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**LETTER TO THE EDITOR**

# Twisted boundary conditions of quantum spin chains near the Gaussian fixed points

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**Abstract.** We consider the Gaussian transition of one-dimensional quantum spin systems. Although the Gaussian transition is the second-order phase transition, the usual finite-size scaling technique does not work well in some cases. Using the conformal field theory, we present a new method which overcomes this difficulty.

In this letter, we propose a method to determine the Gaussian critical point of quantum spin chains. Although the finite-size scaling method is a powerful tool to determine the critical point numerically, difficulty may occur for some Gaussian cases. An example is the transition between the Haldane gap and the large-$D$ phases of the $S = 1$, XXZ spin chains with single-ion anisotropy [1, 2]. It was reported that there are two crossing points of the scaled gaps $L\Delta E(L)$ and $(L+1)\Delta E(L+1)$ ($L$ is the system size, and $\Delta E$ is the energy gap), and the difference of these two points decreases as $L$ increases. As we see below, this behaviour comes from the structure of scaling operators.

For the $S = 1/2$, XXZ spin chain with next-nearest neighbour interactions, the transition between the dimer and the Néel phases is also of Gaussian type. Based on the renormalization group analysis [3], Nomura and Okamoto [4] proposed an elegant method to determine the transition point by crossing of two levels with different symmetry. But, unfortunately, there is a difference between the $S = 1$ and the $S = 1/2$ cases with the periodic boundary condition; that is, the $S = 1/2$ case has an extra $Z_2$ symmetry. So we cannot simply apply the method of Nomura and Okamoto to the $S = 1$ case. By changing the boundary condition, we have the other structure of operators. Therefore, selecting appropriate boundary conditions, we can use the preferable structure to determine the critical point.

As an effective theory of the one-dimensional (1D) quantum spin systems, the following sine–Gordon model (in Euclidean spacetime) has been studied

$$S = \frac{1}{2\pi K}\int d\tau\, dx[(\partial_\tau\phi)^2 + (\partial_x\phi)^2] + \frac{y}{2\pi\alpha^2}\int d\tau\, dx \cos\sqrt{2}\phi \tag{1}$$

where $\alpha$ is a short distance cut-off. The dual field $\theta(\tau, x)$ is defined as

$$\partial_\tau\phi = -\partial_x(iK\theta) \qquad \partial_x\phi = \partial_\tau(iK\theta). \tag{2}$$

We make the identification $\phi \equiv \phi + \sqrt{2}\pi, \theta \equiv \theta + \sqrt{2}\pi$. There exists $U(1)$ symmetry for the field $\theta$, but the second term of equation (1) violates $U(1)$ symmetry for $\phi$. For the

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free-field theory, the scaling dimensions of the spin wave operator $\exp(\pm \mathrm{i} n\sqrt{2}\theta)$ and the vortex operator $\exp(\pm \mathrm{i} m\sqrt{2}\phi)$ are $n^2/2K$ and $Km^2/2$, where the integer variables $n$ and $m$ are electric and magnetic charges in the Coulomb gas picture.

After the scaling transformation $\alpha \to \mathrm{e}^{\mathrm{d}l}\alpha$, we have the following renormalization group equations:

$$\frac{\mathrm{d}K^{-1}}{\mathrm{d}l} = \frac{1}{8}y^2 \qquad \frac{\mathrm{d}y}{\mathrm{d}l} = \left(2 - \frac{K}{2}\right) y.$$

These are the famous recursion relations of Kosterlitz. Up to first order in $y$, we find that $y$ is an irrelevant field for $K > 4$ and relevant for $K < 4$. There is a separatrix $32K^{-1} - 8\ln K^{-1} - y^2 = 8 + 8\ln 4$ which separates the infrared unstable region from the infrared stable region, and on this separatrix the Berezinskii–Kosterlitz–Thouless transition occurs. The Gaussian fixed line lies on $y = 0$. For $K < 4$ and $y \neq 0$, $y$ flows to infinity. For $y > 0$, $\langle\phi\rangle$ is renormalized to $\pi/\sqrt{2}$ as $y \to +\infty$ and for $y < 0$, $\langle\phi\rangle \to 0$ as $y \to -\infty$.

