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LETTER TO THE EDITOR

# Exact transition temperature for an Ising model in three dimensions

D Grensing†, A Huber†, H-U Jüttner†, C Ruge† and M Münier‡

† Institut für Theoretische Physik, Universität Kiel, Olshausenstr. 40-60, D-2300 Kiel, Federal Republic of Germany

‡ Institut für Theoretische Physik, Universität Köln, Zülpicher Str. 77, D-5000 Köln, Federal Republic of Germany

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**Abstract.** For the most general vertex model respecting spin-flip symmetry we obtain on two- and three-dimensional SC lattices all fixed points of the generalised weak-graph transformation. From the result, a phase transition of a constrained Ising model on a three-dimensional lattice is conjectured to occur at coupling strength $\frac{1}{4}\ln(\sqrt{\frac{1}{2}}+\sqrt{\sqrt{2}-\frac{1}{2}})$. We find this value to be consistent with Monte Carlo simulation results, which indicate a first-order phase transition.

We investigate a constrained Ising model (figure 1), with spins $\sigma \in \{+1, -1\}$ situated at (the midpoints of) the bonds of a three-dimensional SC lattice. Euclidean metric is assumed; nearest-neighbour spins interact ferromagnetically with coupling strength $K > 0$. The constraint restricts every product of six spins surrounding a site to be positive.

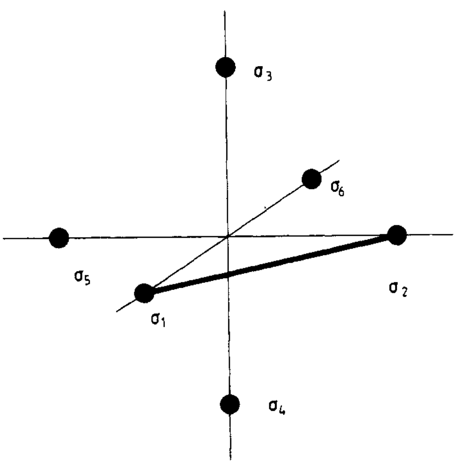


**Figure 1.** The six spins surrounding a site of the SC lattice in three dimensions. The bold line represents the interaction $-K\sigma_1\sigma_2$.

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On simply connected lattices this constraint may be solved by passing to the dual SC lattice (this is an elementary result of algebraic topology, see e.g. [1] in which the application to lattice models is emphasised). The spins, now being situated on faces (figure 2(*a*)), are replaced by a set of new Ising spins on the bonds of this lattice, whose products along the boundary of each face give the value of the original face-spin. The remaining interaction couples the eight spins on the boundary of every two perpendicular faces having a common bond (effectively only six spins are coupled as one spin shows up twice in the product, figure 2(*b*)). For the remainder of our letter we shall, however, refer to the Ising version of the model.

To locate a possible phase transition we look for fixed points of the (duality-like) generalised weak-graph transformation [2-4]. In order to make this transformation applicable note that the constrained Ising model may be viewed as a vertex model on the (original) SC lattice with each site contributing a vertex weight $\omega(\sigma_1, \ldots, \sigma_q)$ depending on the states of the $q = 6$ surrounding spins. Because only products of two or six spins emerge in the vertex weight it is symmetric with respect to flipping all

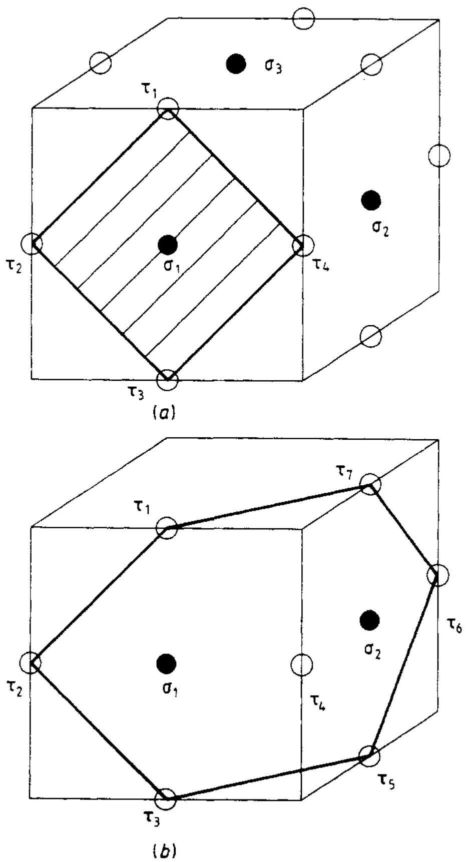


**Figure 2.** (*a*) An elementary cube of the dual lattice. Solid circles represent the original spins $\sigma_1$, $\sigma_2$, $\sigma_3$ (cf figure 1), open circles the new spin-configuration, here denoted by $\tau$. The shaded square corresponds to $\sigma_1 = \tau_1\tau_2\tau_3\tau_4$, which together with analogous relations for $\sigma_2, \ldots, \sigma_6$ solves the constraint of the original model $\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6 = +1$. (*b*) An example of the remaining interaction $-K\sigma_1\sigma_2 = -K\tau_1\tau_2\tau_3\tau_5\tau_6\tau_7$. The spin $\tau_4$ drops out as it occurs twice in this product.

