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COMMENT

The one-dimensional dimerised spin-$\frac{1}{2}$ XY chain with arbitrary boundary conditions and related unitary and non-unitary models

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Abstract. The central charge of the Virasoro algebra of the one-dimensional dimerised XY model with arbitrary boundary conditions is obtained at criticality. We obtain $c = 1 - 12\tau^2$ where $\tau (0 \leq \tau \leq 1/2)$ characterises the boundary conditions. This shift of c yields relations between the XY model and both the q-state Potts model and the O(N) model. We show that the phenomenological renormalisation group equation, which is used to estimate the critical value of the parameter of the system, has no real solution for the range $\tau > 1/2\sqrt{6}$. This corresponds to the non-unitary Potts model ($0 \leq q < 2$) and the O(N) one ($-2 \leq N < 1$).

In this comment, we re-examine some of the results obtained previously with the one-dimensional dimerised XY model with arbitrary boundary conditions (BC) (Spronken and Kemp 1986). One of them is the intriguing result that there are BC for which the phenomenological renormalisation group (PRG) equation (Nightingale 1982), which results from the finite-size scaling hypothesis (Derrida and De Seze 1982), has no real solution for arbitrary large (but finite) size of the linear XY chain. The purpose of the present work is to analyse this result in terms of the theory of conformal invariance (see for instance Cardy (1987) and references therein).

Our aim is twofold. We first obtain the finite-size corrections to the ground-state energy of the system, at criticality. This yields the BC-dependent central charge (or conformal anomaly), c, of the model. This central charge may then be used to relate the XY system to different models like the q-state Potts model ($0 \leq q \leq 4$). We then show that the range of BC for which the PRG equation fails to provide real estimates of the critical parameter corresponds to non-unitary theories (i.e. theories with $c < 1/2$).

In fact, the parameter τ (defined below) that characterises the BC is equivalent to the charge (defect line) introduced in the modified Gaussian model (Blöte *et al* 1986, Dotsenko and Fateev 1984, Cardy 1987). The τ dependence of c, the central charge of the Virasoro algebra (Affleck 1986, Friedan *et al* 1984), is $c = 1 - 12\tau^2$ and one can use the results of Blöte *et al* (1986) (see also Cardy 1987) to relate τ to the q-state Potts model ($0 \leq q \leq 4$). For example one has for $\tau = 1/2\sqrt{6}$, $c = 1/2$ and $q = 2$ (the Ising model) and for $\tau > 1/2\sqrt{6}$, $c < 1/2$ and $q < 2$. This is the range of non-unitary theories. It is precisely for this range of τ (i.e. $\tau > 1/2\sqrt{6}$) that the PRG has no real solution. Using the work of Blöte *et al* (1986), we also give explicit relations between τ and q ($0 \leq q \leq 4$) of the q-state Potts model as well as τ and N of the O(N) model

($|N| \leq 2$). Varying τ from $\tau = 0$ (periodic BC) to $\tau = 1/2$ (antiperiodic BC) (i.e. $-2 \leq c \leq 1$), one obtains the whole set of the dominant corrections to the finite-size scaling for these models.

This comment is organised as follows. We first recall the main results obtained for the one-dimensional dimerised XY model. The ground-state energy is then obtained at criticality and the central charge is calculated. The relations between τ and the parameters of the q-state Potts model and the O(N) model are then established. Using these relations, we show that the XY model with BC such that the PRG has no real solution corresponds to non-unitary models.

The Hamiltonian for the one-dimensional spin-$\frac{1}{2}$ dimerised antiferromagnetic XY model is

$$H = \tfrac{1}{2} \sum_{j=1}^{N} [1-(-1)^j \delta][\sigma_j^+ \sigma_{j+1}^- + \mathrm{cc}] \qquad \sigma_{N+1}^{\pm} = \mathrm{e}^{\pm 2\pi i \tau} \sigma_1^{\pm} \tag{1}$$

where the quantity δ is the dimerisation parameter which is subjected to $|\delta| \leq 1$ and where the boundary conditions are characterised by the parameter τ ($0 \leq \tau \leq 1/2$; $\tau = 0$, periodic BC; $\tau = 1/2$, antiperiodic BC). In equation (1), the σ are the Pauli operators and the factor $\frac{1}{2}$ is a normalisation factor (Hamer 1985). The number of sites, N, is assumed to be even. The XY model whose Hamiltonian is given by (1), has been shown previously (Fields, 1979) to undergo a phase transition in the thermodynamic limit for $\delta = 0$. It also corresponds to the Ashkin–Teller model in the quantum Hamiltonian limit (without interaction, Kohmoto *et al* (1981)).

The Hamiltonian (1) can be rewritten in terms of spinless fermion variables using the Jordan–Wigner transformation (Jordan and Wigner 1928). An additional linear transformation (Lieb *et al* 1961) then yields

$$H = \sum_{k\sigma} \Lambda_k(\delta)(\eta_{k\sigma}^+ \eta_{k\sigma} - \tfrac{1}{2}) \tag{2}$$

where the spin variable $\sigma(\sigma = \uparrow, \downarrow)$ is a dummy index and the elementary excitation operators η are fermion operators. The quantity $\Lambda_k(\delta)$ is given by:

$$\Lambda_k(\delta) = \tfrac{1}{2}[(1-\delta)^2 + (1+\delta)^2 + 2(1-\delta^2)\cos k]^{1/2} \tag{3}$$

and the k depend upon τ through the boundary conditions and also upon the total z component of the spin, Σ_z. The ground state has no elementary excitation ($\Sigma_z = 0$) while the first excited state has one ($\Sigma_z = \pm 1$). The corresponding energies are

$$E_0(\delta, \tau, N) = -\sum_{\substack{m=1\\ \text{odd}}}^{N-1} \left[\delta^2 + (1-\delta^2)\sin^2\left(\frac{m\pi + 2\pi\tau}{N}\right)\right]^{1/2} \tag{4a}$$

$$E_1(\delta, \tau, N) = -\sum_{\substack{m=2\\ \text{even}}}^{N-2} \left[\delta^2 + (1-\delta^2)\sin^2\left(\frac{m\pi + 2\pi\tau}{N}\right)\right]^{1/2}. \tag{4b}$$

