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Finite-size scaling for quantum chains with an oscillatory energy gap

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Abstract. We show that the existence of zeros of the energy gap for finite quantum chains is related to a non-vanishing wavevector. Finite-size scaling ansätze are formulated for incommensurable and oscillatory structures. The ansätze are verified in the one-dimensional XY model in a transverse field.

1. Introduction

Recently two of us (von Gehlen and Rittenberg 1984a) have studied the quantum Hamiltonian of the three-states asymmetric clock model in order to clarify its phase structure. This Hamiltonian was obtained considering the transfer matrix with an asymmetric interaction along the x axis, a symmetric one along the τ axis and taking the continuous τ limit (Kogut 1979). We have then performed a duality transformation in order to get a Hamiltonian which conserves parity. We have computed the spectrum of this Hamiltonian for finite chains in order to apply finite-size scaling (Hamer and Barber 1981, Nightingale 1982) and noticed that the energy gap oscillates. It has zeros and the number of zeros increases with the size N of the chain (the lowest energy states have zero momenta). It was later noticed by von Gehlen (1984) that similar zeroes of the energy gap occur in other 3-states (Howes *et al* 1983) and 4-states (von Gehlen and Rittenberg 1984b) systems. (The latter systems cannot be obtained from the continuous τ limit of two-dimensional spin systems.) We would like to point out that level crossing for finite chains does not imply any pathology. When we have taken the continuous τ limit of the transfer matrix we have neglected terms which would prevent the crossings.

In order to get a better insight into the problem of level crossings and to learn how to apply finite-size scaling for this case, in this paper we consider the transverse XY (TXY) model which also presents an oscillatory energy gap.

The aim of our paper is to use the TXY model as a laboratory from which one can abstract the following information: which conclusions can be drawn about the infinite system from the behaviour of energy crossings of the finite chains. In this way one might settle, for example, the standing controversy about the existence of a Lifshitz point in the 2D asymmetric clock model.

The paper is organised as follows. In § 2 we sum up the known properties of the TXY model. We then illustrate the phenomena of energy crossings for finite chains. In § 3 we apply the ideas of finite-size scaling to systems with energy crossings and notice a hyperscaling-type relation among the critical exponents. In § 4 we re-obtain the critical exponents given in § 2 using the methods of § 3. Our results are summarised in § 5.

As we have already mentioned, we consider the *TXY* model as a toy model for more complex systems. In order to get an insight on the convergence of the finite-size scaling method, in the appendix we study short chains and illustrate the application of the Vanden Broeck and Schwartz (1979) approximants.

2. The transverse *XY* model

2.1. Summary of known results for the thermodynamic limit

The model is defined by the one-dimensional Hamilton operator:

$$H = -g\sum_n \sigma_n^z - \sum_n \left(\frac{1+\gamma}{2}\sigma_n^x\sigma_{n+1}^x + \frac{1-\gamma}{2}\sigma_n^y\sigma_{n+1}^y\right) \tag{2.1}$$

where σ_n^i are Pauli matrices and $0 \leq \gamma \leq 1$. Through a Jordan–Wigner transformation this system can be diagonalised (Katsura 1962, Niemeyer 1967, Barouch and McCoy 1971) and its various properties can be studied analytically. It is known that the Hamiltonian (2.1) commutes with the transfer matrix of the two-dimensional Ising model on a square lattice (Suzuki 1971) for $g^2+\gamma^2>1$ and through a dual transformation with the transfer matrix of the Ising model on a triangular lattice (Stephen and Mittag 1972).

In equation (2.1) the coupling constant g plays the role of a temperature-like variable (Suzuki 1971).

We notice that for $\gamma \neq 0$ the system has Z_2 symmetry since the operator

$$C = \prod_n \sigma_n^z \qquad C^2 = 1 \tag{2.2}$$

commutes with the Hamiltonian. It is convenient to define a charge operator

$$Q = \frac{1-C}{2} \tag{2.3}$$

whose eigenvalues are 0 and 1.

For $\gamma = 0$ the system has a continuous (O(2)) symmetry since in this case also the operator

$$\Sigma^z = \sum_n \sigma_n^z \tag{2.4}$$

commutes with H.

The phase diagram (Barouch and McCoy 1971) of the system (2.1) is shown in figure 1. The line $g=1$ represents an Ising transition which is of no particular interest for us here. We will rather concentrate on the circle $g^2+\gamma^2=1$, which is a type of disorder line on which the nature of the correlation function changes. The line $\gamma=0$ is special (due to a different symmetry) and will be considered separately.

We start with the case $\gamma=0$. Here it is known (Jullien and Pfeuty 1979) that in the vicinity of the critical point $g_c=1$ the energy gap behaves like

$$G = |g-g_c|^s \tag{2.5}$$

with $s=1$.

