The Kinetic Potts Chain and Related Potts Models with Competing Interactions

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Received April 23, 1986; revised June 5, 1986

We consider a general kinetic model for a chain of three-state Potts spins. From the time-evolution operator we infer points in two-dimensional Potts systems where certain spin correlations have one-dimensional character and the model is exactly solvable. This occurs in square lattice models with different kinds of competing interactions.

KEY WORDS: Potts spin systems; vertex systems; competing interactions; kinetic spin models; solubility.

1. INTRODUCTION

In spin systems with competing interactions there can be points in the phase diagram where the spin correlation function changes, e.g., from monotonic to oscillatory behavior. In two dimensions, such "disorder points" were particularly studied in the triangular Ising antiferromagnet.⁽¹⁾ There it was found that right at the disorder point the correlation function becomes a simple exponential. This is typical of a one-dimensional system and, in fact, there is a close connection to a one-dimensional problem at that point⁽²⁾: The relevant eigenvector of the transfer matrix has the form of a one-dimensional Boltzmann factor. In the dual picture it becomes a simple product state. This property is now widely used as the definition of a disorder point. However, we shall use the more precise term "one-dimensional point (or line)" (ODP, ODL). At an ODP not only the correlation, but also the free energy is exactly known and usually very simple. In recent years, such points have been found in a large number of two-dimensional⁽³⁾ and even in three-dimensional^(4,5) systems. Specifically, for Potts spins they were located on Kagomé,⁽⁶⁾ triangular,^(3,6) and checkerboard⁽⁶⁻⁸⁾ lattices.

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There are interesting connections to models of crystal growth,^(3,9,10) cellular automata,⁽⁴⁾ and kinetic spin models⁽²⁾ which can be used to construct systems with ODPs. In the present work we shall use the latter method. It compares the transfer matrix of the two-dimensional system with the time-evolution operator of a suitable one-dimensional kinetic model. Thus, we shall start from a chain of three-state Potts spins, where one spin at a time is allowed to flip. This is a generalization of the kinetic Ising model⁽¹¹⁾ and we shall show that it is equally useful here to find ODPs. We shall locate them in an axial model with competing interactions in one direction and in a model with competition via diagonal crossed bonds. It will turn out that ODPs are in general harder to realize in Potts than in Ising systems.

2. KINETIC POTTS CHAIN

Consider a closed chain of N spins which take the values $\sigma_n = 0, 1, -1$ and are coupled by a nearest neighbor interaction $-J\delta(\sigma_n, \sigma_{n+1})$. The spins are best visualized as vectors in the complex plane which can assume the three directions given by $\omega^{\sigma} = \exp[i(2\pi/3)\sigma]$. The simplest kinetic model is one where single spin rotations (flips) take place with certain rates and in such a way that the system approaches thermodynamic equilibrium. Such models have been studied so far with an emphasis on their dynamical critical behavior.^(12,13) In our case, however, it is the structure of the time evolution operator that is of interest. To specify it, the various processes and their rates have to be fixed. We assume that the rates depend on the relative configuration of the spin in question and its two neighbors, and on the energetics of the transition, but not on the sense of rotation per se. Thus, we distinguish the processes shown in Fig. 1. Detailed balance is already built into our choice of the rates. This guarantees the approach toward equilibrium.

The master equation for the probability $p(\mathbf{\sigma}, t)$ to find a certain spin configuration $\mathbf{\sigma} = \sigma_1, \sigma_2, ..., \sigma_N$ at time t can then be written down. Actually, it is more convenient to work with the reduced probability $\tilde{p}(\mathbf{\sigma}, t) = p(\mathbf{\sigma}, t)/p_0^{1/2}(\mathbf{\sigma})$, where

$$p_0(\boldsymbol{\sigma}) = \exp\left[K\sum_n \delta(\sigma_n, \sigma_{n+1})\right]$$

is the equilibrium distribution and $K = \beta J$. Then the operator T in the master equation

$$\frac{\partial}{\partial t}\,\tilde{p}(\mathbf{\sigma},\,t) = -T\cdot\,\tilde{p}(\mathbf{\sigma},\,t) \tag{2.1}$$



