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LETTER TO THE EDITOR

Exact real space renormalisation group transformation for the dimerised XY chain

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Abstract. An analytical real space renormalisation group transformation is obtained for the one-dimensional spin- $\frac{1}{2}$ antiferromagnetic dimerised XY model. Using the method of Sarker, the recursion relations for the parameters are derived from the mapping between blocks of sizes L and L/b , for arbitrary size L and scale factor b . The results for the gap and for the critical exponent are shown to converge rapidly toward their exact values. The dynamical exponent has $1/L$ corrections ($b \sim 1$) instead of the usual $1/\ln L$ ones ($b = L$). The differential renormalisation group equations are obtained explicitly. We show that the non-analyticity of the scaling function (for the density of energy) stems from a dangerous irrelevant variable, the antiferromagnetic coupling.

The real space renormalisation group (RG) transformation of Sarker (1984) is applied to the dimerised XY system. This method consists of the determination of the recursion relations for the parameters of the model through the mapping between blocks of linear dimensions L and L/b , where b is the scale factor. The details of the calculation will be given below. The procedure reduces to the simple RG transformation when $b = L$ and yields the differential renormalisation group equations in the limit $L \rightarrow \infty$, $b \rightarrow 1$, from which one can infer the scaling properties of the model. Sarker's method does not generate additional parameters and the dimension of the space of parameters is left invariant upon renormalisation. Therefore, the interpretation of the scaling properties of the model in the limit $L \rightarrow \infty$ and $b \rightarrow 1$ is relatively simple. In this letter, we shall obtain the exact RG transformation for arbitrary L and b . The results for the gap, away from criticality, are compared with those obtained by Fields (1979) using the simple RG transformation. The critical exponent which characterises the opening of the gap and the finite-size corrections for the dynamical exponent are calculated. The differential renormalisation group equations are obtained in the limit $L \rightarrow \infty$, $b \rightarrow 1$, and the scaling laws are interpreted using the exact solution.

The letter is organised as follows: the block Hamiltonian for the model is first solved exactly for an arbitrary odd number of sites. (The solution for an even number of sites and for arbitrary boundary conditions can be found in Spronken and Kemp (1986).) The method of Sarker is then briefly recalled and the RG equations are given. The linearisation of these equations is performed and the differential renormalisation transformation upon an infinitesimal change of scale is obtained. Finally, scaling properties are derived and discussed.

The block Hamiltonian for the dimerised XY model is (see, for example, Fields 1979)

$$H(N) = J \sum_{j=1}^{N-1} [1 + (-1)^j \delta] (\sigma_j^+ \sigma_{j+1}^- + c.c.) \quad (1)$$

where the number of sites, N ($N \geq 3$), is assumed to be odd and where the lattice spacing is taken as the unit of distance. The operators σ_j^\pm are the Pauli operators at site j . The spectrum of $H(N)$ is invariant upon the changes $J \leftrightarrow -J$ and $\delta \leftrightarrow -\delta$. We consider an antiferromagnet and therefore $J > 0$ and the dimerisation parameter, δ , is $\delta \geq 0$. When $\delta = 1$, (1) is the Hamiltonian for $(N-1)/2$ non-interacting dimers plus a free spin. This is the trivial case and we shall further restrict the dimerisation parameter to $0 \leq \delta < 1$. Free boundary conditions are imposed upon $H(N)$.

The Hamiltonian (1) can be rewritten in terms of spinless fermion variables using the Wigner-Jordan transformation (Jordan and Wigner 1928). This yields

$$H(N) = \sum_{i=1}^N \sum_{j=1}^N f_i^\dagger (R_N)_{ij} f_j \quad (2)$$

where f_j^\dagger (f_j) is the creation (annihilation) operator for a spinless fermion at site j . The $N \times N$ matrix R_N is a symmetric tridiagonal matrix whose non-vanishing components are

$$(R_N)_{i,i+1} = (R_N)_{i+1,i} = J[1 + (-1)^i \delta] \quad i = 1, 2, \dots, N-1. \quad (3)$$

