

Justification of Vdovichenko's method for the Ising model on a two-dimensional lattice

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1986 J. Phys. A: Math. Gen. 19 1197

(<http://iopscience.iop.org/0305-4470/19/7/021>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 31/05/2010 at 10:58

Please note that [terms and conditions apply](#).

Justification of Vdovichenko's method for the Ising model on a two-dimensional lattice

T Morita

Department of Engineering Science, Faculty of Engineering Tohoku University, Sendai 980, Japan

Received 29 August 1985

Abstract. A detailed proof is presented of Vdovichenko's method giving an exact expression of the free energy of the Ising model on a two-dimensional lattice.

1. Introduction

Kac and Ward (1952) suggested that the exact expression of the free energy of the Ising model on the square lattice, first given by Onsager (1944), is obtained with the aid of a determinant of a matrix inducing the random walk on the lattice. Vdovichenko (1965) gave a method showing that the exact analytic expressions of the free energy obtained in that method are exact for the finite and infinite Ising models. His argument is easy to apply for systems on a two-dimensional lattice even with a large unit cell, and it was taken up by a number of authors (Vaks *et al* 1966, Bryksin *et al* 1980, Kitatani *et al* 1985, Morita 1986). However, it is not easy to see that the method should give exact results. In particular, in the part of his arguments showing cancellations of some diagrams, only simple examples were worked out and their validity for a general case is far from obvious. No discussion was given of the convergence of some limits. Landau and Lifshitz (1968) gave an account of the method in a textbook, but it simply follows the original. The purpose of the present paper is to give a detailed proof showing that his results are exact for finite and infinite systems.

We consider a finite lattice of N lattice sites on a two-dimensional lattice. There is a spin on each lattice site, and the exchange integral between the j th and k th sites is denoted by J_{jk} . It is non-zero only when they are nearest neighbours of each other.

The partition function Z of the system is expressed as follows:

$$\begin{aligned} Z &= \text{Tr} \exp(-\beta H) = \text{Tr} \prod_{(j,k)} \exp(J_{jk} s_j s_k) \\ &= \prod_{(j,k)} \cosh(\beta J_{jk}) \text{Tr} \prod_{(j,k)} [1 + s_j s_k \tanh(\beta J_{jk})], \end{aligned} \quad (1)$$

where the products are over all the pairs of nearest-neighbour lattice sites on the lattice and s_j is the spin variable for the j th site. $\beta = 1/k_B T$, k_B is the Boltzmann constant and T is the temperature. Taking the trace after expanding the last product, we have

$$Z = 2^N \prod_{(j,k)} \cosh(\beta J_{jk}) Z_1(1), \quad (2)$$

where

$$Z_1(t) = 1 + \{\text{the sum of all those single-bonded diagrams on the lattice, that each lattice site is connected to none or an even number of bonds connecting nearest-neighbour sites}\}. \tag{3}$$

A diagram in (3) denotes the product of the factors $\tanh(\beta J_{jk})t$ for (j, k) bonds in it. A parameter t is introduced for the convenience of the proof. An example of the diagrams is shown in figure 1(a).

We follow Vdovichenko (1965) and first show that the sum in (3) is expressed in terms of a sum of connected diagrams in § 2, and then this sum in terms of a determinant of a matrix inducing random walks on the lattice in § 3. In § 4, we assume a translational symmetry and obtain the result in terms of a product of small determinants, and then we can take the thermodynamic limit. Section 5 contains the conclusions. The convergence of a series is proved in appendix 1 and the eigenvalues of a matrix are estimated in appendix 2.

