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Symmetry Relations for the Six-Vertex Model

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The exact solution of the asymmetric six-vertex model is cast in an algebraically simple form in which the extraction of physical quantities is transparent. This is used to derive a symmetry relation corresponding to the exchange of spatial x and y axes. As an application we study the field-induced phase transition of a two-dimensional analogue of spin ice, a frustrated Ising magnet.

KEY WORDS: Six-vertex model; ice model; BCSOS model; spin ice.

1. INTRODUCTION

Exactly solvable models have proved immensely important in the development of the subject of phase transitions and critical phenomena. Among such models in two dimensions, the six-vertex model[1–6] is unique in having been solved for all values of its parameters, including external fields. The various kinds of "frozen order" phase transitions it displays have been explored in detail. As for physical applications, models of this type were originally proposed in the investigation of ferroelectric solids, e.g., potassium dihydrogen phosphate, and date back to Pauling's study of the residual entroy of ice. The six-vertex model is also encountered in studies of the equilibrium shape of crystals, through an exact mapping from the body-centred solid-on-solid (BCSOS) model.[7, 8]

More recently, ice-type models have been proposed in the context of frustrated magnetic systems. In one case of particular interest, known as spin ice,[9–11] and thought to be realized in rare earth titanate materials, magnetic moments, forming a pyrochlore lattice, interact via ferromagnetic exchange and are subject to a specific type of Ising anisotropy. The competition between exchange interactions and anisotropy leads, in a limiting

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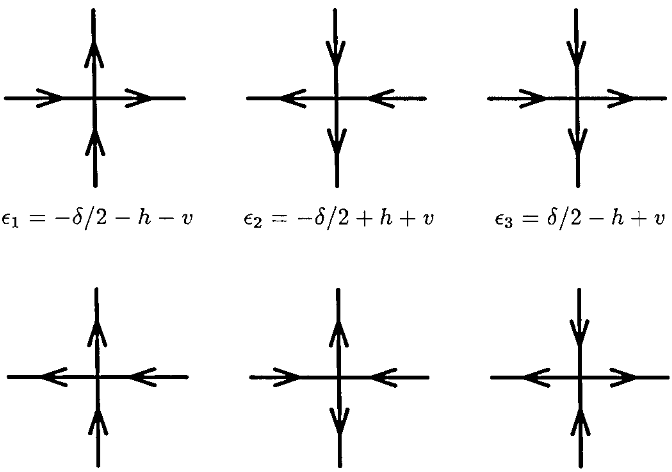
case, to a strict "ice rule" constraint, and to a description by the three-dimensional ice model. The two-dimensional analogue is a special case of the six-vertex model. The behaviour of the system as a function of applied magnetic field is of current interest.[12]

The six-vertex model is defined as follows. On each bond of a square lattice is placed an arrow pointing in either of two directions along the bond. The arrow configuration is required to satisfy the ice rule, which states that there must be two arrows in and two arrows out, at each vertex. This results in six allowed vertex configurations, and these are assigned energies specified, as usual, by four parameters ε, δ, h and v, as shown in Fig. 1. If the arrows represent electric dipole moments in a ferroelectric, h and v are the horizontal and vertical components of the applied electric field. An alternative language, used here as it is appropriate for spin ice (see Section 5), is to refer to the arrows as spins and to h and v as magnetic field components.

The algebraic form of the model's exact solution is cumbersome, especially in the "asymmetric" case where both h and v are nonzero.[7, 13, 14] It takes the form of an integral equation, which, except in special cases, must be solved numerically. One curious feature is that the free energy provided by the exact solution is not the function $f(h, v)$ of external fields, nor is it the Legendre transform $f(x, y)$, where x and y are components of the magnetization (polarization). Rather, it is $f(h, y)$. While this is not a problem of principle, it is at first sight surprising that the components h



$\epsilon_1 = -\delta/2 - h - v$ $\epsilon_2 = -\delta/2 + h + v$ $\epsilon_3 = \delta/2 - h + v$

$\epsilon_4 = \delta/2 + h - v$ $\epsilon_5 = -\epsilon$ $\epsilon_6 = -\epsilon$

Fig. 1. Vertex configurations in the six-vertex model, and their energies.

and v should be treated differently from each other, since the model is symmetric under exchange of coordinate axes, i.e., $x \leftrightarrow y$ and $h \leftrightarrow v$. Certainly, x and v can be obtained from $f(h, y)$, but the obvious method for doing this in practice[7] is quite involved (see Section 2).

