, and proved the renormalizability of these models. But his discussion failed in the region of  $\beta^2 > 8\pi$ . Luther and Emery [19], Halpern [20, 21] and Banks *et al* [22] showed the equivalence between the  $SU(2)$  massless Thirring model and the theory of bosons consisting of a free field plus a  $\beta^2 = 8\pi$  sine–Gordon model, which corresponds to the BKT line. So, there is a hidden  $SU(2)$  symmetry at the BKT transition.

Amit *et al* [23] developed a more systematic field theory treatment of the renormalization group calculation for the sine–Gordon model. By considering the renormalization of the wavefunction, they resolved the problem that Coleman encountered. They calculated the higher terms beyond those of Kosterlitz and found a new universal quantity.

The logarithmic corrections of the  $k = 1$   $SU(2)$  Wess–Zumino–Witten (WZW) model, which has been shown to be equivalent to the  $\beta^2 = 8\pi$  sine–Gordon model, were systematically studied by Affleck *et al* [24]. They found the universal relation of the ratios of logarithmic corrections to scaling amplitudes. This relation was used by Ziman and Schulz [25] for the problem of the  $S = \frac{3}{2}$  quantum Heisenberg chain.

But this  $SU(2)$  symmetry is not apparent in the sine–Gordon model itself and, except for the BKT line, the symmetry is broken to  $U(1) \times \mathbb{Z}_2$ . How does the sine–Gordon model become  $SU(2)$  symmetric on the BKT line? This problem, including the logarithmic corrections, was first treated by Giamarchi and Schulz [26]. They calculated the renormalized correlation functions and found that  $SU(2)$  symmetry for these functions is recovered on the BKT line. In this case the original model is apparently  $SU(2)$  symmetric on the  $\beta^2 = 8\pi$  fixed point.

There are several models that can be mapped onto the sine–Gordon model. Although the mappings are qualitatively correct, since coupling constants and cut-offs are renormalized, one should use numerical results for the determination of the phase diagram. However, near the BKT transition, the divergence of the correlation length is essentially singular and logarithmic corrections exist. Therefore, it is very difficult to find the critical point of a BKT-type transition. In our previous papers [27, 28], by using the level crossing of the eigenvalues of the transfer matrix or the corresponding quantum sine–Gordon Hamiltonian

in 1D, we could easily determine the transition point and identify the universality class. It was based on the  $SU(2)$  symmetry on the BKT transition line.

In this paper we perform a renormalization group calculation of correlation functions which have critical dimensions that become marginal on the BKT line. In the case when  $SU(2)$  symmetry appears on the BKT line, the nine eigenvalues split as five-, three- and one-fold degenerate, i.e. the  $SU(2)$  multiplets structure. Otherwise, the five eigenvalues split as three-, one- and one-fold degenerate, and it is also possible to determine the BKT transition line by the level crossing of the eigenvalues. In addition, new universal relations are found. These may deepen our understanding of the relation between Abelian and non-Abelian bosonization.

This paper is organized as follows. In section 2 the model is introduced, and the symmetry structure is discussed. In section 3 we review the correlation functions which become marginal at  $y_0 = y_\phi = 0$ . In section 4 the renormalization equations are obtained for these functions. The hybridization between the marginal field and the  $\cos \sqrt{8}\phi$  field is important. In section 5 we consider the eigenvalue structure of the transfer matrix and briefly summarize the results of section 4. In section 6 our results are applied to 1D quantum and 2D classical systems. Section 7 is the conclusion.

## 2. Sine-Gordon model

The description of the symmetry and correlation functions of the Gaussian model in this and the following sections is based on [29–31]. We first consider the 2D Gaussian model defined as the Lagrangian

$$\mathcal{L} = \frac{1}{2\pi K} (\nabla\phi)^2. \tag{1}$$

The two-point correlation function for  $\phi$  is

$$2\langle\phi(r_1)\phi(r_2)\rangle = -K \operatorname{Re} \log(z_{12}/\alpha) \tag{2}$$

where  $\alpha$  is a short-distance (ultraviolet) cut-off and  $z \equiv x + iy$ ,  $z_{12} = z_1 - z_2$ . Strictly speaking, a small mass  $\mu$  should be introduced to serve as an infrared cut-off, such as in equation (2.2) in [23]. The logarithmic behaviour of the  $\phi$  correlation function shows that it cannot be directly interpreted as a physical object. However, the exponential operators of  $\phi$  satisfy

$$\langle \exp(i e \phi(r_1)) \exp(-i e \phi(r_2)) \rangle = |z_{12}/\alpha|^{-e^2 K/2} \tag{3}$$

so they are candidates for the correlation functions of the critical theory. A convention needs to be explained regarding this formula. We did not include the divergent ‘self energy’ factors coming from the terms in the exponent where the Green function is to be evaluated at zero. This means that we have really evaluated correlations of the ‘normal ordered’ exponentials:  $\exp(i e \phi)$ .

About the symmetry, the Lagrangian (1) is invariant under  $\phi \rightarrow \phi + \text{constant}$  and  $\phi \rightarrow -\phi$ . This may be used to restrict configurations, with the identification of  $\phi \equiv \phi + 2\pi/\sqrt{2}$ , implying that  $\phi$  takes its values on a circle. In this case, the charges  $e$  are quantized as  $e = \sqrt{2}n$  ( $n$  an integer). One may also introduce the new scaling fields  $\exp(im\sqrt{2}\theta(x))$ , which create a discontinuity of  $\phi$  by  $2\pi m/\sqrt{2}$  around the point  $x$ . The two-point correlation functions are

$$\begin{aligned} 2\langle\theta(r_1)\theta(r_2)\rangle &= -\frac{1}{K} \operatorname{Re} \log(z_{12}/\alpha) \\ 2\langle\phi(r_1)\theta(r_2)\rangle &= -i \operatorname{Im} \log(z_{12}/\alpha) \end{aligned} \tag{4}$$

and furthermore

$$\partial_x \phi = -\partial_y (iK\theta) \quad \partial_y \phi = \partial_x (iK\theta). \quad (5)$$

The field  $\theta$  is called a dual field to  $\phi$ . This model is invariant under the transformations  $\phi \rightarrow \phi + \text{constant}$  and  $\theta \rightarrow \theta + \text{constant}$ , which implies  $U(1) \times U(1)$  symmetry. The full symmetry group is extended to  $O(2) \times O(2)$  by the discrete  $\mathbb{Z}_2$  symmetries  $(z, \phi, \theta) \rightarrow (z, -\phi, -\theta)$  and  $(z, \phi, \theta) \rightarrow (\bar{z}, \phi, -\theta)$ . There is also a dual transformation  $K \leftrightarrow 1/K, \phi \leftrightarrow \theta$ , which exchanges the roles of electric and magnetic excitations. The self-dual point  $K = 1$  is nothing but the  $k = 1$   $SU(2) \times SU(2)$  WZW model. Another point of view is given by a chiral decomposition

$$\Phi_R(z) \equiv \frac{1}{2} \left[ \frac{1}{\sqrt{K}} \phi + \sqrt{K} \theta \right] \quad \Phi_L(\bar{z}) \equiv \frac{1}{2} \left[ \frac{1}{\sqrt{K}} \phi - \sqrt{K} \theta \right]. \quad (6)$$

This system is also chiral invariant.

At this stage, a natural extension of the Gaussian model is to introduce the interaction term  $\cos \sqrt{2}\phi$ . In place of this, we consider the sine-Gordon Lagrangian

$$\mathcal{L} = \frac{1}{2\pi K} (\nabla \phi)^2 + \frac{y_\phi}{2\pi \alpha^2} \cos \sqrt{8}\phi \quad (7)$$

in order to see  $SU(2)$  symmetry on the BKT line explicitly. Note that the  $U(1)$  symmetry of  $\phi$  is explicitly broken to the discrete symmetry  $\phi \rightarrow \phi + 2\pi/\sqrt{8}$ . Since this transformation divides the internal circle of  $\phi$  into two, the symmetry of this model is  $O(2) \times \mathbb{Z}_2 \times \mathbb{Z}_2$ . The interaction term breaks the chiral symmetry. Furthermore, the Lagrangian (7) is invariant under  $\phi \rightarrow \phi + \pi/\sqrt{8}, y_\phi \rightarrow -y_\phi$ . However, calculations in this paper also apply to the usual BKT transition, simply by requiring the periodicity  $\phi \equiv \phi + 2\pi/\sqrt{8}$ . In the latter case, the symmetry is  $O(2) \times \mathbb{Z}_2$ .