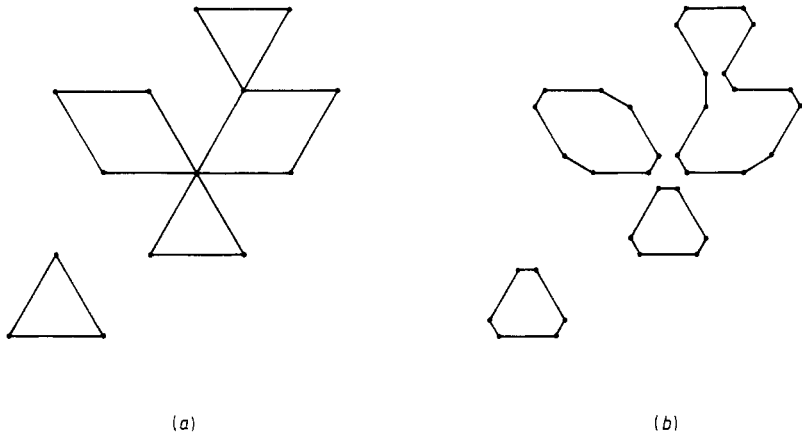


Figure 1. (a) A diagram in the sum of (3) for the system on the triangular lattice. (b) The corresponding term in (4).

2. Expression in terms of connected diagrams

In this section, a diagram is either a loop or a product of loops on a finite lattice. A loop here is via lattice sites and bonds, each connecting a pair of nearest-neighbour lattice sites on the lattice, where the same site or the same pair of sites may be passed an arbitrary number of times. We denote the total number of nearest-neighbour lattice sites on the lattice by M . For a diagram, we shall denote the total number of bonds between the i th pair of nearest-neighbour lattice sites by m_i . The diagram is said to be characterised by the set $\{m_i\}$ of M values m_1, m_2, \dots, m_M . A diagram characterised by the set $\{m_i\}$ is said to be labelled when the m_i bonds are labelled by $1, 2, \dots, m_i$ for each i for which $m_i \geq 2$. Let us label all the bonds of an unlabelled diagram in $\prod_{i=1}^M m_i!$ ways. If there appear N_D distinctive labelled diagrams, the number $\prod_i m_i! / N_D$ is said to be the symmetry number of the unlabelled diagram. The symmetry number for a labelled diagram is one. A diagram in this section represents a product of three factors:

- (i) +1 or -1 according as the parity of the number of crossings of lines is even or odd;
- (ii) the product of $(x_i t)^{m_i}$ for i th pair of nearest neighbours, where $x_i = \tanh(\beta J_{jk})$ if the i th pair is between j th and k th sites;
- (iii) the inverse of the symmetry number.

Here we shall express $Z_1(t)$ given by (3) in terms of loops:

$$Z_1(t) = 1 + \sum_{m_1=0}^1 \sum_{m_2=0}^1 \dots \sum_{m_M=0}^1 S_1\{m_i\}, \tag{4}$$

where

$S_1\{m_i\} = \{$ a product of loops, if such is obtained by drawing a bond between the i th pair if $m_i = 1$, and then connecting them at the edge sites pairwise, in such a way that no crossing occurs, and zero if otherwise $\}$. (5)

In fact, if we connect the bonds at a site next with next, we get such a product from each diagram in the sum of (3); see figure 1(b).

The purpose of this section is to show that $Z_1(t)$ is equal to $Z_2(t)$ which is defined by

$$Z_2(t) = \exp\{\text{the sum of all the loops}\}. \tag{6}$$

In order to confirm this, the exponential is expanded. We denote the sum of all the terms characterised by the same set of $\{m_i\}$ in this expansion by $S_2\{m_i\}$, and put

$$Z_2(t) = 1 + \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \dots \sum_{m_M=0}^{\infty} S_2\{m_i\} \tag{7}$$

$S_2\{m_i\} = \{$ the sum of all the distinct unlabelled diagrams consisting of loops, characterised by the set $\{m_i\}$ $\}$. (8)

Note here that the factorials which occur in the expansion are included in the symmetry number for diagrams. We now show that this sum is zero if there is an i for which m_i is two or more, and that it is equal to one diagram $S_1\{m_i\}$ if all m_i are zero or one. Vdovichenko (1965) and Landau and Lifshitz (1968) gave some arguments to suggest these, which are elaborated here.

