Phase diagram of the Ashkin-Teller quantum spin chain

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We study a one-dimensional quantum Hamiltonian which is related to a highly anisotropic version of the two-dimensional Ashkin-Teller model. We explore the parameter region and complete the ground-state phase diagram. This problem is studied by using duality relations and by series expansions up to seventeenth order. Corresponding critical indices are also calculated. In this parameter region, a line of continuously varying critical indices is found.

I. INTRODUCTION

The two-dimensional Ashkin-Teller model consists of two Ising models coupled by a four-spin interaction.[1] The classical Hamiltonian is given by

$$H = -\sum_{\langle i,j\rangle}\{\, K_2(s_is_j + t_it_j) + K_4 s_is_jt_it_j\}, \qquad (1.1)$$

where $s_i = \pm 1$ and $t_i = \pm 1$ are two kinds of Ising spins at site i on a square lattice and the sum is taken over nearest-neighbor pairs. The K_2 and K_4 denote a two-spin coupling constant and a four-spin one, respectively. When $K_4 = 0$, the model reduces to the two decoupled Ising models with the nearest-neighbor coupling K_2. In the anisotropic case, the Hamiltonian is

$$H = -\sum_{\mathbf{r}}\{K_2^x(s_\mathbf{r}s_{\mathbf{r}+\mathbf{x}} + t_\mathbf{r}t_{\mathbf{r}+\mathbf{x}}) + K_2^\tau(s_\mathbf{r}s_{\mathbf{r}+\tau} + t_\mathbf{r}t_{\mathbf{r}+\tau}) + K_4^x s_\mathbf{r}s_{\mathbf{r}+\mathbf{x}}t_\mathbf{r}t_{\mathbf{r}+\mathbf{x}} + K_4^\tau s_\mathbf{r}s_{\mathbf{r}+\tau}t_\mathbf{r}t_{\mathbf{r}+\tau}\}, \qquad (1.2)$$

where $\mathbf{r} = (i,j)$ is the lattice sites, and $\mathbf{x} = (1,0)$ and $\tau = (0,1)$ are nearest-neighbor displacement vectors.

In this paper, a highly anisotropic version of the Ashkin-Teller model is studied by using the time-continuum Hamiltonian formalism.[2] The two-dimensional classical system is reduced to a one-dimensional quantum system by taking an extreme lattice anisotropic limit.[3] The transfer-matrix method is used to convert a problem of statistical mechanics at a finite temperature in two dimensions into that of a ground state for a one-dimensional quantum Hamiltonian. The Ashkin-Teller quantum chain is obtained by a highly anisotropic limit $K_{2,4}^x \to 0$, $K_{2,4}^\tau \to \infty$.[2] The parametrization is $K_2^x = \tau\beta$, $K_4^x = \tau\beta\lambda$, $K_2^\tau = (\ln\tau^{-1} - \ln\lambda)/4$, and $K_4^\tau = (\ln\tau^{-1} + \ln\lambda)/4$, and takes a limit $\tau \to 0$. The quantum Hamiltonian reads

$$\mathcal{H} = \sum_j\{2(1-\cos p_j) + \lambda(1-\cos 2p_j)\} - \beta\sum_j\{2\cos(\theta_j - \theta_{j+1}) + \lambda\cos(2\theta_j - 2\theta_{j+1})\}. \qquad (1.3)$$

The operator θ_j acts on a site j and has four eigenvalues 0, $\pi/2$, π, and $3\pi/2$. Its conjugate operator p_j changes the eigenstates of the operator θ_j as $e^{inp_j}|\theta_j\rangle = |\theta_j + \pi n/2\rangle$, where n is an integer. They obey the relation $e^{in\theta_k}e^{inp_j} = e^{inp_j}e^{in\theta_k}e^{in\frac{\pi}{2}\delta_{jk}}$. For details, see Sec. II of Ref. 2.

