## Critical Index v of the Vertical-Arrow Correlation Length in the Eight-Vertex Model\*

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We calculate the critical index  $\nu$  of the correlation length between two vertical arrows in the same column for the eight-vertex model and find  $\nu = 1 - \alpha/2$ . We also compute at zero temperature the low-lying excitations of the X-Y-Z model.

Recently, Baxter<sup>1,2</sup> computed the free energy of the zero-field eight-vertex model and the groundstate energy of the X-Y-Z model. This was accomplished by calculating, in the thermodynamic limit, the two eigenvalues largest in magnitude of the transfer matrix for a row of vertices of the eight-vertex model. He determined the critical index  $\alpha$  of the eight-vertex specific heat and found the surprising result that it depended continuously on an interaction parameter. It is of interest to compute the other critical indices of the eightvertex model and to compare them with the predictions of scaling theories of phase transitions.<sup>3</sup> In this note we study  $G_R$ , the correlation function for two vertical arrows in the same column. We also study the low-lying excited states of the X-Y-Z model, which are closely related.

We follow Baxter's notation and denote the pairwise equal weights of the eight-vertex model by a, b, c, and d, and define  $w_1 = \frac{1}{2}(c+d)$ ,  $w_2 = \frac{1}{2}(c-d)$ ,  $w_3 = \frac{1}{2}(a-b)$ , and  $w_4 = \frac{1}{2}(a+b)$ . In terms of these  $w_i$ the partition function Z satisfies the symmetry relations<sup>4</sup>

$$Z(w_1, w_2, w_3, w_4) = Z(\pm w_i, \pm w_j, \pm w_k, \pm w_l), \qquad (1)$$

where i, j, k, l are any permutation of 1,2,3,4. It is therefore sufficient to restrict attention to the fundamental region (FR)  $w_1 > w_2 > w_3 > w_4 > 0$ . The cases of physical interest are

I.  $w_1 > w_4$ ,

$$w_1 > |w_2| > w_4 > |w_3| \quad (T < T_c),$$
 (2a)

$$w_1 > w_4 > |w_2| > |w_3| \quad (T > T_c),$$
 (2b)

$$w_1 > w_4 > |w_3| > |w_2|$$
 (T > T<sub>c</sub>); (2c)

II.  $w_4 > w_1$ ,

$$w_4 > |w_3| > w_1 > |w_2|$$
 (T < T<sub>c</sub>), (3a)

$$w_4 > w_1 > |w_3| > |w_2|$$
 (T > T<sub>c</sub>), (3b)

$$w_4 > w_1 > |w_2| > |w_3| \quad (T > T_c).$$
 (3c)

Using (1) all the cases of physical interest can be reduced to the FR.

The correlation function  $G_R$  given by

$$G_{R}(w_{1}, w_{2}, w_{3}, w_{4}) = Z^{-1} \operatorname{Tr} \left[\sigma^{z} T^{R}(w_{1}, w_{2}, w_{3}, w_{4}) \sigma^{z} T^{N \sim R}(w_{1}, w_{2}, w_{3}, w_{4})\right]$$
(4)

does not possess as much symmetry as Z.  $T(w_1, w_2, w_3, w_4)$  is the transfer matrix of a row and N (even) is the number of rows. In place of (1), we derive

$$G_{R}(w_{1}, w_{2}, w_{3}, w_{4}) = G_{R}(\pm w_{1}, \pm w_{2}, \pm w_{3}, \pm w_{4}) = G_{R}(w_{2}, w_{1}, w_{3}, w_{4}) = (-1)^{R}G_{R}(w_{4}, w_{3}, w_{2}, w_{1}).$$
(5)

Furthermore, using Baxter's expression for T, it may be seen by making a unitary transformation that

$$G_{R}(w_{1}, w_{2}, w_{3}, w_{4}) = Z^{-1} \operatorname{Tr} \left[ \sigma^{y} T^{R}(w_{1}, w_{3}, w_{2}, w_{4}) \sigma^{y} T^{N-R}(w_{1}, w_{3}, w_{2}, w_{4}) \right].$$
(6)

Therefore, unlike Z,  $G_k(w_1, w_2, w_3, w_4)$  cannot be obtained for  $w_i$  in the physical regions from  $G_k$  with  $w_i$  in the fundamental region. However, if we have the required information about matrix elements, then it is only necessary to compute the eigenvalues of T in the FR.