spins: $\omega(-\sigma_1, \ldots, -\sigma_q) = \omega(\sigma_1, \ldots, \sigma_q)$. In what follows the most general two-state vertex model symmetric in this sense will be studied on lattices of coordination numbers $q = 4, 6$.

The generalised weak-graph transformation is a mapping in parameter space

$$\omega^*(\sigma_1, \ldots, \sigma_q) = \sum_{\tau_1, \ldots, \tau_q} V_{\sigma_1\tau_1} \ldots V_{\sigma_q\tau_q} \omega(\tau_1, \ldots, \tau_q) \tag{1}$$

which leaves the partition function of the vertex model invariant. The $y$-parametrised $(2 \times 2)$ matrix

$$V(y) = \frac{1}{\sqrt{1+y^2}} \begin{pmatrix} 1 & y \\ y & -1 \end{pmatrix} \tag{2}$$

exhibits eigenvectors

$$\psi_\varepsilon = \begin{pmatrix} y \\ z_\varepsilon \end{pmatrix} \qquad z_\varepsilon \equiv \varepsilon\sqrt{1+y^2} - 1 \tag{3}$$

corresponding to the eigenvalues $\varepsilon = +1$ and $\varepsilon = -1$ respectively: $V\psi_\varepsilon = \varepsilon\psi_\varepsilon$.

The generalised weak-graph transformation may be viewed as a tensor product $W = V \otimes \ldots \otimes V$ ($q$ factors) of $V$ matrices. Every tensor product $\Psi(\boldsymbol{\varepsilon}) = \psi_{\varepsilon_1} \otimes \ldots \otimes \psi_{\varepsilon_q}$ of eigenvectors of $V$ belonging to eigenvalues $\varepsilon_1, \ldots, \varepsilon_q$ is an eigenvector of $W$ corresponding to the eigenvalue $\lambda(\boldsymbol{\varepsilon}) = \Pi_{i=1}^q \varepsilon_i$. Conversely these tensor products span the (two) eigenspaces of $W$.

The space of vertex weight vectors $\omega$ invariant under the weak-graph transformation is thus spanned by all eigenvectors $\Psi(\boldsymbol{\varepsilon})$ belonging to the eigenvalue $\lambda(\boldsymbol{\varepsilon}) = +1$. Because of the orthogonality property of the eigenvectors this space is equivalently characterised by the eigenvectors $\Psi(\boldsymbol{\varepsilon})$ with eigenvalue $\lambda(\boldsymbol{\varepsilon}) = -1$:

$$\Psi(\boldsymbol{\varepsilon}) \cdot \omega = 0 \qquad \text{for all } \boldsymbol{\varepsilon} \text{ with } \lambda(\boldsymbol{\varepsilon}) = -1. \tag{4}$$

These 'normal vectors' will be used in the following to identify the space of fixed points for parameters $y \neq 0$. (The parameter value $y = 0$ yields a trivial mapping $\omega^*(\sigma_1, \ldots, \sigma_q) = \sigma_1 \ldots \sigma_q \omega(\sigma_1, \ldots, \sigma_q)$, which leaves all vertex weight vectors invariant whose only non-vanishing elements are those with an even number of negative spin-arguments.)

Before applying this technique to the study of the case of $q = 6$, we discuss it for the easier case of $q = 4$. Consider the general sixteen-vertex model without additional symmetry assumptions. There are eight normal vectors: four vectors corresponding to $\boldsymbol{\varepsilon} \in E := \{(-+++), (+-++), (++-+), (+++-)\}$ and four corresponding to $\boldsymbol{\varepsilon}$ with $-\boldsymbol{\varepsilon} \in E$. It will be convenient to compose from these 4+4 normal vectors two new groups (of four vectors each) by

$$\Psi^+(\boldsymbol{\varepsilon}) := \tfrac{1}{2}(\Psi(\boldsymbol{\varepsilon}) + \Psi(-\boldsymbol{\varepsilon})) \tag{5}$$

$$\Psi^-(\boldsymbol{\varepsilon}) := \frac{1}{z_+ - z_-}(\Psi(\boldsymbol{\varepsilon}) - \Psi(-\boldsymbol{\varepsilon})). \tag{6}$$

