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1986 J. Phys. A: Math. Gen. 19 1701

(http://iopscience.iop.org/0305-4470/19/9/040)

J. Phys. A: Math. Gen. 19 (1986) 1701-1708. Printed in Great Britain

Reentrant transition of the Ising model on the centred square lattice

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Received 31 May 1985

Abstract. The Ising model on the centred square lattice (Union Jack lattice) is studied by Vdovichenko's method, for a more general case than Vaks *et al.* The reentrant transition of the system is interpreted in terms of effective interactions. A method of associating a factor −1 to some corners of a loop in Vdovichenko's method is adopted, by which we can obtain the expression of the free energy by calculating a finite number of determinants which consist only of elements of integers.

1. Introduction

The critical temperature of the Ising model on a two-dimensional lattice can be calculated exactly by Vdovichenko's method (Vdovichenko 1965). The method is useful even when the unit cell of repetition in the system is not small, providing the interactions are only between nearest neighbours. An account of the method, closely following the original, is found in a textbook by Landau and Lifshitz (1968). A detailed proof showing that the method is justified is given in a separate paper (Morita 1986).

With the aid of Vdovichenko's method, Vaks *et al* (1966) and Kitatani *et al* (1985) constructed Ising models which show a reentrant transition. The system studied by Vaks *et al* (1966) is the Ising model on the centred square lattice in which the centre of each plaquette of the square lattice is also a site as shown in figure 1. We shall call the original square lattice sublattice A and the sublattice of the centres sublattice B. We denote the interactions between sites on sublattice A by J_1 and J_2, and the interactions of the centres with others by J_3 and J_4. The lattice has the same translational

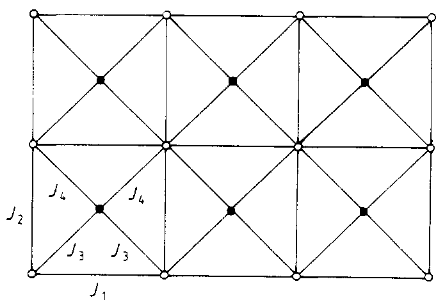


Figure 1. The centred square lattice.

symmetry as the original square lattice. Vaks *et al* (1966) studied the system where $J_2=J_1$ and $J_3=J_4$. We now consider the same system in addition to the system where $J_2=J_1>0$ and $J_4=-J_3<0$. Both systems show a reentrant transition. The purpose of the present paper is to show that this transition can be interpreted in terms of the effective interactions via the centre of the plaquette. In the latter model, the interaction via the centre of the plaquette is antiferromagnetic between horizontal layers on sublattice A and it competes with the ferromagnetic interaction J_2, and there occurs the layered antiferromagnetic (superantiferromagnetic) order.

In § 2, we sketch the method of Vdovichenko (1965) for the Ising model on the square lattice. The method is applied to the system on the centred square lattice in § 3. The effective interactions via the centre of the plaquette are calculated in § 4 and our conclusions are given in § 5.

2. Vdovichenko's method for the square lattice

In Vdovichenko's method, the free energy of an Ising model on a two-dimensional lattice is expressed by a determinant. The determinant is that for the unit matrix minus the matrix which induces directed paths on the lattice. For each step of the path along a bond with interaction J, we have the factor $\tanh \beta J$, where $\beta=1/k_B T$, k_B is the Boltzmann constant and T the temperature. Between each successive pair of steps, we have the factor $\exp(i\theta/2)$ where θ is the angle between the directions of successive steps ($|\theta|<\pi$). This factor $\exp(i\theta/2)$ was introduced to associate the factor -1 with each simple loop (Kac and Ward 1952). Bryksin *et al* (1980) suggested the possibility of associating -1 to some of the successive pairs of steps, e.g. to a step in the right direction either followed by or preceded by a step in the downward direction.