When we consider a sum of unlabelled diagrams, which represents a factor divided by the symmetry number, it is convenient to express it in the form of a sum of labelled diagrams. If an unlabelled diagram in (8) is characterised by $\{m_i\}$ and its symmetry number is S_N , its contribution is

$$\frac{1}{S_N} (\pm 1) \prod_{i=1}^M (x_i t)^{m_i} = \frac{1}{\prod_i m_i!} \frac{\prod_i m_i!}{S_N} (\pm 1) \prod_{i=1}^M (x_i t)^{m_i},$$

which is equal to the sum of all the $\prod_i m_i! / S_N$ distinct labelled diagrams obtained from it, divided by $\prod_i m_i!$. Hence (8) is rewritten as follows:

$$S_2\{m_i\} = \frac{1}{\prod_i m_i!} \{ \text{the sum of all the distinct labelled diagrams of loops, characterised by the set } \{m_i\} \}. \tag{9}$$

We next note that we can obtain all the diagrams in the sum of (9) if we write m_i labelled bonds between the i th pair of nearest neighbours, and connect the edges of the bonds at each site in all the possible ways; see figure 2.

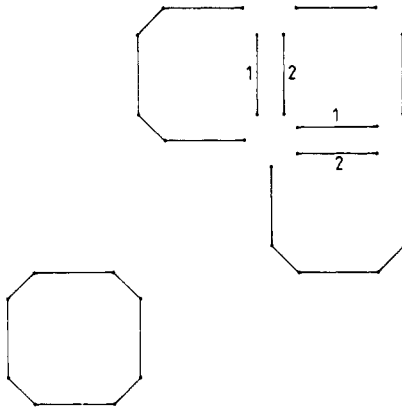


Figure 2. A labelled diagram on the square lattice. $m_i = 2$ for two i , $m_i = 1$ for twelve i and $m_i = 0$ for all other i . The bonds for $m_i = 2$ are labelled by 1 or 2, and all the summands for this $\{m_i\}$ are obtained by connecting the edges of the bonds at each site pairwise in such a way that the bonds for the same pair of sites must not be connected at an edge with each other.

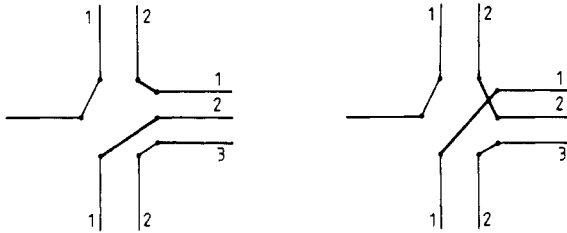


Figure 3. There are eight bonds meeting at a site. The two diagrams in which the connections of the two right bonds labelled by 1 and 2 are exchanged cancel with each other.

We first consider a case where m_i for a pair i of nearest neighbours is two or more; see figure 3. Let us pay attention to a site which is an edge of the i th pair. The edges of the first two of m_i bonds, labelled by 1 and 2, for the i th pair must be connected with other edges of bonds entering the same site. For each of these connections there exists another connection in which the connections are exchanged. The exchange of these connections results in a change of parity of the number of crossings, and the contributions of two diagrams which are different only in these connections cancel with each other. Thus we have $S_2\{m_i\} = 0$ if there exists a pair i of sites for which $m_i \geq 2$.

We now consider a case where m_i is zero or one for all i . We pay attention to a site which connects four or more bonds. We assume that the number is $2m_i$; an example of $2m_i = 6$ is given in figure 4. We label them 1, 2, ..., $2m_i$, in such a way that 1 and 2, 3 and 4, ..., are connected at that site in the diagram $S_1\{m_i\}$. We then ask whether the bonds 1 and 2 in a diagram in $S_2\{m_i\}$ are connected at that site with each other. If not, there exists a diagram in which the connections of 1 and 2 are exchanged at the site. Their contributions cancel with each other. If 1 and 2 are connected, we ask whether 3 and 4 are connected. If not we conclude it cancels with another. If all the pairs 1 and 2, 3 and 4, ..., are connected with each other, then we ask the same thing at another site. After we discard all the cancelled contributions, we are left with one diagram $S_1\{m_i\}$ in the sum $S_2\{m_i\}$ when $m_i = 0$ or 1 for all i . Thus we confirm the desired equality $S_1\{m_i\} = S_2\{m_i\}$, and hence $Z_1(t) = Z'_2(t)$.