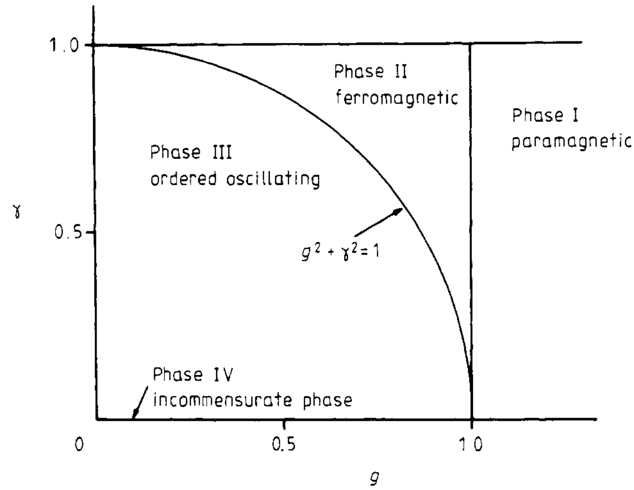

Figure 1. Phase diagram of the transverse XY model.

The specific heat is zero for $g > g_c$ and for $g < g_c$ it is

$$C_v = \frac{-1}{N}\frac{d^2}{dg^2}E = \frac{2}{\pi(g_c^2 - g^2)^{1/2}} \tag{2.6}$$

which implies an exponent $\alpha = \frac{1}{2}$ (E is the ground-state energy). Below g_c, the system is in an incommensurable phase with a wavevector vanishing like

$$K \approx (g_c - g)^{\nu} \tag{2.7}$$

with $\nu = \frac{1}{2}$.

We now consider the case $\gamma \neq 0$. The system has a non-vanishing order parameter below $g = 1$:

$$m_x = \frac{\gamma^{1/4}}{[2(1+\gamma)]^{1/2}}(1 - g^2)^{1/8}. \tag{2.8}$$

(Notice that for $\gamma = 0$, m_x vanishes.)

The two-spins correlation function:

$$\rho^{xx}(R) = \langle 0|\sigma_n^x \sigma_{n+R}^x|0\rangle - |m_x|^2 \tag{2.9}$$

has the following large R behaviour in the three phases:

$$\rho^{xx}(R) \sim A_1 R^{-1/2}\exp(-R/\xi) \qquad g > 1 \tag{2.10a}$$

$$\rho^{xx}(R) \sim A_2 R^{-2}\exp(-2R/\xi) \qquad 1 - \gamma^2 < g^2 < 1 \tag{2.10b}$$

$$\rho^{xx}(R) \sim A_3 R^{-2}\exp(-2R/\xi)\ \mathrm{Re}[B\exp(iKR)] \qquad 0 < g^2 < 1 - \gamma^2. \tag{2.10c}$$

Here A_1, A_2 and B are constants and the correlation length ξ is

$$\xi = \left|\ln\frac{g - (g^2 + \gamma^2 - 1)^{1/2}}{1 - \gamma}\right|^{-1} \qquad g^2 > 1 - \gamma^2 \tag{2.11a}$$

$$\xi = \left|\frac{1}{2}\ln\frac{1+\gamma}{1-\gamma}\right|^{-1} \qquad 0 < g^2 < 1 - \gamma^2. \tag{2.11b}$$

Notice that for $g<(1-\gamma^2)^{1/2}$, the correlation length is independent of g and is g-dependent for $g>(1-\gamma^2)^{1/2}$. If one is interested in the point $g=(1-\gamma^2)^{1/2}$ itself Barouch and McCoy (1971) have shown that in this point all correlation functions are independent of R (the limits $R\to\infty$ and $g\to(1-\gamma^2)^{1/2}$ are not invertible). In conclusion, in the whole region $g<1$, the correlation length is finite. There is however another length which diverges in this region: the inverse of the wavevector which is:

$$L=\frac{1}{K}=\left|\cos^{-1}\frac{g}{(1-\gamma^2)^{1/2}}\right|^{-1}. \tag{2.12}$$

Notice that with $g_c=(1-\gamma^2)^{1/2}$, we have

$$K\sim(g_c-g)^{\nu} \tag{2.13}$$

with $\nu=\frac{1}{2}$. We also have

$$C_v \text{ regular.} \tag{2.14}$$

2.2. *Zeros of the energy gap for finite chains*

We would now like to illustrate how the various phases described above are reflected in the properties of the energy gap for finite chains. If we denote by $E_0(E_1)$ the lowest energy states in the charge sectors 0(1) (see equation (2.3) for the definition of the charge), their expressions can readily be obtained from Katsura (1962):

$$E_0(g_1\gamma_1N)=-\sum_{n=0}^{N-1}\Lambda\left(\frac{2\pi}{N}(n+\tfrac{1}{2})\right) \tag{2.15a}$$

$$E_1(g_1\gamma_1N)=\begin{cases}-\sum_{n=0}^{N-1}\Lambda\left(\frac{2\pi}{N}n\right)+2\Lambda(0) & g\geqslant 1\\ -\sum_{n=0}^{N-1}\Lambda\left(\frac{2\pi}{N}\right) & g<1\end{cases} \tag{2.15b}$$

where

$$\Lambda(\varphi)=[(\cos\varphi-g)^2+\gamma^2\sin^2\varphi]^{1/2} \tag{2.16}$$

(we have taken periodic boundary conditions).