When we have a translational symmetry, we can express the determinant giving the free energy of the system by a product of determinants of a smaller dimension. In the case of the regular Ising model on the square lattice, we have four bonds emanating from a site. The dimension of the smaller determinants is 4×4. In each of these determinants, we have a factor for Fourier transform $p=\exp(2il\pi/L)$, $\bar{p}$, $q=\exp(2im\pi/M)$ or $\bar{q}$ depending on whether the element corresponds to a step in the right, left, up or down direction, where L and M are the total numbers of sites along the horizontal and vertical directions, respectively, on the lattice, and l and m are integers between 0 and $L-1$ and between 0 and $M-1$, respectively. The determinant of the smaller dimension is

$$D(p,q)=\begin{vmatrix} 1-px & -px & 0 & +px \\ -qy & 1-qy & -qy & 0 \\ 0 & -\bar{p}x & 1-\bar{p}x & -\bar{p}x \\ +\bar{q}y & 0 & -\bar{q}y & 1-\bar{q}y \end{vmatrix} \tag{1}$$

where

$$x=\tanh \beta J_x \qquad y=\tanh \beta J_y \tag{2}$$

if J_x and J_y are the interaction of nearest neighbours along the horizontal and the vertical direction, respectively.

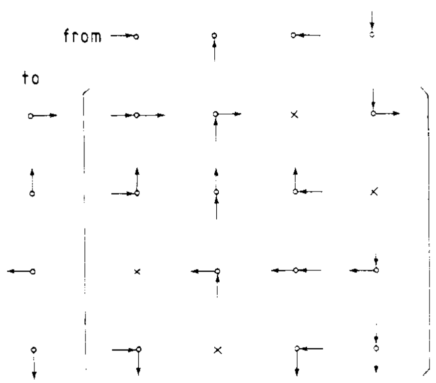


Figure 2. Matrix elements represent an addition of a step of the path. The columns from the left are for the preceding step of right, up, left and down direction, respectively, and the rows from the top are for the succeeding step of right, up, left and down direction, respectively.

Each element in (1) corresponds to a successive pair of steps on the path as shown in figure 2. Equation (1) is rewritten as

$$D(p,q)=x^2y^2\begin{vmatrix} X & 1 & 0 & -1 \\ 1 & Y & 1 & 0 \\ 0 & 1 & \bar{X} & 1 \\ -1 & 0 & 1 & \bar{Y} \end{vmatrix} \tag{3}$$

where

$$X=-(1/px)+1 \qquad Y=-(1/qy)+1. \tag{4}$$

Note that 0 in (3) shows that a doubling back is not allowed in the path, and -1 are the factors giving the factor -1 for each loop.

In the thermodynamic limit of $L\to\infty$ and $M\to\infty$, the free energy per site f is given by

$$-\beta f=\ln 2+\ln\cosh\beta J_x+\ln\cosh\beta J_y$$
$$+\frac{1}{4\pi^2}\int_0^{2\pi}d\theta\int_0^{2\pi}\mathrm{d}\phi\,\tfrac{1}{2}\ln D(\mathrm{e}^{\mathrm{i}\theta},\mathrm{e}^{\mathrm{i}\phi}). \tag{5}$$

The phase transition occurs at the temperature where the determinant (3) is zero for a pair of p and q with $|p|=|q|=1$. The corresponding values of p and q give the pitch of the ordered phase. For the ferromagnetic case, $p=q=1$. For the antiferromagnetic case, $p=q=-1$. For the layered antiferromagnetic case, $p=-q=1$ or $p=-q=-1$. Determinant (3) is expressed as

$$D(p,q)=x^2y^2\{(|X||Y|-2)^2+[4|X||Y|-(X+\bar{X})(Y+\bar{Y})]\} \tag{6}$$

which becomes zero when

$$X=\bar{X} \qquad Y=\bar{Y} \qquad \text{and} \qquad XY=2. \tag{7}$$

From (4) and (7), we obtain the transition temperature and the ordered phase.

3. Vdovichenko's method for the centred square lattice

In the model of figure 1, we have eight bonds emanating from a site of sublattice A and four bonds from a site of sublattice B. We order the 8+4 steps along those bonds as in figure 3. In the present case, the determinant of the smaller dimension, corresponding to (3), is one of 12×12 and is written as

$$D(p,q)=x^2y^2z^4z'^4\begin{vmatrix} X & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 \\ 1 & Y & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & -1 \\ 0 & 1 & \bar{X} & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ -1 & 0 & 1 & \bar{Y} & 0 & 0 & 0 & 0 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & Z_1 & 0 & 0 & 0 & 1 & 1 & 0 & -1 \\ 1 & 1 & 1 & 1 & 0 & Z_2 & 0 & 0 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 & 0 & 0 & Z_2' & 0 & 0 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 & 0 & 0 & 0 & Z_1' & -1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & -1 & \overline{Z_2'} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & \overline{Z_1'} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & \overline{Z_1} & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 & 1 & 0 & 0 & 0 & \overline{Z_2} \end{vmatrix} \tag{8}$$

where

$$\begin{aligned} &X=-(1/px)+1 && Y=-(1/qy)+1 \\ &Z_1=-(1/pqz) && Z_2=-(1/qz) \\ &Z_1'=-(1/pz') && Z_2'=-(1/z') \end{aligned} \tag{9}$$

$$\begin{aligned} &x=\tanh\beta J_1 && y=\tanh\beta J_2 \\ &z=\tanh\beta J_3 && z'=\tanh\beta J_4. \end{aligned} \tag{10}$$