By a nonlocal unitary transformation, this model is mapped to the staggered XXZ model.[2] The Hamiltonian is

$$\mathcal{H} = \sum_j(S_{2j}^xS_{2j+1}^x + S_{2j}^yS_{2j+1}^y + \lambda S_{2j}^zS_{2j+1}^z) + \beta\sum_j(S_{2j-1}^xS_{2j}^x + S_{2j-1}^yS_{2j}^y + \lambda S_{2j-1}^zS_{2j}^z), \qquad (1.4)$$

where $\mathbf{S}$ is the $S = 1/2$ spin operator. When $\lambda = 1$ this model is the $S = 1/2$ alternating Heisenberg chain. This alternating model is equivalent to the $S = 1$ Heisenberg antiferromagnetic chain in the limit $\beta \to -\infty$.[4,5] Haldane pointed out that there are qualitative differences between integer and half-integer Heisenberg antiferromagnetic chains.[6] The above unitary transformation was applied to reveal the hidden $Z_2 \times Z_2$ symmetry of the Haldane-gap problem.[5,7]

In the region $\beta \geq 0$ the phase diagram was first obtained by Kohmoto, den Nijs, and Kadanoff,[2] which was confirmed by several methods.[8] It has a rich structure including a line of continuously varying critical indices. This line is identified with the Gaussian model universality class.[9] There are also investigations based on conformal field theory with the central charge $c = 1$ by several authors.[10–13]

The purpose of the present paper is to determine the phase diagram of the ground state of the Hamiltonian (1.3) in the region $\beta < 0$ quantitatively by a series expansion and duality relations. The critical lines and the critical indices are evaluated by the Padé method.[14] The obtained phase diagram includes a critical line with continuously varying critical indices.

II. DUALITY

This section describes the duality of the Hamiltonian (1.3). This duality is stated as

$$\widetilde{p_j} = \theta_j - \theta_{j+1} - \pi, \quad \widetilde{\theta_j} = \sum_{k>j}(\, p_k + \pi\,), \qquad (2.1)$$

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$$\mathcal{H}(\beta,\ \lambda;\ \theta,\ p\ ) = -\beta\ \mathcal{H}(\ 1/\beta,\ -\lambda;\ \tilde{\theta},\ \tilde{p}\ ). \qquad (2.2)$$

For $\beta < 0$, the ground state is mapped to the ground state in the transformed system. This duality connects the regions (λ, β) and $(-\lambda, \frac{1}{\beta})$. Therefore, if the system is critical at a point (λ, β), the corresponding dual points $(-\lambda, \frac{1}{\beta})$ have the same critical properties.

III. PHASE DIAGRAM

In this section, we describe the phase diagram for negative values of β obtained by the duality and series analysis (see Fig. 1). The phase diagram for positive values of β is described by Kohmoto, den Nijs, and Kadanoff.[2] Therefore, we do not describe it here. The ground states are characterized by their expectation value of the two operators $e^{2i\theta_j}$ and $e^{\pm i\theta_j}$,[2] which are called the polarization operator and the magnetic field operator, respectively. The phase diagram ($\beta < 0$) has four regions: (1) Paramagnetic region, phase I, characterized by $\langle e^{i\theta}\rangle = \langle e^{2i\theta}\rangle = 0$. At point D' (in Fig. 1) the Hamiltonian (1.3) is equivalent to the antiferromagnetic Heisenberg chain with $S = 1$,[4,5] and it is believed that the system has a gap between the ground state and the first excited state.[6] (2) Fully ordered region, phase VI, characterized by $\langle e^{i\theta}\rangle \neq 0$ and $\langle e^{2i\theta}\rangle \neq 0$. This phase is the dual phase of phase I ($\beta < 0$) by (2.2). (3) Partially ordered region, phase VII, characterized by $\langle e^{i\theta}\rangle = 0$ and $\langle e^{2i\theta}\rangle \neq 0$. (4) Partially ordered region, phase VIII, also characterized by $\langle e^{i\theta}\rangle = 0$ and $\langle e^{2i\theta}\rangle \neq 0$.

