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THERMODYNAMIC AVERAGES FOR AN INFINITE PLANE ISING LATTICE

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It is shown that there exist two equally valid variants of calculating statistical averages which lead to two different but equivalent expressions. The first variant was utilized by Kaufman and Onsager[1]. A description is given of the method utilized in the second variant of the calculation which is more convenient for deriving the famous Onsager formula (formula (12) of the present text) for the spontaneous magnetic moment of an infinite Ising lattice.

1. INTRODUCTION

THE present paper is an extension of the work of Kaufman and Onsager[1] devoted to the calculation of thermodynamic averages for an infinite two-dimensional Ising lattice. To facilitate reading and in order not to encumber the present article by references to earlier papers[1,2] we have presented in the appendices a brief exposition of the material which we require, and have focussed our attention on the new material contained in the present paper.

In the papers of Kaufman and Onsager[1,2] the calculation of the partition function Z and of the averages $\langle \mathbf{F} \rangle$ is carried out in accordance with the formulas

$$Z = \mathrm{Sp}(\mathbf{V}_1\mathbf{V}_2)^m, \quad \langle \mathbf{F} \rangle = Z^{-1}\mathrm{Sp}\mathbf{F}(\mathbf{V}_1\mathbf{V}_2)^m. \tag{1}$$

Here $\mathbf{V}_1$, $\mathbf{V}_2$ are two noncommutative 2^n-rowed Hermitian matrices which depend on the temperature and whose form is given in Appendix 1, n is the number of columns and m is the number of rows in the lattice, and we are interested in this paper in the limiting case of an infinite lattice ($n \to \infty$, $m \to \infty$). All three matrices $\mathbf{V}_1$, $\mathbf{V}_2$, $\mathbf{F}$ are functions of the 2n Dirac matrices of dimensionality 2^n: $\mathbf{P}_1\mathbf{Q}_1\ \mathbf{P}_2\mathbf{Q}_2 \ldots \mathbf{P}_n\mathbf{Q}_n$ which satisfy the commutation relations

$$[\mathbf{P}_k\mathbf{P}_l]_+ = 2\delta_{kl}, \quad [\mathbf{Q}_k\mathbf{Q}_l]_+ = 2\delta_{kl}, \quad [\mathbf{P}_k\mathbf{Q}_l]_+ = 0. \tag{2}$$

The characteristic feature of the resultant situation consists of the fact that the system is described by a non-Hermitian statistical operator $\hat{Z} = (\mathbf{V}_1\mathbf{V}_2)^m$ without having a corresponding expression for the Hamiltonian. Therefore, it is convenient to transform formula (1) in a certain manner.

We introduce two Hermitian matrices

$$\mathbf{T}_1 = \mathbf{V}_1^{1/2}\mathbf{V}_2\mathbf{V}_1^{1/2}, \qquad \mathbf{T}_2 = \mathbf{V}_2^{1/2}\mathbf{V}_1\mathbf{V}_2^{1/2} \tag{3}$$

and write the statistical matrix $\hat{Z}$ in two equivalent forms

$$\hat{Z} = (\mathbf{V}_1\mathbf{V}_2)^m = \mathbf{V}_1^{1/2}\mathbf{T}_1^m\mathbf{V}_1^{-1/2},$$
$$\hat{Z} = (\mathbf{V}_1\mathbf{V}_2)^m = \mathbf{V}_2^{-1/2}\mathbf{T}_2^m\mathbf{V}_2^{1/2}. \tag{4}$$

