Studying the Six-Vertex Model with the Yang-Baxter Equation

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We study the six-vertex model, a two-dimensional model of ferroelectric solids, originally solved by Lieb [2] in a restricted case by Bethe ansatz. We construct the phase diagram by deriving and solving the Yang-Baxter equations [5], introduced in statistical physics by Baxter to generate integrable models in two-dimensions. We discuss the significance of the Yang-Baxter equation and comment on the relationship between the six-vertex model and the XXZ quantum spin-chain.

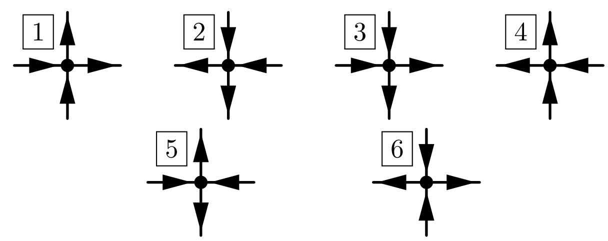
INTRODUCTION

Onsager's solution to the square-lattice Ising model [1] provided the first example of a system exhibiting a finite-temperature, second-order phase transition, whose physical observables could be computed exactly, outside of perturbative treatments. The reason *why* the Ising model was solvable, however, remained unclear for some time. A few decades later, work by Yang on the S-matrix for a one-dimensional Bose gas [3] and by Baxter on the exact solution to another two-dimensional statistical mechanical model [5] shed deep insight on the properties of 'integrable' models, ones with transfer matrices that admit infinitely many conserved quantities, generated by operators that commute with the transfer matrix. The conditions imposed on the transfer matrix, expressed by the Yang-Baxter equation, have since been used to identify models in two-dimensional statistical mechanics that admit non-trivial exact solutions, including the Ising model.

In this paper, we introduce and apply the approach taken by Yang and Baxter – studying the commuting properties of transfer matrices – to analyze the 'six-vertex' model of two-dimensional ferroelectric solids, that was originally solved in a restricted case by Lieb [2] using a lengthy Bethe ansatz approach. Solving the Yang-Baxter equation allows us to find the phase diagram of the model while sidestepping the issue of diagonalizing the transfer matrix, although we comment on how the Yang-Baxter relation can also be used for such a calculation. We conclude by commenting on the equivalence of the six-vertex model to the XXZ quantum spin-chain.

THE SIX-VERTEX MODEL

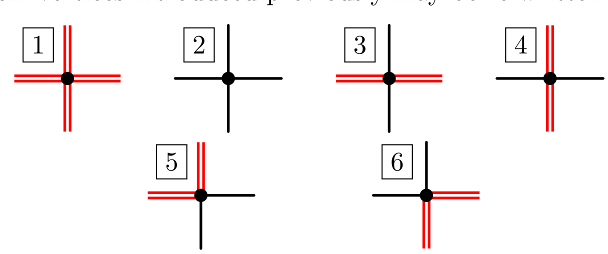
The six-vertex model was originally introduced to understand the statistical mechanics of solids with ferroelectric properties. A prototypical example is given by considering the hydrogen-bond configurations in a two-dimensional sample of ice; when water freezes, local electrical neutrality requires that each oxygen atom is surrounded by four hydrogen ions such that two hydrogen are closer to the oxygen atom, and two are further away. A convenient way to represent the possible configurations surrounding an oxygen atom is to associate an arrow with each bond of an $M \times N$ square lattice, which specifies the state of a hydrogen ion. A Boltzmann weight corresponds to each type of vertex, where four such arrows meet. The 'ice rule' [5] is then enforced by only allowing vertices with zero total 'flux' of arrows through a lattice, resulting in the following six configurations:



Let ϵ_i be the energy of the ith vertex, as numbered above, so that $w_i \equiv e^{-\beta\epsilon_i}$ is the corresponding Boltzmann weight, and n_i is the total number of bonds of type i on the lattice. Since the arrows represent local electrical dipoles, we require that in the absence of an external field, the square lattice is invariant under reversal of *all* of the arrows, which implies that $n_1 = n_2$, $n_3 = n_4$ and $n_5 = n_6$. Alternatively, we may restrict the weights so that $x \equiv w_1 = w_2$, $y \equiv w_3 = w_4$, and $z \equiv w_5 = w_6$. Then the partition function may be written as:

$$Z = \sum_{\{n_i\}} x^{n_1+n_2}\, y^{n_3+n_4}\, z^{n_5+n_6} \tag{1}$$

An interesting feature of the six-vertex model is its sensitivity to boundary conditions. Since specifying the state of a vertex constrains one of bonds on each of the four adjacent vertices, the vertex degrees of freedom are clearly not all independent. To study the effect of periodic boundary conditions, we choose to label vertex states by coloring a bond if the arrow points up or to the right, and leaving the bond empty otherwise. The six vertices introduced previously may be re-written as:



We see that vertices (5) and (6) act as sources and sinks of colored bonds, while the remaining vertices carry zero net bond 'flux'. Imposing periodic boundary conditions then requires that the flux of colored bonds be conserved when traversing the lattice in the horizontal direction, thereby restricting $n_5 = n_6$ *per row* of the lattice. This condition, combined with the fact that configurations (1)-(4) conserve the number of red bonds passing through a lattice point in the vertical direction, leads us to the following important conclusion [6]: in an allowed configuration of bonds on a square lattice with periodic boundary conditions, the number of colored vertical bonds along any row of the lattice must be the same for *all rows.*

This conservation law simplifies the determination of the free energy for the six-vertex model. We define a row-to-row transfer matrix (T) as follows, by specifying the configurations of vertical bonds (e.g. $\alpha \equiv \{\alpha_1, \alpha_2, \ldots, \alpha_N\}$ with $\alpha_i = \pm 1$ depending on the coloring of the bond) both above and below a horizontal row of lattice sites; the elements of the transfer matrix are then given by:

$$T_\alpha^\beta \equiv \langle \alpha \,|\, T \,|\, \beta \rangle = \sum_{\{m_i\}}{}' x^{m_1+m_2} y^{m_3+m_4} z^{2m_5} \tag{2}$$

with m_i denoting the number of vertices of type i in a row, and the sum restricted over configurations of vertices consistent with the states of the vertical bonds α, β. For a square lattice with M rows and N columns, the transfer matrix will have $2^N \times 2^N$ entries, and the partition function is given in the usual prescription by $Z = \mathrm{tr}[T^M]$.

The conservation of colored vertical bonds per row (n) on the square lattice implies that the transfer matrix is block-diagonal for different values of n. In the particularly simple case of $n = 0$, we see that only vertices of type (2) or (3) are allowed on the lattice, and that each row must be composed of the same type of bond. The transfer 'matrix' then has only one element, and we may immediately write down the partition function:

$$Z = (x^N + y^N)^M. \tag{3}$$

For arbitrary n, however, the transfer matrix is not simple to diagonalize. We must instead attempt to derive higher conservation laws that restrict the spectrum of the transfer matrix, to infer the phase diagram of the six-vertex model.

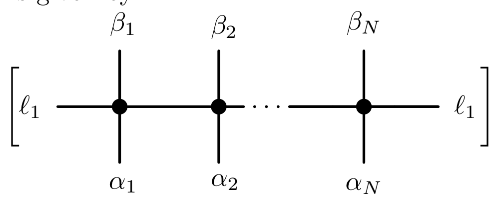
THE YANG-BAXTER EQUATION

The partition function of the six-vertex model was first computed in the restricted case with $x = y = z$ by Lieb [2], using the Bethe ansatz to diagonalize the transfer matrix. Later, Baxter solved a generalization of the six-vertex model [4] using what is now known as the Yang-Baxter relation. The goal in this section will be to apply Baxter's method, and determine under what conditions the transfer matrices parametrized by *different* Boltzmann weights for the six vertices commute, in order to extract the phase diagram of the six-vertex model without lengthy calculation.