The infinite two-dimensional plane can be mapped to a periodic strip of width $L$ by the conformal mapping $w = (L/2\pi)\log z$ $(z = \tau + \mathrm{i}x)$. In the rest of this letter, we consider the boundary effect of this strip system.

First let us consider the following 1D Hamiltonian with the periodic boundary condition [5]

$$H = H_0 + \frac{\lambda}{2\pi}\int_0^L \mathrm{d}x\, \mathcal{O}_1 \tag{3}$$

where $H_0$ is a fixed-point Hamiltonian and $\mathcal{O}_1 (= \mathcal{O}_1^\dagger)$ is a scaling operator whose scaling dimension is $x_1$. According to Cardy [5], the following finite-size dependence of excitation energies up to the first-order perturbation is obtained,

$$\Delta E_n = \frac{2\pi}{L}\left(x_n + \lambda C_{n1n}\left(\frac{2\pi}{L}\right)^{x_1-2} + \cdots\right) \tag{4}$$

where $L$ is the length of the system, $x_n$ is the scaling dimension of the operator $\mathcal{O}_n$. $C_{n1n}$ is the operator product expansion (OPE) coefficient of operators $\mathcal{O}_n$ and $\mathcal{O}_1$ as

$$\mathcal{O}_1(z,\bar{z})\mathcal{O}_n(0,0) = C_{n1n}\left(\frac{\alpha}{z}\right)^{h_1}\left(\frac{\alpha}{\bar{z}}\right)^{\bar{h}_1}\mathcal{O}_n(0,0) + \cdots \tag{5}$$

in which $h_1$ and $\bar{h}_1$ are the conformal weights of $\mathcal{O}_1$ $(x_1 = h_1 + \bar{h}_1)$. From equation (4), we have the following RG equation

$$\frac{\mathrm{d}\lambda}{\mathrm{d}\ln L} = (x_1 - 2)\lambda.$$

When $x_1 < 2$(relevant), the second-order phase transition occurs at $\lambda = 0$, whereas $x_1 > 2$(irrelevant), the second term in equation (4) is the finite-size corrections of the excitation energies of the critical systems. Up to first-order perturbation theory, we find that at the point $\lambda = 0$ the scaled gap $L\Delta E_n$ does not depend on the system size, and the scaled gaps for several $L$ cross linearly at $\lambda = 0$.

On the other hand, when the OPE coefficient $C_{n1n}$ becomes zero for some reason, the above argument is insufficient and we must consider the second-order term of $\lambda$ in equation (4). In this case, the scaled gap $L\Delta E_n$ may have an extremum at the point $\lambda = 0$. In practice, this is not a preferable thing, because the point of extremum is sensitive to finite-size corrections of irrelevant operators such as $L_{-2}\bar{L}_{-2}\mathbf{1}$ $(x = 4)$.

In the sine–Gordon model (1), we substitute the operator $\sqrt{2}\cos\sqrt{2}\phi$ for $\mathcal{O}_1$. In this case, there is no operator $\mathcal{O}_n$ with a non-zero value of $\langle\mathcal{O}_n^\dagger(z_1)\mathcal{O}_1(z_2)\mathcal{O}_n(z_3)\rangle$. (This is related to the charge neutrality conditions in the Coulomb gas picture. Note that the operators $e^{\pm i\phi/\sqrt{2}}$ are not allowed.) Thus the OPE coefficient in (4) is zero. This indicates that we cannot expect the simple behaviour of the finite-size scaling method.