Expressions (4) and (6) are the usual type of relations used to study correlation functions in terms of transfer matrices,<sup>5</sup> and the standard

argument is that for large R

$$G_{k}$$
 - (long-range order) ~  $(\Lambda_{1}/\Lambda_{0})^{k}$ , (7)

where  $\Lambda_0$  is the maximum eigenvalue of T, and  $\Lambda_1$  is the next largest eigenvalue. Here the meaning of "~" is that there may be additional polynomial behavior in R which comes from matrix elements. We will restrict our attention to the

exponential dependence on R, so only the eigenvalues of T are required. Below the critical temperature, we use Eq. (4). The symmetry relations (5) allow us to arrange the arguments of T such that they lie in the FR. The matrix element  $\langle \psi_0^{+} | \sigma^z | \psi_0^{-} \rangle$ , between the eigenvectors  $\psi_0^{\pm}$  of the two eigenvalues  $\pm \Lambda_0$  largest in magnitude, is not zero. Hence, there is long-range order. Above the critical temperature, we use Eq. (6). The symmetry relations (5) allow us to place the arguments of T in the FR. The matrix element  $\langle \psi_0^{+} | \sigma^y | \psi_0^{-} \rangle$  vanishes (since  $\sigma^y$  changes the evenness or oddness of the number of arrows in a row pointing down), so there is no long-range order.

Baxter has shown that the eigenvalues of the transfer matrix can be determined by solving a

set of coupled, nonlinear equations for the zeros of a certain quasiperiodic function. For the two eigenvalues  $\pm \Lambda_0$ , largest in magnitude, all the zeros are real. In the thermodynamic limit, these equations can be approximated by a linear integral equation with difference kernel for the density of these zeros. From previously solved cases,<sup>6</sup> it is reasonable to assume that for  $\mu$  $\leq \pi/2$  the next largest eigenvalues (in magnitude)  $\Lambda_e$  correspond to one of the zeros having imaginary part  $iK_{\mu}/2$ , or to there being a complex-conjugate pair of zeros with imaginary part  $\pm Im\eta$ .<sup>7</sup> In either cases, one can write a linear integral equation for the change of the density of real zeros from the density corresponding to the maximum eigenvalues.<sup>8</sup> We solved the equation by Fourier transform and determined the eigenvalues  $\Lambda_e$ . The result for  $\mu \leq \pi/2$  is

$$\operatorname{Re}\ln\frac{\Lambda_{e}}{\Lambda_{0}} = \alpha_{b} - \lambda + \sum_{m=1}^{\infty} \frac{\sinh m(\alpha_{b} - \lambda) [\cos m\alpha_{1} + \cos m\alpha_{2}]}{m \cosh m\lambda},$$
(8a)

$$\operatorname{Im} \ln \frac{\Lambda_e}{\Lambda_0} = \frac{\alpha_1 + \alpha_2}{2} - \pi (\omega_1 + \omega_2) \sum_{m=1}^{\infty} \frac{\cosh m (\alpha_b - \lambda) [\sin m \alpha_1 + \sin m \alpha_2]}{m \cosh m \lambda},$$
(8b)

where  $0 < \alpha_b < \lambda < \tau$  (FR) and  $-\pi < \alpha_{1,2} \leq \pi$ . Here,  $\omega_1 = 0$  or 2 represents an ambiguity in the choice of a branch of the logarithm, and  $\omega_2 = 0$  or 1 indicates whether one is exciting from  $\pm \Lambda_0$ . For given  $\alpha_1$  and  $\alpha_2$ , there are eight excited states, corresponding to the possible values of  $\omega_1$  and  $\omega_2$  and to whether the excitation is a complexconjugate pair or a zero on  $iK_k'/2$ .