To this end, we begin by introducing a four-index tensor at each site of the square lattice $\mathcal{A}_{\alpha\ell}^{\beta m}$, defined so that taking the trace of a product of tensors along a row of lattice sites yields the transfer matrix:

$$\begin{aligned} T_\alpha^\beta &= \sum_{\ell_1}\sum_{\ell_2}\cdots\sum_{\ell_N} \mathcal{A}_{\alpha_1\ell_1}^{\beta_1\ell_2}\mathcal{A}_{\alpha_2\ell_2}^{\beta_2\ell_3}\mathcal{A}_{\alpha_3\ell_3}^{\beta_3\ell_4}\cdots\mathcal{A}_{\alpha_N\ell_N}^{\beta_N\ell_1} \\ &= \mathrm{tr}\left[\mathcal{A}_{\alpha_1}^{\beta_1}\mathcal{A}_{\alpha_2}^{\beta_2}\cdots\mathcal{A}_{\alpha_N}^{\beta_N}\right] \end{aligned} \tag{4}$$

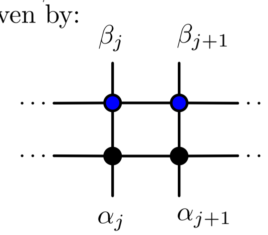
This is similar, in spirit, to the matrix-product-state (MPS) ansatz used to study highly entangled quantum many-body states. Exploiting the analogy further, we introduce a diagrammatic notation for the four-index tensor with four 'legs' protruding from a lattice site, labeled by the tensor indices. The diagrammatic representation of the trace is given by:

$$T_\alpha^\beta = \sum_{\ell_1}\Big[$$


$$\Big]$$

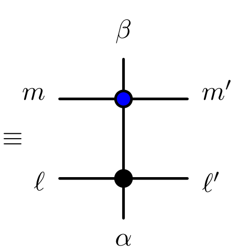
where bonds without labels are assumed to be summed over. The final sum over the ℓ_1 bond imposes periodic boundary conditions in the horizontal direction.

Now consider a second transfer matrix $\tilde{T}$, with different Boltzmann weights x', y', z' for the vertices, so that the transfer matrix admits a decomposition in terms of four-index tensors $\mathcal{B}_{\alpha\beta}^{\ell m}$. The product of these two transfer matrices is given by:

$$\sum_\sigma T_\alpha^\sigma \tilde{T}_\sigma^\beta = \tag{5}$$


$$= \sum_{\{\ell_i\}}\sum_{\{m_i\}} \mathcal{S}_{\ell_1 m_1}^{\ell_2 m_2}(\alpha_1,\beta_1)\,\mathcal{S}_{\ell_2 m_2}^{\ell_3 m_3}(\alpha_2,\beta_2)\cdot\cdot\,\mathcal{S}_{\ell_N m_N}^{\ell_1 m_1}(\alpha_N,\beta_N)$$

with the blue vertices placed on horizontal rows with 'primed' Boltzmann weights. Here, we have defined the components of the two-row transfer matrix by:

$$\mathcal{S}_{\ell\, m}^{\ell' m'}(\alpha,\beta) \equiv$$


$$= \sum_\eta \mathcal{A}_{\alpha\ell}^{\eta\ell'}\,\mathcal{B}_{\eta m}^{\beta m'} \tag{6}$$

We wish to understand what conditions, if any, permit the two distinct transfer matrices to commute. Inverting the order of the matrices, we see that the product $\tilde{T}T$ may be written in the same form as (6), with inverted two-row transfer matrices $\tilde{\mathcal{S}}$ defined by:

$$\tilde{\mathcal{S}}_{\ell m}^{\ell' m'}(\alpha,\beta) = \sum_{\eta} \mathcal{B}_{\alpha\ell}^{\eta\ell'}\, \mathcal{A}_{\eta m}^{\beta m'} \tag{7}$$