Let us return to model (1). If we put artificially half magnetic charges $m = \pm 1/2$ in the system, the OPE relations are

$$\begin{aligned} \mathcal{O}_1(z,\bar{z})\mathcal{O}^e_{1/2}(0,0) &= \frac{\sqrt{2}}{2}\left(\frac{\alpha}{z}\right)^{K/4}\left(\frac{\alpha}{\bar{z}}\right)^{K/4}\mathcal{O}^e_{1/2}(0,0)+\cdots \\ \mathcal{O}_1(z,\bar{z})\mathcal{O}^o_{1/2}(0,0) &= -\frac{\sqrt{2}}{2}\left(\frac{\alpha}{z}\right)^{K/4}\left(\frac{\alpha}{\bar{z}}\right)^{K/4}\mathcal{O}^o_{1/2}(0,0)+\cdots \end{aligned} \tag{6}$$

where

$$\begin{aligned} \mathcal{O}_1 &= \sqrt{2}\cos\sqrt{2}\phi \\ \mathcal{O}^e_{1/2} &= \sqrt{2}\cos\frac{1}{\sqrt{2}}\phi \\ \mathcal{O}^o_{1/2} &= \sqrt{2}\sin\frac{1}{\sqrt{2}}\phi \end{aligned} \tag{7}$$

and there are non-zero OPE coefficients in (4).

For a physical example with half magnetic charges, Alcaraz *et al* [6] studied the $S = 1/2$, XXZ spin chain using the Bethe ansatz

$$H = -\sum_{j=1}^{L}[S^x_j S^x_{j+1} + S^y_j S^y_{j+1} + \Delta S^z_j S^z_{j+1}]$$

with twisted boundary conditions

$$S^x_{L+1} \pm iS^y_{L+1} = e^{\pm i\Phi}(S^x_1 \pm iS^y_1) \qquad S^z_{L+1} = S^z_1.$$

When $\Phi = 0$, this model corresponds to the Gaussian model with $K = \pi/\arccos(\Delta)$, $-1 < \Delta < 1$. According to their numerical results, the twisted boundary conditions change the electric and magnetic charges as

$$n \to n \qquad m \to m + \frac{\Phi}{2\pi}. \tag{8}$$

Hence when the twist angle $\Phi$ is $\pi$, half-integer magnetic charges appear. Recently, Fukui and Kawakami [7] studied this model analytically and their results are consistent with equation (8). However, the off-critical behaviours have not been treated.

To see what happens when the boundary condition is changed in the Coulomb gas picture, we review the case of the following action [8]:

$$S = \frac{1}{2\pi}K\int_{-\infty}^{\infty}d\tau\int_0^L dx[(\partial_\tau\theta)^2 + (\partial_x\theta)^2] + \frac{\Phi}{\sqrt{2}\pi}K\int_{-\infty}^{\infty}d\tau\,\partial_x\theta(\tau,0). \tag{9}$$

Here we write the action with the field $\theta$ which is dual to $\phi$, and we assume the periodic boundary condition $\phi(\tau, L) = \phi(\tau, 0) + \sqrt{2}\pi M$, $\theta(\tau, L) = \theta(\tau, 0) + \sqrt{2}\pi N$, where $M$ and $N$ are integers. If we transform the field $\theta$ as $\theta(\tau, x) \to \theta(\tau, x) - \Phi x/\sqrt{2}L$, then we can eliminate the second term of equation (9) with the additional constant term $\Phi^2 K/2\pi L$, but the boundary condition is changed as $\phi(\tau, L) = \phi(\tau, 0) + \sqrt{2}\pi M$, $\theta(\tau, L) = \theta(\tau, 0) + \sqrt{2}\pi N - \Phi/\sqrt{2}$, which corresponds to the defect line along the imaginary time. When $\Phi = 2N\pi$ ($N$ is an integer), this is the periodic boundary condition.

After the dual transformation (2), the action (9) is transformed as

$$S = \frac{1}{2\pi K}\int_{-\infty}^{\infty}d\tau\int_0^L dx[(\partial_\tau\phi)^2 + (\partial_x\phi)^2] + i\sqrt{2}\left(\frac{\Phi}{2\pi}\right)\int_{-\infty}^{\infty}d\tau\,\partial_\tau\phi(\tau,0). \tag{10}$$