Under a change of the cut-off  $\alpha \rightarrow e^l \alpha$ , the renormalization group equations for the sine-Gordon model (7) are

$$\frac{dy_0(l)}{dl} = -y_\phi^2(l) \quad \frac{dy_\phi(l)}{dl} = -y_\phi(l)y_0(l) \quad (8)$$

where  $K = 1 + \frac{1}{2}y_0$ . For the finite system,  $l$  is related to  $L$  by  $e^l = L$ . There are three critical lines:  $y_\phi = 0 (y_0 < 0)$  corresponding to the Gaussian fixed line; and  $y_\phi = \pm y_0 (y_0 > 0)$  corresponding to the BKT lines. In the region between the two BKT lines ( $|y_\phi| < y_0$ ), all the points will be renormalized to the Gaussian fixed line, so they are massless. The other region is massive, except on the Gaussian fixed line.

### 3. Correlation functions on the Gaussian fixed line

We review the correlation functions on the Gaussian fixed line ( $y_\phi = 0$ ). The correlation functions of the Gaussian model are, in general,

$$\langle O_{n,m}(r_1) O_{-n,-m}(r_2) \rangle = \exp \left[ - \left( n^2 K + \frac{m^2}{K} \right) \log \left( \frac{r_{12}}{\alpha} \right) - 2inm \left( \text{Arg}(r_{12}) + \frac{\pi}{2} \right) \right] \quad (9)$$

$$O_{n,m} \equiv \exp(in\sqrt{2}\phi) \exp(im\sqrt{2}\theta)$$

where  $\text{Arg}(r_{12}) = \text{Im} \log(z_{12})$  is the angle of the  $r_1 - r_2$  vector. Thus,  $O_{n,m}$  has a critical dimension  $x_{n,m}$  and a spin  $l_{n,m}$  given by

$$x_{n,m} = \frac{1}{2} \left( n^2 K + \frac{m^2}{K} \right) \quad l_{n,m} = nm. \quad (10)$$

The expectation value  $\langle \Pi_j O_{n_j, m_j}(r_j) \rangle$  is zero unless the charge and monopole neutrality condition  $\sum n_j = 0, \sum m_j = 0$  are satisfied [14, 15]; this reflects the underlying  $U(1) \times U(1)$  symmetry. Then the fields, which become marginal ( $x = 2$ ) and spin zero at  $y_0 = 0$  ( $K = 1$ ), are four fields of the form  $O_{n,m}$ :

$$\frac{1}{\sqrt{2}}(O_{2,0} + O_{-2,0}) = \sqrt{2} \cos \sqrt{8}\phi \quad \frac{1}{\sqrt{2i}}(O_{2,0} - O_{-2,0}) = \sqrt{2} \sin \sqrt{8}\phi$$

$O_{0,2} \quad O_{0,-2}$  (11)

and four descendent fields, which are expressed as the derivatives of the  $O_{\pm 1, \pm 1}$  fields:

$$\alpha[\bar{\partial} O_{1,1} + \partial O_{-1,1}] \quad \alpha[\bar{\partial} O_{-1,-1} + \partial O_{1,-1}]$$

$$\frac{\alpha}{i}[\bar{\partial} O_{1,1} - \partial O_{-1,1}] \quad \frac{\alpha}{i}[-\bar{\partial} O_{-1,-1} + \partial O_{1,-1}]$$

(12)

where  $\partial \equiv \partial_z$ , and we take the symmetrized and the antisymmetrized forms of the function of  $\phi$ . There is one more field, namely

$$\mathcal{M} = \frac{\alpha^2}{K} \left[ \left( \frac{\partial \phi}{\partial x} \right)^2 + \left( \frac{\partial \phi}{\partial y} \right)^2 \right].$$

(13)

The correlation functions for  $O_{n,m}$  have been shown previously. To calculate the correlation functions for descendent fields, it is enough to know that

$$\alpha^2 \langle \bar{\partial} O_{1,1}(r_1) \bar{\partial} O_{-1,-1}(r_2) \rangle = \frac{\bar{y}_0^2}{8} \left( 1 + \frac{\bar{y}_0^2}{8} \right) \exp \left[ - \left( 4 + \frac{\bar{y}_0^2}{4} \right) \log(r_{12}/\alpha) \right]$$

(14)

where  $\bar{y}_0^2 = 4(K + (1/K) - 2) \simeq y_0^2$ . To calculate the correlation function for the  $\mathcal{M}$  field, we introduce the fields

$$\mathcal{R}^\pm = \frac{\alpha}{\sqrt{K}} \left[ \frac{\partial \phi}{\partial x} \mp i \frac{\partial \phi}{\partial y} \right] = \frac{\alpha}{\sqrt{K}} 2\partial(\bar{\partial})\phi.$$

(15)

Then

$$\langle \mathcal{R}^+(r_1) \mathcal{R}^+(r_2) \rangle = - \left( \frac{z_{12}}{\alpha} \right)^{-2}$$

$$\langle \mathcal{R}^-(r_1) \mathcal{R}^-(r_2) \rangle = - \left( \frac{\bar{z}_{12}}{\alpha} \right)^{-2}$$

$$\langle \mathcal{R}^+(r_1) \mathcal{R}^-(r_2) \rangle = 0.$$

(16)

This means that  $\mathcal{R}^\pm$  are the fields which have critical dimension one and spin  $\pm 1$ . Therefore,

$$\langle \mathcal{M}(r_1) \mathcal{M}(r_2) \rangle = \langle \mathcal{R}^+(r_1) \mathcal{R}^-(r_1) \mathcal{R}^+(r_2) \mathcal{R}^-(r_2) \rangle = \exp[-4 \log(r_{12}/\alpha)]$$

(17)

that is, the critical dimension of this field is always marginal ( $x = 2$ ). Here we have implicitly taken the normal ordered form  $\mathcal{M} =: \mathcal{R}^+ \mathcal{R}^-$  for the marginal field. The field  $\mathcal{M}$  is nothing but the marginal field of Kadanoff *et al* [14, 15]; and our  $\mathcal{R}^{+(-)}$  correspond to their  $F_{1,0}(F_{0,1})$ . Note that, although in these nine fields the critical dimensions of  $O_{n,m}$  and their descendent fields vary with the parameter  $y_0$ , the marginal field  $\mathcal{M}$  always has the critical dimension  $x = 2$ . The equations

$$\langle \mathcal{R}^+(r_1) \phi(r_2) \rangle = - \frac{\alpha \sqrt{K}}{2} \left( \frac{z_{12}}{\alpha} \right)^{-1} \quad \langle \mathcal{R}^\pm \rangle = 0$$

(18)

are useful for further calculations. The three-point functions are

$$\langle \mathcal{M}(r_1) \mathcal{M}(r_2) \mathcal{M}(r_3) \rangle = 0 \quad \langle \mathcal{M}(r_1) \mathcal{M}(r_2) O_{n,m}(r_3) \rangle = 0.$$

(19)

The former comes from Wick's theorem, (17) and (18), and the latter from the neutrality condition.

In the usual BKT transition in which the  $SU(2)$  symmetry is not explicit, the only difference is that the critical dimension of the four descendent fields is  $2 + 1 + \frac{1}{8} = \frac{25}{8}$  at  $y_0 = y_\phi = 0$ . Therefore, only the remaining five fields are marginal at the multi-critical point. The usual BKT transition point can be obtained by 'modding out' the  $SU(2)$  symmetric case with a  $\mathbb{Z}_2$  symmetry [29, 31].