The Hamiltonian (2) can be diagonalised using the canonical transformation

$$f_{2l+1} = \Phi_{2l} \eta + \sum_k (\Phi_{2l}^{k\uparrow} \eta_{k\uparrow} - \Phi_{2l}^{k\downarrow} \eta_{k\downarrow}^\dagger) \quad l = 0, 1, \dots, (N-1)/2 \quad (4a)$$

$$f_{2l} = \sum_k (\Psi_{2l-1}^{k\uparrow} \eta_{k\uparrow} + \Psi_{2l-1}^{k\downarrow} \eta_{k\downarrow}^\dagger) \quad l = 1, 2, \dots, (N-1)/2 \quad (4b)$$

where the new fermion operators, η and $\eta_{k\sigma}$ ($\sigma = \uparrow, \downarrow$), correspond to the elementary excitations of the system, in terms of which the Hamiltonian is

$$H(N) = \Lambda_0 \eta^\dagger \eta + \sum_{k\sigma} \Lambda_k (\eta_{k\sigma}^\dagger \eta_{k\sigma} - \frac{1}{2}). \quad (5)$$

Note that the variable σ in (4) and (5) has no physical meaning. In (4), the Φ and Ψ with different l are the components of the $N \times 1$ column matrices, v and v_k^σ , of the unitary matrix $V = [v, \dots, v_k^\sigma, \dots]$ that diagonalises the Hamiltonian. Here, the transpose of v is $v^T = [\Phi_0, \Psi_1, \Phi_2, \dots, \Phi_{N-1}]$ and $(v_k^\sigma)^T = [\Phi_0^{k\sigma}, \Psi_1^{k\sigma}, \Phi_2^{k\sigma}, \dots, \Phi_{N-1}^{k\sigma}]$. These vectors v and v_k^σ , correspond to the eigenvalues Λ_0 and Λ_k in (5). We shall now obtain the analytical expressions for all these quantities, together with the set of k .

First, $\det(R_N) = 0$ for any N . $\Lambda_0 = 0$ is therefore an eigenvalue of the matrix R_N . The other eigenvalues are obtained as follows. Let $D_{2i+1}(k)$ be the determinant of the $(2i+1) \times (2i+1)$ submatrix $(R_{2i+1} - \lambda_k I_{2i+1})$ involved in the calculation of $\det(R_N - \lambda_k I_N) = 0$, where λ_k is the k th eigenvalue. Here, the matrix I_l stands for the $l \times l$ unit matrix and $\lambda_k = \pm \Lambda_k$, where Λ_k is defined by (Spronken and Kemp 1986)

$$\Lambda_k = J[(1 + \delta)^2 + (1 - \delta)^2 + 2(1 - \delta^2) \cos k]^{1/2}. \quad (6)$$

It is easily shown that the recursion relation for the determinant $D_{2i+1}(k)$ is

$$J^4(1 - \delta^2)^2 D_{2i-3}(k) - 2J^2(1 - \delta^2) \cos(k) D_{2i-1}(k) + D_{2i+1}(k) = 0 \quad (7)$$

where $i = 1, 2, \dots, (N - 1)/2$ and where $D_{-1}(k) = 0$. The solution of (7) is

$$D_{2i+1}(k) = \lambda_k (1 - \delta^2)^i U_i(\cos k) \quad i = 1, 2, \dots, (N - 1)/2 \quad (8)$$

where $U_i(\cos k)$ is the Chebyshev polynomial of the second kind (Gradshteyn and Ryzhik 1980). Setting $D_N(k) = 0$ yields the set of k :

$$k = 2\pi m / (N + 1) \quad m = 1, 2, \dots, (N - 1)/2. \quad (9)$$

The spectrum of the Hamiltonian thus consists of $\Lambda_0 = 0$ and $\pm \Lambda_k$ with k given by (9). The Φ and the Ψ are obtained from the solutions of $R_N v = 0$ and $R_N v_k^\sigma = \lambda_k v_k^\sigma = \alpha_\sigma \Lambda_k v_k^\sigma$ ($\alpha_\uparrow = 1, \alpha_\downarrow = -1$). Straightforward algebra yields (within an arbitrary factor of ± 1)

$$\Phi_{2i}^{k\uparrow} = -\Phi_{2i}^{k\downarrow} = \frac{J}{\Lambda_k} \left(\frac{2}{N+1} \right)^{1/2} [(1 + \delta) \sin ik + (1 - \delta) \sin(i+1)k] \\ i = 0, 1, \dots, (N - 1)/2 \quad (10a)$$