This paper describes a more direct approach, which places the calculation of v and x on an equal footing with h and y. This is done in Section 3 by showing that each pair of variables can be obtained from the solution of an integral equation. A consequence, described in Section 4, is a relationship expressing the symmetry under exchange of coordinate axes in terms of the auxiliary variables (a and b) of the integral equations. This relation agrees in a special case with a conjecture of Bukman and Shore.[13] Finally, in Section 5, the results are applied in a simple calculation for a two-dimensional analogue of "spin ice."

2. EXACT SOLUTION

Details of the Bethe Ansatz technique used to derive the exact solution can be found elsewhere.[5, 6] Here is quoted the final result, for the general case when both h and v are allowed to be nonzero.[4, 7] The solution is couched in terms of several auxiliary quantities: two real parameters, a and b, and a complex function $R(u)$. These satisfy the fundamental integral equation

$$R(u) + \frac{1}{2\pi} \int_{-a}^{a} K(u-v)\, R(v)\, dv = \xi(u) \tag{1}$$

where the kernel K and inhomogeneous part ξ are given functions (see below). The function ξ depends on b. It follows that R depends parametrically on a and b as well as on u. The horizontal field h and vertical magnetization y are found from

$$\frac{\pi}{2}(1-y) - 2i\beta h = g(a) \equiv \gamma \tag{2}$$

where the function g is defined by

$$g(u) = p^0(u) - \frac{1}{2\pi} \int_{-a}^{a} \Theta(u-v)\, R(v)\, dv \tag{3}$$

Here, β is the inverse temperature, and Θ and p^0 are again known functions, which satisfy

$$K(u) = \frac{d\Theta}{du} \qquad \text{and} \qquad \xi(u) = \frac{dp^0}{du} \tag{4}$$

Finally, the free energy (per vertex) is given by

$$-\beta f(h, y) = \max_{\mathrm{R, L}} \left[\pm\beta(\delta/2 + h) + \frac{1}{2\pi} \int_{-a}^{a} \Phi^{\mathrm{R, L}}(u)\, R(u)\, dv \right] \tag{5}$$

where Φ^{R} and Φ^{L} are given functions, and the sign is plus for R and minus for L.

The various functions which occur in the above equations are tabulated in several sources.[5, 7, 13] They take different functional forms depending on whether the parameter

$$\Delta = \tfrac{1}{2}[e^{\beta\delta} + e^{-\beta\delta} - e^{2\beta\varepsilon}] \tag{6}$$

lies in the interval $(-\infty, -1)$, $(-1, 1)$ or $(1, \infty)$. The cases $\Delta = \pm 1$ must also be treated separately. Here they are listed for the case appropriate to spin ice (Section 5), namely $-1 < \Delta < 1$. They are expressed in terms of two additional parameters: μ, defined by $\Delta = -\cos\mu$, and ϕ_0, defined below.

$$\begin{aligned} \Theta &= 2 \arctan(\cot\mu \tanh(u/2)) \\ e^{ip^0} &= \frac{e^{i\mu} - e^{u+ib}}{e^{u+ib+i\mu} - 1} \\ e^{\phi^{\mathrm{R, L}}} &= \frac{e^{u+ib\pm i\mu} - e^{i\phi_0 \mp i\mu}}{e^{i\phi_0} - e^{u+ib}} \\ e^{i\phi_0} &= \frac{1 + e^{\beta\delta + i\mu}}{e^{i\mu} + e^{\beta\delta}} \end{aligned} \tag{7}$$

In (7), the sign is again plus (minus) for the R (L) case.