The normal vectors $\Psi^+$ and $\Psi^-$ serve as the rows of a matrix representing a system of 4+4 homogeneous linear equations for the sixteen vertex weights. The columns are indexed from left to right as $(\sigma_1 \ldots \sigma_4)=(++++)$, $(-+++)$, $(+-++)$, $(++-+)$, $(+++-)$, $(--++)$, $(-+-+)$, $(-++-)$, $(+--+)$, $(+-+-)$, $(++--)$, $(---+)$, $(--+-)$, $(-+--)$, $(+---)$, $(----)$.

$$\begin{pmatrix}
p_0^+ & p_1^+ & p_1^+ & p_1^+ & p_1^+ & -p_0^+ & -p_0^+ & -p_0^+ & p_2^+ & p_2^+ & p_2^+ & -p_1^+ & -p_1^+ & -p_1^+ & p_3^+ & -p_2^+ \\
p_0^+ & p_1^+ & p_1^+ & p_1^+ & p_1^+ & -p_0^+ & p_2^+ & p_2^+ & -p_0^+ & -p_0^+ & p_2^+ & -p_1^+ & -p_1^+ & p_3^+ & -p_1^+ & -p_2^+ \\
p_0^+ & p_1^+ & p_1^+ & p_1^+ & p_1^+ & p_2^+ & -p_0^+ & p_2^+ & -p_0^+ & p_2^+ & -p_0^+ & -p_1^+ & p_3^+ & -p_1^+ & -p_1^+ & -p_2^+ \\
p_0^+ & p_1^+ & p_1^+ & p_1^+ & p_1^+ & p_2^+ & p_2^+ & -p_0^+ & p_2^+ & -p_0^+ & -p_0^+ & p_3^+ & -p_1^+ & -p_1^+ & -p_1^+ & -p_2^+ \\
p_0^- & -p_1^- & p_1^- & p_1^- & p_1^- & -p_0^- & -p_0^- & -p_0^- & p_2^- & p_2^- & p_2^- & -p_1^- & -p_1^- & -p_1^- & p_3^- & -p_2^- \\
p_0^- & p_1^- & -p_1^- & p_1^- & p_1^- & -p_0^- & p_2^- & p_2^- & -p_0^- & -p_0^- & p_2^- & -p_1^- & -p_1^- & p_3^- & -p_1^- & -p_2^- \\
p_0^- & p_1^- & p_1^- & -p_1^- & p_1^- & p_2^- & -p_0^- & p_2^- & -p_0^- & p_2^- & -p_0^- & -p_1^- & p_3^- & -p_1^- & -p_1^- & -p_2^- \\
p_0^- & p_1^- & p_1^- & p_1^- & -p_1^- & p_2^- & p_2^- & -p_0^- & p_2^- & -p_0^- & -p_0^- & p_3^- & -p_1^- & -p_1^- & -p_1^- & -p_2^-
\end{pmatrix}. \tag{7}$$

The polynomials in $y$ constituting the matrix explicitly read

$$\begin{aligned}
p_0^+ &= y^4 & p_0^- &= 0 \\
p_1^+ &= -y^3 & p_1^- &= y^3 \\
p_2^+ &= (y^2+2)y^2 & p_2^- &= -2y^2 \\
p_3^+ &= -(3y^2+4)y & p_3^- &= (y^2+4)y.
\end{aligned} \tag{8}$$

The space of fixed points will in general be $y$ dependent. But returning to the symmetric vertex model this dependence is seen to drop out. We respect the required spin-flip symmetry by adding columns located symmetrically to the centre. After ignoring non-vanishing factors $(y \neq 0)$ common to the matrix elements of some row this yields the matrix

$$\begin{pmatrix}
-1 & P & 0 & 0 & 0 & 1 & 1 & 1 \\
-1 & 0 & P & 0 & 0 & 1 & 1 & 1 \\
-1 & 0 & 0 & P & 0 & 1 & 1 & 1 \\
-1 & 0 & 0 & 0 & P & 1 & 1 & 1 \\
-1 & Q & 0 & 0 & 0 & 1 & 1 & 1 \\
-1 & 0 & Q & 0 & 0 & 1 & 1 & 1 \\
-1 & 0 & 0 & Q & 0 & 1 & 1 & 1 \\
-1 & 0 & 0 & 0 & Q & 1 & 1 & 1
\end{pmatrix} \tag{9}$$

