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The Relation Between Mass-Gap Amplítudes and Critical Exponents in the Heisenberg Model

F.C. ALCARAZ

Departamento de Física, Universidade Federal de São Carlos, Caixa Postal 616, São Carlos, SP, Brasil

and

J.R. DRUGOWICH DE FELÍCIO

Departamento de Física e Ciência dos Materiais, Instituto de Física e Química de São Carlos, USP, Caixa Postal 369, São Carlos, 13560, SP, Brasil

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Abstract We discuss a recent result concerning the universality of the ratio of mass-gap amplitudes using the well known 1-D Heisenberg model which is the quantum version of the two-dimensional eight-vertex model. We confirm the believed extended scaling relation ($x_p=x_\varepsilon/4$) relating the polarization and energy anomalous dimensions. We also obtain the exponent, a, v, γ_m and γ_p by usual phenomenological renormalization group methods.

1. INTRODUCTION

At the begining of the last decade Baxter[1] solved the symmetric 8-vertex model in two-dimensions obtaining for the critical index of the correlation length the result

$$\nu_{8V}^{-1} = \frac{2}{\pi} \cos^{-1} \left(\frac{ab-cd}{ab+cd}\right) = \frac{2}{\pi} \mu \quad , \tag{1}$$

where a, b, c and d are the vertex weights (see Fig. 1). The unexpected critical index dependence on the details of the interaction (Boltzmann weights) was promptly explained by Kadanoff and Wegner[2]. They rewrote the model in a magnetic representation in which the Baxter model can be seen as a Ising one with four-spin coupling which in turn is a marginal operator (it has scale dimension equal to the lattice dimension).

Later, Barber and Baxter have conjectured expressions for the spontaneous magnetization[3] and polarization[4] exponents, namely

$$\beta_m = \pi/16\mu \quad , \tag{2}$$

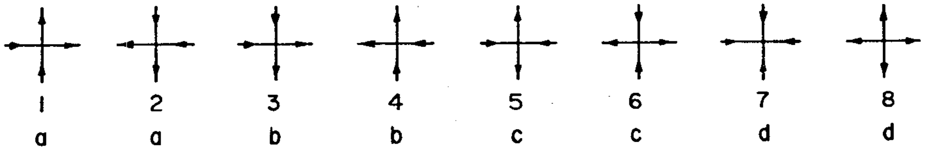

Fig.1 - The eight arrow configurations allowed at a vertex with the corresponding vertex weights.

and

$$\beta_p = -\frac{1}{4} + \frac{\pi}{4\mu} \quad . \tag{3}$$

On the other hand, since Sutherland's work the close relationship betwaen the two-dimensional 8-vertex model and the I-D quantum Heisenberg model

$$H = -\sum_i \left[(1+\lambda)\, S_i^x S_{i+1}^x + (1-\lambda)\, S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z\right] \quad , \tag{4}$$

is well known[6]. The phase diagram of this Hamiltonian is shown in Fig.2, where the critical lines are denoted by heavy lines (in this paper we only study the line (1) since any of them can be mapped on it by convenient transformation). For $|\Delta| < 1$, where the model is massless (critical), a gap develops with respect to A, as

$$G = E_1 - E_0 \sim \xi^{-1} \sim |\lambda|^{\nu} \quad , \tag{5}$$

where

$$\nu^{-1} = \frac{2}{\pi}\cos^{-1}(-\Delta) \quad , \tag{6}$$

and A is directly related to a change of temperature in the 8-vertex model.