These equations constitute a complete solution, which may be approached computationally as follows. Values of a and b are chosen, and (1) solved to obtain the corresponding $R(u)$. This function is then substituted into (3) to obtain the values of y and h from (2), and into (5) to give the free energy. This yields one point on the $f(h, y)$ surface. The procedure is then repeated for a range of values of a and b to map out the function $f(h, y)$.

More effort is required to obtain v and x. These are partial derivatives of the free energy,

$$x = -(\partial f/\partial h)_y = (\partial_a f\, \partial_b y - \partial_b f\, \partial_a y)/d \tag{8}$$

$$v = (\partial f/\partial y)_h = (\partial_a f\, \partial_b h - \partial_b f\, \partial_a h)/d \tag{9}$$

where $d = \partial_a y\, \partial_b h - \partial_b y\, \partial_a h$ and the notation $\partial_a f = (\partial f/\partial a)_b$ is used. The a and b derivatives are obtained by differentiating (2) and (5) to express them in terms of $\partial_a R$ and $\partial_b R$. The latter are, in turn, found by differentiating (1) to obtain integral equations which must be separately solved at each a and b. Complete formulas are provided by Nolden.[7]

3. IDENTITY FOR *x* AND *v*

The procedure just described for calculating v and x is unnecessarily complicated. Here a simpler method is described, which places them on an equal footing with h and y.

This section presents general results which do not depend on the specific form of the kernel and inhomogeneous term of the integral equations, but which follow from only the algebraic structure of Eqs. (1) to (5), together with the following symmetry properties:

$$\Theta(-u) = -\Theta(u)^*, \qquad p^0(-u) = -p^0(u)^*, \qquad \Phi(-u) = \Phi(u)^* \tag{10}$$

where * denotes complex conjugation. It follows from these and (4) that $K(-u) = K(u)^*$, i.e., the kernel is Hermitian.

The main tool in the development is the following consequence of this Hermiticity. Suppose R_1 and R_2 are two functions which obey the integral equation (1) with different inhomogeneous parts, ξ_1 and ξ_2. Then

$$\int_{-a}^{a} R_1(u)\, \xi_2(u)^*\, du = \int_{-a}^{a} R_2(u)^*\, \xi_1(u)\, du \tag{11}$$

The proof is to substitute for each ξ the other side of the corresponding integral equation, leading to several terms which all cancel.

A second useful result is that $g(u)$ itself obeys an integral equation with kernel K. First, by differentiating (3), one finds that $dg/du = R$. Second, integrating the second term of (3) by parts yields

$$g(u) + \frac{1}{2\pi} \int_{-a}^{a} K(u-v)\, g(v)\, dv$$
$$= p^0(u) + \frac{1}{2\pi} \left[\gamma \Theta(a-u) + \gamma^* \Theta(-a-u) \right] \tag{12}$$

where γ is defined in (2). Furthermore, partial derivatives of R also obey integral equations with kernel K; for instance, the equation

$$\partial_a R(u) + \frac{1}{2\pi} \int_{-a}^{a} K(u-v)\, \partial_a R(v)\, dv$$
$$= -\frac{1}{2\pi} [R(a)\, K(a-u) + R(-a)\, K(-a-u)] \tag{13}$$

is obtained by differentiating (1) with respect to a.

Let us now restrict attention to the region of parameter space in which Φ^{R} provides the maximum in (5) which determines the free energy. (The same argument goes through in the L region.) Therefore, the superscript on Φ will be omitted. Now define a function

$$\overline{p^0}(u) = -i\Phi(u)^* \tag{14}$$

The motivation for this definition and the overbar notation will become evident later. As well as $\overline{p^0}$, define $\bar{\xi}$, $\bar{R}$, $\bar{g}$ and $\bar{\gamma}$ by strict analogy with the corresponding unbarred quantities, through (1) to (4).