Fig. 1. Elementary spin-flip processes in the kinetic Potts chain. The middle spin undergoes flips as shown. The rates are given on the right of the figure; they depend on the orientation of the two neighboring spins.

is Hermitian. It is obtained by writing down explicitly all the gain and loss processes shown in Fig. 1. For this task the operators⁽¹⁴⁾

$$\Omega = \begin{pmatrix} 1 & & \\ & \omega & \\ & & \omega^2 \end{pmatrix}, \qquad \Gamma = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$
(2.2)

at each site are necessary and sufficient. The diagonal operators Ω_n can be used to fix the direction of the spins in the initial or final state, while Γ_n

describes a clockwise rotation. A rather long, but straightforward calculation gives T in the form

$$T = -\sum_{n=1}^{N} \sum_{\alpha=1}^{8} v_{\alpha} O_{n}^{\alpha}$$
(2.3)

where the new rates v_{α} and the operators O_n^{α} are given in the Appendix. The first four terms in T contain the rotation operators Γ_n and Γ_n^+ and correspond to the gain processes, while the rest consists of diagonal operators and describes the loss processes. Equation (2.3) generalizes the corresponding Ising result,^(2,15) where instead of Γ_n and Ω_n the Pauli matrices σ_n^{α} and σ_n^{z} appear.

Obviously, the operator T is quite complicated, but by construction the function $p_0^{1/2}(\sigma)$ is an eigenfunction of T with eigenvalue zero. For positive rates α_i it is the lowest state. In this equilibrium state the spin correlation function is

$$C_{n} = \left\langle \exp\left[i\frac{2\pi}{3}\left(\sigma_{k} - \sigma_{k+n}\right)\right]\right\rangle$$
$$= \sum_{\sigma} \exp\left[i\frac{2\pi}{3}\left(\sigma_{k} - \sigma_{k+n}\right)\right]p_{0}(\sigma)$$
$$= \exp(-K^{*}n), \qquad n \ge 0$$
(2.4)

where K^* is the dual coupling of K, defined by

$$e^{-K^*} = (e^K - 1)/(e^K + 2)$$

Normally, one is interested in the dynamics of such a model, i.e., in the time-dependent spin correlation functions. In the Ising case there exist two choices of the rates where the equations of motion close and analytical results are available.^(15,16) Unfortunately, this does not happen in the present problem, because the equation of motion for, say, Ω_n immediately generates a large number of terms.

As it stands, T can also be interpreted as the Hamilton operator of a quantum mechanical spin-one system. The same is true if one performs a dual transformation by introducing bond variables μ_n via

$$\mu_n = \sigma_{n+1} - \sigma_n \pmod{3} \tag{2.5}$$

In terms of the operators this corresponds to the substitutions

$$\Omega_n \Omega_{n+1}^+ \to \Omega_{n+1}^+, \qquad \Gamma_n \to \Gamma_n \Gamma_{n+1}^+ \tag{2.6}$$

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The dual operator T_D then contains at most two-site terms and is of the form

$$T_D = -\sum_{n=1}^{N} T_{n,n+1}$$
(2.7)

where $T_{n,n+1}$ is obtained from $\sum_{\alpha} v_{\alpha} O_n^{\alpha}$ with the help of (2.6). Basically it consists of terms where two neighboring dual spins are rotated plus several pair interactions and a field term linear in Ω_n . Finally, the state $|p_0^{1/2}\rangle$ becomes the simple product state

$$C\prod_{n} \left\{ e^{K/2} \left| \mu_{n} = 0 \right\rangle + \left| \mu_{n} = 1 \right\rangle + \left| \mu_{n} = -1 \right\rangle \right\}$$
(2.8)

Strictly speaking, there is a condition on the possible values of the μ_n because of the cyclic boundary condition $\sigma_{N+1} = \sigma_1$. For large systems, however, we can neglect this effect, The analogue of (2.7) in the Ising case is an operator that describes a spin-1/2 XYZ chain in a field. The product eigenstates of that system were also discovered directly⁽¹⁷⁾ without the route via the kinetic model.

