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$SU(2)/Z_2$ symmetry of the BKT transition and twisted boundary condition

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Abstract. The Berezinskii–Kosterlitz–Thouless (BKT) transition, the transition of the two-dimensional sine-Gordon model, plays an important role in low-dimensional physics. We relate the operator content of the BKT transition to that of the $SU(2)$ Wess–Zumino–Witten model, using twisted boundary conditions. With this method, in order $k-1$ to determine the BKT critical point, we can use the level crossing of the lower excitations instead of those for the periodic boundary case, thus the convergence to the transition point is highly improved. We verify the efficiency of this method by applying it to the $S=1$, 2 spin chains.

1. Introduction

The Berezinskii–Kosterlitz–Thouless (BKT) transition [1–3] plays an important role in 2D classical and one-dimensional (1D) quantum systems, such as the 2D XY spin model, 2D helium film, 2D superconducting film, roughening transition, 1D quantum spin models and 1D electron systems. Furthermore, the BKT transition is a typical instability of the Tomonaga–Luttinger liquid, such as the Mott transition in 1D metal [4].

It was a difficult problem to determine numerically the critical point and the universality class of the BKT transition, because of logarithmic corrections and the slow divergence of the inverse correlation length (or the energy gap) [5]. Moreover, it is hard to distinguish the BKT transition from the second-order transition, by using the conventional finite-size-scaling method [6, 7]. In fact, for the exactly solvable $S=\frac{1}{2}$ XXZ spin chain, where the transition at $\Delta=1$ is of the BKT type, the finite-size scaling method leads to false conclusions [8]. This problem was successfully resolved by the level spectroscopy [9], based on the renormalization group calculation and the $SU(2)/Z_2$ symmetry in the BKT transition.

The $SU(2)$ symmetry inherent in the BKT transition was pointed out by Halpern [10] and Banks *et al* [11]. They showed the equivalence between the $SU(2)$ massless Thirring model and the theory of the bosons consisting of a free field plus a $\beta^2=8\pi$ sine-Gordon model, which corresponds to the BKT line. Another approach was proposed by Ginsparg [12], based on the $c=1$ conformal field theory: modding out the $SU(2)$ symmetry model by Z_2 symmetry gives the structure of the BKT multicritical point.

In this paper we directly relate the $SU(2)/Z_2$ structure of the operator content of the BKT transition to that of the $k=1$ $SU(2)$ Wess–Zumino–Witten (WZW) model, using twisted boundary conditions (TBC). With this method, in order to determine the BKT critical point, we can use the level crossing of the lower excitations than those under the periodic boundary conditions (PBC), thus the convergence to the transition point is highly improved. We then apply the method to the $S = 1$, 2 spin chains.

2. BKT transition and twisted boundary condition

2.1. On the Gaussian line

We consider the 2D Gaussian model defined as the Lagrangian

$$\mathcal{L}_0 = \frac{1}{2\pi K}(\nabla\phi)^2. \tag{1}$$

We compactify ϕ on a circle as $\phi \equiv \phi + 2\pi/\sqrt{2}$. We introduce the dual field θ to ϕ defined as

$$\partial_x\phi = -\partial_y(\mathrm{i}K\theta) \qquad \partial_y\phi = \partial_x(\mathrm{i}K\theta) \tag{2}$$

which has the periodic nature $\theta \equiv \theta + 2\pi/\sqrt{2}$.

The vertex operator defined as

$$O_{m,n} =: \exp(\mathrm{i}m\sqrt{2}\phi)\exp(\mathrm{i}n\sqrt{2}\theta) \tag{3}$$

has a scaling dimension $x_{m,n}$ and a conformal spin $s_{m,n}$

$$x_{m,n}(K) = \frac{1}{2}\left(m^2K + \frac{n^2}{K}\right) \qquad s_{m,n} = mn. \tag{4}$$

There are other types of fields, i.e. the current fields

$$\frac{2\mathrm{i}}{\sqrt{K}}\partial\phi \qquad \frac{2\mathrm{i}}{\sqrt{K}}\bar{\partial}\phi \tag{5}$$

which have $x = 1, s = \pm 1$, and the marginal field

$$\mathcal{M} = -\frac{4}{K}\partial\phi\bar{\partial}\phi = -\frac{1}{K}\left((\partial_x\phi)^2 + (\partial_y\phi)^2\right) \tag{6}$$

which has $x = 2, s = 0$. There also exist descendant fields of them.

About the symmetry, the Gaussian model (1) is invariant under $\phi \to \phi +$constant, $\theta \to \theta +$ constant, which means the $U(1) \times U(1)$ continuous symmetry. There are also the discrete Z_2 symmetries, $T : (z, \phi, \theta) \to (z, -\phi, -\theta)$ and $C : (z, \phi, \theta) \to (\bar{z}, \phi, -\theta)$ (we can also define the redundant symmetry $P = CT : (z, \phi, \theta) \to (\bar{z}, -\phi, \theta)$). The Gaussian model is invariant under the dual transformation $K \leftrightarrow 1/K$, $\phi \leftrightarrow \theta$. The self-dual point $K = 1$ is nothing but the $k = 1$ $SU(2) \times SU(2)$ WZW model, whose symmetry structure is apparent in the conformal dimensions of the vertex, the current, the marginal operators and their descendants. At the point $K = 1$, the number of the marginal operator ($x = 2, s = 0$) is 9.

The $K = 4$ is the BKT multicritical transition point, where the number of the marginal operator ($x = 2, s = 0$) is 5. The correspondence of the scaling dimensions for the WZW point ($K = 1$) with those for the BKT point ($K = 4$) is given by

$$x_{2m,n}(1) = x_{m,2n}(4) \tag{7}$$

and

$$x_{m,2n}(1) = x_{n,2m}(4). \tag{8}$$

Therefore, there is a partial correspondence of the operator content of these two models, reflecting the Z_2 symmetry difference.

Fortunately, introducing a half-integer magnetic charge, one can obtain the full correspondence of the $K = 1$ and $K = 4$ Gaussian models. With twisted boundary conditions on a cylinder, or the cut from 0 to infinity on the complex plane, one can set the arbitrary charges at $\pm\infty$ (on the cylinder) or at $0, \infty$ (on the complex plane) [13–15] (see appendix A). The relation between the twisted boundary condition and the change of the charges has been observed in the Bethe ansatz solvable $S = \frac{1}{2}$ XXZ spin chain [16]. Therefore, with the twist angle $\Phi = \pi$, one can introduce a half-magnetic charge. In that case, we can set

$$x^{\mathrm{TBC}}_{m,n}(K) = x_{m+1/2,n}(K). \tag{9}$$

Then, we obtain

$$x_{2m+1,n}(1) = x^{\mathrm{TBC}}_{m,2n}(4) \tag{10}$$

and

$$x^{\mathrm{TBC}}_{m,2n}(1) = x_{n,2m+1}(4), x^{\mathrm{TBC}}_{m,2n+1}(1) = x^{\mathrm{TBC}}_{n,2m+1}(4) \tag{11}$$

so that we can see the correspondence of all the operator content of $K = 1$ and $K = 4$ points, considering twisted boundary conditions.

2.2. Renormalization

Next we introduce the sine-Gordon-type interaction, that is,

$$\mathcal{L}_I = \frac{y_\phi}{2\pi\alpha^2} : \cos\sqrt{8}\phi : \text{ (for } K = 1) \qquad \frac{y_\phi}{2\pi\alpha^2} : \cos\sqrt{2}\phi : \text{ (for } K = 4) \tag{12}$$

(where α is a short-distance (ultraviolet) cut-off). Here we assume that there is no $\cos\sqrt{2}\phi$ interaction term for the $K = 1$ case, by the symmetry reason (discrete symmetry $\phi \to \phi + \pi/\sqrt{2}$ which corresponds to 'translation by one site' in the half-odd integer spin chain [17]) or adjusting parameters. With the simple transformation $\phi \to 2\phi, \theta \to \theta/2$ or $m \to 2m, n \to n/2$, the sine-Gordon model for $K = 4$ becomes equivalent to the sine-Gordon model for $K = 1$.

About the symmetry, the $U(1)$ symmetry of ϕ is explicitly broken to the discrete symmetry $\phi \to \phi + 2\pi/\sqrt{8} (K = 1)$ or $\phi \to \phi + 2\pi/\sqrt{2} (K = 4)$. Furthermore, the Lagrangian (1) is invariant under $\phi \to \phi + \pi/\sqrt{8}, y_\phi \to -y_\phi (K = 1)$ or $\phi \to \phi + \pi/\sqrt{2}, y_\phi \to -y_\phi (K = 4)$.

Under a change of cut-off $\alpha \to \mathrm{e}^l\alpha$, the renormalization group equations for the sine-Gordon model are [3]

$$\begin{aligned} \frac{\mathrm{d}y_0(l)}{\mathrm{d}l} &= -y_\phi^2(l) \\ \frac{\mathrm{d}y_\phi(l)}{\mathrm{d}l} &= -y_\phi(l)y_0(l) \end{aligned} \tag{13}$$

where $K = 1 + y_0/2$ (around $K = 1$) or $K = 4(1 + y_0/2)$ ($K = 4$). For the finite system, l is related to the system size L by $l = \log(L/\alpha)$. There are three critical lines; $y_\phi = 0$ corresponding to the Gaussian fixed line, and $y_\phi = \pm y_0 (y_0 > 0)$ corresponding to the BKT lines. On the BKT lines, the couplings behave as $y_0(l) = \pm y_\phi(l) = 1/(l + 1/y_0(0)) = 1/\log(L/L_0)$. In the region between the two BKT lines, 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.