$$\Psi_{2i-1}^{k\uparrow} = \Psi_{2i-1}^{k\downarrow} = \left(\frac{2}{N+1} \right)^{1/2} \sin ik \quad i = 1, 2, \dots, (N - 1)/2 \quad (10b)$$

and, corresponding to $\Lambda_0 = 0$,

$$\Phi_{2i} = (-x)^i \left(\frac{1 - x^2}{1 - x^{N+1}} \right)^{1/2} \quad (11a)$$

$$\Psi_{2i-1} = 0 \quad (11b)$$

where the i are identical to those in (10) and where x is defined by

$$x = (1 - \delta) / (1 + \delta). \quad (12)$$

Using (10) and (11), one can show that (with $m = (N - 1)/2$)

$$\sum_{i=0}^m \Phi_{2i}^2 = 1 \quad (13a)$$

$$\sum_{i=0}^m \Phi_{2i} \Phi_{2i}^{k\sigma} = 0 \quad \text{all } k \text{ and } \sigma \quad (13b)$$

$$\sum_{i=0}^m \Phi_{2i}^{k\sigma} \Phi_{2i}^{k'\sigma'} = \frac{1}{2} \alpha_\sigma \alpha_{\sigma'} \delta_{kk'} \quad (13c)$$

$$\sum_{i=1}^m \Psi_{2i-1}^{k\sigma} \Psi_{2i-1}^{k'\sigma'} = \frac{1}{2} \delta_{kk'} \quad \text{all } \sigma \text{ and all } \sigma' \quad (13d)$$

from which one infers that the columns of V form an orthonormal set of eigenvectors. Furthermore one can show, using (4) and (13), that the relation between the operator for the total number of f particles, n , and the operators for the elementary excitations is

$$n = (N - 1)/2 + \eta^\dagger \eta + \sum_{k\sigma} \alpha_\sigma \eta_{k\sigma}^\dagger \eta_{k\sigma} \quad (14)$$

where α_σ has been defined above.

The vacuum state, $|0\rangle$, has no elementary excitation and $\eta|0\rangle = \eta_{k\sigma}|0\rangle = 0$ while the first excited state is $|1\rangle = \eta^\dagger|0\rangle$. Therefore one finds, using (4), (5) and (14)

$$\langle 0|n|0\rangle = (N-1)/2 \quad \langle 1|n|1\rangle = (N+1)/2 \quad (15a)$$

$$\langle 0|f_{2l}|1\rangle = 0 \quad \text{all } l \quad (15b)$$

$$\langle 0|f_{2l+1}|1\rangle = \Phi_{2l} \quad l = 0, 1, \dots, (N-1)/2 \quad (15c)$$

$$\langle 0|H(N)|0\rangle = \langle 1|H(N)|1\rangle = -\sum_k \Lambda_k \quad (15d)$$

where the last equation stems from the symmetry of (2) upon electron-hole exchange. States with $(N \pm 1)/2$ particles are those involved in the simple RG calculation for which a block of linear size L is mapped onto a single site with two levels (Pfeuty *et al* 1982). They also arise in the RG transformation of Sarker which we now recall, for clarity.

Let q and q_b be any initial quantities arising in the block Hamiltonian for block sizes L and L/b , respectively. The use of the simple RG transformation yields $q' = f(L, q)$ and $q'_b = f(L/b, q_b)$. The method of Sarker demands that these quantities be equal. This leads to $q_b = F(q)$ which defines the mapping $L \rightarrow L/b$ for a scale factor b . This will be referred to as the $(L, L/b)$ mapping.

The application of this procedure to the XY model yields, using (15) and (11), the following RG equations:

$$[J(1+\delta)]' = \frac{1-x^2}{1-x^{L+1}} \frac{1-x^{L+b}}{1-x^{2b}} [J(1+\delta)] \quad (16a)$$

$$[J(1-\delta)]' = x^{b-1} \frac{1-x^2}{1-x^{L+1}} \frac{1-x^{L+b}}{1-x^{2b}} [J(1-\delta)] \quad (16b)$$

together with

$$x' = x^b. \quad (17)$$

Equivalently, one has

$$J' = \frac{1-x}{1-x^b} \frac{1-x^{L+b}}{1-x^{L+1}} J \quad (18a)$$

$$\delta' = \frac{(1+\delta)^b - (1-\delta)^b}{(1+\delta)^b + (1-\delta)^b}. \quad (18b)$$

Equations (16) (or (18)) are the RG recursion relations for the mapping $(L, L/b)$. Equation (17) states that $x=0$ ($\delta=1$) is a trivial fixed point and that $x^*=1$ is a critical point ($\delta^*=0$ and, from (18a), $J^*=0$). These results are known (Fields 1979, Matsuyama and Okwamoto 1981). (17) shows that the conjecture of Fields (1979), which has been inferred from numerical calculations with $b=L$, holds for arbitrary scale factor b .