In the following we shall use the direct form (2.3) and the dual form (2.7) to draw conclusions on two-dimensional Potts models.

3. THE ANNNP MODEL

In analogy to the well-known Ising case, $^{(18,19)}$ one can study on a twodimensional square lattice a system of Potts spins that has competing interactions along one (the x) direction and simple ferromagnetic interactions along the other direction. We call this model an axial next nearest neighbor Potts model (ANNNP). As competing interactions we choose a nearest neighbor coupling J_1 , a next nearest neighbor coupling J_2 , and a three-spin coupling J_3 which favors three parallel adjacent spins. The rowto-row transfer matrix in the Hamiltonian limit of strong coupling J_0 in the y direction and weak couplings J_1, J_2, J_3 then has the form $V = \exp(-H)$, where H is a one-dimensional quantum Hamiltonian, which can be expressed in terms of the Ω_n and Γ_n as

$$H = -\sum_{n} \left[\frac{1}{3} K_{0}^{*} (\Gamma_{n} + \Gamma_{n}^{+}) + \left(\frac{1}{3} K_{1} + \frac{2}{9} K_{2} \right) (\Omega_{n} \Omega_{n+1}^{+} + \text{h.c.}) + \left(\frac{1}{3} K_{2} + \frac{1}{9} K_{3} \right) (\Omega_{n} \Omega_{n+2}^{+} + \text{h.c.}) + \left(\frac{1}{3} K_{3} \right) (\Omega_{n} \Omega_{n+1} \Omega_{n+2} + \text{h.c.}) \right]$$
(3.1)

This coincides, up to an additive and a multiplicative constant, with the operator T of Section 2 if $v_2 = v_3 = v_4 = 0$ (which gives $\alpha_i = \alpha$) and if

$$K_1/K_0^* = 2/3(2e^{K/2} - e^{-K/2} - 1)$$
(3.2a)

$$K_2/K_0^* = 1/3(2e^{K/2} - e^K - 1)$$
 (3.2b)

$$K_3/K_0^* = 1/3(3 + e^{\kappa} - 2e^{-\kappa} - 4e^{\kappa/2} + 2e^{\kappa/2})$$
(3.2c)

For this special choice of couplings (which corresponds to $J_1 > 0$, $J_2 < 0$, $J_3 \ge 0$), *H* therefore has the same eigenvalue spectrum as the kinetic model. In particular, the eigenvector of *V* corresponding to the largest eigenvalue is the state $|p_0^{1/2}\rangle$, Thus, the spin correlation function in the *x* direction is given by the simple exponential of Eq. (2.4). The ODL defined by Eqs. (3.2) is best visualized if one plots its projection into the plane of coupling constants. This is shown in Fig. 2, where also the phase boundary at zero temperature is indicated. The ODL exists above the ferromagnetic phase and approaches the boundary to the region with high ground-state degeneracy at low temperatures.

Our result shows a typical difference from the Ising case (ANNNI $model^{(2)}$): Here the balance of three interactions is necessary to give a



Fig. 2. ODL in the ANNNP model, projected down the temperature axis, onto the coupling constant plane. Some values for temperature $t = K_0^*/K_1$ and correlation length are given. The ground states are also indicated, where the label 2 stands for the value $\sigma_n = -1 \pmod{3}$ of the text.

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whole ODL, while in the Ising case two are sufficient. This is intuitively clear, because Potts spins have more freedom and it will in general be harder to obtain the delicate balance corresponding to one-dimensional behavior. For $J_3 = 0$ it can be done only at the one point $J_2/J_1 = -(\sqrt{3}-1)/2$, at one temperature. This ODP is probably located on the true disorder line, which must exist on general grounds also for $J_3 = 0$, but this could be checked only by a numerical calculation.