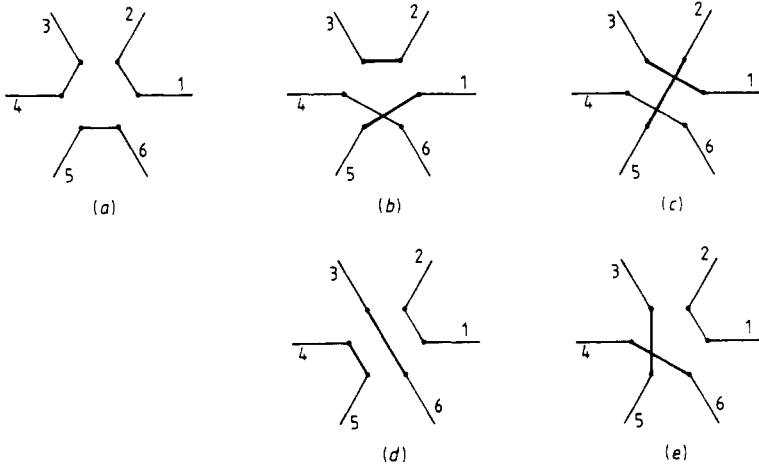


Figure 4. (a) is left uncanceled. (b) and (c) cancel with each other if the connections at the other sites are identical. (d) and (e) cancel with each other.

What remains to be shown is that the quantity $Z_1(t) = Z_2'(t)$ is equal to the limit $Z_2(t)$, which is proven in appendix 1, for t with an absolute value less than $1/2M$.

3. Expression in terms of a determinant

In the preceding section, diagrams are loops of bonds without direction, and their products. We now consider two directions for a bond connecting a pair of nearest-neighbour lattice sites. We call them steps. Since we distinguish them, we have $2M$ kinds of steps. They are labelled by i and i' in this section. A random walk via these steps returning to the starting point is called a directed loop. The diagrams in the present section are directed loops and their products. Equation (6) now reads

$$Z_2(t)^2 = \exp\{\text{the sum of all the directed loops}\}, \tag{10}$$

since we have two loops which are different only in direction, in the present sum.

We introduce a $2M \times 2M$ matrix Λ which induces the random walks. The (i, i') element $a_{i,i'}$ of Λ is

$$a_{i,i'} = x_i \theta_{i,i'} \tag{11}$$

if the step i can follow i' and $|\phi_{i,i'}| < \pi$, and $a_{i,i'} = 0$ otherwise, where $\phi_{i,i'}$ is the angle of the direction of the step i relative to the direction of i' , and $|\phi_{i,i'}| \leq \pi$ and $\theta_{i,i'} = \exp(i\phi_{i,i'}/2)$; here the imaginary unit i must not be confused with the label of a step.

We now consider $\text{Tr } \Lambda^n$ which is expressed as follows:

$$\text{Tr } \Lambda^n = \{\text{the sum of all the distinctive labelled directed loops of } n \text{ steps,} \\ \text{labelled by } 1, 2, \dots, \text{ and } n \text{ along the direction}\}. \tag{12}$$

When we label an unlabelled directed loop along the direction, we have $n/(\text{symmetry number})$ distinct ways, and hence we have

$$\frac{1}{n} \text{Tr } \Lambda^n = \{\text{the sum of all the unlabelled directed loops of } n \text{ steps}\}. \tag{13}$$

The contribution of a diagram in (12) is a product of two factors:

(i') the product of $\theta_{i,r}$ which gives rise to the factor $(-1)^{r+1}$, when there are r crossings;

(ii') the product of x_i for bonds.

See Kac and Ward (1952) and Vdovichenko (1965) for the fact (i'). For a diagram in (13), we have an additional factor:

(iii) the inverse of the symmetry number.