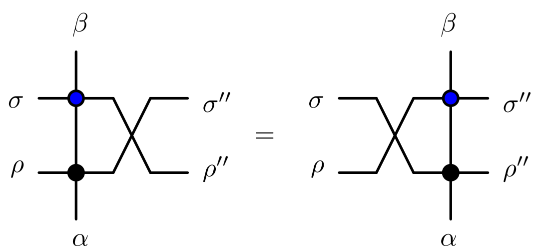
Since the product of two transfer matrices takes the form of a trace of products of the $\mathcal{S}$-matrix, the commutativity of transfer matrices is guaranteed if the corresponding two-row transfer matrices $\mathcal{S}$ and $\tilde{\mathcal{S}}$ are merely related by a change of basis, i.e. if there exists a similarity transformation that takes one matrix to the other by acting on the space of horizontal bonds (the indices of the two-row transfer matrix) [5]. By suppressing the horizontal bond indices, we may write, quite abstractly, that:

$$\tilde{\mathcal{S}}(\alpha,\beta) = \mathcal{R}^{-1}\mathcal{S}(\alpha,\beta)\mathcal{R} \tag{8}$$

with the invertible matrix $\mathcal{R}$ affecting the similarity transformation. More explicitly, the condition may be written in the form:

$$\sum_{\rho',\,\sigma'} \mathcal{S}_{\rho\sigma}^{\rho'\sigma'}(\alpha,\beta)\; \mathcal{R}_{\rho'\sigma'}^{\rho''\sigma''} = \sum_{\rho',\,\sigma'} \mathcal{R}_{\rho\sigma}^{\rho'\sigma'}\; \tilde{\mathcal{S}}_{\rho'\sigma'}^{\rho''\sigma''}(\alpha,\beta) \tag{9}$$

The action of the $\mathcal{R}$ matrix is more intuitively seen by representing the above equation diagrammatically:



(10)

This condition for the commutativity of the transfer matrices is known as the Yang-Baxter equation. The above expression suggests that the $\mathcal{R}$ matrix 'twists' the different transfer matrices together. If solutions to the Yang-Baxter equation exist, then we will have found continuous families of commuting transfer matrices, representing distinct physical realizations of the six-vertex model with different Boltzmann weights. For a given physical system specified by a set (x, y, z) of Boltzmann weights, we will have infinitely many conservation laws that restrict the spectrum of the transfer matrix.

PHASE-DIAGRAM OF THE 6-VERTEX MODEL

Our brief foray into abstraction has given a set of matrix equations whose solutions yield commuting families of transfer matrices. Looking at the diagrammatic form of the Yang-Baxter equation (10), we would now naively conclude that for the six-vertex model, we will have to solve a system of $2^6 = 64$ equations, corresponding to all possible combinations of $\pm$ indices. A variety of simplifications, however, make solving the Yang-Baxter equation surprisingly simple for the six-vertex model. First, note that the four-index tensor $\mathcal{A}_{\alpha\ell}^{\beta m}$ only has six non-vanishing entries:

$$\mathcal{A}_{++}^{++} = \mathcal{A}_{--}^{--} = x \qquad\qquad \mathcal{A}_{+-}^{+-} = \mathcal{A}_{-+}^{-+} = y \tag{11}$$

$$\mathcal{A}_{-+}^{+-} = \mathcal{A}_{+-}^{-+} = z \tag{12}$$

with $+$ $(-)$ representing a colored (uncolored) bond surrounding a vertex.

An important simplification in solving the Yang-Baxter equations arises from assuming that the $\mathcal{R}$ matrix takes the same *form* as the tensor $\mathcal{A}$, with six non-vanishing entries, except with different weights x'', y'' and z'' [5]. In other words, both $\mathcal{A}_{\alpha\ell}^{\beta m}$ and $\mathcal{R}_{\alpha\ell}^{\beta m}$ vanish unless $\alpha + \ell = \beta + m$. Consistently imposing this condition requires that the Yang-Baxter equation (9) is only non-zero if $\alpha + \rho + \sigma = \beta + \rho'' + \sigma''$, which then yields 20 equations relating the components of $\mathcal{S}$ and $\tilde{\mathcal{S}}$. The symmetry of the six-vertex model under switching colored and uncolored bonds (the 'ice rule') further halves the number of independent equations.