Although the renormalization group flow is the same between the $K = 1$ and the $K = 4$ cases, the operator content is different, and in general the correspondences (8), (11) are not

Table 1. Operator content of the sine-Gordon (s-G) model at $K = 1$ and $K = 4$. Here we consider the BKT transition of the $y_\phi(l) = y_0(l)$ branch, and we denote the deviation t from the BKT critical line as $y_\phi(l) = y_0(l)(1+t)$ (for the $y_\phi(l) = -y_0(l)(1+t)$ branch, the role of operators $x^{p0} \leftrightarrow x^{p3}$, $x^{m5,m6} \leftrightarrow x^{m7,m8}$ interchanges).

	Operator in s-G model ($K=1$)	Operator in s-G model ($K=4$)	Renormalized scaling dimension	Dicrete symmetries[b]
x^{p0}	$O_{1,0}+O_{-1,0}$	$O_{1/2,0}+O_{-1/2,0}$(TBC)	$\frac{1}{2}+\frac{3}{4}y_0(l)(1+\frac{2}{3}t)$	$P=T=1$
$x^{p1,p2}$	$O_{0,\pm1}$	$O_{0,\pm2}$	$\frac{1}{2}-\frac{1}{4}y_0(l)$	$P=1$
x^{p3}	$O_{1,0}-O_{-1,0}$	$O_{1/2,0}-O_{-1/2,0}$(TBC)	$\frac{1}{2}-\frac{1}{4}y_0(l)(1+2t)$	$P=T=-1$
x^{c0}	$\frac{2\mathrm{i}}{\sqrt{K}}\partial\phi$	$\frac{2\mathrm{i}}{\sqrt{K}}\partial\phi$	1	
$x^{c1,c2}$	$O_{\pm1,\pm1}$	$O_{\pm1/2,\pm2}$(TBC)	1	
x^{m0}	$-\frac{4}{K}\partial\phi\bar{\partial}\phi$	$-\frac{4}{K}\partial\phi\bar{\partial}\phi$	$2-y_0(l)(1+\frac{4}{3}t)$	$P=T=1$
x^{m1}	$O_{2,0}+O_{-2,0}$	$O_{1,0}+O_{-1,0}$	$2+2y_0(l)(1+\frac{2}{3}t)$	$P=T=1$
x^{m2}	$O_{2,0}-O_{-2,0}$	$O_{1,0}-O_{-1,0}$	$2+y_0(l)$	$P=T=-1$
$x^{m3,m4}$	$O_{0,\pm2}$	$O_{0,\pm4}$	$2-y_0(l)$	$P=1$
$x^{m5,m6}$	$\bar{\partial}O_{\pm1,\pm1}+\partial O_{\mp1,\pm1}$	$\bar{\partial}O_{\pm1/2,\pm2}+\partial O_{\mp1/2,\pm2}$(TBC)	$2+y_0(l)(1+t)$	$P=1$
$x^{m7,m8}$	$\bar{\partial}O_{\pm1,\pm1}-\partial O_{\mp1,\pm1}$	$\bar{\partial}O_{\pm1/2,\pm2}-\partial O_{\mp1/2,\pm2}$(TBC)	$2-y_0(l)(1+t)$	$P=-1$

P, T should be interpreted as $U_{2\pi}T, U_{2\pi}P$ under TBC.
Strictly speaking, the operators (x^{m0}, x^{m1}) are hybridized under renormalization.

satisfied, since the duality relation $K \leftrightarrow 1/K$ does not hold on the BKT lines $y_\phi = \pm y_0$. Fortunately, the correspondences (7), (10) remain correct after the renormalization, since the operator product expansion (OPE) structure of both cases is the same, for example,

$$\begin{array}{rcl} K=1 & & K=4 \\ \langle\cos\sqrt{2}\phi\cos\sqrt{8}\phi\cos\sqrt{2}\phi\rangle & \leftrightarrow & \langle\cos\phi/\sqrt{2}\cos\sqrt{2}\phi\cos\phi/\sqrt{2}\rangle \\ \langle\sin\sqrt{2}\phi\cos\sqrt{8}\phi\sin\sqrt{2}\phi\rangle & \leftrightarrow & \langle\sin\phi/\sqrt{2}\cos\sqrt{2}\phi\sin\phi/\sqrt{2}\rangle \\ \langle\cos\sqrt{8}\phi\mathcal{M}\cos\sqrt{8}\phi\rangle & \leftrightarrow & \langle\cos\sqrt{2}\phi\mathcal{M}\cos\sqrt{2}\phi\rangle \end{array} \tag{14}$$

which can be seen by the mapping $\phi \to 2\phi, \theta \to \theta/2$ (similarly, higher OPEs are the same). The renormalized scaling dimensions are determined by these OPEs [18, 9] (see appendix B). Therefore, using twisted boundary conditions, we can explicitly see the $SU(2)$ structure inherent in the BKT transition.

In table 1 we summarize the operator content of the WZW ($K = 1$) model and that of the BKT ($K = 4$) model, with renormalized scaling dimensions. Note that at the BKT critical line ($y_\phi(l) = y_0(l)$), there are degeneracies of the excitations corresponding to $x^{p1,p2}$, x^{p3} or x^{m0}, $x^{m3,m4}$, $x^{m7,m8}$ or x^{m2}, $x^{m5,m6}$, respectively, reflecting the $SU(2)$ ($SU(2)/Z_2$) symmetry (for the $y_\phi(l) = -y_0(l)$ branch, the role of operators $x^{p0} \leftrightarrow x^{p3}, x^{m5,m6} \leftrightarrow x^{m7,m8}$ interchanges). Thus the level crossing of them can be used to determine the BKT critical point.

In practical systems, there are corrections from the descendant fields of the identity operator $\mathbf{1}$. The most important irrelevant fields in them are $L_{-2}\bar{L}_{-2}\mathbf{1}$, $(L_{-2}^2 + \bar{L}_{-2}^2)\mathbf{1}$ with scaling dimension $x = 4$ [19, 20]. With the twisted boundary conditions, we can use the level crossing of the lower excitations than those with only the periodic boundary conditions. Since the amplitude of the corrections from the irrelevant field becomes smaller with the lower excitations [20], thus the convergence to the transition point is highly improved.

3. Physical examples

3.1. $S = 1$ XXZ chain

As a physical example, let us consider the $S = 1$ XXZ spin chain, described by the Hamiltonian:

$$H = \sum_{j=1}^{L} h_{j,j+1}, h_{j,j+1} = \tfrac{1}{2}(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+) + \Delta S_j^z S_{j+1}^z \tag{15}$$

where we assume that L is even and periodic boundary conditions. This model is invariant under spin rotation around the z-axis, translation ($T_R : S_j^{x,y,z} \to S_{j+1}^{x,y,z}$), space inversion ($P : S_j^{x,y,z} \to S_{L-j+1}^{x,y,z}$), spin reversal ($T : S_j^z \to -S_j^z, S_j^{\pm} \to S_j^{\mp}$). Therefore, energy 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 ($T = \pm 1$).

Note that with the unitary transformation $\exp(\pi \mathrm{i} \sum j S_j^z)$, spin operators change as $S_j^z \to S_j^z, S_j^{\pm} \to (-1)^j S_j^{\pm}$, and the sign of the XY term in (15) reverses. With this transformation the momentum (or the parity) of the eigenstate for the odd $SL + S_t^z$ changes as $q \to q + \pi$ ($P \to -P$), and the spin reversal for the odd SL changes $T \to -T$, from the similar calculation in appendix C and $\exp(2\pi \mathrm{i}(S + S_j^z)) = 1$.

About the spin S XXZ chain, Haldane [21] discussed that for the integer S case, there are two transition points $\Delta_{c1} < 1 < \Delta_{c2}$, where the XY-Haldane transition Δ_{c1} is of the BKT type, and the Haldane–Néel transition point Δ_{c2} is of the 2D Ising universality class, in contrast to the half-odd integer S case where only one transition point exists at $\Delta = 1$ of the $SU(2)$ WZW type.

Numerically Botet and Jullien [22] estimated $\Delta_{c1} \approx 0.1$, Sakai and Takahashi [23] $\Delta_{c1} = -0.01 \pm 0.03$, and Yajima and Takahashi [24] $\Delta = 0.069 \pm 0.003$. Recently, the authors found $\Delta_{c1} = 0$ and checked the universality class [25] using the level spectroscopy [9]. We found the exact degeneracy (at least within numerical accuracy) between the $S_T^z = \pm 4, q = 0, P = 1$ and the $S_T^z = 0, q = 0, P = T = 1$ excitations.

These results are obtained under periodic boundary conditions. To consider a twisted boundary condition, in (15) we replace the boundary term between the Lth site and the first site,

$$h_{L,1} = \tfrac{1}{2}(S_L^+ S_1^- \exp(-\mathrm{i}\Phi) + S_L^- S_1^+ \exp(\mathrm{i}\Phi)) + \Delta S_L^z S_1^z. \tag{16}$$

However, with this boundary condition the Hamiltonian (15) is not translational invariant. The translational invariance can be restored, still maintaining the total angle Φ, by twisting all neighbouring bonds in the chain by an angle Φ/L with the next unitary transformation

$$\begin{gathered} U_\Phi = \exp\left(\mathrm{i}\frac{\Phi}{L}\sum_{j=1}^{L}\left(j - \frac{1}{2}\right) S_j^z\right) \\ U_\Phi S_j^{\pm} U_\Phi^{-1} = S_j^{\pm} \exp(\pm \mathrm{i}(j - \tfrac{1}{2})\Phi/L) \qquad U_\Phi S_j^z U_\Phi^{-1} = S_j^z \end{gathered} \tag{17}$$

(in U_Φ we use $(j - \frac{1}{2})S_j^z$ for the compatibility of the definition of P). Thus, we obtain

$$H_t(\Phi) = \sum h_{j,j+1}^t \qquad h_{j,j+1}^t = \tfrac{1}{2}(S_j^+ S_{j+1}^- \mathrm{e}^{-\mathrm{i}\Phi/L} + S_j^- S_{j+1}^+ \mathrm{e}^{\mathrm{i}\Phi/L}) + \Delta S_j^z S_{j+1}^z. \tag{18}$$