The above relations indicate the 8-vertex model as an interesting laboratory to check new techniques for obtaining critical indices. In this case the Baxter model has been considered by Blöte and Nigthingale[7] to verify a recent conjecture[8] relating critical indices and correlation-length amplitudes of finite systems namely

$$\xi_i^{-1}\,(T=T_c) = A_i/L \tag{7a}$$

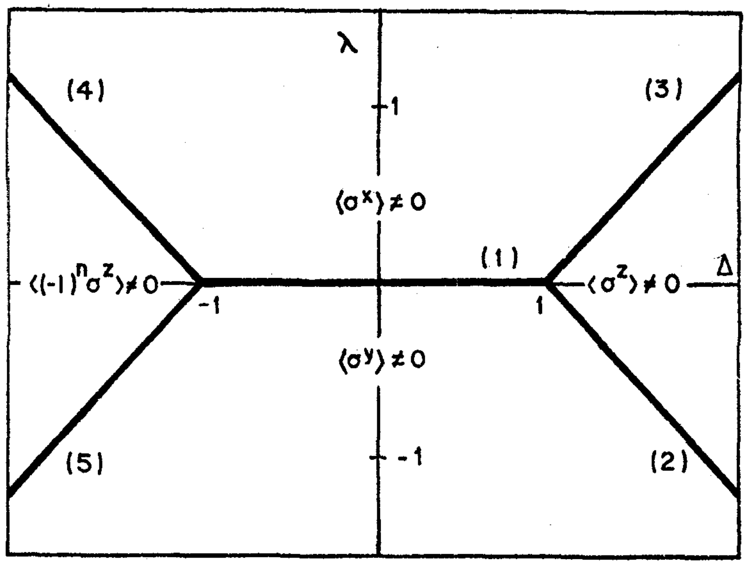

Fig.2 - The phase diagram of the Heisenberg Hamiltonian (Eq. 4).

with

$$A_i = 2\pi\, x_i \tag{7b}$$

where x_i is the anomalous dimension of the operator, whose correlation -function is being calculated.

Recently, several authors have tried to find and equation equivalent to Eq. (7) in the Hamiltonian context. The counterpart of the correlation lengths, in that context, are the mass-gaps. However, as shown by Fradkin and Susskind[10] there is a factor relating those two quantities which, in general, is not under control.

The main purpose of this paper is to study the relationship between critical indices and mass-gap amplitudes in the Heisenberg model. The paper is organized as follows: in section 2 we present the model and identify its operators. Further, a sequence of duality transformations is performed on the original variables to get a Hamiltonian which exhibits the magnetic operator as a local one. Section 3 contains a brief introduction to finite-size scaling (F.S.S.) ideas and the numerical results for the critical indices. Finally, in section 4 we calculate the ratios of mass-gap amplitudes at the critical coupling. Our results are in complete agreement with the exact results of eqs. (2) and (6). In addition they corroborate the conjecture (3) as well as the recent conjecture[9] concerning the universality of mass-gap amplitude ratios.

2. THE MODEL

We will consider the spin-1/2 Heisenberg model inone dimension (eq.4) where S^{α} (a = x,y or z) are Pauli matrices and h, A are coupling constants. The Hamiltonian (4) can be rewritten as

$$H = -\sum_{i} \left[\lambda (S^x_i S^x_{i+1} - S^y_i S^y_{i+1}) + (S^x_i S^x_{i+1} + S^y_i S^y_{i+1}) + \Delta S^z_i S^z_{i+1}\right], \tag{8}$$

which allows us to identify $(S^x_i S^x_{i+1} - S^y_i S^y_{i+1})$ as the energy operator $(O_\varepsilon(i))$ along line (1). Its correlation function, at $\lambda=0$, decays as

$$\langle O_\varepsilon(i)\, O_\varepsilon(i')\rangle \sim |i-i'|^{-2x_\varepsilon} , \tag{9}$$

with

$$x_\varepsilon = 2 - \frac{1}{\nu} . \tag{10}$$

Many other operators can be added to H_{xyz}. the best known isthe polarization operator (S^y) whose correlation function, at $\lambda=0$, decays as

$$\langle S^y_i S^y_{i'}\rangle \sim |i-i'|^{-2x_p} \tag{11}$$

where, according to Eqs. (1), (3), (10), (11) and[11]

$$\beta = \nu(d-2+2x) , \tag{12}$$

x_p is given by

$$x_p = x_\varepsilon/4 . \tag{13}$$

This extended scaling relation can be checked by the method of amplitudes as we will show in section 4. However, eq. (6) which gives ν

