Renormalization-Group Properties of Some Vertex Models

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We use a real-space renormalization-group scheme to obtain exact recursion relations for analyzing the thermodynamic behavior of one-dimensional analogs of six and eight-vertex models. In particular, we show the existence of a smooth flow line and a fixed point to describe the first-order transition of these models. We also show that the method leads to the correct transition temperature of the two-dimensional KDP model.

Six-vertex models were originally proposed to account for the residual entropy in ice and for the ferroelectric phase transition in the hydrogen-bonded crystal KH_2PO_4. Although there are no exact solutions in three dimensions, the transfer matrix method and the Bethe Antatz have been used to obtain complete solutions of a variety of analogs of ferro and antiferroelectric six-vertex models on a square lattice[1]. There is also a famous exact solution of a two-dimensional eight-vertex model, with a continuous phase transition characterized by parameter-dependent critica1 exponents[2]. The two-dimensional version of the simple ferroelectric model for KH_2PO_4 (which we call the KDP model) displays a first-order transition, with a latent heat, at a well defined temperature, while a two-dimensional antiferroelectric six-vertex model (the F-model) displays a subtle infinite-order transition, with a smooth specific heat as a function of temperature. Also, it has been shown that analogs of the KDP model still exhibit a first-order tranrition on d-dimensional lattices[3].

In this paper we use the transfer matrix method and renormalization-group techniques to study a new class of exactly solvable one-dimensional analogs of six and eight-vertex models. The one-dimensional analog of the ferroelectric KDP model, which is more general than a system solved by Nagle[4], displays a first-order transition, with a latent heat, at a finite temperature $T_c = \epsilon/(k_B \ln 2)$, where $c > 0$ is an energy parameter and k_B is Boltzmann's constant. We show the existente of smooth flow lines of the exact renormalization-group recursion relations in a suitable parameter space and a hyperbolic fixed point associated with the first-order transition. The existence of a (first-order) phase transition in the one-dimensional analogs of Baxter's eight-vertex model depends on the ratio between the energy parameters. We show that it is possible to anticipate this kind of behavior from the analysis of the renormalization-group recursion relations. We also generalize the renormalization-group calculations to obtain a set of recursion relations for the two-dimensional KDP model (and calculate the exact value of the transition temperature).

The one-dimensional models considered in this paper are defined on the double-chain lattice illustrated in Fig.(1). Each vertex is bonded to its three nearest neighbors by four hydrogen bonds. We then have an N x 2 lattice, with N sites along one of the horizontal lines and periodic boundary conditions in the vertical direction. This is indeed the building block of the N x M models, which can be obtained by the addition of extra horizontal lines. It is equally easy to obtain the exact thermodynamic functions and the renormalization-group recursion relations for the N x 1 model, as considered by the Nagle[4], and the N x 3 model. If we allow only those configurations with two arrows pointing to each vertex, we have the six-vertex model. If we allow in addition the configurations with four arrows pointing into (or out of) each vertex, we have an eight-vertex model. The energies assigned to these eight types of vertex configurations are given in Fig.(2). For $e_1 = e_2 = 0$, $e_3 = \ldots = e_6 = \epsilon > 0$, and $e_7 = e_8 = \infty$, we have the simple ferroelectric

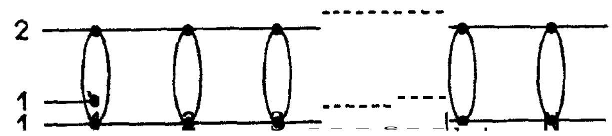

Figure 1: Double-chain lattice ($N \times 2$) for the one-dimensional vertex models.

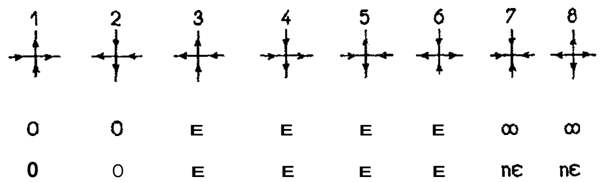

Figure 2: The vertex configurations for the KDP (first line) and the Baxter (second line) models, and their respective energies.