Under this boundary condition, we had better modify the definition of the translational operator $T_R^t \equiv \exp(\mathrm{i}\Phi S_T^z/L) T_R$ (see appendix C). Although there are no discrete symmetries like P, T in general Φ, for the special angle $\Phi = \pi$, the system (18) is invariant under the discrete symmetries $U_{2\pi} P, U_{2\pi} T$. Moreover, it was shown that $U_{2\pi} P, U_{2\pi} T$ are the good

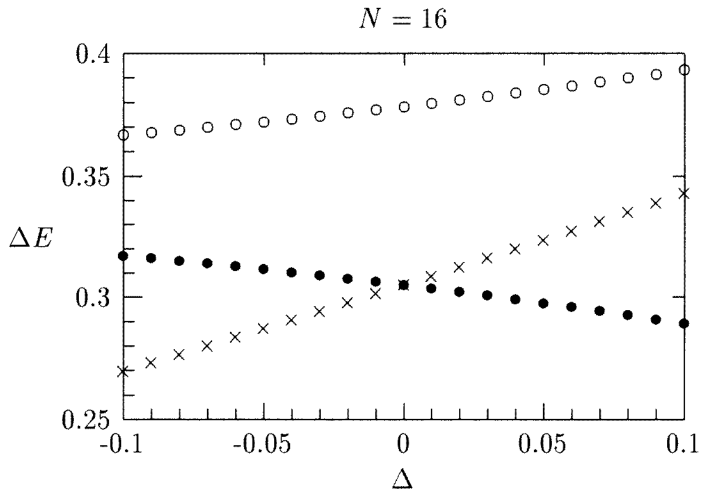

Figure 1. Excitation energies of $S_T^z = \pm 2, q = 0, P = 1$ state with PBC ($\times$), and of $S_t^z = 0, q = 0$ states with TBC ($\bullet : U_{2\pi} P = U_{2\pi} T = -1$ and $\circ : U_{2\pi} P = U_{2\pi} T = 1$).

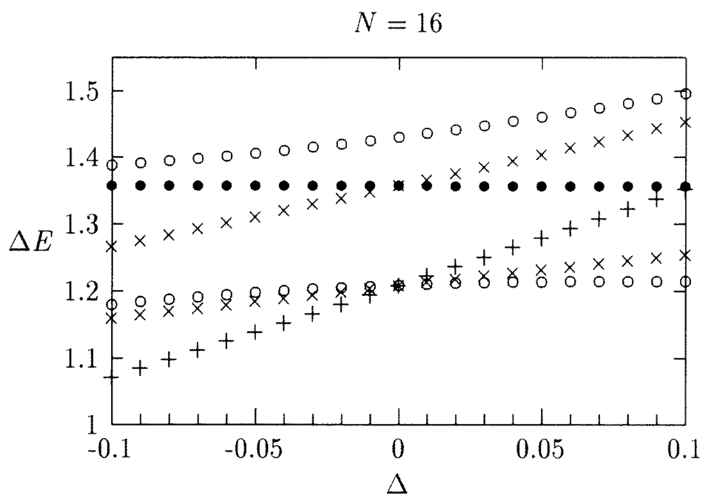

Figure 2. Excitation energies of $S_T^z = 0, q = 0, P = T = 1$ states with PBC ($\circ$), of $S_T^z = 0, q = 0, P = T = -1$ state with PBC ($\bullet$), of $S_T^z = \pm 2, q = 0$ states with TBC ($\times$), and of $S_T^z = \pm 4, q = 0, P = 1$ state with PBC ($+$).

quantum numbers [26] characterizing the generalized $Z_2 \times Z_2$ symmetries [27] (see also appendix C). Thus the twist angle $\Phi = \pi$ has the special meaning in addition to the one discussed in section 2.

Under PBC, the energy eigenvalues E_n are related to the scaling dimension x_n as

$$E_n(L) - E_g(L) = \frac{2\pi v x_n}{L} \tag{19}$$

where v is the spin wave velocity [28]. The conformal anomaly c is related to the ground-state energy [13, 29]

$$E_g(L) = e_g L - \frac{\pi v c}{6L}. \tag{20}$$

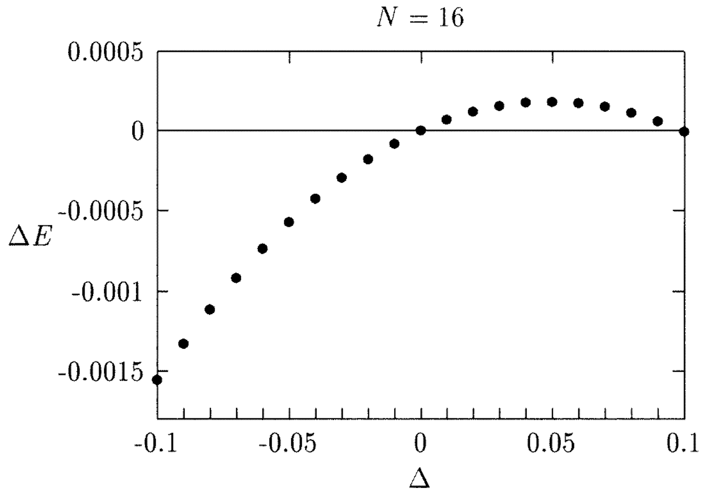

Figure 3. Energy difference $E^{c0} - E^{c1}$ for $L = 16$ systems.

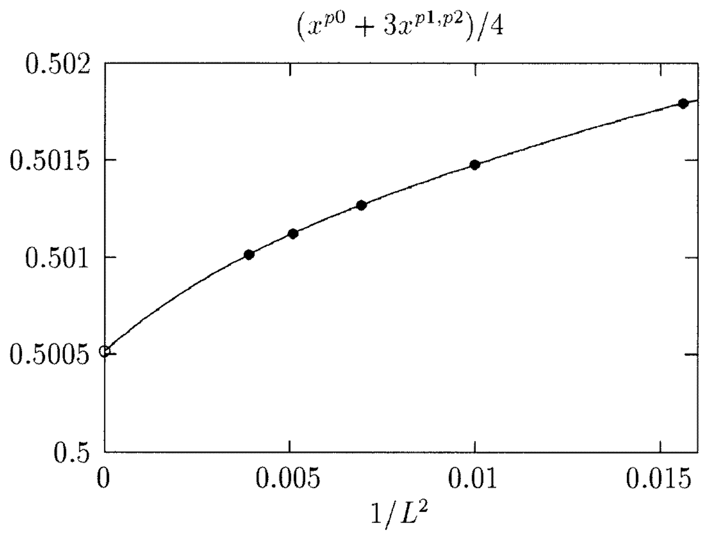

Figure 4. Size dependence of the averaged scaling dimension $(x^{p0} + 3x^{p1,p2})/3$.

In figure 1 we show the excitations corresponding to the scaling dimension $x = \frac{1}{2}$ at the BKT point. The excitation $S_T^z = 0, q = 0, U_{2\pi}P = U_{2\pi}T = -1$ under TBC is exactly degenerate with excitations $S_T^z = \pm 2, q = 0, P = 1$ under PBC at $\Delta = 0$. Figure 2 shows the excitations corresponding to the scaling dimension $x = 2$. At $\Delta = 0$, the excitations $S_T^z = \pm 2, q = 0, U_{2\pi}P = -1$ under TBC are exactly degenerate with excitations $S_T^z = 0, q = 0, P = T = 1$ and $S_T^z = \pm 4, q = 0, P = 1$ under PBC, whereas the excitations $S_T^z = \pm 2, q = 0, U_{2\pi}P = 1$ under TBC are exactly degenerate with the excitation $S_T^z = 0, q = 0, P = T = -1$ under PBC. Figure 3 shows the energy difference between the excitations for $S_T^z = 0$, $q = \pm 2\pi/L$ with PBC, and those for $S_T^z = \pm 2$, $q = \pm 2\pi/L$ with TBC. They are exactly degenerate at $\Delta = 0$.

Table 2. $\mathrm{d}\Delta E/\mathrm{d}\Delta|_{\Delta=0}$ for $L = 16$ system.

Excitations	$\mathrm{d}\Delta E/\mathrm{d}\Delta|_{\Delta=0}$	Expected ratio
p1,p3	0.504 263 15	1/2
m3,m0	1.238 314 39	4/3
m7,m0	0.309 490 32	1/3
m3,m7	0.928 824 06	1
m5,m2	0.938 998 85	1

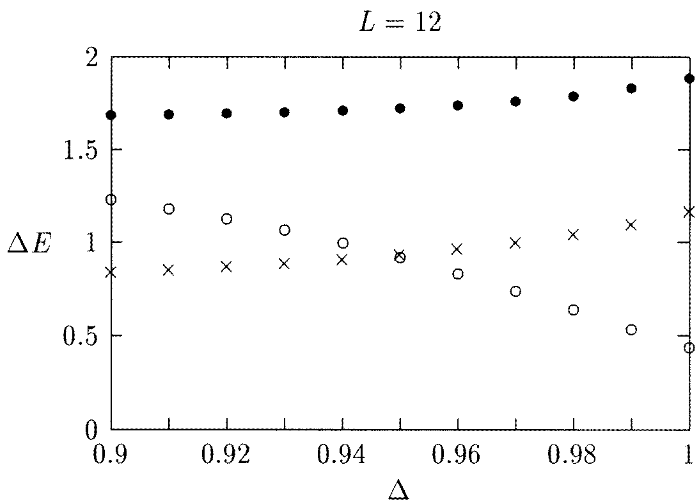

Figure 5. Excitation energies of $L = 12$, $D = 0$ near the XY-Haldane transition point. $\times$'s are $S_T^z = \pm 2$, $q = 0$, $P = 1$ excitations under PBC, $\circ$'s are $S_T^z = 0$, $U_{2\pi}P = U_{2\pi}T = 1$ excitations under TBC, and $\bullet$'s are $S_T^z = 0$, $U_{2\pi}P = U_{2\pi}T = -1$ under TBC.