as a function of λ can be obtained only by the conventional F.S.S. method. To circumvent this difficulty we transform the XYZ Hamiltonian in a sort of Ashkin-Teller one. This transformation is done in two steps[12]: firstly a duality transformation is performed on the S variables (all of them) by introducing a new Pauli set of matrices

$$\mu^{x}_{i+1/2} = S^{z}_{i}\, S^{z}_{i+1} \quad , \tag{14a}$$

$$\mu^{z}_{i+1/2} = \prod_{k\leq i} S^{x}_{k} \quad , \tag{14b}$$

which preserves the spin-1/2 algebra and the number of sites (see Fig. 3). The second step consists of another duality transformation per-

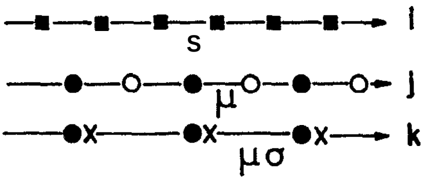

Fig.3 - Before doing the duality transformations we have S variables interacting via eq. (4). After doing the transformations (14) and (15) we get a staggered Ashkin-Teller model.

formed on the odd sites only, preserving commutation relations but reducing the number of sites. The new variables σ are given by

$$\sigma^{x}_{2j} = \mu^{z}_{2j-1}\, \mu^{z}_{2j+1} \tag{15a}$$

$$\sigma_{2j} = \prod_{k\geq j} \mu^{x}_{2k+1} \tag{15b}$$

where $j = i+1/2$. Finally we obtain H in the form

$$H = - \sum_{j} \{ (1+\lambda)\, \mu^{z}_{2j}\mu^{z}_{2j+2} + (1-\lambda)\, \sigma^{z}_{2j}\sigma^{z}_{2j+2} - \Delta\sigma^{z}_{2j}\sigma^{z}_{2j+2}\mu^{z}_{2j}\mu^{z}_{2j+2}$$

$$+ (1+\lambda)\ \sigma^{x}_{2j} + (1-\lambda)\ \mu^{x}_{2j} - \Delta\sigma^{x}_{2j}\mu^{x}_{2j} \} \quad . \tag{16}$$

The advantage of this representation for H is the presence of the magnetic operators σ^{z} and μ^{z} which remind us of the Ising representation of Baxter's model in two-dimensions. According to eqs. (3) and (12) we obtain for $x_m = \eta_m/2$ the value

$$x_m = 1/8 \ , \tag{17}$$

independent of A.

It is this universal behavior which will hep us in extracting the index ν from the mass-gap amplitudes (see section 4).

3. FINITE-SIZE SCALING

a) The Method

The method of finite-size scaling is a powerful tool to analize the critical properties of interacting systems. The method had its genesis in the works of Fisher and collaborators and the most complete review of the theory and its applications has been given recently by Barber[13]. The method is very useful because it does not generate new terms in the Hamiltonian as the other renormalization-group techniques do. The basic FSS assertion (in the transfer-matrix context) is that upon the size change $L \to L'$ the correlation length ξ changes as

$$\xi_L(t) = \frac{L}{L'}\xi_{L'}(t') \quad , \qquad t = (T - T_c)/T_c \tag{18}$$

which becomes at $T=T_c$

$$\frac{\xi_L(T_c)}{L} = \frac{\xi_{L'}(T_c)}{L'} \quad , \tag{19}$$

where T_c is an estimate for the critical temperature. In the case of a quantum Hamiltonian an appropriate form of the FSS can also be stated[14]. Now, the basic quantity which determines the critical behavior is the energy gap $G = E_1 - E_0 \sim \xi^{-1}$ between the ground and first-excited states. In this context, eq. (18) can be reinterpreted as

$$LG_L(\lambda) = L'G_{L'}(\lambda') \quad , \tag{20}$$

and the critical coupling is the solution of

$$LG_L(\lambda_c) = L'G_{L'}(\lambda_c) \quad . \tag{21}$$

This method can also be used to obtain critical exponents. The exponents ν, for example, follows from eq. (20) by taking the derivative with respect to the coupling constant. It results