This shows that there exist magnetic charges $\mp\Phi/2\pi$ at $\tau = \pm\infty$. Thus we obtain the ground-state energy as [6]

$$\frac{L}{2\pi}(E_0(\Phi) - E_0(0)) = \frac{K}{2}\left(\frac{\Phi}{2\pi}\right)^2 \equiv x_0(\Phi) \tag{11}$$

and the conformal anomaly number changes as

$$c(\Phi) = 1 - 12x_0(\Phi) = 1 - 6\left(\frac{\Phi}{2\pi}\right)^2 K. \tag{12}$$

We denote the state corresponding to the primary operator $V_{n,m} = \exp(\mathrm{i}\sqrt{2}n\theta + \mathrm{i}\sqrt{2}m\phi)$ as $|n, m\rangle$. Since there exists a magnetic charge $\Phi/2\pi$ at $\tau = -\infty$, we find the change of this state as

$$|n, m\rangle_\Phi = |n, m + \Phi/2\pi\rangle_{\Phi=0} \tag{13}$$

and because there exists a magnetic charge $-\Phi/2\pi$ at $\tau = \infty$, the conjugate state is

$${}_\Phi\langle n, m| = {}_0\langle n, m + \Phi/2\pi|. \tag{14}$$

Hence we obtain [6]

$$E_{n,m}(\Phi) - E_0(0) = \frac{2\pi}{L}\left(\frac{n^2}{2K} + \frac{K}{2}\left(m + \frac{\Phi}{2\pi}\right)^2\right) \tag{15}$$

or

$$E_{n,m}(\Phi) - E_0(\Phi) = \frac{2\pi}{L}\left(\frac{n^2}{2K} + \frac{K}{2}m\left(m + \frac{\Phi}{\pi}\right)\right). \tag{16}$$

From this equation, we find that the state $|n, 0\rangle_\Phi$ corresponds to $|n, \Phi/2\pi\rangle_0$ which has excitation energy $E_{n,0}(\Phi) - E_0(\Phi) = E_{n,0}(0) - E_0(0)$, and momentum $n\Phi/L$.

Note that Dotsenko and Fateev [9] considered the similar situation

$$S = \frac{1}{2\pi K}\int_{-\infty}^{\infty} \mathrm{d}\tau \int_0^L \mathrm{d}x\, (\partial_\mu\phi)^2 + \mathrm{i}\sqrt{2}\left(\frac{\Phi'}{2\pi}\right)\phi(\tau_0, 0) \qquad (\tau_0 \to \infty) \tag{17}$$

in which the additional charge exists only at $\tau = \infty$ but not at $\tau = -\infty$. If we set $\Phi' = 2\Phi$ [8], the change of conformal anomaly number is the same as equation (12), but the structure of scaling operators is not the same as the case of (9). In the case of (17), $|n, m\rangle_{\Phi'} = |n, m\rangle_0$, and the conjugate state changes as ${}_{\Phi'}\langle n, m| = {}_0\langle n, m + \Phi'/2\pi|$ (which is consistent with (16)). However, in (9) the conjugate relation does not change as equation (13) and (14), and the model is as in $c = 1$ conformal field theory.

In the case of $\Phi = \pi$, we have half-integer magnetic charges effectively. In this case, $|0, -1\rangle_\pi (= |0, -1/2\rangle_0)$ and $|0, 0\rangle_\pi (= |0, 1/2\rangle_0)$ are degenerate for the free-field theory. Introducing the perturbation term of equation (1) and using first-order perturbation theory, we obtain the hybridized states

$$|\psi_1\rangle_\pi = \frac{1}{\sqrt{2}}(|0, -1\rangle_\pi + |0, 0\rangle_\pi) \tag{18}$$

whose parity is even, and

$$|\psi_2\rangle_\pi = \frac{1}{\sqrt{2}\mathrm{i}}(|0, -1\rangle_\pi - |0, 0\rangle_\pi) \tag{19}$$

whose parity is odd. (Note that only when $\Phi = 0$ and $\pi$, parity is a good quantum number.) Using the OPE (6) and setting $\lambda = y/\sqrt{2}$, we obtain the finite-size dependence of energy up to the first-order perturbation as

$$E_1(\pi) - E_0(0) = \frac{2\pi}{L}\left(\frac{K}{8} + \frac{y}{2}\left(\frac{2\pi}{L}\right)^{K/2-2} + \cdots\right)$$
$$E_2(\pi) - E_0(0) = \frac{2\pi}{L}\left(\frac{K}{8} - \frac{y}{2}\left(\frac{2\pi}{L}\right)^{K/2-2} + \cdots\right). \tag{20}$$

Thus we find that the energy eigenvalues of these states cross linearly at $y = 0$.