Finally, the Yang-Baxter equation has a built-in redundancy since exchanging $\alpha \leftrightarrow \beta$, $\rho \leftrightarrow \sigma''$, and $\sigma \leftrightarrow \rho''$ transforms the left diagram in (10) into the one on the right so that four of the remaining equations are trivially satisfied. For the last six equations, we explicitly use the definition of the two-row transfer matrices $\mathcal{S}$ and $\mathcal{S}$ in terms of the four-index tensor, and substitute into the Yang-Baxter relation (9); this then yields three independent equations:

$$xz'x'' = yz'y'' + zx'z'' \tag{13}$$

$$xy'z'' = yx'z'' + zz'y'' \tag{14}$$

$$zy'x'' = zx'y'' + yz'z'' \tag{15}$$

constraining the Boltzmann weights (x, y, z) and $(x', y'.z')$ in terms of the entries of the $\mathcal{R}$-matrix (x'', y'', z''). A non-trivial solution for the entries of the $\mathcal{R}$ matrix exists if the determinant of the coefficient matrix vanishes:

$$\det\begin{bmatrix} xz' & -yz' & -zx' \\ 0 & zz' & yx'-xy' \\ zy' & -zx' & -yz' \end{bmatrix} = \frac{\Delta(x',y',z') - \Delta(x,y,z)}{(xyzx'y'z')^{-1}} = 0$$

with the parameter $\Delta(x, y, z)$ defined as:

$$\Delta(x,y,z) \equiv \frac{x^2+y^2-z^2}{2xy} \tag{16}$$

We are therefore led to conclude that the transfer matrices $T(x, y, z)$ and $\tilde{T}(x', y', z')$ commute so long as $\Delta(x, y, z) = \Delta(x', y', z')$.

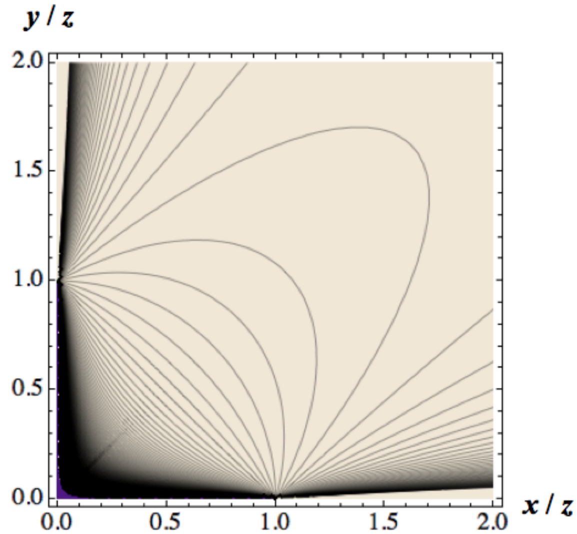


FIG. 1: Lines of constant Δ/z^2 as a function of the ratios x/z, y/z.

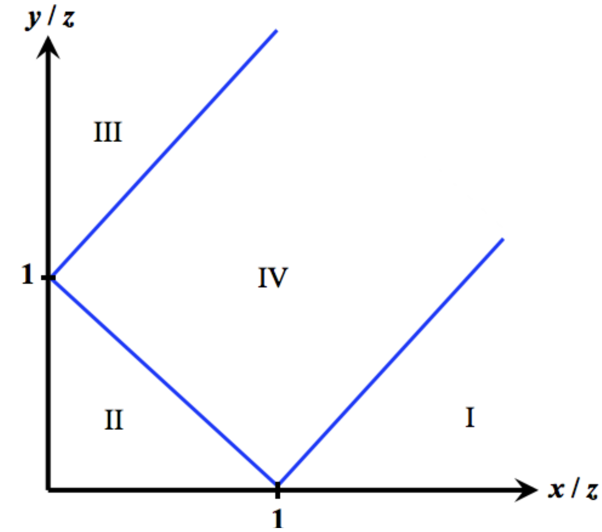


FIG. 2: Phase diagram of the six-vertex model with periodic boundary conditions in the space of Boltzmann weights (x/z, y/z).