Next we discuss the universality relations. The conformal anomaly is estimated $c = 1.000$ in [25]. We can eliminate the logarithmic corrections by taking the appropriate average, for example $(x^{p0} + 2x^{p1} + x^{p3})$ as can be read from table 1. We show the size dependence of $(x^{p0} + 2x^{p1} + x^{p3})/4$ in figure 4; the remaining size dependence is mainly explained by the $x = 4$ irrelevant field. From table 1, in the neighbourhood of the BKT transition, there appear terms linear in the distance t from the BKT line. The ratios of $x^{p3} - x^{p1}$, $x^{m7} - x^{m3}$, $x^{m5} - x^{m2}$, $x^{m0} - x^{m3}$, are $-\frac{1}{2} : -1 : 1 : -\frac{4}{3}$ close to the BKT line. In table 2, we show the coefficients linear in t of the eigenvalues corresponding with $x^{p3} - x^{p1}$, $x^{m7} - x^{m3}$, $x^{m5} - x^{m2}$, $x^{m0} - x^{m3}$.

3.2. $S = 2$ XXZ chain

Next we consider the $S = 2$ XXZ spin chain, described by the Hamiltonian:

$$H = \sum (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z + D(S_j^z)^2). \tag{21}$$

For the isotropic case ($\Delta = 1$, $D = 0$), several studies [30–37] have been done in the relation to the Haldane's conjecture [21]. Although the estimated values of the Haldane gap are widely ranged, they are common on the existence and the smallness of it. Due to the smallness of the Haldane gap, we can expect that the XY-Haldane phase boundary is

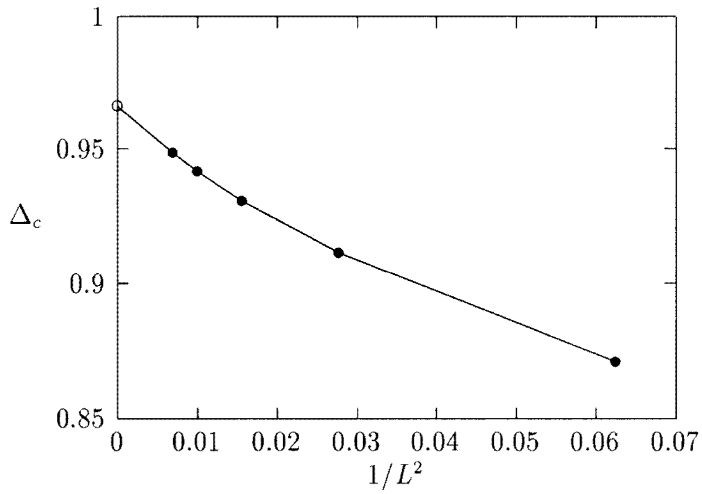

Figure 6. Size dependence of the crossing point. The extrapolated value is $\Delta_c = 0.966$, which is the transition point between the $S = 2$ Haldane gap and the XY phases.

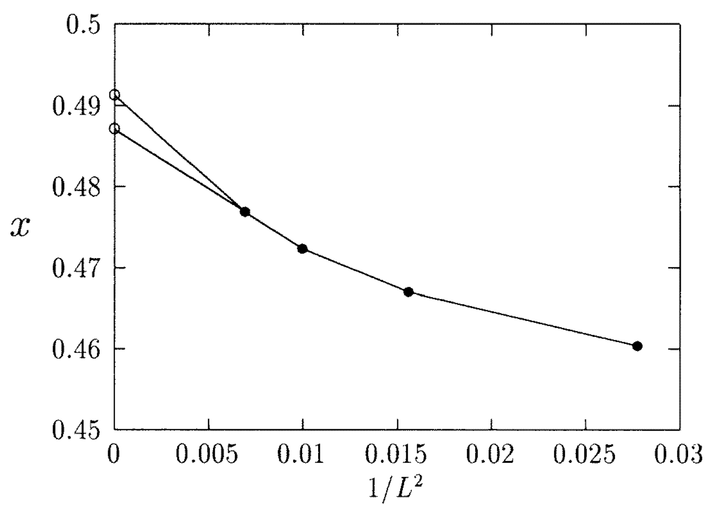

Figure 7. Size dependence of the averaged scaling dimension $(x^{p0} + 3x^{p1})/4$ for Δ_c.

very close to the isotropic point ($\Delta = 1$, $D = 0$), that is $1 - \Delta_c$ ($D = 0$) and D_{c1} ($\Delta = 1$) are very small, compared with the $S = 1$ case [38, 39]. Here we only consider on the line $D = 0$, and on the line $\Delta = 1$ ($D > 0$), to estimate the XY-Haldane and the XY-large D transition points and to determine the universality class.

First we consider on the $D = 0$ line. Figure 5 shows the excitation energies with $S_T^z = \pm 2$, $P = 1$ under PBC, and with $S_T^z = 0$ under TBC for $L = 12$ systems. We can see a level crossing which corresponds to the transition point between the XY and the $S = 2$ Haldane phases, as is expected from table 1. The size dependence of this crossing point is shown in figure 6. The extrapolated value to the thermodynamic limit is $\Delta_c = 0.966$. The conformal anomaly number of this point is estimated as $c = 1.16$. To check the universality class, we show the size dependence of the combination of the scaling

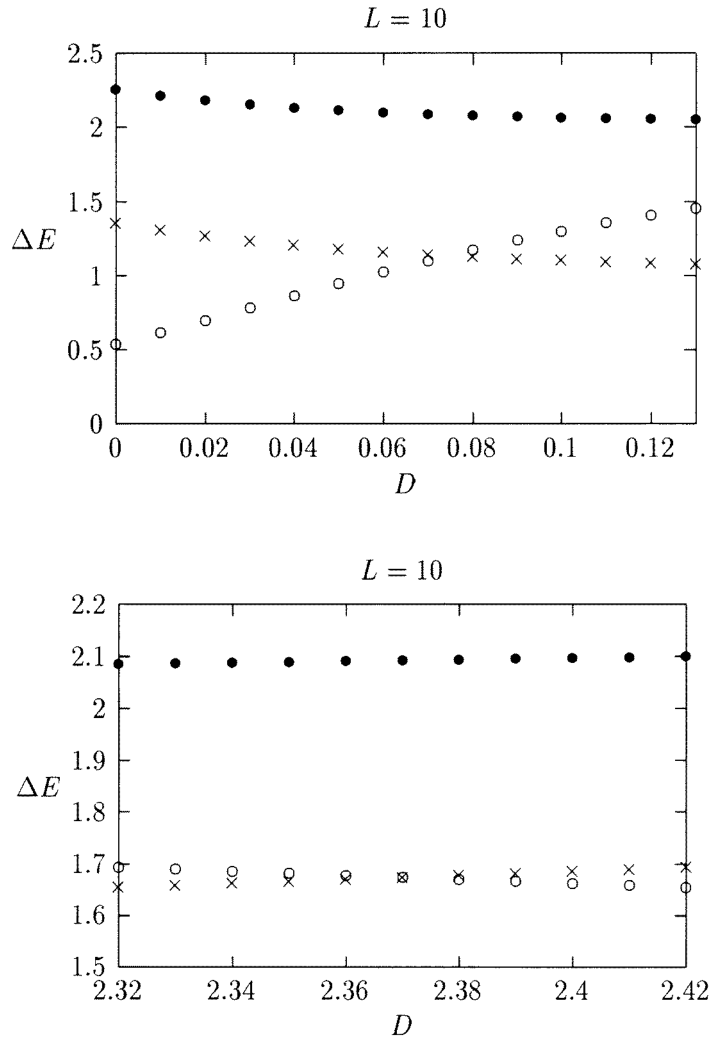

Figure 8. Excitation energies of $L = 10$, $\Delta = 1$ near the Haldane-XY and XY-large D transition points. $\times$'s are $S_T^z = \pm 2$, $q = 0$, $P = 1$ excitations under PBC, $\circ$'s are $S_T^z = 0$, $U_{2\pi}P = U_{2\pi}T = 1$ excitations under TBC, and $\bullet$'s are $S_T^z = 0$, $U_{2\pi}P = U_{2\pi}T = -1$ under TBC.

dimension as $(x^{p0} + 3x^{p1})/4$ in figure 7. We extrapolate the $L \to \infty$ as $x_c(L) = x_c + a_1/L^2$ for $L = 10, 12$ and $x_c(L) = x_c + a_1/L^2 + a_2/L^4$ for $L = 8, 10, 12$, and the obtained values are 0.487 and 0.491 respectively.

Next we show the result on the $\Delta = 1$ ($D > 0$) line. Figure 8 shows the excitation energies with $S_T^z = \pm 2$, $P = 1$ under PBC, and with $S_T^z = 0$ under TBC for $L = 10$ systems. We can recognize the three regions as the $S = 2$ Haldane phase $0 < D < D_{c1}$, the massless XY phase $D_{c1} < D < D_{c2}$, and the large D phase $D_{c2} < D$. The size dependence of crossing points is shown in figures 9 and 10, and the estimated values are $D_{c1} = 0.043$ and $D_{c2} = 2.39$. The estimated conformal anomaly numbers are $c = 1.16$ and 0.998 for D_{c1} and D_{c2} respectively. The transition point between the $S = 2$ Haldane gap and the XY phases (D_{c1}) is consistent with the previously obtained values by Schollwöck and Jolicœur

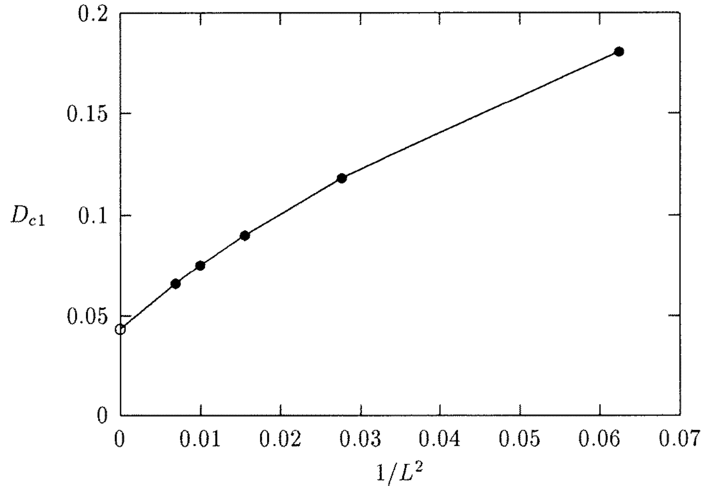

Figure 9. Size dependence of the crossing point. The extrapolated value is $D_{c1} = 0.043$, which is the transition point between the $S = 2$ Haldane gap and the XY phases.