The next step in the argument is to apply the Hermiticity result (11) to the two functions $\partial_a R$ and $\bar{g}$, each of which obeys an integral equation with kernel K, namely (13) and the barred version of (12), respectively. There result several terms, some of which may be simplified using, e.g., the equation resulting from differentiating (3) with respect to a. As the algebra is straightforward we skip the details and write the eventual result:

$$-\mathrm{Im}(\bar{\gamma}\, \partial_a \gamma^*) = \int_{-a}^{a} \partial_a R(u)\, \Phi(u)\, du + R(a)\, \Phi(a) + R(-a)\, \Phi(-a) \tag{15}$$

$$= -2\pi\beta\, \partial_a(f+h) \tag{16}$$

where the second equality follows from differentiating (5) with respect to a.

Very similar reasoning, applying the Hermiticity condition to $\partial_b R$ and $\bar{g}$, and subsequently to R and $\bar{R}$, yields a second result

$$\mathrm{Im}(\bar{\gamma}\, \partial_b \gamma^*) = 2\pi\beta\, \partial_b(f+h) \tag{17}$$

The final step is to observe that, from (2) and (9),

$$\frac{\pi}{2}(1-x) - 2i\beta v = [\partial_a(f+h)\, \partial_b \gamma - \partial_b(f+h)\, \partial_a \gamma]/d \tag{18}$$

Combining this with the expressions derived for the derivatives of $f+h$, together with $\pi\beta d = \mathrm{Im}(\partial_a \gamma^* \, \partial_b \gamma)$, yields

$$\frac{\pi}{2}(1-x) - 2i\beta v = \bar{\gamma} = \bar{g}(a) \tag{19}$$

This is the main result of this section. The purpose of the definition of $\overline{p^0}$ is clear on comparison with (2): barred quantities correspond physically to unbarred ones under the coordinate exchange, $y \to x$, $h \to v$.

Using this result, v and y may be computed in exactly the same way as h and y. An integral equation, (1) with inhomogeneous term given by (14), is solved for $\bar{R}$. This is then used to calculate $\bar{g}(a)$ using the barred version of (3), and v and y follow. There is no need to compute partial derivatives.

A further result derived using the methods of this section is $d = |R(a)|^2/\pi\beta$, which may be of some utility as it is easier to compute than the definition.

4. SYMMETRY RELATIONS

In the previous section it was shown that, just as the horizontal field h and vertical magnetization y can be obtained from the solution of the integral equation (1), the conjugate quantities x and v can be obtained by solving the same equation with a different inhomogeneous part, defined through (14).

Restricting attention to the case $-1 < \Delta < 1$, we now observe from the explicit formulas (7) that the following identity is obeyed:

$$\overline{p^0}(u, b) = -i\Phi^{\mathrm{R}}(u, b)^* = p^0(u, -b-\mu-\phi_0) \tag{20}$$

In other words, the transformation to barred quantities is equivalent to $b \to -b-\mu-\phi_0$, in the R region of free energy, namely $-\mu < b < \phi_0$. This transformation of b maps the R region onto itself. A similar transformation, with $\overline{p^0} = i(\Phi^{\mathrm{L}})^*$, holds in the L region, and thus

$$b \to \begin{cases} -b-\mu-\phi_0, & -\mu < b < \phi_0 \\ -b+\mu+\phi_0, & \phi_0 < b < \mu \end{cases} \tag{21}$$

This simple mapping in the (a, b) plane expresses the symmetry of the model under exchange of coordinate axes.

The other Δ cases also admit symmetry relations. For completeness they are listed below, in the R region. Here, λ and v are the standard names for the parameters analogous to μ in these cases.

$$\begin{aligned} \Delta < -1: &\quad b \to -b - \lambda + \phi_0 \\ \Delta > 1: &\quad b \to -b - v + \phi_0 \\ \Delta = \pm 1: &\quad b \to -b - \tfrac{1}{2} + \phi_0 \end{aligned} \tag{22}$$

The symmetry relation for $\Delta > 1$ has been suggested previously,[13] but not proved.