The energy gap G is

$$G=|\Delta E| \tag{2.17}$$

where

$$\Delta E=E_1-E_0. \tag{2.18}$$

We first start with the case $\gamma=0$. In figure 2 we show the behaviour of E_0 and E_1 as a function of g for $N=8$. One observes that for $g>1$, E_0 is the ground-state energy. With decreasing g, a first crossing occurs at $g=1$ when E_1 becomes the ground-state energy. There is then a change in slope for E_0 (which is the exited state) at $g\approx0.9$ which occurs due to a crossing of levels in the charge zero sector and at $g\approx0.8$, E_0 becomes the ground-state energy, etc. In figure 3 we show ΔE for $N=8$ and 10. We observe that if, for $N=8$, ΔE has changed signs four times then for $N=10$, ΔE changes signs five times. At the same time we see that the first change in signs occurs at $g=1$ in both cases but the next change in signs occurs at a larger value of g for

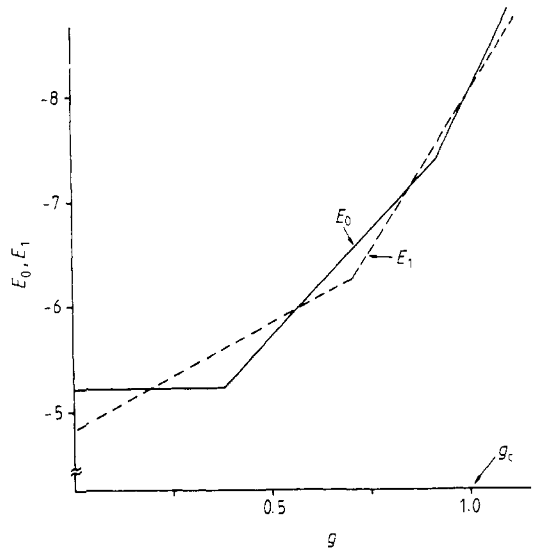

Figure 2. The lowest energy states E_0 and E_1 in the charge sectors 0 and 1 as a function of g for $N = 8$.

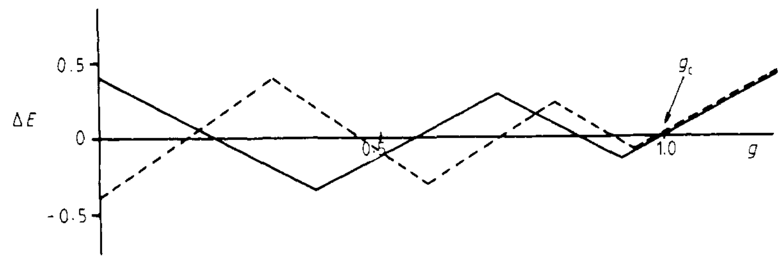

Figure 3. ΔE as a function of g ($\gamma = 0$) for $N = 8$ (——) and 10 (- - -).

$N = 10$ than for $N = 8$. The same trend is observed for larger N: the number of zeros increases and the second zero gets closer to $g = 1$. As will be seen in § 3, all these features can nicely be interpreted in the finite-size scaling property of the energy gap.

We now look at the specific heat

$$C_v = -\frac{1}{N}\frac{d^2 E_N}{dg^2}. \tag{2.19}$$

Here E_N is the ground-state energy of the N sites chain. Since the ground state oscillates between E_0 and E_1 (with straight lines between the crossings as shown in figure 2), the specific heat is a sum of δ functions. This is shown in figure 4 in the case $N = 12$. In order to illustrate how the thermodynamic limit ($N \to \infty$) is obtained, in figure 4 we have smeared the contribution of the δ functions getting step functions. The continuous curve is the thermodynamic limit (see equation (2.6)).