#### 4. Renormalization of correlation functions

In this section we proceed to include the interaction  $y_\phi \cos \sqrt{8}\phi$ . When we calculate correlation functions, divergences appear that come from both short range and long range because of the nature of the 2D Green function. To treat such a problem we use the renormalization procedure. The correlation functions for  $\langle \exp(i\sqrt{8}\theta_1) \exp(-i\sqrt{8}\theta_2) \rangle$  and  $\langle \sqrt{2} \sin(\sqrt{8}\phi_1) \sqrt{2} \sin(\sqrt{8}\phi_2) \rangle$  (for brevity we will use  $\phi_1$  for  $\phi(r_1)$ ) have been obtained by Giamarchi and Schulz [26]. Their results are

$$\begin{aligned} R_2 &\equiv 2 \langle \sin(\sqrt{8}\phi_1) \sin(\sqrt{8}\phi_2) \rangle_I = C_2 \exp \left[ - \int_0^{\ln(r/\alpha)} dl (4 + 2y_0(l)) \right] \\ R_3 &\equiv \langle \exp(i\sqrt{8}\theta_1) \exp(-i\sqrt{8}\theta_2) \rangle_I = C_3 \exp \left[ - \int_0^{\ln(r/\alpha)} dl (4 - 2y_0(l)) \right] \\ R_4 &\equiv \langle \exp(-i\sqrt{8}\theta_1) \exp(i\sqrt{8}\theta_2) \rangle_I = R_3 \end{aligned} \quad (20)$$

where  $C_j$  are the integration constants which depend on the regularization.

##### 4.1. Correlation functions of the marginal and $\cos \sqrt{8}\phi$ fields

The fields  $\mathcal{M}$  and  $\sqrt{2} \cos \sqrt{8}\phi$  become hybridized by the interaction term as

$$\begin{aligned} &\int \frac{d^2 x_3}{\alpha^2} \left\{ \cos \sqrt{8}\phi_1 \mathcal{M}_2 \cos \sqrt{8}\phi_3 \right\} \\ &= \frac{-8}{2 \cdot 2} \int \frac{d^2 x_3}{\alpha^2} \left\{ \mathcal{M}_2 (\phi_1 - \phi_3)^2 \right\} \left\{ \exp(i\sqrt{8}\phi_1) \exp(-i\sqrt{8}\phi_3) \right\} \\ &= -K \int \frac{d^2 x_3}{\alpha^2} \alpha^2 (z_{12}^{-1} - z_{32}^{-1})(\bar{z}_{12}^{-1} - \bar{z}_{32}^{-1}) \exp(-4K \log(r_{31}/\alpha)). \end{aligned} \quad (21)$$

To derive this result we have used Wick's theorem [32], the  $U(1)$  symmetry and (18). Terms which are not invariant under the global transformation  $\phi \rightarrow \phi + \text{constant}$  should be zero. The divergent parts relating to renormalization appear near  $r_{31} \ll r_{12}$  and  $r_{32} \ll r_{12}$ . When  $r_{31} \ll r_{12}$  then  $z_{32}^{-1} \simeq z_{12}^{-1} (1 - z_{31}/z_{12})$  and, therefore, the integrand of (21) is approximately

$$\left| \frac{z_{12}}{\alpha} \right|^{-4} \left| \frac{z_{31}}{\alpha} \right|^2 \exp(-4K \log(r_{31}/\alpha)). \quad (22)$$

When  $r_{32} \ll r_{12}$ , the divergent part of the integrand is

$$\left| \frac{z_{32}}{\alpha} \right|^{-2} \exp(-4K \log(r_{12}/\alpha)) \simeq \left| \frac{z_{12}}{\alpha} \right|^{-4} \left| \frac{z_{32}}{\alpha} \right|^{-2} \exp(-2y_0 \log(r_{12}/\alpha)) \quad (23)$$

where we use  $K = 1 + y_0/2$ . Note that only the terms which contain  $|z_{32}|^{-2}$  contribute to the divergence of the integral; other terms, such as  $z_{32}^{-1}$ , cancel out with the integration. In order to treat these divergences, we exclude two circles of radius  $\alpha$  around  $r_1$  and  $r_2$  from

the domain of integration over  $r_3$ . Then, with the change of cut-off  $\alpha' = \alpha e^{dl}$ , the integral (21) is renormalized as

$$\begin{aligned} & \frac{y_\phi^2}{2\pi} \exp(4 \log(r_{12}/\alpha)) \int_\alpha \frac{d^2x_3}{\alpha^2} \langle \cos \sqrt{8}\phi_1 \mathcal{M}_2 \cos \sqrt{8}\phi_3 \rangle \\ &= \frac{y_\phi^2}{2\pi} \exp(4 \log(r_{12}/\alpha')) \int_{\alpha'} \frac{d^2x_3}{\alpha'^2} \langle \cos \sqrt{8}\phi_1 \mathcal{M}_2 \cos \sqrt{8}\phi_3 \rangle \\ & \quad - 2y_\phi^2 [1 - y_0 \log(r_{12}/\alpha)] dl. \end{aligned} \tag{24}$$

4.1.1. *Near the Gaussian fixed line.* We first treat the case where  $|y_\phi/y_0| \ll 1$ . Let us consider the two hybridized states between the marginal and  $\cos \sqrt{8}\phi$  fields:

$$\begin{aligned} A &= \mathcal{M} + a(y_\phi/y_0) \sqrt{2} \cos \sqrt{8}\phi \\ B &= \sqrt{2} \cos \sqrt{8}\phi + b(y_\phi/y_0)\mathcal{M}. \end{aligned} \tag{25}$$

*The orthogonal condition.* We consider the condition that the correlation function  $\langle A_1 B_2 \rangle_I$  stays zero under renormalization;

$$\begin{aligned} \langle A_1 B_2 \rangle_I &= (y_\phi/y_0) \exp(-4 \log(r_{12}/\alpha)) [a(1 - 2y_0 \log(r_{12}/\alpha)) + b] \\ & \quad - \frac{y_\phi}{2\pi} \int \frac{d^2x_3}{\alpha^2} \sqrt{2} [\langle \cos \sqrt{8}\phi_1 \mathcal{M}_2 \cos \sqrt{8}\phi_3 \rangle + ab(y_\phi/y_0)^2 (1 \leftrightarrow 2)] \\ & \quad + \text{higher order terms.} \end{aligned} \tag{26}$$

By using  $y_\phi(l) \simeq y_\phi(0) \exp(-y_0(0)l)$  and  $y_0(l) \simeq y_0(0)$ , the function defined as

$$F = \langle A_1 B_2 \rangle_I \exp(4 \log(r_{12}/\alpha)) \exp(y_0(0)l) (y_0(0)/y_\phi(0))$$

behaves approximately as a constant  $a + b$  for small enough  $y_0$  and  $y_\phi$ . In order to set  $\langle A_1 B_2 \rangle_I = 0$ , first of all  $a + b$  should be equal to zero. In addition, other terms may appear in the course of the renormalization. For the infinitesimal transformation  $\alpha' = \alpha e^{dl}$ , using equation (24), we obtain

$$F = F' + [-2ay_0 + (y_0/y_\phi)2\sqrt{2}y_\phi(1 + ab(y_\phi/\phi_0)^2)] dl \tag{27}$$

where  $F'$  is the function  $F$  with the new value of  $\alpha'$ . Notice that in the course of the renormalization of  $y_0 \log(r_{12}/\alpha)$ , the term  $y_\phi^2 \log(r_{12}/\alpha) dl$  appears; however this term is cancelled by the identical term in higher order expansions [8, 26]. Thus, the necessary conditions for  $F = 0$  under renormalization are

$$a + b = 0 \quad -2ay_0 + 2\sqrt{2}y_0(1 + ab(y_\phi/\phi_0)^2) = 0. \tag{28}$$

The solution of these equation yields

$$a = -b = \sqrt{2} + O((y_\phi/y_0)^2). \tag{29}$$

*Renormalized correlation function for the marginal-like field.* The correlation function of the marginal  $\mathcal{M}$ -like field is

$$\begin{aligned} \langle A_1 A_2 \rangle_I &= \exp(-4 \log(r_{12}/\alpha)) [1 + a^2(y_\phi/y_0)^2 (1 - 2y_0 \log(r_{12}/\alpha))] \\ & \quad - (y_\phi/y_0) \sqrt{2} a \frac{y_\phi}{2\pi} \int \frac{d^2x_3}{\alpha^2} [\langle \cos \sqrt{8}\phi_1 \mathcal{M}_2 \cos \sqrt{8}\phi_3 \rangle + (1 \leftrightarrow 2)]. \end{aligned} \tag{30}$$