The gap between these states (the fermionic gap, corresponding to the spin–spin correlation of the associated two-dimensional classical spin system (Kohmoto *et al* 1981)) is

$$\Delta_s(\delta, \tau, N) = \sum_{m=1}^{N-1} (-1)^{m+1} \left[\delta^2 + (1-\delta^2)\sin^2\left(\frac{m\pi + 2\pi\tau}{N}\right)\right]^{1/2}. \tag{5}$$

The finite-size corrections to the ground-state energy are now obtained at criticality ($\delta = 0$). This yields the central charge, c, of the model. The PRG equation will be obtained using expression (5) for the fermionic gap.

At the infinite-system critical value of δ, i.e. $\delta = 0$, equation (4a) can be obtained in closed form. The result and its expansion (keeping the dominant terms only when $N \to \infty$) are

$$E_0(0, \tau, N) = -\cos\left(\frac{2\pi\tau}{N}\right) \operatorname{cosec}\left(\frac{\pi}{N}\right) \simeq -\left(\frac{N}{\pi}\right) - \left(\frac{\pi}{6N}\right)(1 - 12\tau^2). \tag{6}$$

The Hamiltonian (1) can be trivially transformed into an equivalent (i.e. with the same spectrum) Hamiltonian with periodic BC (Kolb 1985). One can thus use the formula of Blöte *et al* (1986) to obtain the central charge c. One finds from (6) that $c = 1 - 12\tau^2$.

Other models can then be related to the modified-BC XY model at criticality ($\delta = 0$) through the parameter τ. Since the conformal anomaly c is related to τ through $c = 1 - 12\tau^2$, and since the XY model can be related to the two-dimensional Gaussian model (Kohmoto *et al* 1981), one may infer, from the work of Blöte *et al* (1986) and the result obtained by Kandanoff (this unpublished result was quoted by Cardy (1987; see equation (4.85))), the following relations for the q-state Potts model ($0 \leq q \leq 4$):

$$\sqrt{q} = 2\cos\{\pi\tau[(\tau^2 + 2)^{1/2} - \tau]\} \tag{7a}$$

and, for the O(N) model ($-2 \leq N \leq 2$):

$$N = 2\cos\{\pi\tau[(\tau^2 + 2)^{1/2} + \tau]\}. \tag{7b}$$

In these expressions, $0 \leq \tau \leq 1/2$. Using (5), we now obtain the range of τ for which the PRG has no real solution and from (7), the corresponding values of the parameters q and N of the Potts and the O(N) models.

The value of the critical parameter δ can be obtained using the PRG equation (Nightingale 1982, Derrida and De Seze 1982; note that the gap in the one-dimensional quantum system corresponds to the inverse correlation length in the classical two-dimensional system):

$$N\Delta(\delta, \tau, N) = N'\Delta(\delta, \tau, N'). \tag{8}$$

The solution of (8) yields an estimated value, $\delta_{N,N'}$, of the critical parameter. Using (5) and (8), and the formula

$$\sum_{m=1}^{M-1} \operatorname{cosec}\left(\frac{m+\beta}{M}\pi\right) = \frac{M}{\pi}\left(2\ln\frac{2M}{\pi} - \Psi(1+\beta) - \Psi(1-\beta)\right) + \mathrm{O}(1)$$

one obtains, with $N' = N + 2$ ($N \gg 1$) (keeping the dominant terms only),

$$\delta_{N,N+2} = 2\left(\frac{\pi}{N}\right)^2 D(\tau)(\tfrac{1}{24} - \tau^2)^{1/2} \tag{9}$$

where

$$D(\tau) = \left(\frac{4\tau}{(1-2\tau)} + \Psi(1+\tau) + \Psi(1-\tau) - \Psi(\tfrac{3}{2} - \tau) - \Psi(\tfrac{1}{2} + \tau)\right)^{-1/2}. \tag{10}$$

In these expressions, $\Psi(\ldots)$ is the digamma function. It is straightforward to show that the function $D(\tau)$ is real for the whole range $\tau \leq 1/2$. Therefore, (9) has a real solution for $\tau \leq 1/2\sqrt{6}$ only.

The very puzzling value of $\tau (\tau = 1/2\sqrt{6})$ above which the PRG equation no longer has a real solution thus seems to be related to the assumption made by Friedan *et al* (1984) that only representations corresponding to the central charge $c = 1 - 6/m(m+1)$

(with $m \geq 3$, i.e. $c \geq 1/2$) are allowed when $c < 1$. From the finite-size corrections to the ground-state energy, at criticality, which are given by (6), it follows that $c = 1 - 12\tau^2$. Accordingly we obtain $c = 1/2$ for $\tau = 1/2\sqrt{6}$ and $c < 1/2$ for larger values of τ. The latter corresponds to the non-unitary regime (i.e. model with $c < 1/2$). From (7a) and (7b), one concludes that the XY system then corresponds to the Potts model with $0 \leq q < 2$ and to the O(N) model with $-2 \leq N < 1$.

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