To verify the above things numerically, we study the following $S = 1$ quantum spin chain:

$$H = \sum_{j=1}^{N}(1 - \delta(-1)^j)(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z). \tag{21}$$

The effective action of this model is described as equation (1). For the periodic boundary condition, this model has $U(1)$ symmetry, and this symmetry restricts the operator structure. The whole phase diagram was shown in [10]. The transition between the dimer and the Haldane gap phases is of Gaussian type. Using the Lanczos method, we calculate energy eigenvalues of finite systems ($N = 8, 10, 12, 14, 16$). Figure 1 shows the scaled gap behaviour of $N = 12, 14, 16$ systems with the periodic boundary condition for $\Delta = 0.5$. We can see a minimum of the scaled gap. In figure 2, we show two low-lying energies of the subspace $\sum S^z = 0$ with the boundary conditions $S_{N+1}^x = -S_1^x$, $S_{N+1}^y = -S_1^y$, $S_{N+1}^z = S_1^z$, which correspond to $E_1(\pi)$ and $E_2(\pi)$. We see the expected behaviour (20) for this twisted boundary condition. Figure 3 shows the size dependence of the crossing point. Convergence is very fast. The conformal anomaly number is calculated as $c = 0.998$ for the periodic boundary condition and $c(\pi) = -3.194$ for the $\Phi = \pi$ twisted boundary condition. In table 1, we show some extrapolated scaling dimensions. These numerical

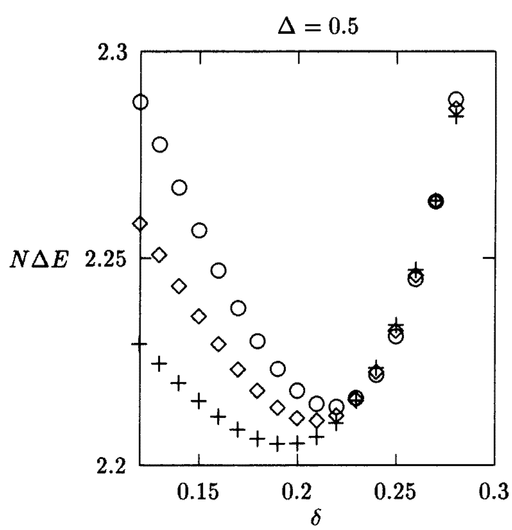


**Figure 1.** The scaled gap behaviour of $N = 12(+)$, $N = 14(\Diamond)$ and $N = 16(\bigcirc)$ systems with the periodic boundary condition for $\Delta = 0.5$.

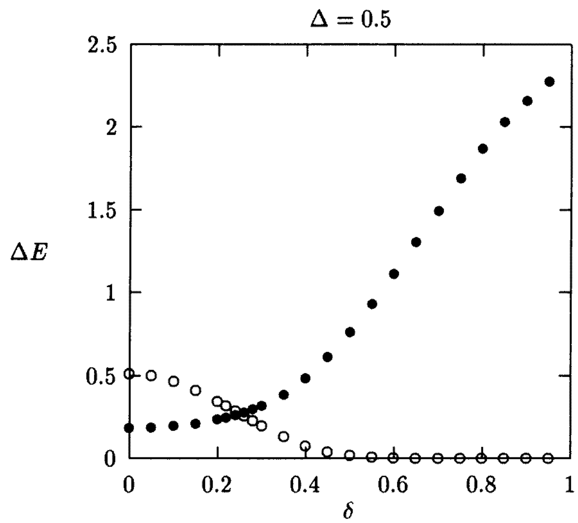


**Figure 2.** The low-lying energies ($E(\Phi = \pi) - E_0(\Phi = 0)$) of the $N = 16$ system for $\Delta = 0.5$. ○s are parity even states ($E_1(\pi)$), and ●s are parity odd states ($E_2(\pi)$).