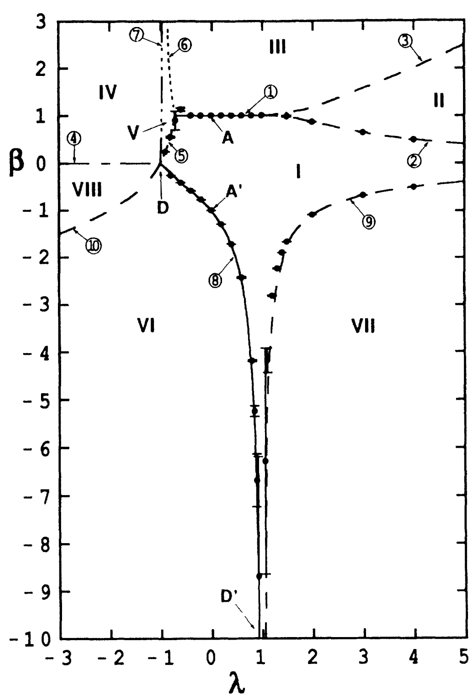

FIG. 1. Ground-state phase diagram of the Ashkin-Teller quantum chain. Estimates of the critical points by a series analysis are shown with error bars. For those without an error bar, the error is smaller than the size of the plotted point. Lines 1 and 8 exhibit continuously varying criticality. Lines 2, 3, 9, and 10 exhibit an Ising transition. Lines 5 and 6 exhibit a Kosterlitz-Thouless transition. Line 4 exhibits a potassium dihydrogen phosphate (KDP) transition. Line 7 is the $\beta = 0$ critical line. The coordinates are $A(0,1)$, $A'(0,-1)$, $D(-1,0)$, and $D'(1,-\infty)$. Region $\beta \geq 0$ was determined by Kohmoto, den Nijs, and Kadanoff (Ref. 2). The plotted points in the region $\beta \geq 0$ are improved estimates from the series analysis up to 17th order.

There is no sign of a "critical fan" in the region $\beta < 0$ within this analysis. A critical fan is a region where a line of continuously varying criticality "fans out" and becomes an area of critical behavior, for example, phase V. However, we cannot discuss the existence of critical fan near point D, because the convergence of the series analysis is poor for $-1 < \lambda < -0.9$.

The regions are separated by critical lines. Line 9 can be understood by examining the limit $\lambda \gg 1$, $\beta\lambda = O(1)$. The second term in the Hamiltonian (1.3) dominates and we can treat the other parts as a perturbation. The effective Hamiltonian is the Ising model in a transverse magnetic field. Therefore, line 9 approaches $\beta = -\frac{2}{\lambda}$ in this limit and belongs to the Ising model universality class. Line 9 is obtained from line 10 by the duality (2.2). Therefore, the boundary of the phases is $\beta = \frac{1}{2}\lambda$, in the limit $|\lambda| \gg 1$ $(\lambda < 0)$.

When $\lambda = 0$, the Hamiltonian (1.4) reduces to the XY model. The Jordan-Wigner transformation maps this model to that of the free fermion.[15] Thus, it is solvable there and is gapless at $\beta = \pm 1$. In the language of the two-dimensional classical Ashkin-Teller model (1.1), the Hamiltonian reduces to the decoupled ferromagnetic Ising models at point A and reduces to the decoupled antiferromagnetic Ising models at point A'. They have the same critical properties and identical critical indices there.

Line 8 is expected to belong to the Gaussian model universality class. The values of critical indices are symmetric under the transformation $\lambda \leftrightarrow -\lambda$ by the duality (2.2). It is natural to consider that lines 8 and 10 meet at point D, because critical lines are not expected to have isolate end points and are expected to be connected to the point with high symmetry, point D in this case. If they meet there, line 9 and another end point of line 8 meet at point D' by the duality (2.2) and the points $(\lambda = -1, -\infty \leq \beta < 0)$ belong to the same phase with a finite excitation gap. It follows that the system exhibits a gap on its corresponding dual points $(\lambda = 1, -\infty < \beta \leq 0)$. Therefore, this result supports Haldane's conjecture.

IV. SERIES EXPANSIONS

We make series expansions with respect to β and obtain series for the specific heat, the magnetization, and the susceptibility to estimate the critical points and critical indices. It is necessary to have long series to extract reliable estimates of the critical points and critical indices. We use the linked cluster expansion method proposed by Kadanoff and Kohmoto.[16] The method of the calculation is exactly the same as that of the previous work of Kohmoto, den Nijs, and Kadanoff.[2] We only describe the definition of the critical indices briefly.