$$\nu = \left[1 + \log(G_L/G_{L'})/\log(L/L')\right]^{-1} . \qquad (22)$$

Analogously we can find the exponent γ of the susceptibility by calculating the second derivative of the free-energy (ground-state of H) with respect to the magnetic field *(h)*. In general, any thermodynamical quantity Q whose infinite lattice behavior is

$$Q(\lambda) \sim (\lambda-\lambda_c)^{-\psi} , \qquad (23)$$

scales in the finite system as

$$Q_L(\lambda_c) \sim L^{\psi/\nu} . \qquad (24)$$

Therefore, by considering a set of finite lattices it is possible to estimate the index ψ/ν by extrapolating the sequence

$$L\{[Q_L(\lambda_c) - Q_{L'}(\lambda_c)]/Q_{L'}(\lambda_c)\} \to \psi/\nu . \qquad (25)$$

b) Numerical Results

We have diagonalized numerically the Hamiltonian (4) for finite lattices of L sites with periodic boundary conditions ($L = 2 \to 18$). The eigenvalues, as well as its derivatives were performed at the true infinite critical coupling $\lambda = 0$ for several values of A. To handle such largematrices we haveused all symmetry properties of the Hamiltonian and employed the Lanczos' algorithm[15] of tridiagonalization (in the Appendix we present a short description of this method).

The critical exponents obtained are shown in Table 1 and 2 together with the exact results given by eq. (6). These exponents were calculated by adequatly choosing the function Q_L (A) in eq. (25). The exponent ν was estimated by using the Beta-function

$$\beta_L(\lambda_c) = \frac{\partial}{\partial\lambda} \log G_L(\lambda)\Big|_{\lambda=0} , \qquad (26)$$

Table 1 - Estimated (F.S.S.) and exact results for the thermal (ν and α) critical exponents of the 1-D Heisenberg model (eq. 4).

Δ	$1/\nu$ (F.S.S.)	$1/\nu$ (EXACT)	α/ν (F.S.S.)	α/ν (EXACT)
-0.50	0.65	0.666	-0.69	-0.67
-0.25	0.838	0.839	-0.34	-0.32
0.25	1.161	1.161	0.32	0.32
0.50	1.332	1.333	0.67	0.67
0.75	1.535	1.540	1.08	1.08
0.90	1.650	1.712	1.30	1.43

Table 2 - Estimated (F.S.S.) and exact results for the electrical susceptibility index (γ_p).

Δ	γ_p/ν (F.S.S.)	γ_p/ν (CONJECTURED)
0.25	1.580	1.580
0.50	1.665	1.667
0.75	1.767	1.769

while the exponent α was obtained by choosing the "specific heat"

$$C_L(\lambda_c) = \left.\frac{\partial^2 E_0}{\partial\lambda^2}\right|_{\lambda=0} , \tag{27}$$

as the Q_L function in eq. (25). In the same fashion to calculate the electrical susceptibility index γ_p we introduce in the Harniltonian (4) an electric field term $E\sum_i S_i^y$ and we use as $Q_L(\lambda)$ the "electric susceptibility"

$$\chi_L^E(\lambda_c) = \left.\frac{\partial^2 E_0}{\partial E^2}\right|_{\lambda=E=0} . \tag{28}$$

We notice a remarkable agreement between the numerical estimates and exact results. The poor convergence in the $\Delta \simeq 1$ region is to be expected since the $\Delta = 1$ value corresponds to a first-order transition (KOP). It is worthwhile to mention that the high precision achieved is due to the use of Vanden Broeck-Schwartz tables[16].

We also calculated the critical indices of the Hamiltonian (16) for lattice size ranging from 2 to 9 sites (4 states per site). The index ν, calculated as before, confirms that both Hamiltonians exhibits the same critical behavior (see Tables 1 and 3).

Table 3 - Mass-gap critical exponent (ν) of the Hamiltonian (16).