One could carry out the same investigation away from the Hamiltonian limit, as in the Ising case, $^{(3)}$ but we shall not pursue this.

4. SQUARE LATTICE POTTS MODEL WITH NEXT NEAREST INTERACTIONS

Competition effects can also arise for spins on a square lattice that are coupled by nearest and next nearest neighbor bonds. The phase diagrams of such a model with Ising spins⁽²⁰⁾ and Potts spins^(21,22) have been studied. An ODL was found in the Ising case, using the diagonal-to-diagonal transfer matrix⁽²³⁾; here we use the same technique to locate an ODL for three-state Potts spins.

Figure 3a shows an elementary square of the lattice with the three couplings we consider. We shall also use the notation

$$u = e^{K_0}$$
 $v_1 = e^{K_1}$ $v_2 = e^{K_2}$

Instead of treating the problem in the spin language,⁽⁸⁾ it is advantageous to go over to a vertex formulation. As in Section 2, bond variables are introduced via $\mu = (\sigma' - \sigma)$, $\mu' = (\sigma'' - \sigma)$, $\mu'' = (\sigma''' - \sigma'')$, and $\mu''' = (\sigma - \sigma''')$. Going once around the square gives the constraint⁽²¹⁾

$$\mu + \mu' + \mu'' + \mu''' = 0 \pmod{3} \tag{4.1}$$



Fig. 3. (a) Labeling of spins and interactions in the square lattice model. (b) Example of a spin configuration and its corresponding vertex configuration.

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This rule determines a vertex model with 27 configurations of the μ 's. It is best visualized by associating an in-going arrow with $\mu = -1$, an outgoing one with $\mu = +1$, and no arrow with $\mu = 0$. Figure 3b shows an example which has the Boltzmann weight uv_2 . Choosing μ , μ' as an incoming variables defines the elementary (9×9) transfer matrix $V(\mu, \mu'/\mu'', \mu''')$. The complete transfer matrix consists of two rows of V's. Calling the bond variables in a row $\mu_1, \mu_2, ..., \mu_N$ and writing $V_{m,m+1} = V(\mu_m, \mu_{m+1}/\mu'_m, \mu'_{m+1})$, one has the complete transfer matrix as

$$V = \left(\prod_{n} V_{2n,2n+1}\right) \left(\prod_{n} V_{2n+1,2n+2}\right)$$
(4.2)

We now look for the possibility of having an eigenvector of the form (2.8) giving the largest eigenvalue of V. One way is to write down $V_{m,m+1}$ explicitly in terms of the operators Ω and Γ at sites m, m+1. Then one finds that $V_{m,m+1}$ has precisely the form of $T_{m,m+1}$ that appears in the dual version of the kinetic model. The constants v_{α} are now determined by u, v_1 , and v_2 and are given in the Appendix. Now, a product state is an eigenstate of each individual $V_{m,m+1}$ or $T_{m,m+1}$. Therefore, if T has such an eigenvector, then V also has it, provided the constants $v_1, ..., v_7$ in the two models coincide up to a common factor (the constant v_8 multiplying the unit operator is irrelevant). This gives the following two conditions for a product eigenvector:

$$v_{1} = \frac{v_{2} + uv_{2} + u + [(v_{2} - uv_{2} - u)^{2} + 8u]^{1/2}}{u^{2}v_{2} + v_{2} + 1 + [(u^{2}v_{2} - v_{2} - 1)^{2} + 8u^{2}]^{1/2}}$$
(4.2a)
$$\{(u^{2}v_{2} - v_{2} - 1) + [(u^{2}v_{2} - v_{2} - 1)^{2} + 8u^{2}]^{1/2}\}$$
$$\times \{(v_{2} - uv_{2} - u) + [(v_{2} - uv_{2} - u)^{2} + 8u]^{1/2}\}^{2} = 8u^{2}$$
(4.2b)