where $P=(p_3^+ + p_1^+)/(p_2^+ - p_0^+) = -2(y^2+1)/y$ and $Q=(p_3^- - p_1^-)/(p_2^- - p_0^-) = -2/y$. After subtracting the first four equations from the last four these read

$$\begin{aligned}
\omega(-+++) &= \omega(+---) = 0 & \omega(+-++) &= \omega(-+--) = 0 \\
\omega(++-+) &= \omega(--+-) = 0 & \omega(+++-) &= \omega(---+) = 0
\end{aligned} \tag{10}$$

the first equalities expressing the spin-flip symmetry. The remaining four equations all read

$$a = b + c + d \tag{11}$$

where the Baxter-like definitions

$$
\begin{aligned}
a &= \omega(++++) = \omega(----) \qquad & c &= \omega(-+-+) = \omega(+-+-) \\
b &= \omega(-++-) = \omega(+--+) \qquad & d &= \omega(--++) = \omega(++--)
\end{aligned}
\tag{12}
$$

were used.

Thus for spin-flip symmetric $(q=4)$-vertex models the space of fixed points becomes independent of $y$ as anticipated, and coincides with a hyperplane of phase transition points of the zero-field eight-vertex model [5].

We now turn to the case of $(q=6)$-vertex models respecting spin-flip symmetry (this includes the constrained Ising model). The vertex weights will be denoted as

$$
\begin{aligned}
a &= \omega(++++++) = \omega(------) & c_{10} &= \omega(++--++) = \omega(--++--) \\
b_1 &= \omega(-+++++) = \omega(+-----) & c_{11} &= \omega(++-+-+) = \omega(--+-+-) \\
b_2 &= \omega(+-++++) = \omega(-+----) & c_{12} &= \omega(++-++-) = \omega(--+--+) \\
b_3 &= \omega(++-+++) = \omega(--+---) & c_{13} &= \omega(+++--+) = \omega(---++-) \\
b_4 &= \omega(+++-++) = \omega(---+--) & c_{14} &= \omega(+++-+-) = \omega(---+-+) \\
b_5 &= \omega(++++-+) = \omega(----+-) & c_{15} &= \omega(++++--) = \omega(----++) \\
b_6 &= \omega(+++++-) = \omega(-----+) & d_1 &= \omega(---+++) = \omega(+++---) \\
c_1 &= \omega(--++++) = \omega(++----) & d_2 &= \omega(--+-++) = \omega(++-+--) \\
c_2 &= \omega(-+-+++) = \omega(+-+---) & d_3 &= \omega(--++-+) = \omega(++--+-) \\
c_3 &= \omega(-++-++) = \omega(+--+--) & d_4 &= \omega(--+++-) = \omega(++---+) \\
c_4 &= \omega(-+++-+) = \omega(+---+-) & d_5 &= \omega(-+--++) = \omega(+-++--) \\
c_5 &= \omega(-++++-) = \omega(+----+) & d_6 &= \omega(-+-+-+) = \omega(+-+-+-) \\
c_6 &= \omega(+--+++) = \omega(-++---) & d_7 &= \omega(-+-++-) = \omega(+-+--+) \\
c_7 &= \omega(+-+-++) = \omega(-+-+--) & d_8 &= \omega(-++--+) = \omega(+--++-) \\
c_8 &= \omega(+-++-+) = \omega(-+--+-) & d_9 &= \omega(-++-+-) = \omega(+--+-+) \\
c_9 &= \omega(+-+++-) = \omega(-+---+) & d_{10} &= \omega(-+++--) = \omega(+---++).
\end{aligned}
\tag{13}
$$

As in (7) we construct a matrix whose rows $\Psi^+$, $\Psi^-$ span the orthocomplement to the $\lambda=+1$ eigenspace. When treated analogously to the case of $q=4$, it breaks up into two submatrices which coupled weights of

(i) type $a$ and type $c$,

(ii) type $b$ and type $d$,

respectively. Among the equations (i) there are only six independent ones, which we choose to be

$$
\begin{aligned}
a &= c_5 + c_9 + c_{12} + c_{14} + c_{15} \\
0 &= c_1 + c_5 + c_9 - c_{10} - c_{11} - c_{13} \\
0 &= c_2 + c_4 + c_{11} - c_7 - c_9 - c_{14} \\
0 &= c_3 + c_4 + c_{13} - c_6 - c_9 - c_{12} \\
0 &= c_3 + c_5 + c_{14} - c_6 - c_8 - c_{11} \\
0 &= c_4 + c_5 + c_{15} - c_6 - c_7 - c_{10}.
\end{aligned}
\tag{14}
$$