KDP model. The antiferroelectric F-model is defined by the choice $e_1 = ... = e_4 = \epsilon > 0$, $e_5 = e_6 = 0$, and $e_7 = e_8 = \infty$. Finally, the Baxter eight-vertex model is given by $e_1 = e_2 = 0$, $e_3 = ... = e_6 = \epsilon > 0$, and $e_7 = e_8 = n\epsilon$, with $n > 0$. The energy of a microscopic state of the lattice is given by the sum of the energies of the vertex configurations. We can use the transfer matrix method to obtain the exact thermodynamic potential of these models[1,5]. Let ϕ_i and ϕ_{i+1} be the states of two successive columns of horizontal bonds. With periodic boundary conditions in the horizontal direction, the partition function can be written as

$$Z = \sum_{\{\phi\}} T(\phi_1, \phi_2) T(\phi_2, \phi_3) \cdots T(\phi_N, \phi_1) = \mathrm{Tr}\mathbf{T}^N, \tag{1}$$

where the first sum is over the states of the columns and T is a transfer matrix. For the six-vertex KDP model, it is convenient to write the transfer matrix in the form

$$\mathbf{T}_6 = [1 + \exp(-2\beta\epsilon)] \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & K_1 & K_2 & 0 \\ 0 & K_2 & K_1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{2}$$

where

$$K_1 = 2\exp(-\beta\epsilon)[1 + \exp(-2\beta\epsilon)]^{-1}, \tag{3}$$

and

$$K_2 = \exp(-2\beta\epsilon)[1 + \exp(-2\beta\epsilon)]^{-1}, \tag{4}$$

with $\beta = 1/k_B T$. It is well known that the block-diagonal nature of the transfer matrix for the six-vertex models is related to a law of conservation of the left-ward (or rightward) arrows. For an N × M lattice, the first block is 1 × 1, and the second largest M × M block is amenable to a renormalization-group treatment. It is easy to show that there is a competition between the largest eigenvalues of $\mathbf{T}_6$. At high temperatures, there is a single well defined functional form of the largest eigenvalue. At low temperatures, however, there is another functional form of a double-degenerate largest eigenvalue. The first-order transition occurs at $T_c = \epsilon/(k_B \ln 2)$. It is also simple to write the analogous expression for the transfer matrix of the antiferroelectric F-model. In this case, however, the largest eigenvalue is non-degenerate for all finite temperatures, and there is no phase transition.

The transfer matrix for the N x 2 eight-vertex model may be written in the form

$$\mathbf{T}_8 = [1 + \exp(-2\beta\epsilon)] \begin{pmatrix} 1 & K_3 & 0 & 0 \\ K_3 & 1 & 0 & 0 \\ 0 & 0 & K_4 & K_5 \\ 0 & 0 & K_5 & K_4 \end{pmatrix}, \tag{5}$$

where

$$K_3 = 2\exp(-\beta\epsilon - \beta n\epsilon)[1 + \exp(-2\beta\epsilon)]^{-1}, \tag{6}$$

$$K_4 = 2\exp(-\beta\epsilon)[1 + \exp(-2\beta\epsilon)]^{-1}, \tag{7}$$

$$K_5 = [\exp(-2\beta\epsilon) + \exp(-2\beta n\epsilon)][1 + \exp(-2\beta\epsilon)]^{-1}. \tag{8}$$

For $n \leq 2$, as the largest eigenvalue of $\mathbf{T}_8$ is non-degenerate for all finite temperatures, there is no phase transition. However, for $n > 2$, as in the case of the ferroelectric KDP model, we have a transition temperature given by the equation

$$\exp(-\beta n\epsilon) - 2\exp(-\beta\epsilon) + 1 = 0. \tag{9}$$

The two-dimensional Baxter model displays a critical temperature, for all values of n, given by an expression very similar to Eq. 9, the only difference being a change of sign in one of the terms.

To use the real-space renormalization-group scheme, consider the transfer matrix T as a function of the set of parameters $\vec{K} = (K_1, K_2, ..., K_m)$. Also, suppose that we can write the relation