Let us consider the function  $F = \langle A_1 A_2 \rangle_I \exp(4 \log(r_{12}/\alpha))$ . In the absence of  $y_\phi$ ,  $F$  reduces to the constant 1. For the infinitesimal transformation  $\alpha' = \alpha e^{dl}$ , using equation (24), we obtain

$$F = \exp([-2a^2(y_\phi/y_0)^2 y_0 + 2a^2(y_\phi/y_0)^2 y_0 + 4\sqrt{2}a(y_\phi/y_0)y_\phi]) dl \times F' \\ = \exp(8y_0(y_\phi/y_0)^2 dl) \times F'. \tag{31}$$

As a result,

$$R_0 \equiv \langle A_1 A_2 \rangle_I = C_0 \exp \left[ - \int_0^{\ln(r/\alpha)} dl [4 - 8y_0(l)(y_\phi/y_0)^2] \right]. \tag{32}$$

*Renormalized correlation function for the  $\cos\sqrt{8}\phi$ -like field.* The correlation function of the  $\cos\sqrt{8}\phi$ -like field is

$$\langle B_1 B_2 \rangle_I = \exp(-4 \log(r_{12}/\alpha)) [1 - 2y_0 \log(r_{12}/\alpha) + b^2(y_\phi/y_0)^2] \\ - (y_\phi/y_0) \sqrt{2}b \frac{y_\phi}{2\pi} \int \frac{d^2x_3}{\alpha^2} [(\cos\sqrt{8}\phi_1 \mathcal{M}_2 \cos\sqrt{8}\phi_3) + (1 \leftrightarrow 2)]. \tag{33}$$

Let us consider the function  $F = \langle B_1 B_2 \rangle_I \exp(4 \log(r_{12}/\alpha))$ . For the infinitesimal transformation  $\alpha' = \alpha e^{dl}$ ,

$$F = \exp([-2y_0 + (y_\phi/y_0)^2 y_0 (2b^2 + 4\sqrt{2}b)]) dl \times F' \\ = \exp([-2y_0 - 4y_0(y_\phi/y_0)^2]) dl \times F'. \tag{34}$$

As a result,

$$R_1 \equiv \langle B_1 B_2 \rangle_I = C_1 \exp \left[ - \int_0^{\ln(r/\alpha)} dl [4 + 2y_0(l)(1 + 2(y_\phi/y_0)^2)] \right]. \tag{35}$$

*4.1.2. Near the BKT transition line.* Next we treat the case near the BKT transition, where  $y_\phi = \pm y_0(1 + t)$ ,  $|t| \ll 1$ . With this parametrization,  $t$  plays the role of the deviation from the critical point, such as  $(T - T_c)/T_c$ . Let us consider the two combinations of the marginal and  $\cos\sqrt{8}\phi$  fields:

$$A = \mathcal{M} + a \sqrt{2} \cos\sqrt{8}\phi \quad B = \sqrt{2} \cos\sqrt{8}\phi + b\mathcal{M}. \tag{36}$$

*The orthogonal condition.* The correlation function  $\langle A_1 B_2 \rangle_I$  is obtained by setting  $y_\phi/y_0 = 1$  in the previous subsection. Let us consider the function  $F = \langle A_1 B_2 \rangle_I \exp(4 \log(r_{12}/\alpha))$ . The conditions for  $F = 0$  under renormalization are

$$a + b = 0 \quad -2ay_0 + 2\sqrt{2}y_\phi(1 + ab) = 0. \tag{37}$$

The solution of these equations yields

$$a = -b = \pm \frac{1}{\sqrt{2}} \quad \text{for } y_\phi = \pm y_0(1 + t). \tag{38}$$

*Renormalized correlation function for the marginal-like field.* Let us consider the function  $F = \langle A_1 A_2 \rangle_I \exp(4 \log(r_{12}/\alpha))/(1 + a^2)$ . For the infinitesimal transformation  $\alpha' = \alpha e^{dl}$ ,

$$F = \exp \left( \left[ \frac{-2a^2 y_0 + 4\sqrt{2} a y_\phi}{1 + a^2} \right] dl \right) \times F' \\ = \exp[2y_0(1 + \frac{4}{3}t) dl] \times F'. \tag{39}$$

As a result,

$$R_0 \equiv \langle A_1 A_2 \rangle_I = C_0 \exp \left[ - \int_0^{\ln(r/\alpha)} dl [4 - 2y_0(l)(1 + \frac{4}{3}t)] \right]. \tag{40}$$

Renormalized correlation function for the  $\cos\sqrt{8}\phi$ -like field. Let us consider the function  $F = \langle B_1 B_2 \rangle_I \exp(4 \log(r_{12}/\alpha))/(1 + b^2)$ . For the infinitesimal transformation  $\alpha' = \alpha e^{dl}$ ,

$$F = \exp\left(\left[\frac{-2y_0 + 4\sqrt{2}by_\phi}{1 + b^2}\right] dl\right) \times F'$$

$$= \exp[-4y_0(1 + \frac{2}{3}t) dl] \times F'. \tag{41}$$

As a result,

$$R_1 \equiv \langle B_1 B_2 \rangle_I = C_0 \exp\left[-\int_0^{\ln(r/\alpha)} dl [4 + 4y_0(l)(1 + \frac{2}{3}t)]\right]. \tag{42}$$

4.2. Correlation functions of the descendent fields

The renormalization calculations for the descendent fields ( $\partial O_{1,1}$  etc) are a straightforward extension of the method of Giamarchi and Schulz [26]:

$$\alpha^2 \langle (\bar{\partial} O_{1,1} + \partial O_{-1,1})(r_1) (\partial O_{1,-1} + \bar{\partial} O_{-1,-1})(r_2) \rangle_I$$

$$= \alpha^2 \langle \bar{\partial} O_{1,1}(r_1) \bar{\partial} O_{-1,-1}(r_2) \rangle + \alpha^2 \langle \partial O_{-1,1}(r_1) \partial O_{1,-1}(r_2) \rangle$$

$$- \frac{y_\phi}{2\pi} \int \frac{d^2x_3}{\alpha^2} \alpha^2 \langle \bar{\partial} O_{1,1}(r_1) \partial O_{1,-1}(r_2) O_{2,0}(r_3) \rangle. \tag{43}$$

The first two terms have been calculated in (14). Therefore, it is enough to estimate the divergent part of the integrand of the third term:

$$\alpha^2 \langle \bar{\partial} O_{1,1}(r_1) \partial O_{1,-1}(r_2) O_{2,0}(r_3) \rangle$$

$$= \left(\frac{z_{31}}{\alpha}\right)^{-2} \left(\frac{\bar{z}_{32}}{\alpha}\right)^{-2} \left[ \frac{1}{2} \left(y_0 - \frac{y_0^2}{4}\right) \frac{\alpha}{z_{12}} + \frac{1}{2} y_0 \frac{\alpha}{z_{31}} \right]$$

$$\times \left[ -\frac{1}{2} \left(y_0 - \frac{y_0^2}{4}\right) \frac{\alpha}{z_{12}} + \frac{1}{2} y_0 \frac{\alpha}{z_{32}} \right]$$

$$\times \exp\left[\pi i + \left(y_0 - \frac{y_0^2}{4}\right) \log(r_{12}/\alpha) - y_0 \log(r_{31}/\alpha) - y_0 \log(r_{32}/\alpha)\right]. \tag{44}$$

This expression diverges near  $r_{31} \ll r_{12}$  and  $r_{32} \ll r_{12}$ . In the case where  $r_{31} \ll r_{12}$  then  $z_{32}^{-1} \simeq z_{12}^{-1}(1 - z_{31}/z_{12})$  and, thus, the divergent part is

$$\frac{y_0^2}{4} \left|\frac{z_{31}}{\alpha}\right|^{-2-y_0} \left|\frac{z_{12}}{\alpha}\right|^{-4} \exp\left[-\frac{y_0^2}{4} \log(r_{12}/\alpha)\right]. \tag{45}$$

Note that only the terms which contain  $|z_{31}|^{-2}$  contribute to the divergence. The divergent part of the integrand near  $r_{32} \ll r_{12}$  is of the same form.