Equations (ii) reduce to

$$\left(y-\frac{1}{\sqrt{3}}\right)b_1=0$$
$$-b_1=-b_2=-b_3=-b_4=-b_5=-b_6=d_1=d_2=d_3=d_4=d_5=d_6=d_7=d_8=d_9=d_{10} \qquad (15)$$

so that, for non-negative vertex weights, all weights with an odd number of equal spin-arguments have to vanish just as in the case of $q=4$. The remaining sixteen weights of the spin-flip symmetric 64-vertex model are constrained by (14) to a ten-dimensional manifold of fixed points.

This general result is now applied to the constrained Ising ferromagnet introduced at the beginning of our letter. Its non-vanishing vertex weights are

$$a=\exp(12K)$$
$$c_1=c_2=c_3=c_4=c_6=c_7=c_9=c_{11}=c_{12}=c_{13}=c_{14}=c_{15}=1 \qquad (16)$$
$$c_5=c_8=c_{10}=\exp(-4K).$$

Fixed points under the generalised weak-graph transformation for this model have to satisfy (14) which in this case reduces to

$$\exp(12K)=4+\exp(-4K) \qquad (17)$$

the only real solution of which is

$$K_f=\tfrac{1}{4}\ln(\sqrt{\tfrac{1}{2}}+\sqrt{\sqrt{2}-\tfrac{1}{2}})=0.12719367\ldots. \qquad (18)$$

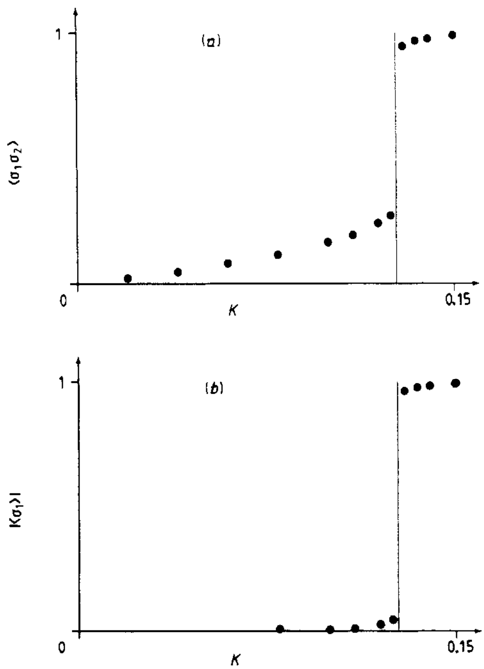


**Figure 3.** Monte Carlo simulation results of the constrained Ising model. The observables shown, plotted against the coupling strength, are ($a$) the nearest-neighbour spin correlation (which is proportional to the internal energy) and ($b$) the magnetisation per spin. The fine vertical line is the location of the coupling strength $K_f$, obtained exactly in this letter. The results indicate a first-order phase transition at this point.

Using standard arguments for fixed points of duality-like transformations we conjecture this value to be the exact location of the phase transition for this model if it exhibits one and only one transition. The results of a (preliminary) Monte Carlo simulation we performed for the constrained Ising model strongly support this conjecture. The internal energy and the magnetisation (normalised to the interval [0, 1]) both seem to have a discontinuity at the expected coupling strength $K_f$ (figure 3). Thus the constrained Ising model undergoes a first-order phase transition at this point.

Finally we show that (14), (15) describe a manifold of phase transitions for a different case, too. The $(q=6)$-vertex model with spin-flip symmetry may be interpreted as a ferroelectric model by the usual transition of terminology from bond spins to arrows on bonds representing electric dipoles. We generalise the ice-rule to the case of $q=6$ by allowing only vertex configurations with exactly three in-going arrows. Thus all vertices of type $b$ and $d$ vanish (i.e. (15) is satisfied) and, in addition,

$$c_1 = c_2 = c_6 = c_{13} = c_{14} = c_{15} = 0. \tag{19}$$

If we associate an energy $E$ (i.e. a weight $\exp(-\beta E)$) with the remaining vertices of type $c$ and zero energy (weight 1) with vertices of type $a$, then (14) yields for this model one fixed point at

$$\beta_f E = \ln 3. \tag{20}$$

That there is indeed a first-order phase transition at this point can be shown by extending a proof by Nagle [6] from $q=4$ to $q=6$ [7]. Thus, in the sector of vertex weights specified above our assumption that phase transition points will be fixed points of the generalised weak-graph transformation, has been explicitly verified.

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