The Hamiltonian for the XY model studied by Fields (1979) differs slightly from (1). Both Hamiltonians can be related through the change of variable $J = \tilde{J}/(1+\delta)$. The RG recursion equation for the variable \tilde{J} can be obtained from (16a). One has

$$\tilde{J}' = \frac{1-x^2}{1-x^{L+1}} \frac{1-x^{L+b}}{1-x^{2b}} \tilde{J}. \quad (19)$$

The iteration of equations (18a) and (19) yields

$$J^\infty/J = 1 - x = 2\delta/(1 + \delta) \tag{20a}$$

$$\tilde{J}^\infty/\tilde{J} = 1 - x^2 \tag{20b}$$

when $L \gg 1$ and $x \neq 1$. The gap in the spectrum of the Hamiltonian (1) is $\Delta/2J = \delta^\nu$ or, in terms of the variable \tilde{J} , $\Delta/2\tilde{J} = \frac{1}{2}(1 - x)^\nu$. Here $\nu = 1$ and these expressions for the gap hold for the whole range $0 \leq \delta \leq 1$ (i.e. $0 \leq x \leq 1$) (Fields 1979). The results (20) state that the quantity $\frac{1}{2}(1 + \delta)J^\infty/J$ is more suitable to study the behaviour of the gap away from criticality than the quantity $\frac{1}{2}\tilde{J}^\infty/\tilde{J}$ used by Fields (1979). Typical results plotted in figure 1 illustrate this point. We have plotted the quantities $\frac{1}{2}\tilde{J}^\infty/\tilde{J}$ and $\frac{1}{2}J^\infty/J$ as a function of x for several mappings. The curves A, B and C refer to the first quantity while the curves D, E and F refer to the second one. They correspond to the mappings $(L, L/b) = (3, 1)$ (curves A and D), $(7, 1)$ (curves B and E) and $(15, 13)$ (curves C and F). The curves A and B correspond to the calculation of Fields (1979). The curves C and F do not differ much, on the scale of the figure, from the quantities $\frac{1}{2}(1 - x^2)$ and $\frac{1}{2}(1 - x)$, respectively. We have checked that the quantity $\frac{1}{2}J^\infty/J$ computed with different mappings $(L, L - 2)$ (i.e. $b = L/(L - 2)$), with $L = 3, 5, 7, 9, 11, 13$, converges rapidly to the results shown for $(15, 13)$. For example, the estimate of the index ν gives $\nu = 0.76$ (3, 1), 0.90 (5, 3), 0.94 (7, 5), 0.96 (9, 7), 0.97 (11, 9), 0.99 (13, 11).