$$\mathbf{T}^2(\vec{K}) = A(\vec{K})\mathbf{T}\left(\vec{K'}\right), \tag{10}$$

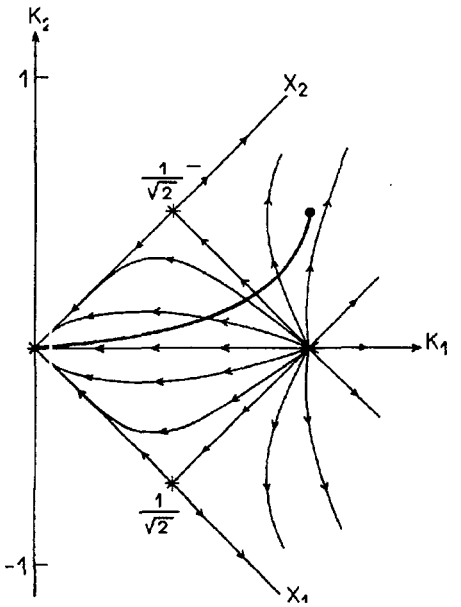

Figure 3: Flow lines and fixed points of the exact renormalization-group recursion relations for the KDP model on the N x 2 lattice. The stars indicate the fixed points, and the heavy line represents the physical curve.

where $\boldsymbol{A}\left(\overrightarrow{K}\right)$ is a regular function of $\overrightarrow{K}$, and $\overrightarrow{K'}$ depends on $\overrightarrow{K}$ through the recursion relations

$$\overrightarrow{K'} = \mathbf{R}\left(\overrightarrow{K}\right). \tag{11}$$

Now we can use the standard renormalization-group scheme. The transformation R may be associated with a variety of fixed points. The only relevant fixed points should be reached from successive applications of R , beginning from a physically acceptable state $\overrightarrow{K_0}$. If we start with the system at the transition temperature, represented by the state $\overrightarrow{K_c}$, we must be led to a hyperbolic unstable fixed point $\overrightarrow{K^*}$ of R which cannot be reached otherwise.

For the KDP model, since the regular term $[1+\exp(-2\beta\epsilon)]$ can be factorized from the transfer matrix, the recursion relations are given by

$$K_1' = K_1^2 + K_2^2 \quad \text{and} \quad K_2' = 2K_1K_2. \tag{12}$$

The analysis of these relations becomes easier if we rotate to the new set of variables $x_1 = (K_1 - K_2)/\sqrt{2}$ and $x_2 = (K_1 + K_2)/\sqrt{2}$. Thus we have

$$x_1' = 2^{1/2}x_1^2 \quad \text{and} \quad x_2' = 2^{1/2}x_2^2. \tag{13}$$

Some flow lines, and the fixed points, $(0,0)$, $(0,1/\sqrt{2})$, $(1/\sqrt{2},0)$, and $(1/\sqrt{2},1/\sqrt{2})$, of these recursion relations are shown in Fig.(3). The initial values of K_1 and K_2 belong to the physical curve,

$$K_1^2 - 4K_2^2(1-K_2) = 0, \tag{14}$$

which is obtained through the elimination of the factor $\exp(-\beta\epsilon)$ from Eqs. 3 and 4. In the physical region, $0 \le K_1$, $2K_2 \le 1$, we can either flow to infinity or to the fixed points $(0,0)$ and $(K_1^* = 1/\sqrt{2}, K_2^* = 1/\sqrt{2})$. The stable fixed point $(0,0)$ is associated with the trivial behavior at zero temperature. The hyperbolic unstable fixed point can be reached from initial conditions such that

$$2^{1/2}x_2 = K_1 + K_2 = 1, \tag{15}$$

which already leads to the correct transition temperature of the KDP model. In fact, from Eqs.14 and 15 we find the solutions $K_2 = 1/5$, which gives the transition temperature, and $K_2 = 1$, which is unphysical.

A slightly more complicated set of recursion relations can be written for the N x 2 eight-vertex model. As in the last paragraph, we work with a matrix V which is defined by $\mathrm{T} = [1+\exp(-2\beta\epsilon)]\,\mathrm{V}$, where a regular term has been factorized from the transfer matrix. Now, if we factorize another regular term $(1+K_3^2)$ at each iteration, it is easy to write