Compared with (i) and (ii) for the contribution of the same diagram in (10), the sign is different in (i') and the factor t is missing for each of n steps in (ii'). Hence we have

$$Z_2(t)^2 = \exp\left(-\sum_{n=1}^{\infty} \frac{1}{n} \text{Tr} \Lambda^n t^n\right) = \exp\left(-\sum_{n=1}^{\infty} \frac{1}{n} \sum_{k=1}^{2M} \lambda_k^n t^n\right)$$

where λ_k is the k th eigenvalue of the matrix Λ . In appendix 2, we show that $|\lambda_k| < 2M$ for all k , so that the last summation is absolute convergent when $|t| < 1/2M$ and then the exchange of the two summations in the last term of the preceding equation is allowed. As a result, we get

$$Z_2(t)^2 = \exp\left(\sum_{k=1}^{2M} \ln(1 - \lambda_k t)\right) = \prod_{k=1}^{2M} (1 - \lambda_k t) = \det(\mathbf{I} - \Lambda t), \tag{14}$$

where \mathbf{I} is the unit matrix of order $2M$.

Since we have proved that $Z_1(t) = Z_2(t)$ for $|t| < 1/2M$, we now have

$$Z_1(t)^2 = \det(\mathbf{I} - \Lambda t) \tag{15}$$

for these t . Since both sides are polynomials of variable t of degree $2M$ or less and hence they are entire functions of t if we regard them as functions of a complex variable t , and they are equal to each other for a region $|t| < 1/2M$, they are identical for all t values by the identity theorem (Titchmarsh 1968).

4. Expression in terms of small determinants

In the present section, we consider a system which consists of N' unit cells, and there are $z/2$ pairs of nearest neighbours per unit cell, so that $2M = N'z$ kinds of steps in the system. When the step i represents a μ th step for the j th unit cell, i is denoted by $j\mu$. The exchange integral between the two sites connected by the step $j\mu$ is denoted by $J_{j\mu}$ in this section. The matrix element $t_{j\mu, k\nu}$ of $\mathbf{I} - \Lambda$ is given by

$$\begin{aligned} t_{j\mu, k\nu} &= 1 && \text{if } j\mu = k\nu, \\ t_{j\mu, k\nu} &= -\tanh(\beta J_{j\mu}) \theta_{\mu\nu} \end{aligned} \tag{16}$$

if the step $j\mu$ can follow $k\nu$ and $|\phi_{\mu\nu}| < \pi$, and it is 0 otherwise, where $\phi_{\mu\nu}$ is the direction of the step $j\mu$ relative to the direction of $k\nu$, and $|\phi_{\mu\nu}| \leq \pi$ and $\theta_{\mu\nu} = \exp(i\phi_{\mu\nu}/2)$.

The next step in Vdovichenko's argument is to call attention to the fact that $\det(\mathbf{I} - \Lambda)$ can be expressed as a product of small determinants, when we adopt a periodic boundary condition on the lattice. The representative position of the j th cell is denoted by \mathbf{R}_j . We consider N' wavevectors \mathbf{Q} for which $\exp(i\mathbf{Q} \cdot \mathbf{R})$ is periodic with respect to the representative position \mathbf{R} of a unit cell. We introduce $N'z \times N'z$ matrices Ψ , $\tilde{\Psi}'$ and $\tilde{\mathbf{T}}$ as follows. The $(\mathbf{Q}\mu, j\mu')$ element of Ψ and the $(k\nu, \mathbf{Q}\nu')$ element of $\tilde{\Psi}'$ are

given by

$$(1/\sqrt{N'}) \exp(i\mathbf{Q} \cdot \mathbf{R}_j) \delta_{\mu,\mu'}, \quad (1/\sqrt{N'}) \exp(-i\mathbf{Q} \cdot \mathbf{R}_k) \delta_{\nu,\nu'}, \quad (17)$$

respectively, and $\tilde{\mathbf{T}}$ is given by a product of the matrices:

$$\tilde{\mathbf{T}} = \Psi(\mathbf{I} - \Lambda)\tilde{\Psi}'. \quad (18)$$

The $(\mathbf{Q}\mu, \mathbf{Q}'\nu)$ element of $\tilde{\mathbf{T}}$ is given by