It is obvious that the matrices $\mathbf{T}_1$ and $\mathbf{T}_2$ are similar, and that the partition function Z can be calculated in two equivalent forms:

$$Z = \mathrm{Sp}\,\mathbf{T}_1, \qquad Z = \mathrm{Sp}\,\mathbf{T}_2. \tag{5}$$

We meet an analogous situation also in the evaluation of averages and obtain for them two equivalent expressions:

$$\langle \mathbf{F} \rangle = Z^{-1}\,\mathrm{Sp}\,\mathbf{F}\mathbf{V}_1^{1/2}\mathbf{T}_1^m\mathbf{V}_1^{-1/2} = Z^{-1}\,\mathrm{Sp}\,(\mathbf{V}_1^{-1/2}\mathbf{F}\mathbf{V}_1^{1/2})\mathbf{T}_1^m, \tag{6a}$$

$$\langle \mathbf{F} \rangle = Z^{-1}\,\mathrm{Sp}\,\mathbf{F}\mathbf{V}_2^{-1/2}\mathbf{T}_2^m\mathbf{V}_2^{1/2} = Z^{-1}\,\mathrm{Sp}\,(\mathbf{V}_2^{1/2}\mathbf{F}\mathbf{V}_2^{-1/2})\mathbf{T}_2^m. \tag{6b}$$

In the literature there are given two formulas for the correlation of spins $\langle \mathbf{S}_k\mathbf{S}_{k+1} \rangle$ in the same row.

The first one was obtained by Onsager and Kaufman[1] and has the form [1)]

$$(-1)^k\langle \mathrm{S}_1\mathrm{S}_{1+k}\rangle = \mathrm{ch}^2 H^*\Delta_k - \mathrm{sh}^2 H^*\Delta_{-k}, \tag{7*}$$

where H* is the temperature parameter (cf., Appendix 1); Δ_k and Δ_{-k} are two Toeplitz determinants:

$$\Delta_k = \begin{vmatrix} \Sigma'(1)\ \Sigma'(2) \ldots \Sigma'(k) \\ \Sigma'(0)\ \Sigma'(1) \ldots \Sigma'(k-1) \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \Sigma(2-k) \ldots\ldots \Sigma'(1) \end{vmatrix}, \quad \Delta_{-k} = \begin{vmatrix} \Sigma'(-1) \ldots\ldots \Sigma'(-k) \\ \Sigma'(0) \ldots\ldots \Sigma'(1-k) \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \Sigma'(k-2) \ldots\ldots \Sigma'(-1) \end{vmatrix}, \tag{8}$$

1)There is an error in sign in[1].
*sh = sinh, ch = cosh.

and the matrix elements $\Sigma'(k)$ are defined in the limit ($n \to \infty$, $m = \infty$) by the formula

$$\Sigma'(k) = \frac{1}{2\pi} \int_0^{2\pi} \cos(k\omega + \delta'(\omega))\, d\omega. \qquad (9)$$

The second formula was obtained by Potts and Ward[3,4] and is derived with the aid of a technique which is different from that utilized in[1]. It has the form

$$\langle S_1 S_{k+1} \rangle = \begin{vmatrix} \Sigma^*(0)\, \Sigma^*(1) \ldots \Sigma^*(k-1) \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \Sigma^*(1-k) \ldots\ldots \Sigma^*(0) \end{vmatrix}, \qquad (10)$$

$$\Sigma^*(k) = \frac{1}{2\pi} \int_0^{2\pi} \cos(k\omega + \delta^*(\omega))\, d\omega. \qquad (11)$$

A mathematical proof of the equivalence of the two formulas is given in an appendix to[4]. The functions $\delta'(\omega)$ and $\delta^*(\omega)$ appearing in formulas (9) and (11) are internal angles of a hyperbolic triangle and are expressed in terms of the sides $2H^*$ and $2H'$ by means of formulas (2.5) of hyperbolic trigonometry given in Appendix 2.

The object of the present paper consists of showing that in choosing for our calculations either the matrix $\mathbf{T}_1$ or the matrix $\mathbf{T}_2$ we arrive either at formula (7) or at formula (10), so that the equivalence of the two formulas becomes obvious and follows from formula (6).