Now Re  $\ln(\Lambda_0/\Lambda_1)$  is given by (8a), with  $\alpha_1 = \alpha_2 = \pi$ . To calculate the critical index  $\nu$ , we perform a Poisson summation on (8a), with  $\alpha_1 = \alpha_2 = \pi$ , and we find that Re  $\ln(\Lambda_0/\Lambda_1) \sim |T - T_c|^{\pi/2\mu}$  for  $T \rightarrow T_c$ .

$$\nu = \pi/2\mu. \tag{9}$$

Since Baxter has found  $\alpha = 2 - \pi/\mu$ ,

$$\nu = 1 - \alpha/2, \tag{10}$$

which is the usual prediction of scaling.<sup>3</sup>

We have been careful in the above not to make the identification  $\xi^{-1} = \operatorname{Re} \ln(\Lambda_0/\Lambda_1)$ , because it is not valid for our calculation. This can be most easily seen by considering the decoupling limit  $\mu = \pi/2$  and taking *R* even. Then by looking at the underlying Ising lattice, equivalent to the eightvertex model,<sup>9</sup> one can prove that the verticalarrow correlation function for a row, C(R)=  $\langle 0|\sigma_0^{z}\sigma_R^{z}|0\rangle$ , is equal to the vertical-arrow correlation function  $G_R$  for a column. (Both are equal to the square of the Ising-model two-spin correlation function along a diagonal.) Now  $|0\rangle$ is an eigenvector of *T* and is independent<sup>1</sup> of  $\alpha_b$ . Therefore, C(R) and hence its correlation length are independent of  $\alpha_b$ . However, Re  $\ln(\Lambda_0/\Lambda_1)$  is obviously dependent on  $\alpha_b$ , so  $\xi^{-1} \neq \text{Re } \ln(\Lambda_0/\Lambda_1)$ . The critical indices of  $\xi$  and Re  $\ln(\Lambda_0/\Lambda_1)$  are still believed to be equal and, in fact, they can be shown to be equal in the case  $\mu = \pi/2$  by comparing with known results.<sup>10</sup>

In the region  $\mu > \pi/2$ , to proceed as outlined above leads to difficulties with the choice of branches. However, all plausible choices of branches lead to an expression of the form

$$\operatorname{Re}\ln\frac{\Lambda_e}{\Lambda_0} = \sum_{i} \sum_{m=-\infty}^{\infty} C_m \frac{i \operatorname{cosm} \alpha_i}{\operatorname{cosh} m \lambda}$$

Assuming that the  $C_m^i$  fall off sufficiently rapidly, one finds  $\nu = \pi/2\mu$  for  $\mu > \pi/2$ .

We conclude by using the above results to study the low-lying excitations of the X-Y-Z model. The Hamiltonian we consider is

$$H = -\frac{1}{2} \sum_{j=1}^{N} (J_{x} \sigma_{j}^{x} \sigma_{j+1}^{x} + J_{y} \sigma_{j}^{y} \sigma_{j+1}^{y} + J_{z} \sigma_{j}^{z} \sigma_{j+1}^{z})$$

with a periodic boundary condition and with  $J_z$  $\langle J_y \langle -|J_x|$ . A useful parametrization<sup>11</sup> is  $J_x/J_z$ = cn(2 $\zeta$ , l) and  $J_y/J_z$ =dn(2 $\zeta$ , l), where for the above restriction on the J's the parameters  $\zeta$  and l are in the FR.