The unperturbed system [(1.3) with $\beta = 0$] has the ground state which is a collection of uncorrelated local states, $|p_j = 0\rangle$. It is disordered in the sense that the expectation values of the local order parameters vanish. Thus, we consider the disorder operators $\mathcal{O}_\pm = \frac{1}{M}\sum_j \prod_{k>j} \cos p_k$ and $\mathcal{O}_2 = \frac{1}{M}\sum_j \prod_{k>j} e^{2ip_k}$, where M is the number of sites, which have nonzero expectation values in disordered phases and disappear in an ordered phase. They are the disorder operators[17,18] corresponding to the magnetic field operator and the polarization operator, respectively. To calculate series for the magnetization of the operators $\mathcal{O}_m$ ($m = \pm$ or 2), we modify the Hamiltonian to $\mathcal{H} + h\mathcal{O}_m$. The ground-state energy in the presence of h is calculated in a power series of β and h as $E(\lambda;\beta,h) = \sum_{n=0}\sum_{m=0} E^{(n,m)}(\lambda)\beta^n h^m$. The specific heat is obtained by $C = \partial_\beta^2 E(\lambda;\beta,h=0)$. The expectation value of the magnetization and the susceptibility is given by $\langle\mathcal{O}_m\rangle = \partial_h E(\lambda;\beta,h)|_{h=0}$ and $\partial_h\langle\mathcal{O}_m\rangle = \partial_h^2 E(\lambda;\beta,h)|_{h=0}$, respectively. We use the Dlog Padé method[14] to estimate the critical points β_c and critical indices. The definition of critical indices are $C(\lambda;\beta) \sim |\beta_c-\beta|^{-\alpha}$, $\langle\mathcal{O}_m\rangle \sim |\beta_c-\beta|^{-\beta_m}$, and $\partial_h\langle\mathcal{O}_m\rangle \sim |\beta_c-\beta|^{-\gamma_m}$, $(\beta\to\beta_c)$, where m is $\pm$ or 2.

The quantities calculated by series expansions are the specific heat (15 terms), the magnetization (17 terms), and the susceptibility (15 terms). The estimates for the quantities are obtained by averaging the three or four highest-order elements $[n-1,n]$, $[n,n]$, and $[n+1,n]$ of the Padé tables. Error bars are set to include these three or four values.

For $-1 < \lambda < 1$, the best estimates for the critical points are obtained from series for $\langle\mathcal{O}_2\rangle$. They show good convergence in almost all of this region. The poor convergence near $\lambda = 1$ is due to the large values of β_c. Phase I is the disordered phase and phase VI is the fully ordered one. In general, it is possible that a partially ordered phase exists between these phases. For example, see the relation among phases I, II, and III. At a fixed value of λ, an analysis of the series for $\langle\mathcal{O}_\pm\rangle$ and $\langle\mathcal{O}_2\rangle$ shows that there is one critical point, their values are same, and these values are the same as that of $\frac{1}{\beta_c}$ at $-\lambda$ within the error bars. Therefore the above possibility is denied and we conclude there is one critical line.

For $\lambda > 1$, the best estimates for the critical points are obtained from the series for $\langle\mathcal{O}_\pm\rangle$. As λ becomes large the Padé tables become extremely stable. For example, at $\lambda = 4$ we estimate $\beta_c = -0.506\,385\,75(1)$. The series analysis shows that line 9 approaches the line $\beta = -\frac{2}{\lambda}$, which is consistent with the results in Sec. III.

For $\lambda < -1$, we determine line 10 from line 9 by the duality (2.2).

In Figs. 2 and 3, the critical indices $\beta_\pm$ and $\gamma_\pm$ are shown, respectively. The critical indices β_2, γ_2, and α are shown in Figs. 4 and 5, respectively.

At $\lambda = 0$, the system reduces to decoupled Ising models. Therefore, we know the exact critical indices $\alpha = 0$, $\beta_\pm = \frac{1}{8}$, and $\beta_2 = \frac{1}{4}$ which is due to two pieces of Ising models. We obtain the values $\gamma_\pm = \frac{7}{4}$ and $\gamma_2 = \frac{3}{2}$ with the help of the standard scaling relations. These values are also obtained from those at point A (see Ref. 2 and references therein). We know the exact critical point $\beta_c = -1$. Instead of evaluating residues at the poles, we

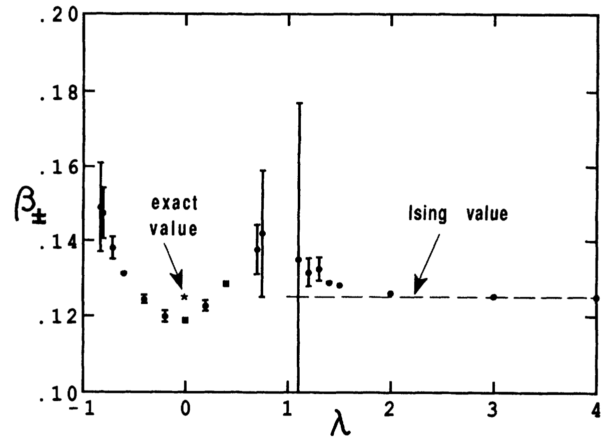

FIG. 2. Critical index $\beta_\pm$ as a function of λ on lines 8 and 9.

can improve the estimates of the critical indices by evaluating the Padé approximants at $\beta = \beta_c$. The estimated values of the critical indices from the series analysis are $\alpha = 0.18(5)$, $\beta_\pm = 0.122(2)$, $\gamma_\pm = 1.74(2)$, $\beta_2 = 0.246(1)$, and $\gamma_2 = 1.43(2)$.