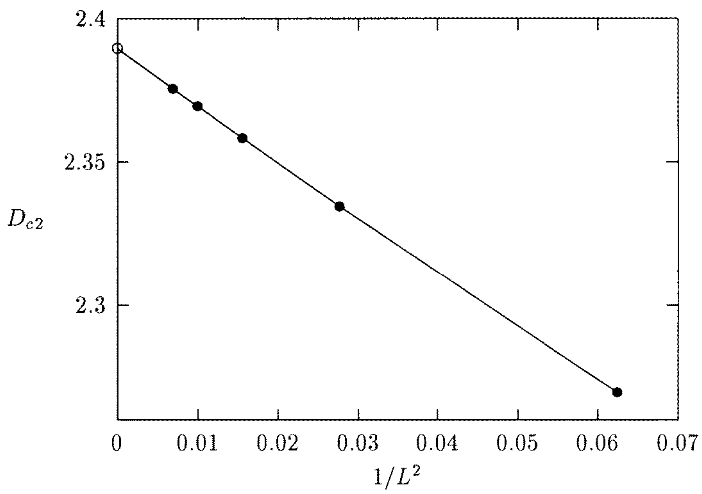

Figure 10. Size dependence of the crossing point. The extrapolated value is $D_{c2} = 2.39$, which is the transition point between the XY and the large D phases.

[34] ($D_{c1} = 0.04(2)$), but the transition point between the XY and the large-D phases (D_{c2}) deviates from their value ($D_{c2} \approx 3$). Figures 11 and 12 show the size dependence of $(x^{p0} + 3x^{p1})/4$. The extrapolated values for D_{c1} are 0.489 for $L = 10, 12$ and 0.493 for $L = 8, 10, 12$. For D_{c2} the values are 0.5005 for $L = 10, 12$ and 0.5006 for $L = 8, 10, 12$.

The conformal anomaly numbers and the scaling dimensions for the critical points $(\Delta, D) = (\Delta_c, 0)$ and $(1, D_{c1})$ deviate somewhat from the ideal value $c = 1$ and $x = \frac{1}{2}$. We think that at these points the BKT transition points are very close to the 2D Ising transition line between the $S = 2$ Haldane and the antiferromagnetic phases [34], so that the crossover effect is very large for these points. In fact, at the BKT transition point $(\Delta, D) = (1, D_{c2})$ where the 2D Ising transition line is far, these values are consistent with

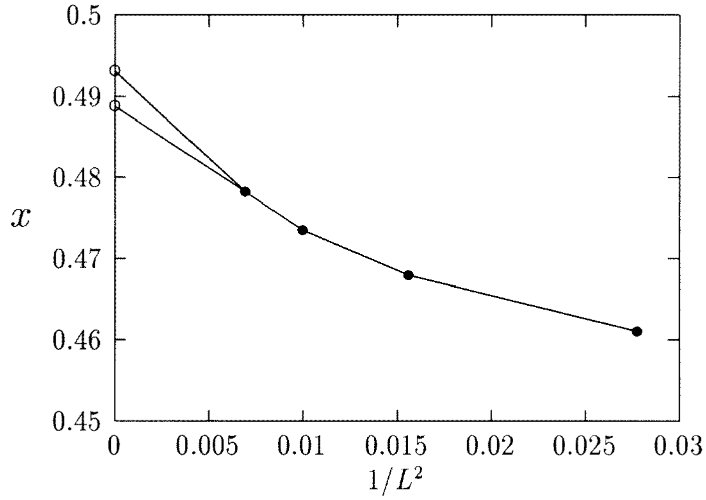

Figure 11. Size dependence of the averaged scaling dimension for D_{c1}.

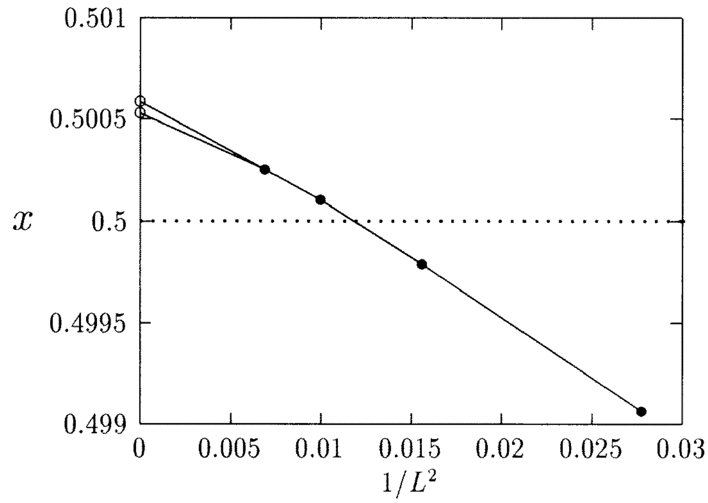

Figure 12. Size dependence of the averaged scaling dimension for D_{c2}.

the ideal values.

In the XY phase on the $\Delta = 1$ line, we find that under TBC the energy levels with $S_T^z = 0, U_{2\pi}P = U_{2\pi}T = 1$ and with $S_T^z = 0, U_{2\pi}P = U_{2\pi}T = -1$ cross twice (see figure 13). These two points correspond to the Gaussian fixed points [15], so that there are two Gaussian fixed lines in the whole phase diagram of (21). This may be the 'indirect' evidence of the intermediate-D phase, predicted by Oshikawa [27]. To see the intermediate-D phase, Oshikawa *et al* [40] studied the line $\Delta = 1$ with the quantum Monte Carlo method. However, we cannot find that phase, and we think that in order to find the intermediate-D phase, one needs to study the region with larger values of Δ (>1).

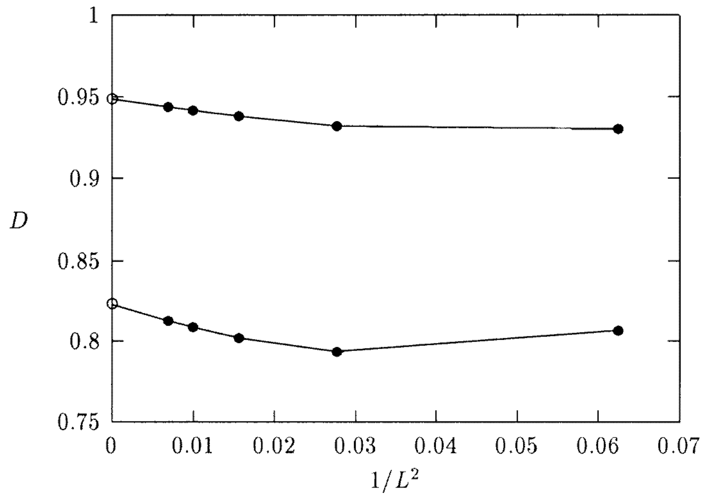

Figure 13. Size dependence of the Gaussian fixed points in XY phase on the $\Delta = 1$ line.

Finally we make the following remark. From the large S mapping onto the anisotropic nonlinear sigma model by Haldane [21], $1 - \Delta + D$ is proportional to the anisotropy of it. Numerical values $1 - \Delta_c = 0.034$ and $D_{c1} = 0.043$ are comparable, thus it is consistent with Haldane's arguments.

4. Conclusion

Physical properties of the BKT transition, including the renormalization group properties and the $SU(2)$ or the $SU(2)/Z_2$ symmetry, have been well investigated in the field theory. However, the mapping from the various models to the field theoretical models, such as the sine-Gordon model or the WZW model, is neither simple nor quantitatively correct. Fortunately, the symmetry structure and the sum rule at the BKT phase transition point survive after the mapping. Therefore, using these properties, we can determine the BKT critical point and the universality class.

In numerical calculations, $SU(2)$ symmetry has been used to determine the BKT-type critical line in [41], $SU(2)/Z_2$ symmetry has been used in [9], and the sum rule to eliminate logarithmic corrections in [42]. Recently, introducing the half-magnetic charges by twisting boundary condition, one of the authors has developed a method to determine the Gaussian fixed line and its universality class for the non-integrable models [15]. In this paper, using the twisted boundary condition, we explicitly relate the energy eigenvalue structure to the $SU(2)$ symmetry of the BKT transition. At the same time, we can improve the convergence of the physical quantities to the thermodynamic limit, in comparison with the original level spectroscopy [9].

Our method is applicable not only to the quantum problems, but also to the classical models, treating the eigenvalue structure of the transfer matrix.