This condition already allows us to derive the phase diagram of the six-vertex model. Since T and $\tilde{T}$ commute when $\Delta = \Delta'$, the two matrices must have the same eigenvectors. Furthermore, since the two matrices belong to a *continuous* family of transfer matrices, there can be no level-crossings in the eigenvalue spectrum of the two matrices as the parameters (x, y, z) are tuned to (x', y', z'), keeping $\Delta = \Delta'$ constant. In other words, the free energy must take the same analytic form along lines of constant Δ in the space of Boltzmann weights, so that the system must be in the *same phase* along such contours. This further implies that the boundary separating distinct phases must be given by a line of constant Δ.

In Figure 1, we have plotted the lines of constant Δ/z^2 as a function of the ratios x/z and y/z. We note that the character of the curves changes drastically as we tune Δ; for $\Delta < 1$, the constant-Δ contours are curves of finite-length connecting the points $(0, 1)$ and $(1, 0)$, while for $\Delta > 1$, the curves are no longer bounded, connecting each of these points to $x/z \to \infty$ or $y/z \to \infty$. Since these two classes of curves clearly correspond to distinct phases, it is natural to take the curve $|\Delta| = 1$ to define the phase boundary of the six-vertex model. This curve is shown in Figure 2, splitting the region of Boltzmann weights into four distinct spaces; the phases corresponding to each region may be extracted by considering the asymptotic behavior of the Boltzmann weights in each region.

- Region I: Here, $\Delta > 1$ and $x > y$, z. Therefore, a thermodynamically large portion of the vertices will all be of the form (1) or (2) as numbered previously. Returning to the 'arrow' representation of the six vertices, we see that the type-(1) and (2) vertices have a net electric dipole moment pointing vertically and to the right or down and to the left, respectively. We thus conclude that in Region I, the lattice is *ferroelectrically-ordered.* In fact, we have already computed the partition function in this region of the phase-diagram, since a lattice with all type-(2) vertices corresponds to the case with $n = 0$ colored vertical bonds per row so that the free energy per site $\beta f = -\ln[x]$ throughout the *entire* region, in the thermodynamic limit.

- Region II: Here, $\Delta < -1$ so that $z > x + y$. As a result, an extensive number of vertices will be of the type (5) or (6). In the 'arrow' representation of vertices, we see that neither vertex carries a net electric dipole moment. Furthermore, the vertices must alternate between lattice sites. We then conclude that the lattice exhibits *anti-ferroelectric order* in this region.

- Region III: The same analysis as in Region I holds; the system consists of all type-(3) or (4) vertices and is therefore ferroelectrically-ordered, with a net moment pointing up and to the left or down and to the right. Again, the free energy $\beta f = -\ln[y]$ in the thermodynamic limit.

- Region IV: Here, $-1 < \Delta < 1$ and $x + y + z > 2x$, $2y$ and $2z$. We see that this region of the phase diagram includes the line $\Delta = 1/2$, corresponding to $x = y = z$, which is always true in the limit of infinite temperature. Then we conclude that this is the *disordered phase* with no ferroelectric order and arbitrary vertex configurations proliferating throughout the lattice.

With the exception of our analysis in Region IV of the phase diagram, the remaining analysis turns out to be exactly the case when comparing our solution via the Yang-Baxter equation with the lengthier Bethe ansatz approach, in which the transfer matrix is explicitly diagonalized. It turns out that while Region IV is, in fact a 'disordered phase', it is possible to show that correlation functions decay as power-laws in this region [5]; in fact, Baxter has shown [4] that this region corresponds to the critical behavior of the more general 'eight-vertex model', of which the six-vertex model is a special case.