Let us consider the function

$$F = \langle (\bar{\partial} O_{1,1} + \partial O_{-1,1})(r_1) (\partial O_{1,-1} + \bar{\partial} O_{-1,-1})(r_2) \rangle_I \left(2\frac{y_0^2}{8} \left(1 + \frac{y_0^2}{8}\right)\right)^{-1}$$

$$\times \exp\left[\left(4 + \frac{y_0^2}{4}\right) \log(r_{12}/\alpha)\right] \tag{46}$$

which reduces to the constant 1 when  $y_\phi = y_0 = 0$ . Then, considering renormalization behaviour, we obtain, as before,

$$F = \exp(-2y_\phi dl) \times F'. \tag{47}$$

As a result,

$$\begin{aligned} R_5 &\equiv \alpha^2 \langle (\bar{\partial} O_{1,1} + \partial O_{-1,1})(r_1) (\partial O_{1,-1} + \bar{\partial} O_{-1,-1})(r_2) \rangle_I \\ &= C_5 \exp \left[ - \int_0^{\log(r_{12}/\alpha)} (4 + 2y_\phi(l)) dl \right] \end{aligned} \quad (48)$$

$$R_6 \equiv \alpha^2 \langle (\partial O_{1,-1} + \bar{\partial} O_{-1,-1})(r_1) (\bar{\partial} O_{1,1} + \partial O_{-1,1})(r_2) \rangle_I = R_5.$$

Except for the sign of  $y_\phi$ , the calculation is the same for the antisymmetric combination.

$$\begin{aligned} R_7 &\equiv -\alpha^2 \langle (\bar{\partial} O_{1,1} - \partial O_{-1,1})(r_1) (\partial O_{1,-1} - \bar{\partial} O_{-1,-1})(r_2) \rangle_I \\ &= C_7 \exp \left[ - \int_0^{\log(r_{12}/\alpha)} (4 - 2y_\phi(l)) dl \right] \end{aligned} \quad (49)$$

$$R_8 = R_7.$$

## 5. Eigenvalue structure

Conformal field theory [33, 34] is an efficient method for determining critical dimensions of 2D systems. One of the most useful applications of this theory is with respect to finite-size scaling. When we denote the transfer matrix of a strip of width  $L$  with periodic boundary condition by  $\exp(-H)$ , then the eigenvalues  $E_n$  are related to the scaling dimension  $x_n$  ( $= \eta_n/2$ ) as [35]:

$$E_n(L) - E_g(L) = \frac{2\pi x_n}{L} \quad (50)$$

in the limit of  $L \rightarrow \infty$ . However, this relation is exact only at the fixed point. In general, there are corrections resulting from the irrelevant (marginal) fields.

It is possible to relate the eigenvalues of the transfer matrix to the renormalized correlation functions obtained in the previous section. The renormalized critical exponents  $\eta_n(l)$  are related to the correlation functions as [32]:

$$R_n = \exp \left[ - \int_0^{\ln(r/a)} dl \eta_n(l) \right] \quad (51)$$

and by using equation (50), we obtain

$$\frac{L \Delta E_n}{2\pi} = x_n(l) = \frac{1}{2} \eta_n(l). \quad (52)$$

Although equation (50) is satisfied under the condition of scale invariance, we use the renormalization group to extend relation (50) to the region where the system size is much smaller than the bulk correlation length  $\xi$ . The renormalized critical dimensions are (close to the BKT transition)

$$\begin{aligned} x_0(l) &= 2 - y_0(l) \left(1 + \frac{4}{3}t\right) \\ x_1(l) &= 2 + 2y_0(l) \left(1 + \frac{2}{3}t\right) \\ x_2(l) &= 2 + y_0(l) \\ x_3(l) &= x_4(l) = 2 - y_0(l) \end{aligned} \quad (53)$$

and

$$\begin{aligned} x_5(l) &= x_6(l) = 2 + y_\phi(l) = 2 \pm y_0(1+t) \\ x_7(l) &= x_8(l) = 2 - y_\phi(l) = 2 \mp y_0(1+t). \end{aligned} \quad (54)$$

These results mean that on the BKT transition line (for example  $y_\phi(l) = y_0(l)$ ) the eigenvalues of the transfer matrix corresponding to the fields  $x_0(l)$ ,  $x_3(l)$ ,  $x_4(l)$  and  $x_7(l)$ ,  $x_8(l)$  become degenerate, as well as those corresponding to  $x_2(l)$  and  $x_5(l)$ ,  $x_6(l)$ . This  $SU(2)$  multiplets structure reflects the fact that the  $\beta^2 = 8\pi$  sine-Gordon model corresponds to the  $SU(2)$  massless Thirring model [22] or to the  $SU(2)$   $k = 1$  WZW model [24]. On the BKT line,  $y_0(l)$  is renormalized as  $y_0(l) \simeq 1/\log L$ . The ratios of the logarithmic correction terms in  $x_3(l)$ ,  $x_2(l)$  and  $x_1(l)$  are  $-1:1:2$ , in agreement with the  $SU(2)$   $k = 1$  WZW model [24]. Although the convergence of the logarithmic term is very slow, the ratios of the logarithmic corrections can be used to eliminate them [25, 28].

In the neighbourhood of the BKT transition line, in  $x_0(l)$ ,  $x_1(l)$  and  $x_5(l)$ ,  $x_6(l)$ ,  $x_7(l)$ ,  $x_8(l)$ , terms linear in the distance  $t$  from the BKT line appear, and their ratios are  $-\frac{4}{3}:\frac{4}{3}:1:-1$ , indicating new universal relations. Moreover,  $x_0(l) - x_3(l)$ , for example, is linear in  $t$ , a useful relation for determining the BKT critical line. This describes how the  $SU(2)$  symmetry breaks down to  $U(1) \times \mathbb{Z}_2$  in Abelian bosonization.

Close to the Gaussian fixed line, the only differences are

$$x_0(l) = 2 - 4y_0(l)(y_\phi(l)/y_0(l))^2 \quad x_1(l) = 2 + y_0(l)[1 + 2(y_\phi(l)/y_0(l))^2] \quad (55)$$

and therefore the ratios of the  $(y_\phi/y_0)^2$  terms are  $-4:2$ . In this case, the difference  $x_5(l) - x_7(l)$  is linear in the deviation from the Gaussian fixed line  $y_\phi$ , since they are interchanged under the transformation  $\phi \rightarrow \phi + \pi/\sqrt{8}$ . Furthermore, the difference  $x_1(l) - x_2(l)$  is quadratic in  $y_\phi$ . This relation may be used to determine the Gaussian fixed line.

Finally, we comment on the symmetry. The symmetry structure of the model (7) at  $y_0 = y_\phi = 0$  is  $SU(2) \times SU(2) \times \mathbb{Z}_2$ . The additional  $\mathbb{Z}_2$  symmetry is needed to inhibit the  $SU(2)$  symmetric relevant field [36]. In general, for an  $SU(n)$  critical model, an additional  $\mathbb{Z}_n$  symmetry is necessary to stabilize the massless phase [37]. On the BKT line where the chiral invariance is broken, the symmetry becomes  $SU(2) \times \mathbb{Z}_2 \times \mathbb{Z}_2$ .