Let us consider the case $\gamma \neq 0$. In figure 5 we show ΔE as a function of g for various N in the case $\gamma = 0.707$. We observe that for $g \leq g_c = (1 - \gamma^2)^{1/2}$ the pattern of the zeros is similar to the case $\gamma = 0$ (figure 3). Two major differences can, however, be noticed. First we see that the amplitudes of the oscillations decrease much faster

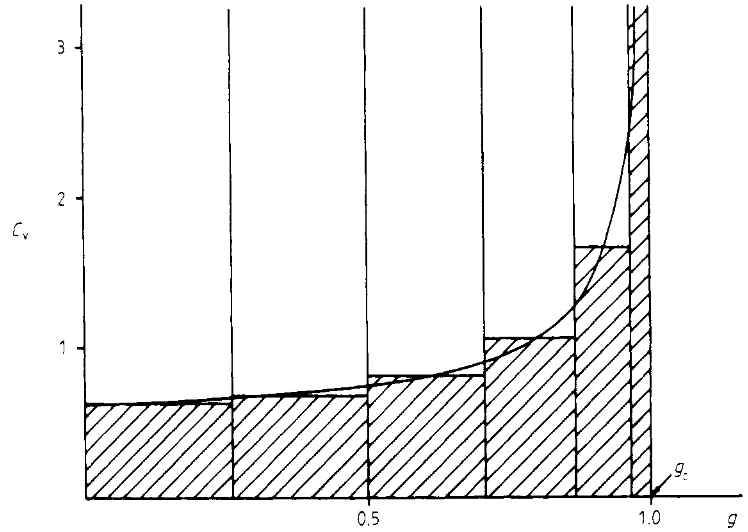

Figure 4. The specific heat C_v for $N = 12$ is a succession of δ functions. Smearing out the contributions of the δ functions one gets a good approximation to the thermodynamic limit (smooth curve).

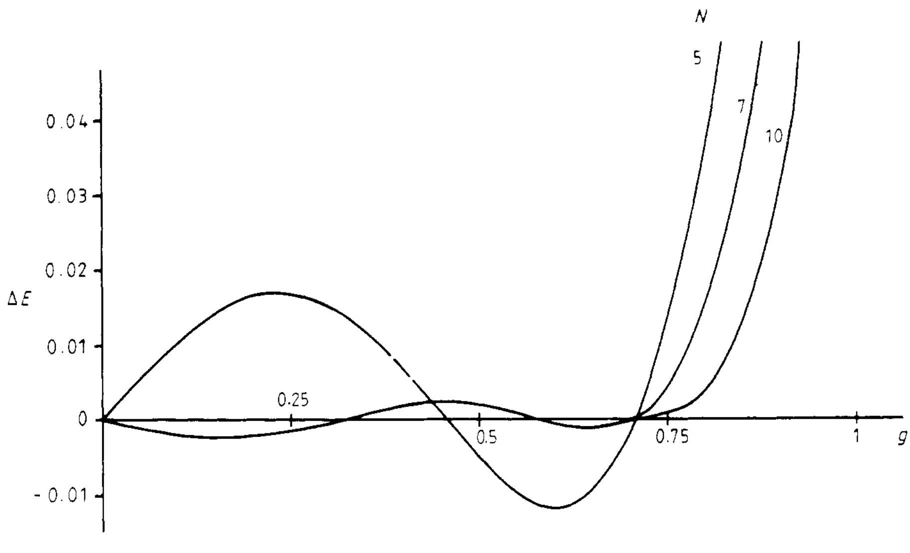

Figure 5. ΔE as a function of g for $N = 5$, 7 and 10. $\gamma = 0.707$, $g_c = (1 - \gamma^2)^{1/2}$.

with N than in figure 3. Actually the decrease is exponential in one case and algebraic in the other. The second difference is that there are no more energy crossings within the same charge sector (ΔE is obtained through the interplay of just two energy levels). This makes the ΔE function to be smooth in g.

In order to illustrate the fact that the oscillations of the energy gap are not an artefact of our choice of periodic boundary, in figure 6 we show ΔE for $\gamma = 0.707$ and $N = 9$ in the case of free boundary conditions. The oscillations are there all right, the

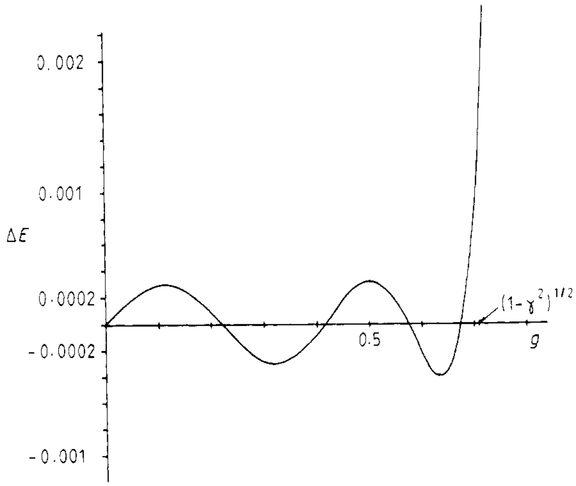

Figure 6. ΔE as a function of g for $N=9$ and $\gamma=0.707$ (free boundary conditions).

single difference is that the first zero does not appear at $g=g_c$ but at a slightly smaller value of g.