The factor -1 is introduced for an addition of each of the steps shown in figure 4. There are 2^{12} determinants which are obtained by replacing the diagonal elements with

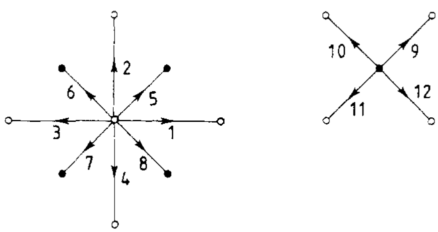


Figure 3. Twelve kinds of steps on the centred square lattice. Steps 1-8 are from a site on sublattice A and steps 9-12 are from a site on sublattice B.

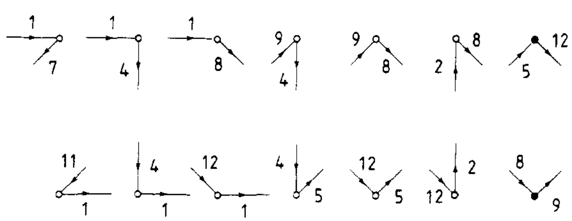


Figure 4. The additions of a step which has a downward component is preceded by one not having a downward component and has a direction rotated clockwise less than 180° from the preceding one, and the inverse additions of these steps.

0 or 1. All of them are calculated, and the result is used to give the following explicit form of $D(p, q)$:

$$
\begin{aligned}
D(e^{i\theta}, e^{i\phi}) = {} & \{(1+x)[4zz'+y(1+z^2)(1+z'^2)]-(1-x)(1-z^2)(1-z'^2)\}^2 \\
& +2(1-x^2)[4zz'+y(1+z^2)(1+z'^2)](1-z^2)(1-z'^2)(1-\cos\phi) \\
& +2(1-y^2)[(z+z')^2+x(1+zz')^2][(1-zz')^2+x(z-z')^2](1-\cos\theta) \\
& -4(1-x^2)(1-y^2)zz'(1-z^2)(1-z'^2)(1-\cos\phi)(1-\cos\theta).
\end{aligned} \tag{11}
$$

The free energy per pair of sites f is given by

$$
\begin{aligned}
-\beta f = {} & \ln 2+\ln\cosh\beta J_1+\ln\cosh\beta J_2+2\ln\cosh\beta J_3+2\ln\cosh\beta J_4 \\
& +\frac{1}{4\pi^2}\int_0^{2\pi} d\theta \int_0^{2\pi} d\phi\, \tfrac{1}{2}\ln D(e^{i\theta}, e^{i\phi}).
\end{aligned} \tag{12}
$$

When $z=z'$ and $x=y$, this expression reduces to the one obtained by Vaks *et al* (1966).

In the cases of $p=1$, $q=\pm1$, the determinant is expressed as follows:

$$D(1, \pm1)=\{(1+x)[4zz'+y(1+z^2)(1+z'^2)]\mp(1-x)(1-z^2)(1-z'^2)\}^2. \tag{13}$$

At the zero of these expressions, the phase transitions to the ferromagnetic and the layered antiferromagnetic order, respectively, occur.

In the case of $p=q=-1$,

$$D(-1, -1)=\{(1+x)[(1+z^2)(1+z'^2)+4yzz']+(1-x)y(1-z^2)(1-z'^2)\}^2. \tag{14}$$

At the zero of this expression, the phase transition to the antiferromagnetic state occurs.

We now examine the systems with $x=y$ and $z'=\pm z$.

(*a*) *Ferromagnetic transition when $J_4=J_3$*

Putting $x=y=\tanh\beta J_1$ and $z=z'=\tanh\beta J_3$, the zero of (13) with the upper sign gives

$$\tanh^2\beta J_3=\frac{4-8^{1/2}(1+x)}{1-2x-x^2}-1. \tag{15}$$

Calculating J_3/J_1 for given values of $k_B T_c/J_1$, we obtain the curve for the part of $J_4/J_1=J_3/J_1>0$ in figure 5(*a*) and the curve between the paramagnetic phase (P) and ferromagnetic phase (F) in figure 6(*a*).