From (10) one can in a fairly elementary manner derive the famous Onsager formula[4] for the spontaneous magnetic moment of an infinite two-dimensional Ising lattice (cf., Appendix 5):

$$(M/M_0)^2 = \lim \langle S_1 S_{1+k} \rangle$$

$$= (1 - \mathrm{sh}^{-2} 2H' \,\mathrm{sh}^{-2} 2H)^{1/4} \text{ for } T < T_{\mathrm{cr}}, \qquad (12)$$

$$(M/M_0)^2 = 0 \text{ for } T > T_{\mathrm{cr}}. \qquad (13)$$

2. REDUCTION OF THE MATRICES T_1 AND T_2 TO DIAGONAL FORM

In accordance with the basic formulas of the theory of Dirac matrices

$$\mathbf{P}_k' = e^{-ix\mathbf{P}_k\mathbf{Q}_l}\,\mathbf{P}_k e^{ix\mathbf{P}_k\mathbf{Q}_l} = \mathbf{P}_k \,\mathrm{ch}\, 2x + i\mathbf{Q}_l \,\mathrm{sh}\, 2x,$$

$$i\mathbf{Q}_l' = e^{-ix\mathbf{P}_k\mathbf{Q}_l}\,(i\mathbf{Q}_l)\, e^{ix\mathbf{P}_k\mathbf{Q}_l} = \mathbf{P}_k \,\mathrm{sh}\, 2x + i\mathbf{Q}_l \,\mathrm{ch}\, 2x, \qquad (14)$$

the matrix $\mathbf{T}_1$ is a 2^n-rowed representation of a certain rotation $R(\mathbf{T}_1)$ (Lorentz transformation) in the 2n-dimensional space of the basis vectors $(\mathbf{P}_k, i\mathbf{Q}_l)$. It is obvious that this rotation $R(\mathbf{T}_1)$ can be represented as a product of n consecutive commuting rotations in the nonintersecting planes $(\overline{\mathbf{P}}_1, i\overline{\mathbf{Q}}_1)(\overline{\mathbf{P}}_2, i\overline{\mathbf{Q}}_2) \ldots (\overline{\mathbf{P}}_n, i\overline{\mathbf{Q}}_n)$ through certain hyperbolic angles $\gamma_1, \gamma_2, \ldots \gamma_n$.

The 2^n-rowed representation of this rotation $R(\overline{\mathbf{T}}_1)$ will be expressed by the 2^n-rowed matrix:

$$\overline{\mathbf{T}}_1 = \prod_{\alpha=1}^{n} \exp\left(\frac{1}{2} i\gamma_\alpha \overline{\mathbf{P}}_\alpha \overline{\mathbf{Q}}_\alpha\right) = \prod_{\alpha=1}^{n} \exp\left(\frac{1}{2}\gamma_\alpha \overline{\mathbf{C}}_\alpha\right), \qquad (15)$$

which is obtained as the result of a certain canonical transformation of the initial system of basis vectors $(\mathbf{P}_k, i\mathbf{Q}_l)$ into the new system of unit vectors $(\overline{\mathbf{P}}_\alpha, i\overline{\mathbf{Q}}_\beta)$.

Since in the new system of basis vectors the matrix $\overline{\mathbf{T}}_1$ is a function of n commuting matrices $\overline{\mathbf{C}}_\alpha$ which we can choose to be diagonal with eigenvalues equal to ± 1, the matrix $\mathbf{T}_1$ is a diagonal matrix with the eigenvalues

$$\lambda_\nu = \exp[{}^1\!/_2(\pm\gamma_1 \pm \gamma_2 \pm \cdots \pm \gamma_n)], \qquad (16)$$

where the subscript ν runs through all the 2^n possible choices of sign in the exponent. Geometrically the parameter γ_α turns out to be the third side of a hyperbolic triangle (diagram in Appendix 2).