Δ	$1/\nu$ (F.S.S.)	$1/\nu$ (EXACT)
-0.50	0.663	0.666
-0.35	0.771	0.772
-0.25	0.839	0.839
0.25	1.161	1.161
0.50	1.335	1.333

In this new version it is difficult to calculate the index y_p because the polarization operator S^y has a non-local representation in terms of σ's and μ's. The opposite happens for γ_m which is easy to calculate in the new representation by adding to the Hamiltonian (16) a magnetic field

$$- h \sum_i (\sigma_i^z + \mu_i^z) \qquad (29)$$

which breaks explicitly the $Z(2)$ symmetry of the Hamiltonian. Finally we use the magnetic susceptibility

$$\chi_L^m = \left. \frac{\partial^2 E_0}{\partial h^2} \right|_{\lambda=h=0} \qquad (30)$$

in eq. (25) to calculate γ_m (see Table 4). Our results confirm the uni-

Table 4 - Magnetical susceptibility index (γ_m).

Δ	γ_m/ν (F.S.S.)	γ_m/ν (EXACT)
-0.50	1.73	1.750
-0.25	1.73	1.750
0.25	1.750	1.750
0.50	1.750	1.750
0.75	1.751	1.750
1.00	1.74	1.750

versal behavior of η given by

$$\eta_m = 2 - \frac{\gamma_m}{\nu} = 0.250 \tag{31}$$

4. MASS-GAP AMPLITUDES

In the finite-size scaling theory for continuous transitions the inverse correlation length vanishes at critical temperature, as

$$\xi^{-1}(T=T_c) = A/L \tag{32}$$

where A is the so-called amplitude of correlation length. Recently an interesting conjecture has been proposed claiming that the amplitude A is related to critical exponents, namely

$$A = \pi\eta \tag{33}$$

where η is the exponent of the spin-spin correlation-function. Later[7], this conjecture was extended to include anisotropic models as well as other correlation-lengths. In the case of a quantum Hamiltonian instead of the several correlation-lengths we have the various mass-gaps

$$G_i = E_i - E_0 = A_i/L \quad , \tag{34}$$

and the universal quantities seem to be[9] the ratios of mass-gap amplitudes. The relation (7b) is now replaced by

$$A_i/A_j = x_i/x_j \tag{35}$$

where $x_i (x_3)$ is the anomalous dimension of the operator related to the corresponding mass gap $G_i (G_3)$.

For the Hamiltonian (4) the ratio A_1/A_2 is related to x_p/x_ε since the polarization operator is linear in S^y while the energy one is bilinear in S^y. So, for any value of A we expect to obtain $A_1/A_2 = 1/4$ according to eq. (13). In fact as shown in Table 5 our numerical calculations are in complete agreement with this result. It is worthwhile to mention that to obtain the exponent ν we need to consider Hamiltonian (16) which contains the magnetic operator whose anomalous dimension does not depend[3] on coupling constant ($x_m = 1/8$). Then, by considering the first and third mass-gap of Hamiltonian (16) we find the ratio

Table 5 - Mass-gap amplitude ratio (A_1/A_2), for several values of coupling Δ, of the Hamiltonian (4).

Δ	A_1/A_2	x_p/x_ε (CONJECTURED)
-0.50	0.2542	0.250
-0.25	0.2527	0.250
0.25	0.2515	0.250
0.50	0.2510	0.250
0.75	0.2506	0.250

$$\frac{x_m}{x_\varepsilon^{AT}(-\Delta)} = x_m \cdot x_{CR}^{AT}(-\Delta) \quad , \tag{36}$$

where x_ε^{AT} (x_{CR}^{AT}) is the anomalous dimension of the energy (crossover) operator of the Ashkin-Teller model, which in turn is related to the anomalous dimension of the eight-vertex one[17] by

$$x_{CR}^{AT}(-\Delta) = x_\varepsilon^{8V}(\Delta) . \tag{37}$$

Thus, we obtain

$$A_1/A_3 = x_m x_\varepsilon^{8V} = \frac{1}{8}\left[2 - \frac{1}{\nu}\right] \ . \tag{38}$$

In Table 6 we show the mass-gap amplitude ratios together with the exact results.

Table 6 - Mass-gap amplitude ratio (A_1/A_3), for several values of coupling Δ, of the Hamiltonian (16).