In the usual BKT transition in which  $SU(2)$  symmetry is not explicit, the only difference is that the critical dimension of the descendent fields is  $\frac{25}{8}$ , so they are no longer marginal. Nevertheless, including the logarithmic term, a degeneracy remains between the  $\exp(\pm i\sqrt{8}\theta)$  fields and the marginal-like field on the BKT line which can be used to determine the BKT transition point from the eigenvalues.

## 6. Physical systems

The sine-Gordon model can be related to a variety of 1D quantum or 2D classical systems. As an example of the sine-Gordon model with an  $O(2) \times \mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry, we consider the  $S = 1/2$  XXZ spin chain with next-nearest neighbour interactions (NNNI). For the sine-Gordon model with a simple  $O(2) \times \mathbb{Z}_2$  symmetry, we treat a bond-alternation  $S = \frac{1}{2}$  XXZ spin chain. Finally, we treat the 2D classical  $p$ -clock model as an example of the sine-Gordon model with an  $O(2) \times \mathbb{Z}_2 \times \mathbb{Z}_p$  symmetry.

### 6.1. $S = \frac{1}{2}$ XXZ spin chain with next-nearest-neighbour interaction

In our previous works [27, 28], we studied the  $S = \frac{1}{2}$  XXZ spin chain with competing interactions:

$$H = \sum_{j=1}^L (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) + \alpha \sum_{j=1}^L (S_j^x S_{j+2}^x + S_j^y S_{j+2}^y + \Delta S_j^z S_{j+2}^z) \quad (56)$$

with the periodic boundary condition  $S_{L+1} = S_1$ ,  $L$  being the number of spins ( $L$  even).

This model is exactly solvable on the lines  $\alpha = 0$  and  $\alpha = \frac{1}{2}$ . On the line  $-1 < \Delta \leq 1, \alpha = 0$ , the ground state is the spin-fluid state, characterized by a gapless excitation spectrum and power-law decaying correlation functions. In the region  $\Delta > 1, \alpha = 0$ , this system is Néel ordered and it has a two-fold degenerate ground state with an energy gap [38, 39]. On the line  $\alpha = \frac{1}{2}$ , the ground state is purely dimerized [40, 41]. The existence of the energy gap and the uniqueness of the two-fold degenerate ground state have been proven [42]. The dimer state is characterized by the excitation gap, the exponential decay of the spin correlation function, and the dimer long-range order.

Let us examine the symmetry of the Hamiltonian (56). This model is invariant under spin rotation around the  $z$ -axis, translation ( $S_j^{x(y,z)} \rightarrow S_{j+1}^{x(y,z)}$ ), space inversion ( $S_j^{x(y,z)} \rightarrow S_{L-j+1}^{x(y,z)}$ ), spin reversal ( $S_j^z \rightarrow -S_j^z, S_j^\pm \rightarrow -S_j^\mp$ ), and conjugation ( $S_j^z \rightarrow S_j^z, S_j^\pm \rightarrow S_j^\mp$ ). Therefore, eigenstates are characterized by the  $z$ -component of the total spin ( $S_T^z = \sum S_j^z$ ), wavenumber ( $q = 2\pi k/L$ ), parity ( $P = \pm 1$ ), spin reversal ( $T = \pm 1$ ), and charge conjugation  $C$ . The charge conjugation  $C$  is redundant because of the identity  $CPT = 1$ , as will be shown later. For  $L = 4n$ , the ground state is a singlet ( $S_T^z = 0, q = 0, P = 1, T = 1$ ). The symmetries of several low-energy excitations are classified in table 1. The operators in spin representation are also shown.

**Table 1.** Identification of eigenstates of the XXZ spin model in the sine-Gordon language.

$q$	Symmetries of eigenstate			Identification in spin language	Identification in sine-Gordon model
	$S_T^z$	$T$	$P$		
0	0	1	1	1	1
$\pi$	1	*	-1	$(-1)^j S_j^+$	$O_{0,1}$
$\pi$	0	-1	-1	$(-1)^j S_j^-$	$O_{1,0} + O_{-1,0} = 2 \cos \sqrt{2}\phi$
$\pi$	0	1	1	$(-1)^j (S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+)$	$\frac{1}{2}[O_{1,0} - O_{-1,0}] = 2 \sin \sqrt{2}\phi$
$2\pi/L$	0	-1	*	$\exp(2\pi i j/L) S_j^z$	$\partial\phi$
$2\pi/L$	1	*	*	$\exp(2\pi i j/L) S_j^+$	$O_{1,1}$
0	2	*	1	$S_j^+ S_{j+1}^+$	$O_{0,2}$
0	1	*	1	$S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+$	$\bar{\partial}O_{1,1} + \partial O_{-1,1}$
0	0	1	1	a part of the Hamiltonian	$\mathcal{M}$
0	1	*	-1	$S_j^+ S_{j+1}^+ S_{j+2}^- - S_j^- S_{j+1}^- S_{j+2}^+$	$\frac{1}{4}[\bar{\partial}O_{1,1} - \partial O_{-1,1}]$
0	0	-1	-1	$S_j^z (S_{j+1}^+ S_{j+2}^- + S_{j+1}^- S_{j+2}^+)$	$\frac{1}{4}[O_{2,0} - O_{-2,0}]$
0	0	1	1	$-(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+) S_{j+2}^z$	
0	0	1	1	a part of the Hamiltonian	$O_{2,0} + O_{-2,0}$

Next we consider a corresponding sine-Gordon model. After a Jordan-Wigner transformation, the model (56) is transformed to the 1D spinless fermion system. Its continuum limit is a Tomonaga-Luttinger liquid [43] or, equivalently, a sine-Gordon model [44]. Using the same procedure, we associate expressions in the sine-Gordon model with the spin operators (table 1). The marginal-like field and the  $\cos \sqrt{8}\phi$ -like field are parts of the Lagrangian, so they have the same symmetry as the ground state and the corresponding spin operators are parts of the Hamiltonian with the same symmetry. Except for the Gaussian fixed line, a hybridization occurs between the marginal and the  $\cos \sqrt{8}\phi$  fields. Note that the fields in the sine-Gordon model are defined on the infinite plane, whereas operators in the spin model are defined on the cylinder. The former can be mapped to the latter by  $f(z) = L/2\pi \log(z)$ . The symmetry operation in the sine-Gordon model corresponding to

the spin reversal ( $T$ ) is

$$\phi \rightarrow -\phi + \pi/\sqrt{2} \quad \theta \rightarrow -\theta + \pi/\sqrt{2} \tag{57}$$

the operation corresponding to the space inversion ( $P$ ) is

$$\phi \rightarrow -\phi + \pi/\sqrt{2} \quad \theta \rightarrow \theta + \pi/\sqrt{2} \quad z \rightarrow \bar{z} \tag{58}$$

and the operation corresponding to the charge conjugation ( $C$ ) is

$$\phi \rightarrow \phi \quad \theta \rightarrow -\theta \quad z \rightarrow \bar{z}. \tag{59}$$

Therefore, successive transformations yield the identity  $CPT = 1$ . In addition, the operation corresponding to the translation by one site is

$$\phi \rightarrow \phi + \pi/\sqrt{2} \quad \theta \rightarrow \theta + \pi/\sqrt{2}. \tag{60}$$

The symmetry breaking is related to the phase transition as follows. In the spin-fluid region, no symmetry breaking occurs because  $y_\phi$  is renormalized to zero. In the dimer region  $y_\phi \rightarrow +\infty$  and, therefore, one has a long-range order in the  $\phi$  field, whereas correlations of  $\theta$  decay exponentially. The average value of the ordered field is  $\langle \phi \rangle = \pi/\sqrt{8}$ . In the spin system this means that there is symmetry breaking of the translation invariance. In the Néel region  $y_\phi \rightarrow -\infty$ ,  $\langle \phi \rangle = 0$ . This corresponds to the symmetry breaking of the translation invariance, space inversion and spin reversal.