All the above also refers to the matrix $\mathbf{T}_2$, which is similar to the matrix $\mathbf{T}_1$ and which, consequently, has the same eigenvalues (16) as the matrix $\mathbf{T}_1$. Consequently, there exists a system of basis vectors $(\overline{\overline{\mathbf{P}}}_\alpha, i\overline{\overline{\mathbf{Q}}}_\beta)$ in terms of which the matrix $\mathbf{T}_2$ assumes the form:

$$\overline{\overline{\mathbf{T}}}_2 = \prod_1^n \exp({}^1\!/_2 i\gamma_\alpha \overline{\overline{\mathbf{P}}}_\alpha \overline{\overline{\mathbf{Q}}}_\alpha) = \prod_1^n \exp({}^1\!/_2 \gamma_\alpha \overline{\overline{\mathbf{C}}}_\alpha). \qquad (17)$$

The transitions $\mathbf{T}_1 \to \overline{\mathbf{T}}_1$ and $\mathbf{T}_2 \to \overline{\overline{\mathbf{T}}}_2$ are accomplished by means of two canonical transformations of the initial system of basis vectors $(\mathbf{P}_k, i\mathbf{Q}_l)$ into the systems of basis vectors $(\overline{\mathbf{P}}_\alpha, i\overline{\mathbf{Q}}_\beta)$ or $(\overline{\overline{\mathbf{P}}}_\alpha, i\overline{\overline{\mathbf{Q}}}_\beta)$. The first of these transformations has the form[2)]

$$\mathbf{P}_k = \sum_{(\alpha)} (\sigma_{k\alpha} \overline{\mathbf{P}}_\alpha + \tau_{k\alpha} \overline{\mathbf{Q}}_\alpha), \qquad \mathbf{Q}_k = \sum_{(\alpha)} (\sigma'_{k\alpha} \overline{\mathbf{P}}_\alpha + \tau'_{k\alpha} \overline{\mathbf{Q}}_\alpha),$$

$$\sigma_{k\alpha} = \frac{1}{n^{1/2}} \cos\left[\frac{2\pi\alpha k}{n} + \frac{\delta'(\alpha)}{2}\right],$$

$$\tau_{k\alpha} = -\frac{1}{n^{1/2}} \sin\left[\frac{2\pi\alpha k}{n} + \frac{\delta'(\alpha)}{2}\right],$$

$$\sigma_{k\alpha}' = \frac{1}{n^{1/2}} \sin\left[\frac{2\pi\alpha k}{n} - \frac{\delta'(\alpha)}{2}\right],$$

$$\tau_{k\alpha}' = \frac{1}{n^{1/2}} \cos\left[\frac{2\pi\alpha k}{n} - \frac{\delta'(\alpha)}{2}\right]. \qquad (18)$$

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2)There is an error in sign in[2] in formula (58) and in[1] in the case of $\tau_{k\alpha}$.

Since we need formulas also for the second canonical transformation $(P_k, iQ_l) \to (\bar{\bar{P}}_\alpha, i\bar{\bar{Q}}_\beta)$, we have given in Appendix 3 a new derivation of the formulas for both transformations and we have obtained the formulas

$$P_k = \sum_{(\alpha)} (\lambda_{k\alpha} \bar{\bar{P}}_\alpha + \mu_{k\alpha} \bar{\bar{Q}}_\alpha), \qquad Q_k = \sum_{(\alpha)} (\lambda_{k\alpha}' \bar{\bar{P}}_\alpha + \mu_{k\alpha}' \bar{\bar{Q}}_\alpha).$$

$$\lambda_{k\alpha} = \frac{1}{n^{1/2}} \cos\left[\frac{2\pi\alpha}{n}\left(k - \frac{1}{2}\right) - \frac{\delta^*(\alpha)}{2}\right],$$
$$\mu_{k\alpha} = \frac{1}{n^{1/2}} \sin\left[\frac{2\pi\alpha}{n}\left(k - \frac{1}{2}\right) - \frac{\delta^*(\alpha)}{2}\right],$$
$$\lambda_{k\alpha}' = \frac{1}{n^{1/2}} \sin\left[\frac{2\pi\alpha}{n}\left(k + \frac{1}{2}\right) + \frac{\delta^*(\alpha)}{2}\right],$$
$$\mu_{k\alpha}' = -\frac{1}{n^{1/2}} \cos\left[\frac{2\pi\alpha}{n}\left(k + \frac{1}{2}\right) + \frac{\delta^*(\alpha)}{2}\right]. \quad (19)$$