(*b*) *Ferromagnetic transition when $J_4=-J_3$*

Putting $x=y=\tanh\beta J_1$ and $z=-z'=\tanh\beta J_3$, the zero of (13) with the upper sign gives

$$\tanh^2\beta J_3=\frac{[8x(1-x^2)]^{1/2}-4x}{1-2x-x^2}-1. \tag{16}$$

The boundary between P and F in the region of $J_4/J_1<0$ in figure 5(*a*) is plotted as the solution of (16).

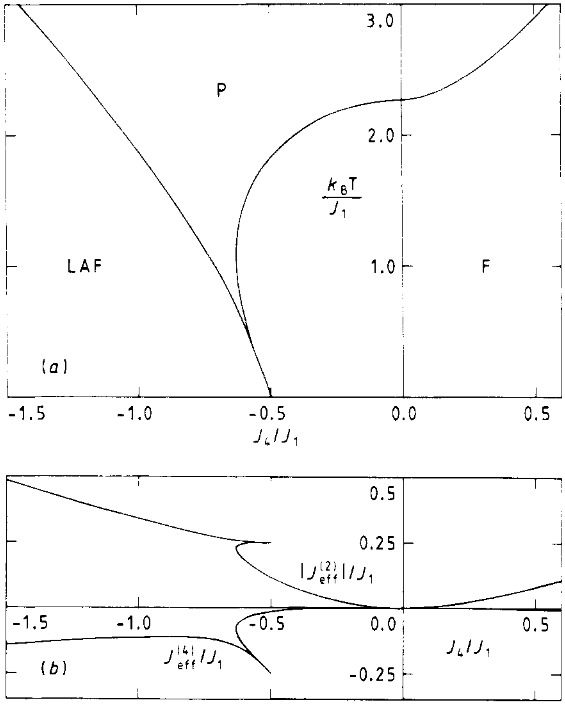


Figure 5. (a) The transition temperatures as a function of J_4/J_1, where $J_2=J_1>0$ and $J_3=\pm J_4>0$. P, F and LAF denote the paramagnetic, ferromagnetic and layered antiferromagnetic phases, respectively. (b) Effective two- and four-spin interactions between the corners on a plaquette, via the centre of the plaquette, along the transition lines.

(c) *Antiferromagnetic transition when $J_4=-J_3$*

When $J_2=J_1>0$, the antiferromagnetic transition occurs only when J_3 and J_4 are of opposite signs. Now we put $q=-1$ and $J_4=-J_3$ and hence $x=y=\tanh\beta J_1$, $z=-z'=\tanh\beta J_3$. The zero of (13) with the lower sign gives

$$\tanh^2\beta J_3=\frac{4-[8(1-x^2)]^{1/2}}{1+x^2}-1. \tag{17}$$

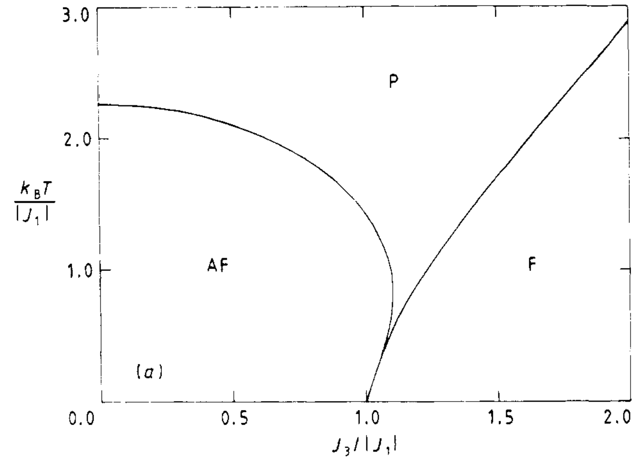
The boundary of the paramagnetic phase (P) and the layered antiferromagnetic phase (LAF) in figure 5(a) is obtained as a solution of (17).