We can now bring together the two halves of this section with an interesting conclusion: *the energy gap oscillates in the regions with a non-vanishing wavevector.* Based on this observation we are going to write the finite-size scaling prescriptions for the phase transition which occurs where the wavevector vanishes. This is the circle $g^2+\gamma^2=1$ in our model.

3. Finite-size scaling

We now formulate the finite-size scaling ansatz in the case where the wavevector K vanishes like

$$K=(g_c-g)^{\nu}.$$

We are going to distinguish between two cases. In the first one (this corresponds to $\gamma=0$ in our toy model) the correlation function has an algebraic decay (there is no correlations length). The second case ($\gamma\neq 0$ in our model) corresponds to a situation where the correlation length ξ is finite at the critical point and equal to ξ_c.

3.1. The incommensurable phase

We define a scaling variable in the standard way:

$$z=N^{1/\nu}(g_c-g) \tag{3.1}$$

and make the usual ansatz for the scaling limit of the specific heat:

$$C_v(g,N)=N^{\alpha/\nu}F(z) \tag{3.2}$$

($N\to\infty$, z fixed). We also assume as usual that

$$\lim_{z\to\infty} F(z)=Az^{-\alpha}. \tag{3.3}$$

We now characterise the incommensurate phase through the specific expression of $F(z)$:

$$F(z)=\sum_{k=0}^{\infty}\tilde{c}_k\delta(z-z_k) \tag{3.4}$$

where $\tilde{c}_k$ are constants.

In order to match equations (3.3) and (3.4) we have

$$\lim_{k\to\infty}\tilde{c}_k\propto k^{\lambda_1} \qquad \lim_{k\to\infty}z_k\propto k^{\lambda_2} \qquad \tfrac{1}{2}(\lambda_2-\lambda_1+1)=\alpha.$$

The specific heat for a chain with N sites has the expression

$$C_v(g,N)=\sum_{k=0}^{n(N)}C_k(N)\delta(g-g_k(N)). \tag{3.5}$$

Here $n(N)+1$ represents the number of zeros of the energy gap (the zeros are located at $g_k(N)$). In writing equation (3.5) we have disregarded the smooth part of $C_v(g,N)$.

We now compare equations (3.2), (3.4) and (3.5) and obtain

$$g_k(N)=g_c-z_kN^{-1/\nu} \tag{3.6a}$$

$$C_k(N)=\tilde{C}_kN^{(\alpha-1)/\nu}. \tag{3.6b}$$

Equations (3.6) allow us to determine ν and α. Let $g_0(N)$ and $g_1(N)$ be the positions of the first two zeros of the energy gap and $Z(N)$ their difference:

$$Z(N)=g_0(N)-g_1(N). \tag{3.7}$$

From equations (3.6a) and (3.7) we get estimates for ν:

$$\nu_N=\frac{\ln((N-1)/N)}{\ln(Z(N)/Z(N-1))}. \tag{3.8}$$

The value of g_c can be obtained using equation (3.6a) and the values of $g_0(N)$. Making a fit to $g_0(N)$ one determines g_0, z_0 and one gets an independent determination of ν.

We now use equation (3.6b) in order to get estimates for the critical exponent α:

$$\alpha_N=1+\nu_N\frac{\ln(C_k(N)/C_k(N-1))}{\ln(N/(N-1))}. \tag{3.9}$$

We now consider the function $\Delta E(g,N)$ (see equation (2.18)). In the scaling limit we have

$$\Delta E(g,N)=N^{-s/\nu}E(z) \tag{3.10}$$

where $E(z)$ is an oscillating function with zeros at z_k. For large value of z we have

$$E(z)=A_1z^{s_1}h(z) \tag{3.11}$$

where $h(z)$ is an oscillating function with $|h(z)|\leqslant 1$. If in the vicinity of $z=0$ we have

$$h(z)=A_2z^{s_2} \tag{3.12}$$

then

$$s=s_1+s_2 \tag{3.13}$$

and

$$\Delta E(g, N\to\infty) = A_1 A_2 (g_c - g)^s. \tag{3.14}$$

From equation (3.10) we can get estimates for the critical exponent s:

$$s_N = 1 - \nu_N \ln\left(\frac{d}{dg}\Delta E(g_k(N), N) \Big/ \frac{d}{dg}\Delta E(g_k(N-1), N-1)\right)(\ln(N/N-1))^{-1}. \tag{3.15}$$

Let us observe that the coefficients $c_k(N)$ in equation (3.5) are

$$c_k(N) = \frac{1}{N^d}\left|\frac{d}{dg}E_0 - \frac{d}{dg}E_1\right| = \frac{1}{N^d}\left|\frac{d}{dg}\Delta E(g_k(N), N)\right| \tag{3.16}$$

where d is the number of dimensions of the quantum chain. The first equality in (3.16) implies the assumption that E_0 and E_1 are smooth functions at $g = g_k$. If we introduce the expression (3.16) for $c_k(N)$ in equation (3.9) and compare the result with the expression (3.15) we obtain (see also Hornreich *et al* 1975)

$$\alpha = 2 - s - d\nu \tag{3.17}$$

for any N.