$$\delta_{\mathbf{Q},\mathbf{Q}'} \tilde{t}_{\mu\nu}(\mathbf{Q}) \quad (19)$$

where

$$\begin{aligned} \tilde{t}_{\mu\nu}(\mathbf{Q}) &= \sum_j t_{j\mu,k\nu} \exp[i\mathbf{Q} \cdot (\mathbf{R}_j - \mathbf{R}_k)] \\ &= \begin{cases} \delta_{\mu,\nu} - \tanh(\beta J_{j\mu}) \exp[i\mathbf{Q} \cdot (\mathbf{R}_j - \mathbf{R}_k)] \theta'_{\mu\nu} & (|\phi_{\mu\nu}| < \pi), \\ 0 & (|\phi_{\mu\nu}| = \pi). \end{cases} \end{aligned} \quad (20)$$

In the last term of (20), if there exist such a pair of j and k that the step $j\mu$ can follow $k\nu$, $\theta'_{\mu\nu} = \theta_{\mu\nu}$ and j and k are this pair, and if otherwise, $\theta'_{\mu\nu} = 0$.

Now that the product $\Psi\tilde{\Psi}'$ is a unit matrix, we have

$$\det(\mathbf{I} - \Lambda) = \det(\tilde{\mathbf{T}}). \quad (21)$$

Since $\tilde{\mathbf{T}}$ takes the form (19), $\det(\tilde{\mathbf{T}})$ is equal to the product of the small determinants of $z \times z$ matrices ($\tilde{t}_{\mu\nu}(\mathbf{Q})$) for N' values of \mathbf{Q} :

$$\det(\mathbf{I} - \Lambda) = \prod_{\mathbf{Q}} \det(\tilde{t}_{\mu\nu}(\mathbf{Q})). \quad (22)$$

Now, using this result (22) in (2) and (15), we have

$$\frac{1}{N'} \ln Z = \frac{N}{N'} \ln 2 + \frac{1}{2} \sum_{\mu=1}^z \ln \cosh(\beta J_{j\mu}) + \frac{1}{2N'} \sum_{\mathbf{Q}} \ln \det(\tilde{t}_{\mu\nu}(\mathbf{Q})). \quad (23)$$

In the second term on the right-hand side, we have a factor $\frac{1}{2}$ since the summation is taken for steps and hence the same pair of lattice sites is covered twice.

5. Conclusion

Equation (23) is the desired result. The notation occurring in it is explained in § 4. In the preceding sections, (23) is shown to be exact for a finite Ising model on a two-dimensional lattice, when a periodic boundary condition is assumed. The thermodynamic limit $N' \rightarrow \infty$ in the van Hove sense changes the summation with respect to \mathbf{Q} divided by N' into an integral.

The factor $\theta_{\mu\nu}$ induces a factor -1 to each crossing of closed random walks. This results in the cancellation of unnecessary loops which appear because of the definition of determinant (Kac and Ward 1952, Vdovichenko 1965). Bryksin *et al* (1980) suggested the possibility of associating -1 with some of the successive pairs of steps, e.g. with the step of the right direction either followed by or preceded by a step in the downward direction, in the case of the square lattice. Then $\theta_{\mu\nu}$ is put equal to -1 for these steps

and 1 for the other steps. As a result, we can obtain an analytic expression of the free energy by calculating a number of determinants of elements 0, 1 or -1 (Morita 1986).

Appendix 1. The convergence of (6) to (4)

Equation (6) is written as

$$\exp\left(\sum_{n=1}^{\infty} a_n t^n\right) \tag{A1.1}$$

and (4) is written as

$$1 + \sum_{m=1}^M b_m t^m. \tag{A1.2}$$

The argument in § 2 shows that, if we expand (A1.1) in powers of t and compare with (A1.2), we obtain the equalities

$$\sum_{\{n_k\}}^* \left(\prod_{k=1}^m n_k!\right)^{-1} a_k^{n_k} = \begin{cases} b_m & (m = 1, 2, \dots, M), \\ 0 & (m = M + 1, M + 2, \dots), \end{cases} \tag{A1.3}$$

where the asterisk (*) indicates the restriction $\sum_{k=1}^m kn_k = m$ for the summation. a_n is estimated as

$$|a_n| < M^n, \tag{A1.4}$$

considering that it is a sum of loops of n bonds on the lattice of M pairs of nearest neighbours, and that the absolute value of the factor, excluding t , for a bond is less than unity.