For $-1 < \lambda < 1$, the critical indices vary continuously. They show good convergence near $\lambda = 0$, for example, $\beta_\pm = 0.1285(6)$ at $\lambda = 0.4$. However, we cannot determine the values accurately near $\lambda = -1$ and 1 due to the poor convergence of the critical points there.

For $\lambda > 1$, line 9 belongs to the Ising model universality class (see Sec. III). Therefore, the critical indices α, $\beta_\pm$, and $\gamma_\pm$ must be 0, $\frac{1}{8}$, and $\frac{7}{4}$, respectively. The critical indices $\beta_\pm$ and $\gamma_\pm$ obtained from series analysis show good agreement with the Ising value, for example, $\beta_\pm = 0.12507956(4)$ and $\gamma_\pm = 1.736(3)$ at $\lambda = 4$. The convergence becomes poor around $\lambda = 1$ due to the poor convergence of the critical points.

V. DISCUSSION AND SUMMARY

We studied the ground-state properties of the Ashkin-Teller quantum chain in the region of $\beta < 0$. The ground-state phase diagram is obtained by series expansions and the critical indices on the critical points are also

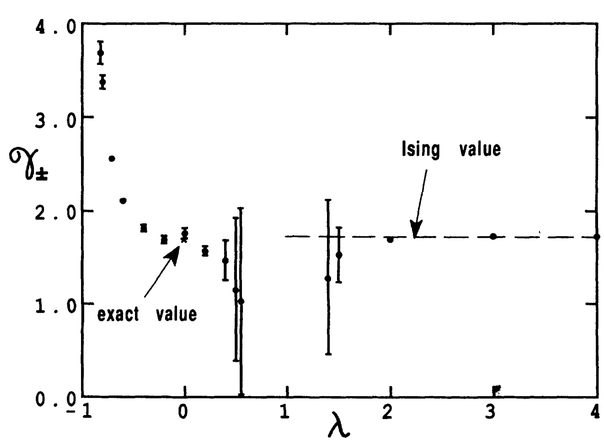

FIG. 3. Critical index $\gamma_\pm$ as a function of λ on lines 8 and 9.

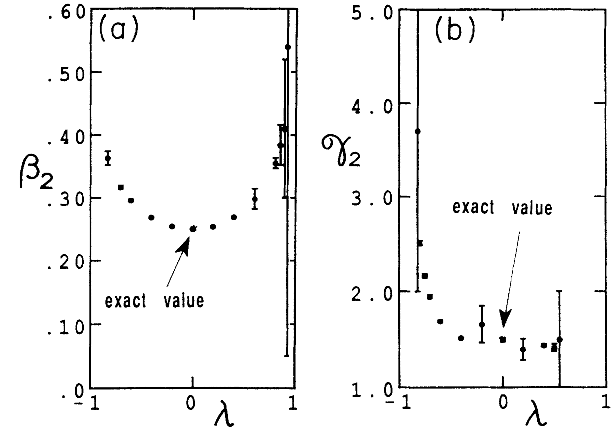

FIG. 4. Critical indices β_2 (a) and γ_2 (b) as a function of λ on line 8.

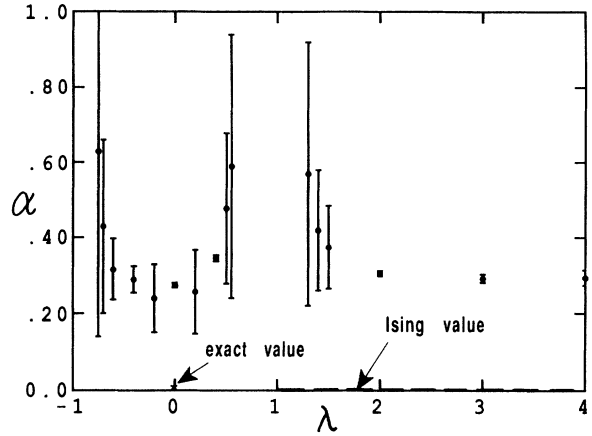

FIG. 5. Critical index α as a function of λ on lines 8 and 9.

evaluated.[19] In the region $\beta < 0$ and $|\lambda| < 1$, we find the critical line of continuously varying critical indices (line 8). This line is expected to belong to the Gaussian model universality class. A more detailed investigation on line 8 will be reported elsewhere.[20] For $\lambda > 1$ and $\lambda < -1$, each region has one critical line and these lines belong to the Ising model universality class. In the region $\beta > 0$, there is a critical fan[2] (phase V in Fig. 1). On the other hand, there is no sign of a critical fan in the region $\beta < 0$ within our analysis.