This relation is of course verified by the critical exponents of the *TXY* model with $\gamma = 0$.

3.2. *The oscillatory phase*

Since in this phase the correlation length is non-zero at g_c but equal to ξ_c, we will make a different ansatz for the scaling functions. We will replace equation (3.10) by the assumption

$$\Delta E(g, N) = N^{-\omega}\exp(-N/\xi_c)\tilde{E}(z) \tag{3.18}$$

where ω is unknown. The function $\tilde{E}(z)$ will again have zeros at z_k. The critical exponent ν and the critical point g_c can be determined as in § 3.1 (one uses equations (3.6*a*) and (3.8)). The values of ξ_c and ω can be determined from a fit at fixed z.

4. Application of finite-size scaling to the *TXY* model

In this section we verify the finite-size scaling ansatz of § 3 in the case of the *TXY* model. We consider separately the cases $\gamma = 0$ and $\gamma \neq 0$.

4.1. *The $\gamma = 0$ case*

From equations (2.15) and (2.16) we conclude that for a given N, ΔE has $[\frac{1}{2}(N+1)]$ zeros ($[l]$ denotes the integer part of l) that we are going to denote by $g_0, g_1, \ldots, g_{[(N+1)/2]}$. The first zero is fixed (independent of N):

$$g_0 = 1. \tag{4.1}$$

From equation (3.6*a*) we conclude that

$$g_c = 1 \qquad z_0 = 0. \tag{4.2}$$

For the other zeros we have

$$g_{2n}(N)=2\sum_{j=1}^{n}\left(\cos\frac{\pi}{N}2j-\cos\frac{\pi}{N}(2j-1)\right)+1$$
$$g_{2n+1}(N)=2\sum_{j=0}^{n}\left(\cos\frac{\pi}{N}(2j+1)-\cos\frac{\pi}{N}2j\right)+1. \tag{4.3}$$

We now take the large N limit of equation (4.3) and get

$$1-g_k(N)=z_kN^{-1/\nu}=\frac{\pi^2}{2}k(k+1)N^{-2}. \tag{4.4}$$

Thus we have

$$\nu=\frac{1}{2} \qquad z_k=\frac{\pi^2}{2}k(k+1). \tag{4.5}$$

The value obtained for ν is in agreement with equation (2.7).

The expression of the specific heat is

$$C_v(g,N)=\frac{2}{N}\sum_{k=0}^{[(N-1)/2]}\delta(g-g_k(N)). \tag{4.6}$$

This implies (see equation (3.5)) that

$$C_k(N)=2/N \tag{4.7}$$

and using equation (3.6*b*)

$$\tilde{C}_k=2 \qquad \alpha=\tfrac{1}{2} \tag{4.8}$$

We also have (see equation (3.5))

$$\lambda_1=0 \qquad \lambda_2=2. \tag{4.9}$$

The scaling function $F(z)$ from equation (3.2) is

$$F(z)=2\sum_{k=0}^{\infty}\delta(z-z_k). \tag{4.10}$$

One can use equation (3.17) to get $s=1$.

Finally, in figure 7 we show the scaling function $E(z)$. In agreement with equation (3.13) one finds

$$s_1=s_2=\tfrac{1}{2}. \tag{4.11}$$

We have thus shown that for the one-dimensional TXY model finite-size scaling works and gives the correct critical exponents. In the appendix we discuss different aspects of the convergence of the estimates ν_N for ν obtained from short chains.

4.2. The $\gamma\neq 0$ case

In figure 8 we show the locations of the zeros of ΔE for $N=9$ as a function of γ. One observes that their number for $\gamma\neq 0$ is the same as for $\gamma=0$. In the appendix we show that using equation (3.6*a*) one finds $\nu=\frac{1}{2}$ in agreement with equation (2.13). In order to check in detail our ansatz (3.18) for the case $\gamma=0.707$ we have fitted ξ_c and

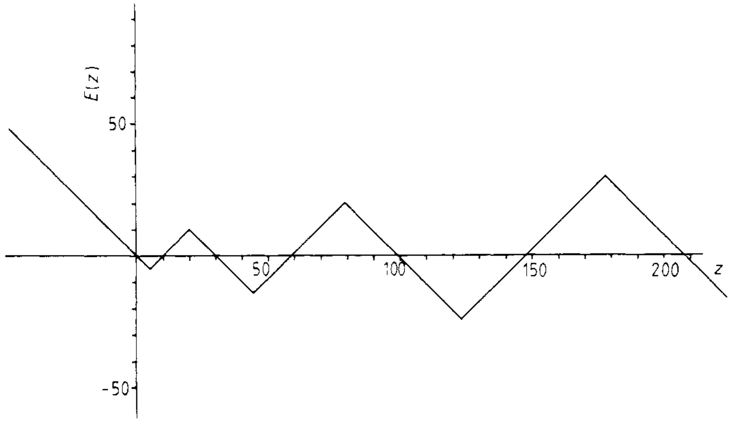

Figure 7. The scaling function $E(z)$ from $\Delta E(g, N) = N^{-2}E(z)$ $(\gamma = 0)$.