$$K_3' = \frac{2K_3}{1+K_3^2}, \tag{16}$$

$$K_4' = \frac{K_4^2 + K_5^2}{1+K_3^2}, \tag{17}$$

and

$$K_5' = \frac{2K_4K_5}{1+K_3^2}. \tag{18}$$

In the physical region of the (K_3, K_4, K_5) parameter space, there are two trivial stable fixed points, $(0,0,0)$ and $(1,0,0)$, and two hyperbolic unstable fixed points: (i) $(0,1/2,1/2)$, which can be reached through the straight line $K_3 = 0$ and $K_4 + K_5 = 1$, and (ii) $(1,1,1)$, which can be reached through the plane $K_4 + K_5 - K_3 = 1$. Since the parameters K_3, K_4, and K_5 are not independent, the initial values lie on a physical curve as in the case of the KDP model. This curve depends on the ratio n of the excited energy levels. For $n \le 2$, it is possible to show that we cannot reach the hyperbolic unstable fixed points. For $n > 2$, the hyperbolic unstable fixed point $(0,1/2,1/2)$ is still unaccessible, but we can reach the fixed point $(1,1,1)$. Thus, the

transition temperature of the N x 2 eight-vertex model is given by the expression

$$K_4 + K_5 - K_3 = 1, \tag{19}$$

which is identical with the exact result obtained from Eq. 9. In the $n \to \infty$ limit, as we regain the ferroelectric KDP model, the only relevant fixed point becomes $(0, 1/2, 1/2)$, which could not have been reached otherwise.

At this point, let us make some considerations on the N x M ferroelectric KDP model. The transfer matrix is block-diagonal, and we can as usual factorize the element of the 1×1 block. In principle, all blocks can be parametrized, and we can think about parameter spaces, flow lines, and fixed points for each of them separately. If we start at the transition temperature of the model, we may suppose that, by successive applications of the renormalization-group transformations, the parameters of each block will flow, within their respective parameter spaces, to the proper hyperbolic unstable fixed points.Of course, except for the 1 x 1 block, the other blocks of the transfer matrix may be very complicated to deal with. Fortunately, the second largest block is an M x M cyclic matrix, with the elements of the first line given by

$$K_1 = [\exp(-\beta\epsilon) + \exp(-\beta\epsilon M + \beta\epsilon)] [1 + \exp(-M\beta\epsilon)]^{-1}, \tag{20}$$

$$K_2 = \exp(-2\beta\epsilon)\,[1 + \exp(-M\beta\epsilon)]^{-1}, \tag{21}$$

$$K_3 = \exp(-3\beta\epsilon)\,[1 + \exp(-M\beta\epsilon)]^{-1}, \tag{22}$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$K_M = \exp(-M\beta\epsilon)\,[1 + \exp(-M\beta\epsilon)]^{-1}. \tag{23}$$

Since the square of a cyclic matrix is still a cyclic matrix, we can work in an M-dimensional space of parameters, and write the corresponding M recursion relations. Indeed, these relations, which are a straightforward generalization of Eq.12, can be written in the compact form

$$\vec{K'} = \mathrm{M}\vec{K}, \tag{24}$$

where the cyclic matrix M is the transpose of the M x M block of the original factorized transfer matrix. Now it is easy to use the properties of cyclic matrices to diagonalize the recursion relations for obtaining the analogs of Eq.14. Thus, we have a set of relations of the type $x_i' = x_i^2$, for $i = 1, \ldots, M$, where x_i is a suitable linear combination of the elements K_i . In analogy with the case of the $N \times 2$ KDP model, it is possible to show that the physically relevant fixed point is given by

$$x_1 = K_1 + K_2 + \ldots + K_M = 1, \tag{25}$$

and $x_2 = x_3 = \ldots = x_M = 0$. It is remarkable that the transition temperature of the two-dimensional KDP model is indeed a solution of Eq. 25. Moreover, at this transition temperature, we have $|x_i| < 1$, for $i = 2, 3, \ldots, M$, which assures that one really flow to the hyperbolic unstable fixed point. Although it has been fortunate to obtain this result, we have not been able to go beyond the $M \times M$ block. The peculiar features of the thermodynamic behavior of the two-dimensional ferroelectric KDP model are not expected to be revealed unless we are able to deal with the innermost blocks of the transfer matrix.

As a final remark, let us say that the $N \times 2$ F-model can also be treated by this renormalization-group scheme. As the non-trivial fixed points cannot be reached, this antiferroelectric model does not exhibit a phase transition in one dimension.The same treatment of the last paragraph can be applied to the M x M block of the transfer matrix associated with the two-dimensional F-model. Again, there is no possibility of flow to a hyperbolic unstable fixed point. This is an indication that the phase transition of the two-dimensional F-model is too subtle to be described by our renormalization-group treatment.

References

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