By taking a derivative<sup>2</sup> of the expression (8a) for Re  $\ln(\Lambda_e/\Lambda_0)$ , we obtain (for  $\mu \leq \pi/2$ ) the energy difference  $\Delta E$  between the first excited states and ground state as a function of  $\alpha_1$  and  $\alpha_2$ . Baxter<sup>2</sup> has shown that the transfer matrix  $T(\alpha_b = \lambda)$ is equal to  $2^N$  times the cyclic shift operator that moves all spins one site to the left. Therefore, from Im  $\ln(\Lambda_e/\Lambda_0)$ , calculated at  $\alpha_b = \lambda$ , one can extract the momentum difference  $\Delta P$  between the excited states and the ground state in terms of  $\alpha_1$  and  $\alpha_2$ . We define two new variables  $q_1$  and  $q_2$  by

$$q_i = \int_{-K_m}^{K_m \alpha_i/\pi} \mathrm{dn}(\varphi, m) \, d\varphi.$$

Then

$$\Delta P = q_1 + q_2 - (\omega_1 + \omega_2)\pi - \pi,$$
(11a)

$$\Delta E = -J_z \operatorname{sn}(2\xi, l) K_m(K_l')^{-1}$$
$$\times [(1 - m^2 \cos^2 q_1)^{1/2} + (1 - m^2 \cos^2 q_2)^{1/2}], (11b)$$

where *m* is determined from  $K_m'/K_m = \lambda/\pi$ . The range of the  $q_i$  is  $0 \le q_i \le \pi$ . For a given value of  $q_1$  and  $q_2$ , there are eight states, and the statistics of the excitations is believed to be of the Fermi-Dirac type.

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<sup>7</sup>Here we are using Baxter's parametrization *a*:*b*:*c*:*d* = sn( $v + \eta$ , k):sn( $v - \eta$ , k):sn( $2\eta$ , k):k sn( $2\eta$ , k) sn( $v - \eta$ , k) × sn( $v + \eta$ , k) and defining  $\pi\eta = i\lambda K_k$ ,  $\pi v = i\alpha_b K_k$ ,  $2\pi\eta = i\mu K_k'$ , and  $2K_k\tau = \pi K_k'$ .

<sup>8</sup>We wish to remark that the whole integral equation formalism suffers from ambiguities in that the branches of the logarithms appearing in the formalism are not *a priori* specified. We have chosen these branches such that the known results in the decoupling  $(\mu \rightarrow \pi/2)$  and ice limits are recovered and the excitation energies of the X-Y-Z model are correct in the X-Y and Heisenberg-Ising limits.

<sup>9</sup>L. P. Kadanoff and F. J. Wegner, Phys. Rev. B <u>4</u>, 3989 (1971); F. Y. Wu, Phys. Rev. B <u>4</u>, 3212 (1971). <sup>10</sup>E. Barouch, Phys. Lett. <u>34A</u>, 347 (1971). <sup>11</sup>ζ and *l* are related to  $\lambda$  and *k* by l = (1 - k)/(1 + k) and  $K_l'\lambda = \pi \zeta$ .

## Quadrupole Moment of the Deuteron\*

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The electric field gradient in the HD and  $D_2$  molecules has been calculated from 87term wave functions of the James and Coolidge type. With the use of experimental values of the quadrupole interaction constant, the electric quadrupole moment of the deuteron is found to be 0.2875 F<sup>2</sup> which is 2% larger than the most recent values. The estimated error is 0.002 F<sup>2</sup>.

The quadrupole moment of the deuteron, Q, has long served as a touchstone for models of the nucleon-nucleon interaction because of its connection with the tensor force, without which Qwould vanish. At the present time Q cannot be directly determined experimentally; it can be extracted from the electric quadrupole interaction constant eqQ/h with the aid of a theoretically calculated field gradient q. However, quantitative calculation of the field gradient<sup>1-5</sup> for such simple molecules has proved difficult. Code and Ramsey<sup>6</sup> cast doubt on the most recent calculation<sup>5</sup> by showing that the results were not consistent with their  $D_2(J=1)$  and the earlier<sup>7</sup> HD(J=1) interaction constants. Signell and Parker<sup>8</sup> have noted the extent and aspects of the seriousness