FURTHER POINTS OF INTEREST

Here, we note two incredibly useful features of the Yang-Baxter equation that we are unable to derive and discuss in detail in the interest of space. First, the Yang-Baxter equation can also be used to explicitly find all eigenvalues of the transfer matrix for the six-vertex model. Baxter [5] demonstrated via a careful analysis, that a solution to the Yang-Baxter equation also implies the existence of a family of matrices Q that commutes with the transfer matrix, whose product with the transfer matrix can be expanded as a sum of these matrices. Explicitly parametrizing the eigenvalues of the Q-matrix then leads to two sets of equations, yielding the eigenvalues of both the Q and T matrices [7]. It is the remarkable equivalence between these equations and what was derived in the Bethe ansatz approach [2] [7] that first suggested that the success of the ansatz generally implied some deeper integrable structure.

The six-vertex model can also be mapped to an interacting quantum spin-chain. We note that the four-index symbol $\mathcal{A}_{\alpha\ell}^{\beta m}$ may be written as a 4×4 matrix, after suppressing vertical bond indices [6]:

$$\mathcal{A}_\ell^m = \begin{bmatrix} x & 0 & 0 & 0 \\ 0 & z & y & 0 \\ 0 & y & z & 0 \\ 0 & 0 & 0 & x \end{bmatrix} \tag{17}$$

However, this four-by-four matrix may be equivalently expanded in terms of products of Pauli matrices as $\mathcal{A}_\ell^m = \frac{x}{2}\left(1-\sigma_\ell^z\sigma_m^z\right) - y\left(\sigma_\ell^+\sigma_m^- + \sigma_m^+\sigma_\ell^-\right) + \frac{z}{2}\left(1+\sigma_\ell^z\sigma_m^z\right)$. Now, consider letting $x = 1+\delta_x$, $y = \delta_y$, $z = 1+\delta_z$ so that δ_x, δ_y, $\delta_z << 1$ and $\mathcal{A}$ is close to the identity. Since the transfer matrix is just a product of the $\mathcal{A}$ matrices over a closed horizontal loop, we may then write that:

$$T = C + H_{XXZ} + O(\delta_x^2, \delta_y^2, \delta_z^2) \tag{18}$$

where C is a constant and the operator H_{XXZ} given by the following expression, up to an overall constant normalization factor:

$$H_{XXZ} \propto \sum_n \left[2\delta_y\left(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y\right) + \frac{\delta_x-\delta_z}{2}\sigma_n^z\sigma_{n+1}^z \right]$$

which we recognize as the Hamiltonian for the XXZ quantum spin-chain. Since we have expanded the parameters (x, y, z) around the tricritical point in the phase diagram for the six-vertex model, separating regions I, II and IV, we are then led to conjecture that the critical behavior of the six-vertex model is the same as that of the XXZ spin-chain. More generally, it is possible to show that at *every* point in phase diagram, there exists an XXZ spin-chain Hamiltonian $H_{XXZ}(x, y, z)$ that commutes with the transfer matrix $T(x, y, z)$ and is therefore diagonalized by the same unitary transformation [4]. The two models are therefore equivalent and share the same phase diagram.

CONCLUSION

We have extracted the phase diagram of the six-vertex model by deriving the conditions under which transfer matrices parametrized by different Boltzmann weights commute, thereby solving the six-vertex model for a wide-class of physical realizations. We also discussed how the Yang-Baxter equation could be used to extract the eigenvalues of the transfer matrix, allowing for a direct calculation of the free energy and correlation functions in the thermodynamic limit, and demonstrated that the model can be mapped exactly onto the XXZ quantum spin-chain. The Yang-Baxter approach provides a powerful method for extracting exact solutions to problems in two-dimensional statistical mechanics. It would be interesting to see if 'integrability' can arise in a similar fashion in higher-dimensional systems.

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