(d) *Antiferromagnetic transition when $J_4=J_3$, $J_2=J_1<0$*

This transition is obtained by putting $x=y=\tanh\beta J_1$ and $z=z'=\tanh\beta J_3$. The zero of (14) gives

$$\tanh^2\beta J_3=-\frac{4x^2+8^{1/2}x(1+x)}{1+2x-x^2}-1. \tag{18}$$

The boundary of the paramagnetic phase (P) and the antiferromagnetic phase (AF) in figure 6(a) is obtained as the solution of (18).



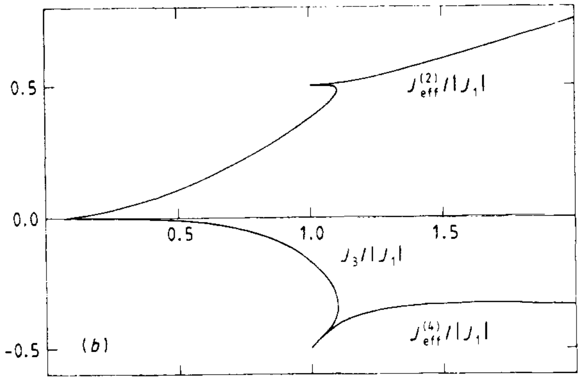


Figure 6. (*a*) The transition temperatures as a function of $J_3/|J_1|$, where $J_2 = J_1 < 0$ and $J_3 = J_4 > 0$. AF denotes the antiferromagnetic phase. (*b*) Effective two- and four-spin interactions between the corners of a plaquette, via the centre of the plaquette, along the transition line.

4. Effective interactions

If we take the summation with respect to the spin variables for the sites at the centres of the plaquettes on the square lattice, we can regard the system as an Ising model on the square lattice, where every pair and all four of the corners of a plaquette have an effective interaction. When $J_4 = J_3$, these interactions $J_{\text{eff}}^{(2)}$ and $J_{\text{eff}}^{(4)}$ are given by

$$\exp[\beta J_{\text{eff}}^{(2)}(s_1s_2 + s_1s_3 + s_1s_4 + s_2s_3 + s_2s_4 + s_3s_4) + \beta J_{\text{eff}}^{(4)} s_1s_2s_3s_4]$$
$$= C \sum_{s'=\pm 1} \exp[\beta J_3 s'(s_1 + s_2 + s_3 + s_4)] \tag{19}$$

where C is a constant, and s_1, s_2, s_3 and s_4 take the values ± 1. The values of the effective interactions are functions of J_3 and the temperature T.

For the case of $J_4 = -J_3$, the values $J_{\text{eff}}^{(2)}$ and $J_{\text{eff}}^{(4)}$ along the transition lines are plotted in figure 5(*b*). $J_{\text{eff}}^{(2)}$ between the corners on different layers must be taken to be of minus sign. In this case, we shall disregard the effects of $J_{\text{eff}}^{(4)}$, since it favours equally the ferromagnetic phase and the antiferromagnetic or layered antiferromagnetic phase.

We notice that the value of $J^{(2)}_{\text{eff}}/J_1$ is nearly equal to -0.25 around the point $k_B T/J_1 \sim 0$ and $J_4/J_1 \sim -0.5$. For each plaquette, there are four pairs of corners on different layers. The value $J^{(2)}_{\text{eff}}/J_1 \times 4$ just offsets the value $J_2/J_1 = 1$, resulting in the reentrant transition to the paramagnetic phase and then to the antiferromagnetic phase, as the temperature is lowered when $J_4/J_1 \leqslant -0.5$.

For the case of $J_4 = J_3$ and $J_2 = J_1 < 0$, the effective interactions are plotted in figure 6(*b*). At $J_3/|J_1| \geqslant 1.0$, $J^{(2)}_{\text{eff}}/|J_1|$ become 0.5 at very low temperatures. There are two effective interactions between a nearest-neighbour pair of sites on sublattice A and hence the value 0.5 just offsets $J_2/|J_1| = -1$, causing the reentrant transition from the antiferromagnetic state to the paramagnetic and then to the ferromagnetic state as the temperature is lowered.

5. Conclusion

The exact expression for the free energy of the Ising model on the centrec square lattice is obtained for a more general case than the case studied by Vaks *et ıl* (1966) by the method of Vdovichenko (1965). In the calculation, we compute $2^{1\cdot}$ 1.terminants with elements of integers. We see that the system with competing interactions also shows a reentrant transition in a different situation. Ve see that the reentrant transition occurs when the effective pair interactions via the centre of a plaquette exactly cancel the interaction J_2.

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