At $\lambda = 1$ the Hamiltonian (1.3) is mapped to the $S = 1/2$ alternating Heisenberg chain by a unitary transformation.[2] This alternating model is equivalent to the $S = 1$ antiferromagnetic Heisenberg chain in the limit $\beta \to -\infty$.[4,5] On the line $\lambda = 1$ $(-\infty \leq \beta < 1)$, it is expected that the system belongs to the same phase as the Haldane phase.[4,5,7] The series analysis here shows that the system is in the same phase on the line $\lambda = 1$ $(-\infty \leq \beta < 1)$. It supports the results by several authors.[4,5,7]

Several authors discussed the Haldane-gap problem with the Hamiltonian (1.4) in the limit $\beta \to -\infty$.[4,5,7] We can view it from another standpoint. The duality (2.2) tells us that the phase structure around point D' is mapped to that around point D. It is expected that the critical line does not cross the line $\lambda = -1$ $(\beta < 0)$. Therefore the system has a finite excitation gap on the line $\lambda = 1$ $(\beta \leq 0)$. This observation provides support of Haldane's conjecture.[6]

ACKNOWLEDGMENTS

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[1] J. Ashkin and E. Teller, Phys. Rev. **64**, 178 (1943).
[2] M. Kohmoto, M. den Nijs, and L.P. Kadanoff, Phys. Rev. B **24**, 5229 (1981).
[3] For a review see J.B. Kogut, Rev. Mod. Phys. **51**, 659 (1979).
[4] K. Hida, Phys. Rev. B **45**, 2207 (1992); **46**, 8268 (1992); J. Phys. Soc. Jpn. **62**, 1463 (1993); **62**, 1466 (1993); **62**, 3357 (1993).
[5] M. Kohmoto and H. Tasaki, Phys. Rev. B **46**, 3486 (1992).
[6] F.D.M. Haldane, Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983). For a review, see I. Affleck, J. Phys. Condens. Matter **1**, 3047 (1989).
[7] M. Yamanaka, Y. Hatsugai, and M. Kohmoto, Phys. Rev. B **48**, 9555 (1993).
[8] F. Iglói and J. Sólyom, J. Phys. A **17**, 1531 (1984); F.C. Alcaraz and J.R.D. Felício, *ibid.* L561 (1984); S. Yoshida and K. Okamoto, J. Phys. Soc. Jpn. **58**, 4367 (1989).
[9] L.P. Kadanoff and A.C. Brown, Ann. Phys. (N.Y.) **121**, 318 (1979).
[10] G. von Gehlen and V. Rittenberg, J. Phys. A **19**, L1039 (1986); **20**, 227 (1987); F.C. Alcaraz, M.N. Barber, and M.T. Batchelor, Phys. Rev. Lett. **23**, 771 (1987).
[11] H. Saleur, J. Phys. A **20**, L1127 (1987).
[12] S.K. Yang, Nucl. Phys. **B285**[FS19], 183 (1987); **B285**[FS19], 639 (1987); S.K. Yang and H.B. Zheng, *ibid.* **B285**[FS19], 410 (1987).
[13] P. Ginsparg, Nucl. Phys. **B295**[FS21], 153 (1988).
[14] G.A. Baker, Jr., Phys. Rev. **124**, 768 (1961). For an example, see D.S. Gaunt and A.J. Guttmann, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1974), Vol. 3.
[15] P. Jordan and E. Wigner, Z. Phys. **47**, 631 (1928).
[16] L.P. Kadanoff and M. Kohmoto, J. Phys. A **14**, 1291 (1981).
[17] L.P. Kadanoff and H. Ceva, Phys. Rev. B **3**, 3918 (1971).
[18] L.P. Kadanoff and M. Kohmoto, Nucl. Phys. **B190**[FS3], 671 (1981).
[19] For the numerical diagonalization studies, see M. Yamanaka *et. al.* (unpublished).
[20] M. Yamanaka and M. Kohmoto (unpublished).