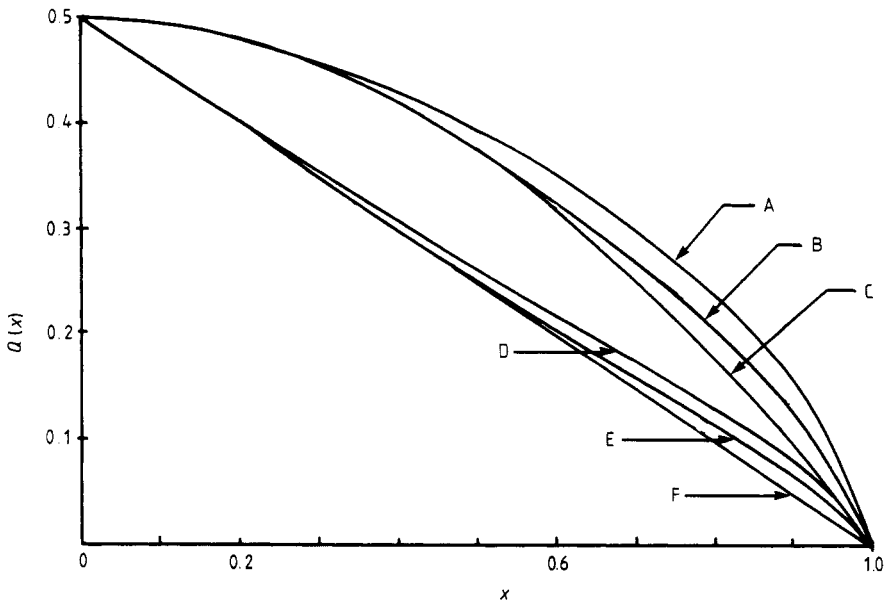


Figure 1. Plot of the quantity $Q(x)$ as a function of x for several mappings $(L, L/b)$. $Q(x) = \frac{1}{2}\tilde{J}^\infty/\tilde{J}$ for the curves A(3, 1), B(7, 1), C(15, 13), and $Q(x) = \frac{1}{2}J^\infty/J$ for the curves D(3, 1), E(7, 1), F(15, 13).

This critical index can also be obtained from the linearisation of the RG equations at the critical point ($\delta^* = J^* = 0$). The linearisation yields (Fisher 1982)

$$\delta' = b\delta = b^\nu\delta \tag{21a}$$

$$J' = (L + b)/[b(L + 1)]J = b^{-\tau}J \tag{21b}$$

from which one finds that $\nu = 1$ and that the dynamical exponent, z , is given by

$$z = 1 - \frac{1}{\ln b} \ln[(L + b)/(L + 1)]. \quad (22)$$

The finite-size corrections for z can then be estimated. One finds

$$z = 1 - O(\ln 2/\ln L) \quad L \gg 1, b = L \quad (23)$$

in the case of the simple RG transformation $(L, 1)$ and

$$z = 1 - O(1/L) \quad L \gg 1, b \sim 1 \quad (24)$$

in the case of the RG transformation of Sarker $(L, L/b)$. For example, a $(15, 1)$ mapping yields $z = 0.77$ and a $(15, 13)$ gives $z = 0.93$. The errors are of the same order of magnitude as those indicated in (23) and (24).

The differential renormalisation group equations are obtained from (21) taking the limit $L \rightarrow \infty, b \rightarrow 1$. One finds

$$dJ(l)/dl = -J(l) \quad (25a)$$

$$d\delta(l)/dl = \delta(l) \quad (25b)$$

where we have set $b = e^l$. The field $J(l)$ is thus an irrelevant field with the exponent $-z = -1$. The quantity $\delta(l)$ is the only relevant field (with the exponent $\nu = 1$). Note that the quantity $J(l)\delta(l)$ is left invariant upon an infinitesimal change of scale. The solutions of the linear differential equations (25) are

$$\delta(l) = \delta e^l \quad (26a)$$

$$J(l) = J e^{-l} \quad (26b)$$

and $J(l)\delta(l) = J\delta$. The scaling laws for the gap and for the singular part of the ground-state energy density (respectively, the analogues of the inverse of the correlation length and of the singular part of the free energy density for two-dimensional systems (Kogut 1979)) are

$$\Delta(\delta) = e^{-l} \Delta(\delta e^l, e^{-l}) \quad (27a)$$

$$f_s(\delta) = e^{-2l} f(\delta e^l, e^{-l}) \quad (27b)$$

where J has been taken as the unit of energy. Choosing l to satisfy $\delta e^l = 1$ yields

$$\Delta(\delta) = \delta \Delta(1, \delta) \quad (28a)$$

$$f_s(\delta) = \delta^2 f(1, \delta). \quad (28b)$$

A comparison with the exact solution (Fields 1979) shows that $\Delta(1, 0)$ is a constant while $f(1, \delta) \sim \ln \delta$, i.e. the scaling function $f(1, \delta)$ is non-analytic at the critical point. Therefore $J(l)$ is a dangerous irrelevant field (Fisher 1982).

Of course the procedure of Sarker for constructing the RG equations discards other irrelevant variables. The above result indicates, however, that the coupling constant is the leading irrelevant one. The rapid convergence of the results for the gap to the exact value, away from criticality, supports this.

In conclusion, we have shown that the RG method of Sarker is a reliable real space method which is able to describe quantitatively the properties of the dimerised XY system for the whole range of dimerisation parameter. This method, which, until now, has not been widely applied, should be applicable to other Hamiltonians.

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