Acknowledgments

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Appendix A. Free boson on the complex plane

We briefly review the free boson theory on the complex plane [43] and the relation between the half-odd magnetic monopole and twisted boundary conditions [14]. The equation of motion $\partial\bar{\partial}\phi = 0$ for (1) allows the chiral decomposition

$$\phi(z, \bar{z}) = \frac{\sqrt{K}}{2}(\varphi(z) + \bar{\varphi}(\bar{z})) \tag{22}$$

where we introduce the two independent complex coordinates $z = x + \mathrm{i}y$, $\bar{z} = x - \mathrm{i}y$ and use the notation $\partial = (\partial_x - \mathrm{i}\partial_y)/2$, $\bar{\partial} = (\partial_x + \mathrm{i}\partial_y)/2$. Then the action can be written

$$S = \int \mathcal{L} = \frac{1}{2\pi}\int \frac{\mathrm{i}\mathrm{d}z \wedge \mathrm{d}\bar{z}}{2}\partial\varphi\bar{\partial}\bar{\varphi}. \tag{23}$$

The two point functions are

$$\langle\varphi(z)\varphi(w)\rangle = -\log(z - w) \qquad \langle\bar{\varphi}(\bar{z})\bar{\varphi}(\bar{w})\rangle = -\log(\bar{z} - \bar{w}). \tag{24}$$

A.1. Chiral current

Here we introduce the $U(1)$ chiral current as

$$J(z) = \mathrm{i}\partial\varphi(z). \tag{25}$$

The chiral current has a leading short distance expansion

$$J(z)J(w) = \frac{1}{(z - w)^2} + \cdots \tag{26}$$

inferred by taking two derivatives of (24). We introduce the mode expansion of the current

$$J(z) = \sum_n z^{-n-1}\alpha_n \qquad \alpha_n = \oint \frac{\mathrm{d}z}{2\pi\mathrm{i}} z^n J(z). \tag{27}$$

Using the short distance expansion (26) and the radial quantization, we obtain the commutation relation

$$[\alpha_m, \alpha_n] = m\delta_{m+n,0} \tag{28}$$

which means the $U(1)$ current algebra. Note that α_0 is the conserved charge of the $U(1)$ current.

A.2. Stress–energy tensor

From the Noether theorem, the stress–energy tensor is written as

$$T(z) = \tfrac{1}{2} : J(z)J(z) : . \tag{29}$$

Using the short distance expansion (26) and Wick's theorem, we obtain the OPE of the $T(z)$, $T(w)$

$$T(z)T(w) = \frac{\frac{1}{2}}{(z - w)^4} + \frac{2T(w)}{(z - w)^2} + \frac{\partial T(w)}{z - w} + \text{reg.} \tag{30}$$

which means that this satisfies the $c = 1$ Virasoro algebra. Similarly, the OPE of the $T(z)$, $J(w)$

$$T(z)J(w) = \frac{J(w)}{(z-w)^2} + \frac{\partial J(w)}{z-w} + \text{reg.} \tag{31}$$

means that $J(z)$ is the primary field with the conformal dimension (1,0). The mode expansion of $T(z)$ is

$$T(z) = \sum_n z^{-n-2} L_n \tag{32}$$

where L_n can be written

$$L_n = \frac{1}{2}\sum_m :\alpha_{m+n}\alpha_{-m}: \tag{33}$$

especially

$$L_0 = \frac{1}{2}\alpha_0^2 + \sum_{n=1}^{\infty} :\alpha_{-n}\alpha_n: . \tag{34}$$

A.3. Vertex operator

The vertex operator is defined as $:\exp(\mathrm{i}\alpha\varphi(z)):$. The OPE of the vertex operator and the current is

$$J(z) : \mathrm{e}^{\mathrm{i}\alpha\varphi(w)} := \frac{\alpha}{z-w} : \mathrm{e}^{\mathrm{i}\alpha\varphi(w)} : +\text{reg.}. \tag{35}$$

The OPE of the vertex operator and the stress–energy tensor is

$$T(z) : \mathrm{e}^{\mathrm{i}\alpha\varphi(w)} := \frac{\alpha^2/2}{(z-w)^2} : \mathrm{e}^{\mathrm{i}\alpha\varphi(w)} : + \frac{\partial_w : \mathrm{e}^{\mathrm{i}\alpha\varphi(w)} :}{z-w} + \text{reg.} \tag{36}$$

therefore the vertex operator is a primary field with conformal dimension $h = \alpha^2/2$.

A.4. Highest weight states

When we define the state

$$|\alpha\rangle \equiv \lim_{w\to 0} : \mathrm{e}^{\mathrm{i}\alpha\varphi(w)} : |0\rangle \tag{37}$$

it is the highest weight state of the $U(1)$ current algebra,

$$\alpha_0|\alpha\rangle = \alpha|\alpha\rangle \qquad \alpha_n|\alpha\rangle = 0 \qquad (n > 0) \tag{38}$$

from equation (35). This is also the highest weight state of the Virasoro algebra

$$L_0|\alpha\rangle = \frac{\alpha^2}{2}|\alpha\rangle \qquad L_n|\alpha\rangle = 0 \qquad (n > 0). \tag{39}$$

A.5. Compactification of the internal space

The compactification of the internal space $\phi \equiv \phi + 2\pi/\sqrt{2}$ restricts the eigenvalues $\alpha, \bar{\alpha}$ of the $U(1) \times U(1)$ charges $\alpha_0, \bar{\alpha}_0$. First we note that

$$\begin{aligned} \varphi(z) &= q - \mathrm{i}\alpha_0 \log z + \mathrm{i} \sum_{n \neq 0} \frac{1}{n} z^{-n} \alpha_n \\ \bar{\varphi}(\bar{z}) &= \bar{q} - \mathrm{i}\bar{\alpha}_0 \log \bar{z} + \mathrm{i} \sum_{n \neq 0} \frac{1}{n} \bar{z}^{-n} \bar{\alpha}_n \end{aligned} \tag{40}$$

where $q, \bar{q}$ are zero modes and satisfy the commutation relation

$$[q, \alpha_0] = [\bar{q}, \bar{\alpha}_0] = \mathrm{i}. \tag{41}$$

Rotating around the origin 0, there appears a phase factor $\pm 2\pi\mathrm{i}$ in the function $\log(z)(\log(\bar{z}))$. Thus, considering the periodic nature of ϕ, we obtain

$$\alpha - \bar{\alpha} = \sqrt{\frac{2}{K}} n \qquad (n : \text{integer}) \tag{42}$$

for the requirement of the uniqueness of the vertex operator under the change $\phi \equiv \phi + 2\pi/\sqrt{2}$,

$$\alpha + \bar{\alpha} = \sqrt{2K} m \qquad (m : \text{integer}). \tag{43}$$

In one word, eigenvalues for $\alpha_0, \bar{\alpha}_0$ are

$$\alpha = \sqrt{\frac{K}{2}} m + \sqrt{\frac{1}{2K}} n \qquad \bar{\alpha} = \sqrt{\frac{K}{2}} m - \sqrt{\frac{1}{2K}} n. \tag{44}$$

Since $L_0 \pm \bar{L}_0$ are the generators of dilatation and rotation, we identify $(\alpha^2 \pm \bar{\alpha}^2)/2$ as the scaling dimension and the conformal spin of the state $|\alpha, \bar{\alpha}\rangle$. Finally, by defining the dual field θ to ϕ as

$$\theta = \frac{1}{2\sqrt{K}} (\varphi(z) - \bar{\varphi}(\bar{z})) \tag{45}$$

θ has a periodicity $2\pi/\sqrt{2}$.

A.6. Twisted boundary conditions and background charge

To any conformal operator $f(\alpha_0, \bar{\alpha}_0)$, we can associate a twisted operator

$$\begin{aligned} f_{\Theta\bar{\Theta}}(\alpha_0, \bar{\alpha}_0) &= \exp(-\mathrm{i}(\Theta q + \bar{\Theta}\bar{q})) f(\alpha_0, \bar{\alpha}_0) \exp(\mathrm{i}(\Theta q + \bar{\Theta}\bar{q})) \\ &= f(\alpha_0 + \Theta, \bar{\alpha}_0 + \bar{\Theta}). \end{aligned} \tag{46}$$

Here we set

$$\Theta = \bar{\Theta} = \sqrt{\frac{K}{2}} \frac{\Phi}{2\pi}. \tag{47}$$

On the one hand, from equations (40) this means

$$\phi \to \phi - \mathrm{i}\frac{K}{\sqrt{2}} \frac{\Phi}{2\pi} \log|z| \qquad \theta \to \theta - \mathrm{i}\frac{1}{\sqrt{2}} \frac{\Phi}{2\pi} \left(\frac{1}{2} \log \frac{z}{\bar{z}} \right) \tag{48}$$

that is, there is a cut for θ.

Mapping from the plane to the cylinder by $w \equiv u + \mathrm{i}v = (L/2\pi) \log z$, we obtain

$$\phi \to \phi - \mathrm{i}\frac{K}{\sqrt{2}} \frac{\Phi}{L} u \qquad \theta \to \theta + \frac{1}{\sqrt{2}} \frac{\Phi}{L} v \tag{49}$$

that is, twisted boundary conditions for θ in the v direction.

On the other hand, the change (46), (47) with equations (42), (43) means the change of the magnetic charges

$$m \to m + \frac{\Phi}{2\pi} \qquad n \to n. \tag{50}$$

This can be interpreted to set a magnetic monopole $\Phi/2\pi$ at the origin $z = 0$, and a magnetic monopole $-\Phi/2\pi$ at the infinity $z = \infty$.