5. TWO-DIMENSIONAL SPIN ICE

We close with a simple application. Spin ice[9–12] consists of magnetic moments (spins) arranged in a pyrochlore lattice, a structure formed of corner-sharing tetrahedra. Its characteristic feature is strong Ising anisotropy, with a specific geometry which implies that the configuration of spins in a single tetrahedron, minimizing the local energy, consists of two spins pointing in towards the centre, and two pointing out. In the limit of infinite exchange coupling, J, this results in a strict local "two in, two out" condition identical to that in ice.

Recent work[12] has identified unusual behaviour of spin ice in magnetic fields applied along various directions. An especially interesting case is when the field is along the lattice [1 0 0] direction, a high symmetry axis forming the same angle with all the Ising spins. Monte Carlo simulations[12] appear to show a phase transition, in which the magnetization abruptly saturates at a critical value of the applied field. The transition occurs along a line in the (T, h)-plane, ending at a critical point located at a temperature of order J.

To further understanding of this phenomenon, it is useful to study an exactly soluble case. Here we consider the two-dimensional analogue, where the tetrahedra of spins are flattened into squares and linked into a square lattice. Further, we take the limit $J \to \infty$, where the ice rule is strictly enforced. The model thus obtained is the two-dimensional ice model, which is a special case ($\delta = \varepsilon = 0$) of the six-vertex model. The axis analogous to the pyrochlore [1 0 0] direction lies at 45 degrees to the spins, so consider the symmetric field, $h = v$. This case has apparently not been examined in detail previously in the literature.

The results of Sections 3 and 4 are particularly useful when $h = v$. Since this corresponds to a fixed point of the coordinate exchange transformation, we deduce at once that $b = \pm(\phi_0 + \mu)/2$. It is, of course, extremely

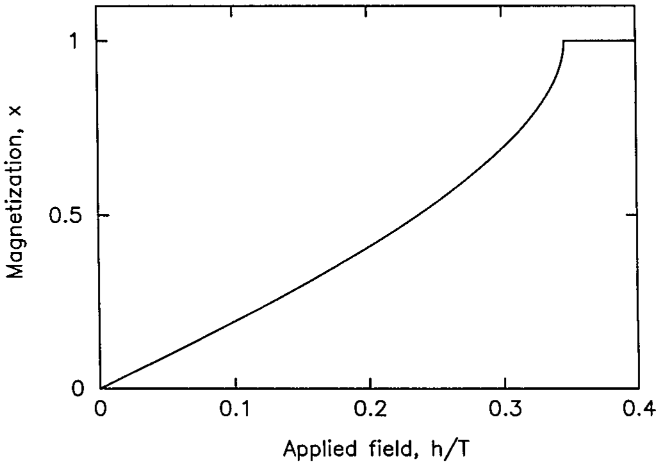


Fig. 2. Magnetization curve for two-dimensional spin ice, which is the six-vertex model with $\delta = \varepsilon = 0$ and $h = v$.

useful in practice to be able to restrict computations to a line of constant b. Further, since $\gamma = \bar{\gamma}$, it is sufficient to solve a single integral equation, for each a, to obtain the dependence of magnetization x on external field h.

This has been carried out for the case ($\Delta = 1/2$, $\phi_0 = 0$) of interest, and the result is shown in Fig. 2, in a plot of magnetization against applied field. There is indeed a phase transition to saturated magnetization, i.e., "frozen" order, occuring at $h/T = \frac{1}{2} \log 2$.

The singularity at the transition is of square root type, $1 - x \propto (h - h_c)^{1/2}$. Because of the trivial temperature dependence in this model, following from $\delta = \varepsilon = 0$, the specific heat (at constant field) is proportional to $(h/T)^2$ times the isothermal susceptibility, and both of these diverge with an inverse square root singularity below the transition, and are zero above it. These properties are similar to those of the KDP model of ferroelectrics.[3]

The present calculation confirms the results of ref. 12 in the limit $J \gg h, t$. Unfortunately, the six-vertex model does not provide information about the case of finite J. If the ice condition is not enforced, it is necessary to consider the sixteen-vertex model,[5] about which little is known. A discussion of the physics of this general case is left for a future publication.

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