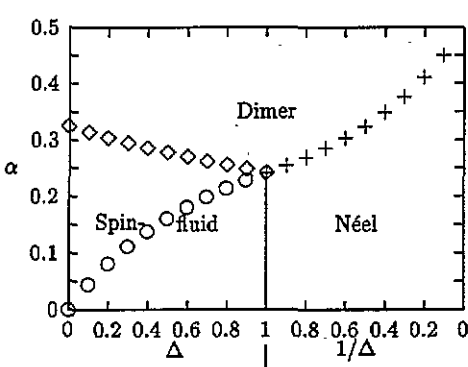


Figure 1. Phase diagram of the  $S = \frac{1}{2}$  NNNI model. Néel-dimer critical points (+); dimer-fluid critical points ( $\diamond$ ); Gaussian fixed points ( $\circ$ ).

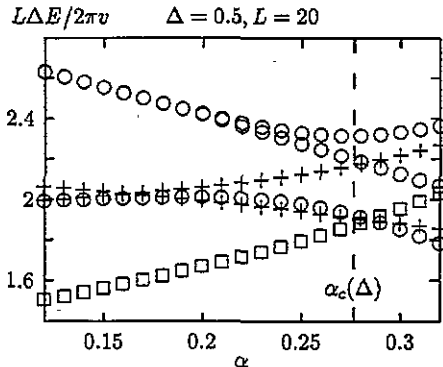
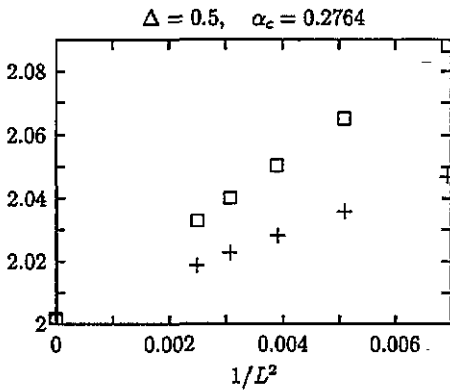


Figure 2. The normalized excitation energies.  $S_T^Z = 0$  ( $\circ$ );  $S_T^Z = \pm 1$ ; (+);  $S_T^Z = \pm 2$  ( $\square$ ).

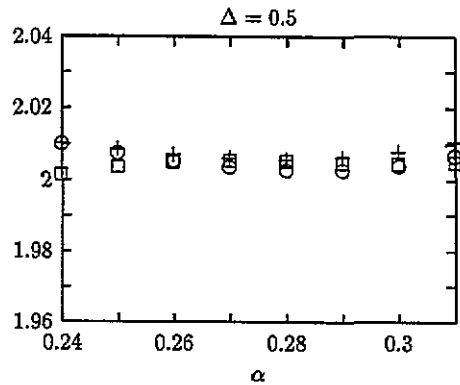
We compare the renormalization calculations in sections 4 and 5 with numerical results. The whole phase diagram is shown in figure 1. The normalized excitations  $L\Delta E/2\pi v$  for  $\Delta = 0.5$  are shown in figure 2. The general behaviour is consistent with the renormalization results. One sees that  $SU(2)$  symmetry appears on the BKT line [28]. Next we investigate the ratios of logarithmic terms. On the BKT line ( $t = 0$ ), by using equations (53) and by taking the averages

$$\frac{1}{2}[x_2(l) + x_3(l)] \quad \frac{1}{3}[x_1(l) + 2x_3(l)] \tag{61}$$

we can eliminate the contribution of the logarithmic corrections, and at the same time we can confirm their ratios. In figure 3 these averages are shown as a function of system size  $L$ . As expected, they converge to a value of two. The  $1/L^2$  corrections are due to the irrelevant field  $L_{-2}\bar{L}_{-2}1$  ( $x = 4$ ) [35]. The extrapolated values are taken to be two within a 0.2% error, compared with the bare values of  $x_n(l)$  (5–15% error). Finally, we examine



**Figure 3.** The ratios of logarithmic terms. By taking the averages  $\frac{1}{2}[x_2(l) + x_3(l)]$  (□) and  $\frac{1}{3}[x_1(l) + 2x_3(l)]$  (+), the logarithmic terms cancel each other.



**Figure 4.** The ratios of terms linear in  $t$ . By taking the averages  $\frac{1}{3}[x_0(l) + x_1(l) + x_3(l)]$  (○),  $\frac{1}{2}[x_5(l) + x_7(l)]$  (+) and  $\frac{1}{2}[\frac{3}{4}x_0(l) + x_7(l) + \frac{1}{4}x_3(l)]$  (□), the  $t$  linear terms cancel each other.

the ratios of the terms linear in  $t$  of the critical dimensions. From equations (53) and (54), by taking the averages

$$\frac{1}{3}[x_0(l) + x_1(l) + x_3(l)] \quad \frac{1}{2}[x_5(l) + x_7(l)] \quad \frac{1}{2}[\frac{3}{4}x_0(l) + x_5(l) + \frac{1}{4}x_3(l)] \quad (62)$$

the terms linear in  $t$  should be annihilated. In fact, as is shown in figure 4, in the neighbourhood of the critical point  $\alpha_c = 0.2764$ , the linear components of  $t$  are almost absent (the points have already been extrapolated as  $1/L^2$ ). The coefficients of the terms linear in  $t$  are at least  $10^{-2}$  less than those in the raw data  $x_n(l)$ .

**6.2. Bond-alternation  $S = \frac{1}{2} XXZ$  spin chain**

This model is described by the Hamiltonian

$$H = \sum_j (1 + \delta(-1)^j)(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z). \quad (63)$$

After bosonization, we obtain

$$\mathcal{L} = \frac{1}{2\pi K} (\nabla\phi)^2 + \frac{y_\phi}{2\pi\alpha^2} \sin\sqrt{2}\phi. \quad (64)$$

The correspondence between the spin model and the sine-Gordon model is the same as before (table 1). The symmetry structure in this model is a simple  $O(2) \times \mathbb{Z}_2$ . At  $\Delta = -1/\sqrt{2}$  and  $\delta = 0$ , the critical dimension of  $\sin\sqrt{2}\phi$  becomes marginal. Therefore, in the neighbourhood of this point, the BKT transition appears [45]. Although higher terms such as  $\cos\sqrt{8}\phi$  exist, we neglect them for simplicity.

After a simple transformation of the fields  $\phi \rightarrow 2\phi$ ,  $\theta \rightarrow \theta/2$ , we can use the results of sections 4 and 5, except that the critical dimension of the descendent fields is  $x = \frac{25}{8}$  at  $y_0 = y_\phi = 0$ . The corresponding spin operators, which become marginal at  $y_0 = y_\phi = 0$ , are  $(-1)^j S_j^z$ ,  $(-1)^j (S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+)$ ,  $S_j^+ S_{j+1}^+ S_{j+2}^+ S_{j+3}^+$  ( $S_1^z = 4, q = 0, P = 1$ ) and the operator corresponding to the marginal field.

In the spin-fluid region,  $y_\phi$  is renormalized to zero so that symmetry breaking does not occur. As for the region where  $y_\phi$  flows to infinity, one has long-range order of the  $\phi$  field ( $\phi \rightarrow \mp\pi/\sqrt{8}$  for  $y_\phi \rightarrow \pm\infty$ ). Via the symmetry considerations of the previous subsection, this corresponds to breaking the translation symmetry. However, since the

translation invariance is already broken in the original model, there is no spontaneous symmetry breaking in the whole region.