A second way, which is also instructive, is to diagonalize $V_{m,m+1}$ explicitly. This is easy, because $V_{m,m+1}$ decomposes into three (3×3) problems. Two of them are identical, which reflects the symmetry of the problem under arrow reversal $(\mu = 1 \leftrightarrow \mu = -1)$. One finds three non-degenerate eigenvalues

$$\varepsilon_{1} = v_{1}(v_{2} - 1)$$

$$\varepsilon_{2,3} = \frac{v_{1}}{2} \left\{ (u^{2}v_{2} + v_{2} + 1) \pm \left[(u^{2}v_{2} - v_{2} - 1)^{2} + 8u^{2} \right]^{1/2} \right\}$$
(4.3a)

and three doubly degenerate ones

$$\varepsilon_{4} = u(v_{2} - 1)$$

$$\varepsilon_{5,6} = \frac{1}{2} \left\{ (uv_{2} + u + v_{2}) \pm [(uv_{2} - v_{2} - 1)^{2} + 8u]^{1/2} \right\}$$
(4.3b)

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In general, the eigenvectors do not have the form (2.8). However, if $\varepsilon_2 = \varepsilon_5 \equiv \varepsilon$ [which is Eq. (4.2a)], the largest eigenvalue becomes triply degenerate. Equation (4.2b) then guarantees that one can form a linear combination that has the desired product form. Such a state leads to a spin correlation function of the form (2.4) along a horizontal zigzag line, with the parameter K determined by

$$\exp(-K) = \frac{\varepsilon - u^2 v_1 v_2}{2u v_1} \tag{4.4}$$

Furthermore, the partition function per site is simply ε .



Fig. 4. ODL in the anisotropic square lattice; see caption of Fig. 2. The indicated temperature here is $t = 1/K_0$. The ground states to the left are highly degenerate.

Equations (4.2) can be solved explicitly for the triangular lattice that results for $J_2 = 0$, $v_2 = 1$. Then one recovers the known expression^(3,6,7) for the ODL,

$$v_1 = (1+2u)/(2+u^2) \tag{4.5}$$

and furthermore $K = K_0$. Equation (4.5) always gives $v_1 < 1$, which corresponds to an antiferromagnetic diagonal bond J_1 competing with the bond J_0 , which can be of either sign here. A similar formula even holds for arbitrary Potts spins.

In general, Eqs. (4.2) have to be solved numerically. One then finds the ODL shown in Fig. 4, again projected onto the plane of coupling constants, using $J_0 > 0$. We see that it lies above the ferromagnetic phase in the region $J_2 > 0$. Thus, $J_1 < 0$ competes against the combined effects of J_0 and J_2 . Contrary to the Ising case,⁽²¹⁾ there is no ODL (but there will be a disorder line) for the isotropic system with $J_1 = J_2 < 0$. This shows again that in general the balance of three different couplings is necessary to produce an ODL in the Potts case. For large values of J_2 (and high temperatures) the ODL approaches the asymptote $J_1/J_0 = -(\sqrt{3}-1)$. This is related to the results of Section 3. In fact, for $J_2 \rightarrow \infty$ the present model is equivalent to an ANNNP model in the Hamiltonian limit with couplings $J_0^A = J_2$, $J_1^A = 2J_0$, $J_2^A = J_1$, $J_3^A = 0$. The ODP in this case was found exactly at the value of J_1/J_0 given above.

The model we treated here is similar, but not identical to the checkerboard lattice. In that case, ODPs were found using the spin picture and the formulation as an IRF model.⁽⁸⁾ Our procedure is somewhat more explicit and also could be applied to other situations, for example, including fourspin couplings.