The geometric meaning of the angles $\delta'(\alpha)$ and $\delta^*(\alpha)$ appearing in formulas (18) and (19) is given in Fig. 1 of Appendix 2. Expressions for them are given in Appendices 2 and 5.

3. "INTERMEDIATE" AVERAGES

We find it convenient to introduce two "intermediate" averages of the quantity F by means of the formulas

$$\{F\}_1 = Z^{-1}\,\mathrm{Sp}\,FT_1^m, \qquad \{F\}_2 = Z^{-1}\,\mathrm{Sp}\,FT_2^m, \quad (20)$$

in terms of which, taking (6) into account, we shall express the true average:

$$\langle F\rangle = \{V_1^{-1/2} F V_1^{1/2}\}_1, \quad \langle F\rangle = \{V_2^{1/2} F V_2^{-1/2}\}_2. \quad (21)$$

We write formulas (20) in terms of the systems of basis vectors which diagonalize either T_1, or T_2:

$$\{F\}_1 = Z^{-1}\,\mathrm{Sp}\,F(\bar{P}, \bar{Q}) \prod_1^n \exp(\gamma(\alpha)\bar{C}_\alpha / 2),$$
$$\{F\}_2 = Z^{-1}\,\mathrm{Sp}\,F(\bar{\bar{P}}, \bar{\bar{Q}}) \prod_1^n \exp(\gamma(\alpha)\bar{\bar{C}}_\alpha / 2). \quad (22)$$

We see that only those terms of the matrix F will give a non-zero contribution to $\{F\}_1$, or $\{F\}_2$, which are expressed in terms of the paired operators $\bar{C}_\alpha = i\bar{P}_\alpha \bar{Q}_\alpha$ or $\bar{\bar{C}}_\alpha = i\bar{\bar{P}}_\alpha \bar{\bar{Q}}_\alpha$. Thus, for example

$$P_k Q_l = \sum_{\alpha,\beta} \{\sigma_{k\alpha}\sigma'_{l\beta}\bar{P}_\alpha\bar{P}_\beta + \tau_{k\alpha}\tau'_{l\beta}\bar{Q}_\alpha\bar{Q}_\beta + (\sigma_{k\alpha}\tau'_{l\beta} - \tau_{k\alpha}\sigma'_{l\beta})\bar{P}_\alpha\bar{Q}_\beta\} = \sum_{\alpha,\beta} \{\lambda_{k\alpha}\lambda'_{l\beta}\bar{\bar{P}}_\alpha\bar{\bar{P}}_\beta + \mu_{k\alpha}\mu'_{l\beta}\bar{\bar{Q}}_\alpha\bar{\bar{Q}}_\beta + (\lambda_{k\alpha}\mu'_{l\beta} - \mu_{k\alpha}\lambda'_{l\beta})\bar{\bar{P}}_\alpha\bar{\bar{Q}}_\beta\}$$

and, consequently,

$$\{iP_kQ_l\}_1 = \sum_{(\alpha)} (\sigma_{k\alpha}\tau'_{l\alpha} - \tau_{k\alpha}\sigma'_{l\alpha})\{\bar{C}_\alpha\}_1, \quad (23a)$$

$$\{iP_kQ_l\}_2 = \sum_{(\alpha)} (\lambda_{k\alpha}\mu'_{l\alpha} - \mu_{k\alpha}\lambda'_{l\alpha})\{\bar{\bar{C}}_\alpha\}_2. \quad (23b)$$