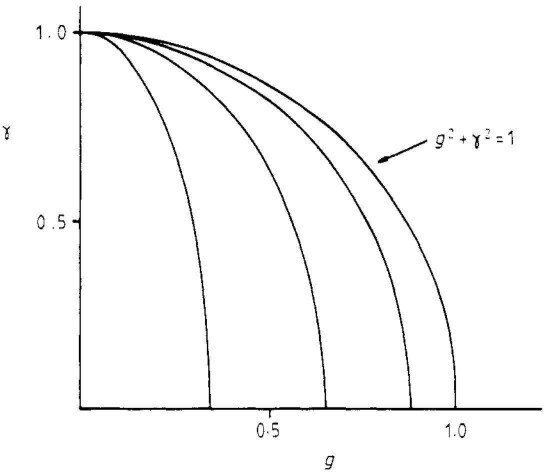

Figure 8. The locations of the zeroes of ΔE in the γ, g plane for $N = 9$.

ω for the point $z = 0.5$. One finds

$$\xi_c^{-1} = 0.8815 \pm 0.0007 \qquad \omega = 1.00 \pm 0.02. \tag{4.12}$$

The value for ξ_c is in excellent agreement with the value derived from equation (2.11*b*) which is $\xi_c^{-1} = 0.881\,16$.

With ξ_c and ω known, one can derive the scaling function $\tilde{E}(z)$ of equation (3.18). This function is shown in figure 9.

5. Conclusions

We have shown that in a phase with a non-vanishing wavevector K which vanishes at the critical point like $K = (g_c - g)^{\nu}$, one can make finite-size scaling ansatz both for incommensurate phases as well as for oscillatory phases (in this case the correlation

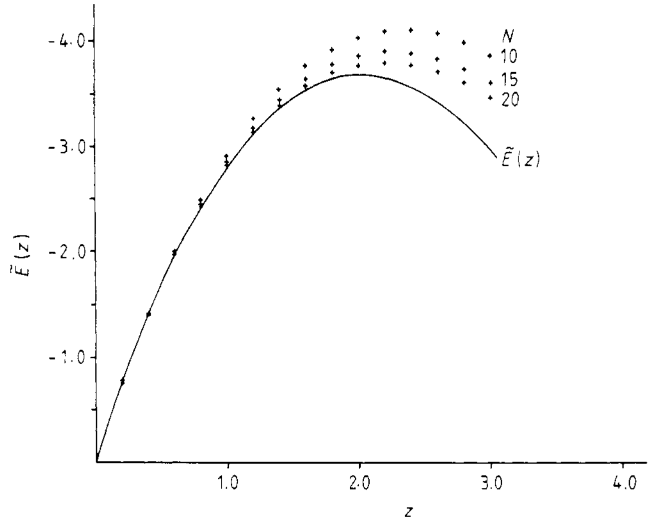

Figure 9. The scaling function $\tilde{E}(z)$ from $\Delta E(g, N) = \exp(-N/\xi_c)E(z)/N$ in the case $\gamma = 0.707$.

length stays finite at g_c). The derivation of the critical exponents exploits the fact that the energy gap has zeros whose number depends on the number N of sites in the quantum chain.

An interesting open question is to find out up to how many dimensions finite-size scaling works in this case.

The methods presented in this paper have been applied by von Gehlen *et al* (1984) to the 3-states asymmetric clock model. This study is complementary to the work of Duxbury *et al* (1984) where the transfer matrix was taken in the orthogonal direction.

Acknowledgments

We would like to thank P M Duxbury, M Henkel and W Selke for discussions.

Appendix. Determination of the critical exponent ν from short quantum chains

The aim of this appendix is to find out the convergence of the estimates for the critical exponents of the *TXY* model. This exercise is interesting because we have in mind applications to many-states systems where it is very difficult to diagonalise long chains. We are going to consider only estimates for ν.