A.7. Discrete symmetries

For the Gaussian model (23), besides continuous $U(1) \times U(1)$ symmetries, there are discrete symmetries

$$T : (\varphi, \bar{\varphi}) \to (-\varphi, -\bar{\varphi}) \qquad C : (z, \varphi) \to (\bar{z}, \bar{\varphi}). \tag{51}$$

Appendix B. Calculation of the renormalized scaling dimensions

In this appendix, we calculate the correction of scaling dimensions in table 1, up to the first order of y_0, y_ϕ in some degenerate cases. The derivation here is simpler than the original one [18, 9]. Let us consider the following 1D quantum Hamiltonian

$$H = H_0 + \frac{\lambda_1}{2\pi} \int_0^L \mathrm{d}v \mathcal{O}_1 \tag{52}$$

where H_0 is a fixed point Hamiltonian, L is the system size (in table 1 l is related with L as $l = \log(L/\alpha)$), and $\mathcal{O}_1 (= \mathcal{O}_1^\dagger)$ is a scaling operator whose scaling dimension is x_1. We set the short-range cut-off as 1. According to Cardy [19], the size dependence of excitation energies up to the first-order perturbation is given by

$$\Delta E_n(L) = \frac{2\pi}{L}(x_n + C_{n1n}\lambda_1(L) + \cdots) = \frac{2\pi}{L} x_n(L) \tag{53}$$

where x_n is the scaling dimension of the operator $\mathcal{O}_n$, C_{n1n} is the OPE coefficient of operators $\mathcal{O}_n$ and $\mathcal{O}_1$ as

$$\mathcal{O}_1(z, \bar{z})\mathcal{O}_n(0, 0) = C_{n1n} z^{-h_1} \bar{z}^{-h_1} \mathcal{O}_n(0, 0) + \cdots$$

in which $h_1 (= \bar{h}_1)$ is the conformal weight of $\mathcal{O}_1$ ($x_1 = 2h_1$). We used the notation

$$\lambda_1(L) = \lambda_1 \left(\frac{2\pi}{L}\right)^{x_1 - 2}$$

which comes from the renormalization group equation.

For the sine-Gordon model, we denote

$$K = \frac{4}{m^2}\left(1 + \frac{1}{2} y_0\right)$$

near $K = 1$ ($m = 2$) or $K = 4$ ($m = 1$). We can rewrite the Lagrangian density as

$$\mathcal{L}(z, \bar{z}) = \mathcal{L}_0(z, \bar{z}) + \mathcal{L}_I(z, \bar{z}) \tag{54}$$

where

$$\mathcal{L}_0(z, \bar{z}) = \frac{m^2}{8\pi}(\nabla\phi)^2$$

and

$$\mathcal{L}_I(z,\bar{z}) = \frac{y_0}{4\pi}\mathcal{M} + \frac{y_\phi}{2\sqrt{2}\pi}\sqrt{2}\cos\sqrt{2}m\phi \tag{55}$$

and we set

$$\lambda_0 = \frac{y_0}{2} \qquad \lambda_\phi = \frac{y_\phi}{\sqrt{2}}. \tag{56}$$

B.1. x^{p0} and x^{p3}

We calculate x^{p0} and x^{p1} up to the first order of y's. We denote operators $\sqrt{2}\cos m\phi/\sqrt{2}$ (whose scaling dimension is x^{p0}) and $\sqrt{2}\sin m\phi/\sqrt{2}$ (whose scaling dimension is x^{p3}) as $\mathcal{O}_c$ and $\mathcal{O}_s$ respectively. We have the following OPE's

$$\mathcal{M}(z,\bar{z})\mathcal{O}_{c,s}(0,0) = \frac{1}{2}\frac{1}{|z|^2}\mathcal{O}_{c,s} + \cdots \tag{57}$$

$$\sqrt{2}\cos\sqrt{2}m\phi(z,\bar{z})\mathcal{O}_{c,s}(0,0) = \pm\frac{1}{\sqrt{2}}\frac{1}{|z|^2}\mathcal{O}_{c,s}(0,0) + \cdots \tag{58}$$

where + is for $\mathcal{O}_c$ and − is for $\mathcal{O}_s$. From these OPEs and equation (53), we can obtain the scaling dimensions,

$$x^{p0}(L) = \frac{1}{2} + \frac{1}{2}\frac{y_0(L)}{2} + \frac{1}{\sqrt{2}}\frac{y_\phi(L)}{\sqrt{2}} \tag{59}$$

for $\sqrt{2}\cos m\phi/\sqrt{2}$, and

$$x^{p3}(L) = \frac{1}{2} + \frac{1}{2}\frac{y_0(L)}{2} - \frac{1}{\sqrt{2}}\frac{y_\phi(L)}{\sqrt{2}} \tag{60}$$

for $\sqrt{2}\sin m\phi/\sqrt{2}$. Setting $y_\phi = y_0(1+t)$, we have the scaling dimension described in table 1. These are consistent with the results obtained by Giamarchi and Schulz [18].

Similar calculation can be applied to $x^{m5,m6,m7,m8}$.

B.2. Marginal operators

For the BKT transition, there exists a hybridization between the marginal field $\mathcal{M}$ and the operator $\sqrt{2}\cos\sqrt{2}m\phi$ ($m = 2$ for $K = 1$, and $m = 1$ for $K = 4$) [9]. These two operators have the same scaling dimension and symmetries at $K = 1$ or $K = 4$. Treating $\mathcal{L}_I$ as the perturbation term, we have the following OPE's

$$\begin{aligned}\mathcal{L}_I(z,\bar{z})\mathcal{M}(0,0) &= \frac{y_\phi\sqrt{2}}{2\pi|z|^2}\sqrt{2}\cos\sqrt{2}m\phi(0,0) + \cdots\\ \mathcal{L}_I(z,\bar{z})\sqrt{2}\cos\sqrt{2}m\phi(0,0) &= \frac{y_0}{2\pi|z|^2}\sqrt{2}\cos\sqrt{2}m\phi(0,0) + \frac{y_\phi\sqrt{2}}{2\pi|z|^2}\mathcal{M}(0,0) + \cdots.\end{aligned} \tag{61}$$

Setting $y_\phi = y_0(1+t)$, and diagonalizing these equations, we have the orthogonal operators,

$$\sqrt{\tfrac{2}{3}}(1 - \tfrac{1}{9}t)\mathcal{M} + \sqrt{\tfrac{1}{3}}(1 + \tfrac{2}{9}t)\sqrt{2}\cos\sqrt{2}m\phi \tag{62}$$

with the scaling dimension (up to the first order of y_0 and t)

$$x^{m0}(L) = 2 - y_0(L)(1 + \tfrac{4}{3}t)$$

and

$$\sqrt{\tfrac{2}{3}}(1 - \tfrac{1}{9}t)\sqrt{2}\cos\sqrt{2}m\phi + \sqrt{\tfrac{1}{3}}(1 + \tfrac{2}{9}t)\mathcal{M} \tag{63}$$

with the scaling dimension

$$x^{m1} = 2 + 2y_0(L)(1 + \tfrac{2}{3}t).$$

These scaling dimensions are consistent with the results obtained by one of the authors [9].

Appendix C. Symmetry in twisted boundary conditions

In equation (17), we showed the unitary transformation of TBC for spin operators. In this appendix we discuss the unitary transformation of other operators T_R, P, T. They are not well defined except for the special Φ, in contrast to the spin operators.

C.1. Translation operator

The unitary operator U_Φ of the twisted boundary condition (17) is transformed with the translation as

$$\begin{aligned} T_R U_\Phi [T_R]^{-1} &= \exp\left(\frac{\mathrm{i}\Phi}{L}\sum_{j=1}^{L}(j-\tfrac{1}{2})S^z_{j+1}\right) \\ &= U_\Phi \exp\left(-\frac{\mathrm{i}\Phi}{L}S^z_T\right)\exp(\mathrm{i}\Phi S^z_1) \end{aligned} \tag{64}$$

therefore, we obtain

$$U_\Phi T_R [U_\Phi]^{-1} = \exp(-\mathrm{i}\Phi S^z_1) T^t_R \tag{65}$$

where we introduce the operator $T^t_R \equiv \exp(\mathrm{i}\Phi S^z_T/L)T_R$. The operator $\exp(-\mathrm{i}\Phi S^z_1)$ is not well defined except for $\Phi = 2\pi l (l$: integer)

$$U_{2\pi l} T_R [U_{2\pi l}]^{-1} = (-1)^{2Sl} T^t_R. \tag{66}$$

In the notation T^t_R, the periodicity of the energy and the momentum eigenvalue under $\Phi \to \Phi + 2\pi (S$: integer) or $\Phi \to \Phi + 4\pi (S$: half-odd integer) [44, 45] becomes apparent, in contrast to [46, 47]. Note that when we define the wavenumber $q' \equiv q + \Phi S^z_T/L$ as

$$T^t_R |\psi(q, S^z_T, \Phi)\rangle = \exp(\mathrm{i}(q + \Phi S^z_T/L))|\psi(q, S^z_T, \Phi)\rangle \tag{67}$$

$Lq'/2\pi$ is not integer in general, although it corresponds to the eigenvalue $mn + n\Phi/2\pi$ of the conformal spin operator $L_0 - \bar{L}_0$ under TBC (see equations (39), (42), (43), (50)), and T^t_R has a more natural symmetry structure than T_R, as will be seen later.

C.2. Discrete symmetries P, T

The unitary operator U_Φ is transformed with the parity as

$$\begin{aligned} P U_\Phi P &= \exp\left(\frac{\mathrm{i}\Phi}{L}\sum_{j=1}^{L}(j-\tfrac{1}{2})S^z_{L+1-j}\right) \\ &= U_{-\Phi}\exp(\mathrm{i}\Phi S^z_T) \end{aligned} \tag{68}$$

therefore, we obtain

$$U_\Phi P [U_\Phi]^{-1} = U_{2\Phi} P \exp(-\mathrm{i}\Phi S^z_T). \tag{69}$$

The operator $\exp(\mathrm{i}\Phi S^z_T)$ is not well defined except for $\Phi = \pi l (l$:integer)

$$U_{\pi l} P [U_{\pi l}]^{-1} = (-1)^{S^z_T l} U_{2\pi l} P \tag{70}$$

where we use that S_T^z is integer. In this case, we obtain

$$(U_{2\pi l}P)^2 = 1. \tag{71}$$

Similarly, we obtain

$$U_\Phi T[U_\Phi]^{-1} = U_{2\Phi}T \tag{72}$$

and

$$(U_{2\Phi}T)^2 = 1. \tag{73}$$

For the twist angle $\Phi = \pi l$, Hamiltonian (18) commutes with the operators $U_{2\pi l}P, U_{2\pi l}T$. Moreover, these operators forms Z_2 group, that is, the eigenvalue of $U_{2\pi}P, U_{2\pi}T$ is ± 1.