For an integer K greater than M , we have

$$\begin{aligned} & \left| \exp\left(\sum_{n=1}^K a_n t^n\right) - 1 - \sum_{m=1}^M b_m t^m \right| \\ &= \left| \prod_{n=1}^K \exp(a_n t^n) - 1 - \sum_{m=1}^M b_m t^m \right| \\ &= \left| \sum_{m=K+1}^{\infty} \left(\sum_{\{n_k\}^\dagger} \prod_k \frac{a_k^{n_k}}{n_k!}\right) t^m \right| < \sum_{m=K+1}^{\infty} (2M|t|)^m, \end{aligned} \tag{A1.5}$$

where the dagger (†) denotes the restriction $\sum_{k=1}^K kn_k = m$ for the summation. Here (A1.3) and (A1.4) are used and the number of those ways of distributing m indistinguishable objects for which n_k boxes include k objects for $k = 1, 2, \dots$, and K , is overestimated by 2^m . If $|t| < 1/2M$, this quantity tends to zero as $K \rightarrow \infty$. This shows that the limit (A1.1) exists and is equal to (A1.2) if $|t| < 1/2M$.

Appendix 2. Estimate of the eigenvalues of a matrix

When (x_j) is a normalised eigenvector of an $n \times n$ matrix (a_{ij}) and λ is the corresponding

eigenvalue

$$\sum_{j=1}^n a_{ij}x_j = \lambda x_i \quad i = 1, 2, \dots, n,$$

$$\sum_{i=1}^n \bar{x}_i x_i = 1.$$

Multiplying the first equation by \bar{x}_i and summing with respect to i , we have

$$\lambda = \sum_{i=1}^n \sum_{j=1}^n a_{ij} \bar{x}_i x_j.$$

If we regard the right-hand side as a scalar product of two vectors (a_{ij}) and $(\bar{x}_i x_j)$ of n^2 elements, the Schwarz inequality gives us

$$|\lambda|^2 \leq \sum_{i=1}^n \sum_{j=1}^n a_{ij}^2. \quad (\text{A2.1})$$

If $|a_{ij}| < a_M$, this gives

$$|\lambda| < na_M. \quad (\text{A2.2})$$

Λ in § 3 is a $2M \times 2M$ matrix of elements given by (11), so that $n = 2M$ and $a_M = 1$ and the absolute value of an eigenvalue λ_k of Λ is less than $2M$.

Note added in proof. The proofs in the text are performed for a system in a plane. We would get Onsager's result if we could apply (23) to a system satisfying a periodic boundary condition in two directions, which is a system with nearest-neighbour interactions on a torus but not in a plane. We need some more arguments to complete the justification of Vdovichenko's method. This will be taken up in a future paper.

References

- Bryksin V V, Gol'tsev A Yu and Kudinov E E 1980 *J. Phys. C: Solid State Phys.* **13** 5999-6007
 Kac M and Ward J C 1952 *Phys. Rev.* **88** 1332-7
 Kitatani H, Miyashita S and Suzuki M 1985 *Phys. Lett.* **108A** 45-9
 Landau L D and Lifshitz E M 1968 *Statistical Physics* 2nd edn (Oxford: Pergamon) pp 447-54
 Morita T 1986 *J. Phys. A: Math. Gen.* **19** to appear
 Onsager L 1944 *Phys. Rev.* **65** 117-49
 Titchmarsh E C 1968 *The Theory of Functions* 2nd edn (Oxford: Oxford University Press) pp 88-9
 Vaks V G, Larkin A I and Ochinnikov Yu N 1966 *Sov. Phys.-JETP* **22** 820-6
 Vdovichenko N V 1965 *Sov. Phys.-JETP* **20** 477-9