### 6.3. *p*-clock model

We consider the case of the  $O(2) \times \mathbb{Z}_2 \times \mathbb{Z}_p$  symmetric sine-Gordon model

$$\mathcal{L} = \frac{1}{2\pi K} (\nabla\phi)^2 + \frac{y_\phi}{2\pi\alpha^2} \cos p\sqrt{2}\phi. \tag{65}$$

This is invariant under  $\phi \rightarrow \phi + 2\pi/p\sqrt{2}$ , i.e. shifting the circle coordinate  $\phi$  by  $1/p$  times its period ( $2\pi/\sqrt{2}$ ). The  $\cos p\sqrt{2}\phi$  term becomes marginal at  $y_\phi = 0$ ,  $K = 4/p^2$ . By parametrizing  $Kp^2/4 = 1 + y_0/2$ , the renormalization equations are the same as (8). There are three fields that are marginal at  $y_0 = y_\phi = 0$ , namely,  $\cos p\sqrt{2}\phi$ ,  $\sin p\sqrt{2}\phi$  and  $\mathcal{M}$ . Their renormalization behaviour has been described in sections 4 and 5. There is no degeneracy on the BKT line. However, the renormalized critical dimension for  $O_{0,m}$  [26] is

$$x'_m(l) = \frac{m^2 p^2}{8} (1 - \frac{1}{2}y_0(l)). \tag{66}$$

Therefore, the ratio of  $x_0(l)$  and  $x'_m(l)$  is  $2:m^2 p^2/8$ , including logarithmic corrections. This may be used to determine the BKT critical line because  $x_0(l) - 16x'_m(l)/m^2 p^2$  is linear in the deviation  $t$  from the BKT line. The ratios of the logarithmic corrections are useful in determining the critical dimensions and in checking the consistency.

When  $p$  is even, an additional relation appears. The renormalized critical dimension for  $\cos p\phi/\sqrt{2}$  is [26]

$$\begin{aligned} x'(l) &= \frac{1}{2}(1 + \frac{1}{2}y_0(l) + y_\phi(l)) \\ &= \begin{cases} \frac{1}{2}(1 + \frac{3}{2}y_0(l)(1 + \frac{2}{3}t)) & \text{for } y_\phi = y_0(1 + t) \\ \frac{1}{2}(1 - \frac{1}{2}y_0(l)(1 + 2t)) & \text{for } y_\phi = -y_0(1 + t) \end{cases} \end{aligned} \tag{67}$$

and the renormalized critical dimension for  $\sin p\phi/\sqrt{2}$  is

$$x'(l) = \begin{cases} \frac{1}{2}(1 - \frac{1}{2}y_0(l)(1 + 2t)) & \text{for } y_\phi = y_0(1 + t) \\ \frac{1}{2}(1 + \frac{3}{2}y_0(l)(1 + \frac{2}{3}t)) & \text{for } y_\phi = -y_0(1 + t). \end{cases} \tag{68}$$

Therefore, the lower part of these relations can be used to determine the BKT line as  $x_0(l) - 4x'(l)$ .

What are the corresponding real systems? One candidate is the  $p$ -clock model [12] in which the spins at each site can take only  $p$  discrete angles  $2\pi l/p$ ,  $l = 1, \dots, p$ . The 2D classical Hamiltonian is such that

$$H = -K \sum_{\langle r, r' \rangle} \cos \frac{2\pi}{p} [l(r) - l'(r')] \tag{69}$$

where the sums over  $r$  index the sites of a 2D lattice, the symbol  $\langle r, r' \rangle$  indicates a sum over nearest-neighbour lattice sites only, and  $K = J/k_B T$ .

José *et al* [12] showed that  $\mathbb{Z}_p$  perturbations on the 2D XY model are irrelevant for a range of temperatures below the critical temperature  $T_c$  of the 2D XY model, provided  $p > 4$ . Thus, these models should undergo two phase transitions as a function of temperature. For  $T < T_{c1}$ , the  $\mathbb{Z}_p$  symmetry is broken and the correlation length is finite. For  $T_{c1} < T < T_{c2}$  the symmetry is unbroken and the correlation length  $\xi$  is infinite, while for  $T > T_{c2}$  we have a disordered phase with a finite  $\xi$ . Elitzur *et al* [46] showed that this is also the behaviour of the pure  $\mathbb{Z}_p$  clock model in which the strength of the above mentioned breaking term



is infinite. In considering the  $\mathbb{Z}_p$  invariant Villain-type model [11], they established the existence of the intermediate massless phase using self-duality and Griffiths-type inequalities [47, 48].

From renormalization group considerations [12, 46] the  $\mathbb{Z}_p$  model corresponds to the sine-Gordon model as follows. The upper critical point  $T_{c2}$  is described by the usual  $O_2 \times \mathbb{Z}_2$  BKT transition, whereas the universality class of the lower critical point  $T_{c1}$  is the  $O_2 \times \mathbb{Z}_2 \times \mathbb{Z}_p$  BKT transition described in this subsection.

We add here a comment on the antiferromagnetic (AF)  $\mathbb{Z}_p$  clock models with  $p$  odd. These models have a high degree of degeneracy in the ground state. According to Berker and Kadanoff [49], in such a system a critical low-temperature phase may appear, with an infinite correlation length, similar to the 2D XY model. In contrast, Cardy [50] claimed that AF  $\mathbb{Z}_p$  models with  $p$  odd belong to the same universality class as F  $\mathbb{Z}_{2p}$  clock models, so that there is an ordered low-temperature phase with  $\mathbb{Z}_{2p}$  symmetry breaking. However, this argument was criticized by den Nijs [51]. At  $T = 0$  the model reduces to the six-vertex model at the so called ice point, which means that zero temperature would be located inside the intermediate massless phase of the  $\mathbb{Z}_{2p}$  clock models and, therefore, there is no  $\mathbb{Z}_{2p}$  symmetry breaking.

## 7. Conclusions: level spectroscopy

The idea that the level crossings of the low-energy excitations can be used to determine the critical point (hereafter called ‘level spectroscopy’) originates from the work by Giamarchi and Schulz [26] who studied how the sine-Gordon model becomes  $SU(2)$  symmetric on the BKT line from the anisotropic phase. This was used for the problem of the  $S = \frac{1}{2}$  NNNI spin chain [28]. Another technique, namely taking the appropriate average of the eigenvalues to eliminate logarithmic corrections, comes from the work by Ziman and Schulz [25] who studied the  $S = \frac{3}{2}$  isotropic spin chain on the basis of conformal field theory and the renormalization group. In this paper we have developed these methods to the case where  $SU(2)$  symmetry is not apparent on the BKT line by considering the hybridization between the marginal and the  $\cos\sqrt{8}\phi$  fields.

The level spectroscopy method is completely different from the finite-size scaling method [52, 53]; and for the BKT problem the former is superior to the latter. In finite-size scaling one uses the data from several lengths to construct a scaling flow relation and to search the fixed point. However, in the BKT problem there are continuous fixed points below the critical temperature, so it is difficult to determine the BKT critical point by the finite-size scaling. Moreover, there is the problem that the correlation length diverges singularly, and of the logarithmic corrections. In fact, as was noticed by Bonner and Müller [54], Sólyom and Ziman [55], and in [27, 28], the finite-size scaling method may lead to false conclusions for the BKT-type transition, at least for the simple  $S = \frac{1}{2}$  XXZ chain where exact results are known by the Bethe ansatz. Naively implemented finite-size scaling would predict the critical point  $\Delta_c = 0.4-0.5$ , although it is known to be exactly  $\Delta_c = 1$ . In addition, Roomany-Wyld approximants for the  $\beta$  function [56, 57], which converge remarkably quickly for the conventional second-order transition, converge slowly to an infinite limit in the  $S = \frac{1}{2}$  XXZ case [55].

In contrast, in level spectroscopy the symmetry structure of the eigenvalues of the transfer matrix is used to determine the critical point and to obtain the critical dimensions. The renormalization process is already performed explicitly, not by the numerical data. Moreover, the singular behaviour of correction terms can be eliminated. In principle only the data at one length are needed. Generally there are corrections from the irrelevant field

$L_{-2}\bar{L}_{-2}1(x=4)$  and, therefore, extrapolations are needed. Nevertheless the convergences are extremely fast.

Finally, although it is possible to consider the sine-Gordon model with  $O(2) \times \mathbb{Z}_2 \times \mathbb{Z}_p$  symmetry, the  $SU(2)$  symmetry appears on the BKT line only in the  $O(2) \times \mathbb{Z}_2 \times \mathbb{Z}_2$  case. Such a symmetry does not occur in other cases. The usual  $O(2) \times \mathbb{Z}_2$  BKT critical point is also special, because at this point the Gaussian and the orbifold model are equivalent [29, 30].

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