We start with the $\gamma = 0$ case (periodic boundary conditions). One uses equations (3.7) and (3.8) with $g_0(N) = 1$ and one finds the estimates given in table A1. One can get better estimates if one considers the quantities

$$X(N) = (N^2 - 9)\left(\frac{1}{g_k(N)} - 1\right) \tag{A1}$$

where

$$\lim_{N\to\infty} X(N) = AN^{2-1/\nu}. \tag{A2}$$

Table A1. Estimates for $\nu(\gamma=0$ and periodic boundary conditions). ν_N is defined by equation (3.8) and $\tilde{\nu}_N$ by equation (A2).

N	$\tilde{\nu}_N-0.5$	$\nu_N-0.5$
4	2.15070×10^{-3}	
5	1.24314×10^{-3}	2.18223×10^{-2}
6	8.13857×10^{-4}	1.42565×10^{-2}
7	5.75416×10^{-4}	1.00680×10^{-2}
8	4.28837×10^{-4}	7.49800×10^{-3}
9	3.32142×10^{-4}	5.80462×10^{-3}
10	2.64937×10^{-4}	4.62861×10^{-3}
11	2.16307×10^{-4}	3.77812×10^{-3}

The quantities $X(N)$ contain the information that for $N=3$, $g_1(3)=0$. Other threshold factors like $N(N-3)$ instead of N^2-9 can be used as well. We denote by $\tilde{\nu}_N$ the estimates obtained from equation (A2) and their values are also shown in table A1. One notices that they are closer to the correct value $\nu=\frac{1}{2}$ than the estimates ν_N.

In order to improve the estimates we have tried the Vanden Broeck and Schwartz (1979) method (see also Hamer and Barber 1981). We denote by $[N, L]$ $(L=1,2,\ldots)$ the Lth approximants. They are defined through the recurrence relations:

$$[N,-1]=\infty \qquad [N,0]=\nu_N$$

$$([N,L+1]-[N,L])^{-1}+([N,L-1]-[N,L])^{-1} = ([N+1,L]-[N,L])^{-1}+([N-1,L]-[N,L])^{-1}. \tag{A3}$$

In tables A2 and A3 we give the approximants up to $L=4$ and one notices that their precision is remarkable.

In table A4 we give the estimates ν_N and $\tilde{\nu}_N$ in the case of free boundary conditions $(\gamma=0)$. As usual they are poorer than those for periodic boundary conditions. The estimates $\tilde{\nu}_N$ are better than ν_N. An amusing phenomenon appears now if one takes the Vanden Broeck-Schwartz approximants for ν_N and $\tilde{\nu}_N$: they are excellent for ν_N and poor for $\tilde{\nu}_N$.

Table A2. Vanden Broeck-Schwartz approximants for $\nu_N-0.5$ (table A1).

4.87322×10^{-3}		
3.41716×10^{-3}	2.21677×10^{-5}	
2.53353×10^{-3}	1.35230×10^{-5}	2.1029×10^{-6}
1.95548×10^{-3}	8.6124×10^{-6}	
1.55602×10^{-3}		

Table A3. Vanden Broeck-Schwartz approximants for $\tilde{\nu}_N-0.5$ (table A1).

2.77502×10^{-4}		
1.94953×10^{-4}	1.1589×10^{-6}	
1.44708×10^{-4}	7.065×10^{-7}	1.078×10^{-7}
1.11777×10^{-4}	4.492×10^{-7}	
8.89909×10^{-5}		

Table A4. Estimates for ν ($\gamma = 0$ and free boundary conditions).

N	$\tilde{\nu}_N - 0.5$	$\nu_N - 0.5$
3	-5.46228×10^{-2}	2.58162×10^{-1}
4	-5.16952×10^{-2}	1.72746×10^{-1}
5	-4.79833×10^{-2}	1.29399×10^{-1}
6	-4.43840×10^{-2}	1.03282×10^{-1}
7	-4.11175×10^{-2}	8.58634×10^{-2}
8	-3.82136×10^{-2}	7.34340×10^{-2}
9	-3.56457×10^{-2}	6.41268×10^{-2}

We now consider the $\gamma \neq 0$ case. In table A5 we give the estimates for ν_N and $\tilde{\nu}_N$ for $\gamma = 0.707$. The quality of the estimates compares with that of the case $\gamma = 0$ with free boundary conditions. In fact, we have also taken much longer chains and got very close to $\nu = 0.5$.

Table A5. Estimates for ν ($\gamma = 0.707$ and periodic boundary conditions).

N	$\nu_N - 0.5$	$\tilde{\nu}_N - 0.5$
5	-1.5648×10^{-2}	2.8765×10^{-2}
6	-2.2135×10^{-2}	2.8506×10^{-2}
7	-2.4447×10^{-2}	2.7740×10^{-2}
8	-2.4930×10^{-2}	2.6655×10^{-2}
9	-2.4561×10^{-2}	2.5427×10^{-2}
10	-2.3784×10^{-2}	2.4167×10^{-2}
11	-2.2856×10^{-2}	2.2936×10^{-2}

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