Further, we express $\{F\}_1$ and $\{F\}_2$ in terms of the eigenvalues of the matrices T_1 and T_2 by means of the formulas:

$$\{F\}_1 = \Sigma(\nu|F|\nu)_1\lambda_\nu^m / \Sigma\lambda_\nu^m,$$
$$\{F\}_2 = \Sigma(\nu|F|\nu)_2\lambda_\nu^m / \Sigma\lambda_\nu^m, \quad (24)$$

where $(\nu|F|\nu)_1$ and $(\nu|F|\nu)_2$ are diagonal matrix elements of the operator F in those representations in which either T_1 or T_2 are diagonal.

Let λ_{max} be the maximum eigenvalue of the matrices T_1 and T_2. Without loss of generality we can always choose representations for $\bar{C}_\alpha$, or for $\bar{\bar{C}}_\alpha$ such that for all α we will have either

$$(\lambda_{max}|\bar{C}_\alpha|\lambda_{max})_1 = 1, \quad \text{or} \quad (\lambda_{max}|\bar{\bar{C}}_\alpha|\lambda_{max})_2 = 1. \quad (25)$$

Dividing the numerator and the denominator in (24) by λ_{max}^m and letting $m \to \infty$, we obtain

$$\{F\}_1 = (\lambda_{max}|F|\lambda_{max})_1, \quad \{F\}_2 = (\lambda_{max}|F|\lambda_{max})_2. \quad (26)$$

Using this formula for the calculation of the "intermediate" averages in accordance with formula (23) we obtain, taking (25) into account,

$$\{iP_kQ_l\}_1 = \sum_\alpha (\sigma_{k\alpha}\tau'_{l\alpha} - \tau_{k\alpha}\sigma'_{l\alpha}) = \frac{1}{n}\sum_{(\alpha)} \cos\left[\frac{2\pi}{n}\alpha(k-l) + \delta'(\alpha)\right],$$

$$-\{iP_kQ_l\}_2 = -\sum_\alpha (\lambda_{k\alpha}\mu'_{l\alpha} - \mu_{k\alpha}\lambda'_{l\alpha}) = \frac{1}{n}\sum_{(\alpha)} \cos\left[\frac{2\pi\alpha}{n}(l-k+1) + \delta^*(\alpha)\right]. \quad (27)$$

Carrying out calculations in accordance with this scheme we easily obtain

$$\{iP_kP_l\}_1 = \sum_{(\alpha)} (\sigma_{k\alpha}\tau_{l\alpha} - \tau_{k\alpha}\sigma_{l\alpha}) = 0,$$

$$\{iP_kP_l\}_2 = \sum_{(\alpha)} (\lambda_{k\alpha}\mu_{l\alpha} - \mu_{k\alpha}\lambda_{l\alpha}) = 0,$$

$$\{iQ_kQ_l\}_1 = \sum_{(\alpha)} (\sigma'_{k\alpha}\tau'_{l\alpha} - \tau'_{k\alpha}\sigma'_{l\alpha}) = 0,$$

$$\{iQ_kQ_l\}_2 = \sum_{(\alpha)} (\lambda'_{k\alpha}\mu'_{l\alpha} - \mu'_{k\alpha}\lambda'_{l\alpha}) = 0. \quad (28)$$