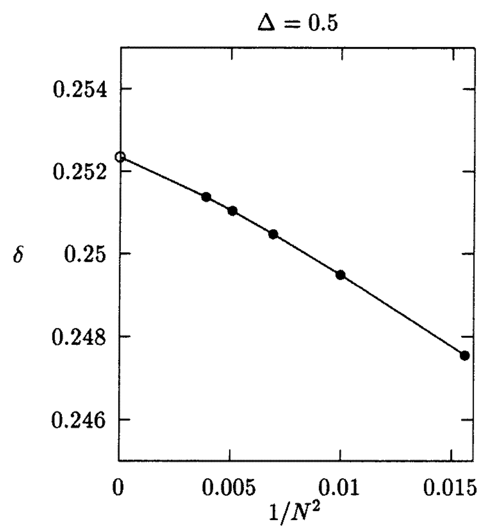


**Figure 3.** Size dependence of the crossing points. The extrapolated value is $\delta_c = 0.2524$.

values are consistent with equations (11), (12), and (15). With this method, we can also determine the Gaussian fixed line in the massless XY phase [11] and apply the approach to the $S = 1$ spin chains with single-ion anisotropy [1, 2].

Lastly we consider the difference between the $S = 1$ models and the model treated by Nomura and Okamoto [4]. The continuum effective action of the latter model is written as

$$S = \frac{1}{2\pi K} \int d\tau\, dx [(\partial_\tau \phi)^2 + (\partial_x \phi)^2] + \frac{y_2}{2\pi\alpha^2} \int d\tau\, dx \cos\sqrt{8}\phi \qquad (22)$$

**Table 1.** Scaling dimensions at the critical point $\Delta = 0.5$, $\delta = 0.2524$. Here we have extrapolated the corrections from the irrelevant field $L_2\bar{L}_2\mathbf{1}$ ($x = 4$). For the value of $x_{0,1}$, we take the average of the scaling dimensions of $2\cos\sqrt{2}\phi$ and $2\sin\sqrt{2}\phi$.

| | $x_{1,0} = 1/2K$ | $x_{0,1} = K/2$ | $x_{0,1/2} (= x_0(\pi))$ |
|---|---|---|---|
| Scaling dimension | 0.1786 | 1.400 | 0.3497 |
| $K$ | 2.799 | 2.801 | 2.798 |

with the identification $\phi = \phi + \sqrt{2}\pi$, $\theta = \theta + \sqrt{2}\pi$. For $K < 1$, the operator $\sqrt{2}\cos\sqrt{8}\phi$ is relevant and the second-order (Gaussian) transition occurs at $y_2 = 0$. In this case, the three-point function

$$\langle e^{\pm i\sqrt{2}\phi(z_1)}\sqrt{2}\cos\sqrt{8}\phi(z_2)e^{\pm i\sqrt{2}\phi(z_3)}\rangle_0$$

is not zero, so it is enough to consider the periodic boundary condition. The action (22) is invariant under $\phi \to \phi + \pi/\sqrt{2}$, and this $Z_2$ symmetry separates the even and the odd magnetic charge operators. However, the action (1) does not have this type of $Z_2$ symmetry. For the case of (1), if we see the operator structure as the sum of the one with the periodic boundary condition and the one with the $\Phi = \pi$ twisted boundary condition,

$$[\mathrm{PBC}(n, m = \text{integer})] \oplus [\pi\mathrm{TBC}(n = \text{integer}, m = \text{half integer})] \tag{23}$$

the invariance $\phi \to \phi + \sqrt{2}\pi$ separates the integer and the half-integer magnetic charge operators. Therefore, the twisted boundary condition for (1) is needed to add an additional $Z_2$ symmetry. Consequently, the OPE structure of (1) with the periodic and the $\Phi = \pi$ twisted boundary conditions becomes the same as (22) (at least relating to $\phi$).

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