Δ	A_1/A_3	$x_m . x_\varepsilon^{8V}$ (EXACT)
-0.50	0.1618	0.1666
-0.25	0.1447	0.1451
0.00	0.1259	0.1250
0.25	0.1057	0.1049
0.50	0.0839	0.0833

APPENDIX

In this appendix we discuss the Lanczos scheme of tri-diagonalization which has been so useful in finite-size studies of quantum 1-D Hamiltonians. In this method we seek a unitary transformation

$$U^+ H U = T \quad , \quad U^+ U = I \tag{A.1}$$

where T is tridiagonal, real and symmetric:

$$T = \begin{pmatrix} a_1 & b_1 & & & & \\ b_1 & a_2 & b_2 & & & \\ & b_2 & a_3 & b_3 & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot \\ & & & & \cdot & \cdot & \cdot \end{pmatrix} \tag{A.2}$$

Writing U as a series of columm vectors

$$U = (u_1, u_2, u_3, \dots) \tag{A.3}$$

with

$$u_i^+ u_j = \delta_{ij} \tag{A.4}$$

we obtain from (A.1)

$$Hu_1 = a_1 u_1 + b_1 u_2$$

$$Hu_i = b_{i-1} u_{i-1} + a_i u_i + b_i u_{i+1} \tag{A.5}$$

$$Hu_N = b_{N-1} u_{N-1} + a_N u_N$$

These questions can be used recursively to calculate all the coefficients $\{a_i, b_i\}$ which appear in T.

The advantage of the Lanczos algorithm over other methods is that it does not require the matrix H to be stored in a large $N \times N$ array which is "filled in" by the calculation even if H has a large number of zero elements. We only require storage space for 3 Lanczos' vectors and a subroutine to multiply a vector by H. Further we calculate the scalar product

$$u_i^+ H u_i$$

which equals a_i as a consequence of the herrniticity of H and of the orthonormalization of u_i. Finally we get

$$b_i u_{i+1} = Hu_i - b_{i-1} u_{i-1} - a_i u_i$$

The main property of Lanczos' method is that the low-lying eigenvalues of H can be obtained after 30 or 40 steps (even for systems with 2^{18} degrees of freedom). One can monitor the convergence by comparing the eigenvalues obtained after n steps with those calculated after $(n-1)$ Lanczos steps.

To implement this scheme in the computer it is convenient to represent a quantum state by an integer number (or a combination of integers) which in turn is a sequence of 1's and O's in the binary code. The effect of the Hamiltonian on a quantum state can be obtained by using logical built-in functions usually available in advanced computer languages. If, for example, we want to act on the state $\downarrow\uparrow\uparrow\downarrow\uparrow \equiv$ (01101) by the operator $\sigma^x(3)\ \sigma^x(2)$ all we have to do is to form the logical

EXCLUSIVE OR (IEOR) function of the original state 13 with the number 6(00110). The result is 11 (01011) ≡ ↓↑↓↑↑. The diagonal part of the Hamiltonian can be implemented by the BITEST function which returns "true" if the bit is 1 and "false" in any other case.

Because of round-off errors, the state u_{n+1} may not be orthogonal to , , ..., in consequence, spurious eigenvalues (ghosts) can be obtained. Fortunately these ghosts can be recognized because we assume H to be nondegenerate. The spurious eigenvalues can also be recognized by comparing with the eigenvalues of the tridiagonal matrix formed from the f'irst $(N-1)$ interactions.

We are grateful to Prof. R.Köberle for useful discussions

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Resumo

Discutimos nesse trabalho um resultado recente que relaciona os expoentes críticos de um modelo com as amplitudes das lacunas de massa da Hamiltoniana associada. Nós usamos como teste o modelo de Heisenberg unidimensional que é a versão quântica do modelo de oito-vértices (Baxter) em duas dimensões. São obtidos, pelo método usual do grupo de renormalização fenomenológico, os índices ν, a, γ_m e γ_p. Os resultados confirmam a universalidade da razão das amplitudes mencionadas.