5. CONCLUSION

We have shown how it is possible to connect kinetic spin chains, quantum Hamiltonians, and two-dimensional transfer matrices for the case of Potts spins with q = 3. We have found new ODPs and noticed that they are somewhat rarer here than in the corresponding Ising models. Our aim was not to give particularly simple criteria for the ODPs, but to display the structure of the operators involved and to use this information. We also have distinguished ODPs (which are rather special phenomena) from the disorder points (which are a more common feature of systems with competing interactions). The ODPs we studied represent only the simplest type. Others would correspond to staggered or to helical correlations in certain directions of the lattice.

APPENDIX

The terms in the time-evolution operator (2.3) are explicitly as

$$9v_{1} = (\alpha_{1} + 2\alpha_{3}) + 2(\alpha_{2} + 2\alpha_{4})$$

$$9v_{2} = (\alpha_{1} + 2\alpha_{3}) - (\alpha_{2} + 2\alpha_{4})$$

$$9v_{3} = (\alpha_{1} - \alpha_{3}) + 2(\alpha_{2} - \alpha_{4})$$

$$9v_{4} = (\alpha_{1} - \alpha_{3}) - (\alpha_{2} - \alpha_{4})$$

$$9v_{5} = -2(\alpha_{1} - \alpha_{2}) - 2\alpha_{3}(e^{K} + e^{-K}) + 2\alpha_{4}(e^{K/2} + e^{-K/2})$$

$$9v_{6} = (\alpha_{1} + 2\alpha_{2}) + \alpha_{3}(e^{K} - 2e^{-K}) - 2\alpha_{4}(2e^{K/2} - e^{-K/2})$$

$$9v_{7} = (\alpha_{1} - \alpha_{2}) + \alpha_{3}(e^{K} - 2e^{-K}) + \alpha_{4}(2e^{K/2} - e^{-K/2})$$

$$9v_{8} = -2(\alpha_{1} + 2\alpha_{2}) - 2\alpha_{3}(e^{K} + e^{-K}) + 4\alpha_{4}(e^{K/2} + e^{-K/2})$$

$$O_{n}^{1} = \Gamma_{n} + \Gamma_{n}^{+}$$

$$O_{n}^{2} = (\Omega_{n-1}\Omega_{n+1}^{+} + h.c.)(\Gamma_{n} + \Gamma_{n}^{+})$$

$$O_{n}^{3} = (\omega^{*}\Omega_{n-1}\Omega_{n}\Omega_{n+1} + h.c.)\Gamma_{n} + h.c.$$

$$O_{n}^{4} = [\omega(\Omega_{n-1} + \Omega_{n+1})\Omega_{n}^{+} + h.c.]\Gamma_{n} + h.c.$$

$$O_{n}^{5} = \Omega_{n-1}\Omega_{n}\Omega_{n+1} + h.c.$$

$$O_{n}^{7} = (\Omega_{n-1} + \Omega_{n+1})\Omega_{n}^{+} + h.c.$$

$$O_{n}^{7} = (\Omega_{n-1} + \Omega_{n+1})\Omega_{n}^{+} + h.c.$$

$$O_{n}^{8} = 1$$

with h.c. denoting the Hermitian conjugate. The dual form of the operators follows from the substitutions (2.6) and the relations $\Omega^2 = \Omega^+$ and $\Omega^3 = 1$.

For the elementary transfer matrix $V_{n,n+1}$ of Section 4 the coefficients $v_1, ..., v_4$ are obtained by setting

$$\alpha_1 = v_1;$$
 $\alpha_2 = u;$ $\alpha_3 = uv_1;$ $\alpha_4 = \sqrt{u}$

in the above equations. The remaining coefficients are given by

$$9v_5 = v_1v_2(2+u^2) - v_2(1+2u)$$

$$9v_6 = v_1v_2(u^2-1) + 2v_2(1-u)$$

$$9v_7 = v_1v_2(u^2-1) - v_2(1-u)$$

$$9v_8 = v_1v_2(2+u^2) + 2v_2(1+2u)$$

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