Next for the twist angle $\Phi = \pi l$, we discuss the relation between the operator $U_{2\pi l}P$ and the translation operator T_R^t. Using (64), we obtain

$$\begin{aligned} T_R^t U_{2\pi l} P T_R^t &= \exp\left(\frac{2\pi \mathrm{i} l}{L} S_T^z\right) T_R U_{2\pi l}[T_R]^{-1} T_R P T_R \\ &= \exp(2\pi \mathrm{i} S_1^z l) U_{2\pi l} P. \end{aligned} \tag{74}$$

Since the operator $\exp(2\pi \mathrm{i} S_1^z)$ is $\pm I$ for S integer or half-integer, this means

$$T_R^t(U_{2\pi l}P) = (-1)^{2Sl}(U_{2\pi l}P)(T_R^t)^{-1} \tag{75}$$

that is, in the momentum space for the even-integer $2Sl$, the spectrum is symmetric with respect to $q = 0, \pi$, whereas for the odd-integer $2Sl$, the spectrum is symmetric with respect to $q = \pm\pi/2$. For the half-odd integer S case, under TBC ($\Phi = \pi$) the ground state ($q = 0$) is exactly degenerate with a state $q = \pi$ [46], which is related to the Gaussian transition [26].

C.3. Valence bond solid states

As an application of the previous sections, we discuss the generalized $Z_2 \times Z_2$ symmetries or valence bond solid (VBS) [27] under the twisted boundary condition. It was shown that under the twisted boundary conditions the quantum numbers P, T are the good quantum numbers characterizing the generalized $Z_2 \times Z_2$ symmetries [26]. Here we generalize these results for the twisted boundary conditions with the translational invariant case.

The spin variable can be represented by the Schwinger bosons as follows

$$S_j^z = \tfrac{1}{2}(a_j^+ a_j - b_j^+ b_j) \qquad S_j^+ = a_j^+ b_j \qquad S_j^- = a_j b_j^+ \tag{76}$$

with the constraint that the boson occupation number at each site $a_j^+ a_j + b_j^+ b_j$ is $2S$.

The VBS states with the TBC can be written as

$$\begin{aligned} |S, M, TBC(\Phi = \pi)\rangle = {} & (a_L^+ b_1^+ \mathrm{e}^{-\mathrm{i}\pi/2L} - b_L^+ a_1^+ \mathrm{e}^{\mathrm{i}\pi/2L})^{S-M} \\ & \times \prod_{j=1}^{L/2-1} (a_{2j-1}^+ b_{2j}^+ \mathrm{e}^{-\mathrm{i}\pi/2L} - b_{2j-1}^+ a_{2j}^+ \mathrm{e}^{\mathrm{i}\pi/2L})^{S+M} \\ & \times (a_{2j}^+ b_{2j+1}^+ \mathrm{e}^{-\mathrm{i}\pi/2L} - b_{2j}^+ a_{2j+1}^+ \mathrm{e}^{\mathrm{i}\pi/2L})^{S-M} \\ & \times (a_{L-1}^+ b_L^+ \mathrm{e}^{-\mathrm{i}\pi/2L} - b_{L-1}^+ a_L^+ \mathrm{e}^{\mathrm{i}\pi/2L})^{S+M} |0\rangle \end{aligned} \tag{77}$$

where M is an integer for the integer S, or a half-odd integer for the half-odd integer S (here we include bond-alternating cases). First we make a parity transformation for the VBS state

$$P|S, M, TBC(\Phi = \pi)\rangle = (-1)^{SL}|S, M, TBC(\Phi = -\pi)\rangle \tag{78}$$

where we use $P|0\rangle = |0\rangle$. Then twisting with $U_{2\pi}$, we obtain

$$U_{2\pi} P|S, M, TBC(\Phi = \pi)\rangle = (-1)^{SL-S+M}|S, M, TBC(\Phi = \pi)\rangle \qquad (79)$$

where we use $U_{2\pi}|0\rangle = |0\rangle$, and $U_{2\pi} a_L^+ b_1^+ U_{2\pi}^{-1} = a_L^+ b_1^+ \exp(2\pi \mathrm{i}(L-1)/2L)$. The same discussion applies for $U_{2\pi} T$. Therefore, each M-VBS states is characterized by the discrete quantum numbers $U_{2\pi} P = U_{2\pi} T = (-1)^{SL-S+M}$.

Similarly we can classify the intermediate large D phase with the discrete quantum number $U_{2\pi} P$, $U_{2\pi} T$ under TBC.

References

[1] Berezinskii V L 1971 *Zh. Eksp. Teor. Fiz.* **61** 1144 (Engl. transl 1972 *Sov. Phys.–JETP* **34** 610)
[2] Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181
[3] Kosterlitz J M 1974 *J. Phys. C: Solid State Phys.* **7** 1046
[4] Giamarchi T 1991 *Phys. Rev.* B **44** 2905
Giamarchi T 1992 *Phys. Rev.* B **46** 342
[5] For example Gupta R, DeLapp J, Batrouni G G, Fox G C, Baillie C F and Apostolakis J 1988 *Phys. Rev. Lett.* **61** 1996
[6] Seiler E, Stamatescu I O, Patrascioiu A and Linke V 1988 *Nucl. Phys.* B **305** 623
[7] Edwards R G, Goodman J and Sokal A D 1991 *Nucl. Phys.* B **354** 289
[8] Sólyom J and Ziman T A L 1984 *Phys. Rev.* B **30** 3980
[9] Nomura K 1995 *J. Phys. A: Math. Gen.* **28** 5451
[10] Halpern M B 1975 *Phys. Rev.* D **12** 1684
Halpern M B 1976 *Phys. Rev.* D **13** 337
[11] Banks T, Horn D and Neuberger H 1976 *Nucl. Phys.* B **108** 119
[12] Ginsparg P 1988 *Nucl. Phys.* B **295** 153
[13] Blöte H W J, Cardy J L and Nightingale M P 1986 *Phys. Rev. Lett.* **56** 742
[14] Destri C and de Vega H J 1989 *Phys. Lett.* B **223** 365
[15] Kitazawa A 1997 *J. Phys. A: Math. Gen.* **30** L285
[16] Alcaraz F C, Barber M N and Batchelor M 1987 *Phys. Rev. Lett.* **58** 771
Alcaraz F C, Barber M N and Batchelor M 1988 *Ann. Phys.* **182** 280
[17] Affleck I 1985 *Phys. Rev. Lett.* **55** 1355
[18] Giamarchi T and Schulz H J 1989 *Phys. Rev.* B **39** 4620
[19] Cardy J L 1986 *Nucl. Phys.* B **270** 186
[20] Reinicke P 1987 *J. Phys. A: Math. Gen.* **20** 5325
[21] Haldane F D M 1983 *Phys. Lett.* **93A** 464
Haldane F D M 1983 *Phys. Rev. Lett.* **50** 1153
[22] Botet R and Jullien R 1983 *Phys. Rev.* B **27** 613
[23] Sakai T and Takahashi M 1990 *J. Phys. Soc. Japan* **59** 2688
[24] Yajima M and Takahashi M 1994 *J. Phys. Soc. Japan* **63** 3634
[25] Kitazawa A, Nomura K and Okamoto K 1996 *Phys. Rev. Lett.* **76** 4038
[26] Kitazawa A and Nomura K 1997 *J. Phys. Soc. Japan* **66** 3944
Kitazawa A and Nomura K 1997 *J. Phys. Soc. Japan* **66** 3379
[27] Oshikawa M 1992 *J. Phys.: Condens. Matter* **4** 7469
[28] Cardy J L 1984 *J. Phys. A: Math. Gen.* **17** L385
[29] Affleck I 1986 *Phys. Rev. Lett.* **56** 746
[30] Hatano N and Suzuki M 1993 *J. Phys. Soc. Japan* **62** 1346
[31] Deisz J, Jarrell M and Cox D L 1993 *Phys. Rev.* B **48** 10 227
[32] Sun G 1995 *Phys. Rev.* B **51** 8370
[33] Nishiyama Y, TotsukaK, Hatano N and Suzuki M 1995 *J. Phys. Soc. Japan* **64** 414
[34] Schollwöck U and Jolicœur Th 1995 *Europhys. Lett.* **30** 493
[35] Yamamoto S 1995 *Phys. Rev. Lett.* **75** 3348
[36] Qin S, Ng T K and Su Z B 1995 *Phys. Rev.* B **52** 12 844
[37] Qin S, Liu Y L and Yu L 1997 *Phys. Rev.* B **55** 2721
[38] Nightingale M P and Blöte H W 1986 *Phys. Rev.* B **33** 650
[39] White S R 1992 *Phys. Rev. Lett.* **69** 2863
White S R 1993 *Phys. Rev.* B **48** 10 345

[40] Oshikawa M, Yamanaka M and Miyashita S 1995 *Preprint* (cond-mat/9507098)
[41] Nomura K and Okamoto K 1994 *J. Phys. A: Math. Gen.* **27** 5773
[42] Ziman T A L and Schulz H J 1987 *Phys. Rev. Lett.* **59** 140
[43] Ginsparg P 1990 *Fields, Strings, and Critical Phenomena (Les Houches XLIX)* ed E Brézin and J Zinn-Justin (Amsterdam: North Holland)
[44] Sutherland B and Shastry B S 1990 *Phys. Rev. Lett.* **65** 1833
[45] Fukui T and Kawakami N 1996 *J. Phys. Soc. Japan* **65** 2824
[46] Kolb M 1985 *Phys. Rev.* B **31** 7494
[47] Fáth G and Sólyom J 1993 *Phys. Rev.* B **47** 872