We shall refer to expressions (27) and (28) as the pairing of the corresponding operators. In going in (27) to the limit $n \to \infty$ we obtain (since the argument of the cosine contains odd functions of ω)

$$\{i\,\mathbf{P}_k\,\mathbf{Q}_l\}_1 = \frac{1}{2\pi}\int_{-\pi}^{\pi}\cos\left[\omega(k-l)+\delta'(\omega)\right]d\omega$$

$$= \frac{1}{\pi}\int_0^{\pi}\cos\left[\omega(k-l)+\delta'(\omega)\right]d\omega$$

$$= \frac{1}{2\pi}\int_{-\pi}^{\pi}\exp i\left[\omega(k-l)+\delta'(\omega)\right]d\omega = \Sigma'(k-l),$$

$$-\{i\,\mathbf{P}_k\,\mathbf{Q}_l\}_2 = \frac{1}{2\pi}\int_{-\pi}^{\pi}\cos\left[\omega(l-k+1)+\delta^*(\omega)\right]d\omega$$

$$= \frac{1}{\pi}\int_0^{\pi}\cos\left[\omega(l-k+1)+\delta^*(\omega)\right]d\omega$$

$$= \frac{1}{2\pi}\int_{-\pi}^{\pi}\exp i\left[\omega(l-k+1)+\delta^*(\omega)\right]d\omega$$

$$= \Sigma^*(l-k+1). \quad (29)$$

We now express in terms of pairings the true averages $\langle i\mathbf{P}_k\mathbf{Q}_l\rangle$, $\langle i\mathbf{P}_k\mathbf{P}_l\rangle$, and $\langle i\mathbf{Q}_k\mathbf{Q}_l\rangle$. In accordance with formulas (14) we have

$$\mathbf{V}_1^{-1/2}\mathbf{P}_k\mathbf{V}_1^{1/2} = \operatorname{ch}H^*\mathbf{P}_k + \operatorname{sh}H^* i\mathbf{Q}_k,$$
$$\mathbf{V}_1^{-1/2}\mathbf{Q}_l\mathbf{V}_1^{1/2} = \operatorname{sh}H^*\mathbf{P}_l + \operatorname{ch}H^* i\mathbf{Q}_l,$$
$$\mathbf{V}^{1/2}\mathbf{P}_k\mathbf{V}_2^{-1/2} = \operatorname{ch}H'\mathbf{P}_k + i\mathbf{Q}_{k-1}\operatorname{sh}H',$$
$$\mathbf{V}_2^{1/2} i\mathbf{Q}_l\mathbf{V}_2^{-1/2} = \operatorname{sh}H'\mathbf{P}_{l+1} + i\mathbf{Q}_l\operatorname{ch}H'. \quad (30)$$

Consequently, in accordance with formulas (21), (27), and (28) ($k \neq l$)

$$\langle\mathbf{P}_k\mathbf{P}_l\rangle = \operatorname{sh}H^*\operatorname{ch}H^*[\Sigma'(k-l)-\Sigma'(l-k)] = -\langle\mathbf{Q}_k\mathbf{Q}_l\rangle,$$
$$\langle\mathbf{P}_k\mathbf{P}_l\rangle = -\operatorname{sh}H'\operatorname{ch}H'[\Sigma^*(l-k)-\Sigma^*(k-l)]$$
$$= -\langle\mathbf{Q}_k\mathbf{Q}_l\rangle, \quad (31)$$
$$\langle i\mathbf{P}_k\mathbf{Q}_l\rangle = \operatorname{ch}^2 H^*\Sigma'(k-l) - \operatorname{sh}^2 H^*\Sigma'(l-k),$$
$$\langle i\mathbf{P}_k\mathbf{Q}_l\rangle = -\operatorname{ch}^2 H'\Sigma^*(l-k+1)$$
$$+\operatorname{sh}^2 H'\Sigma^*(k-l-1). \quad (32)$$

In particular, from (32) it follows that

$$\langle\mathbf{S}_1\mathbf{S}_2\rangle = \langle -i\mathbf{P}_2\mathbf{Q}_1\rangle = -\operatorname{ch}^2 H^*\Sigma'(1) + \operatorname{sh}^2 H^*\Sigma'(-1),$$
$$\langle\mathbf{S}_1\mathbf{S}_2\rangle = \langle -i\mathbf{P}_2\mathbf{Q}_1\rangle = \Sigma^*(0). \quad (33)$$

In [1] a proof is given of a theorem, analogous to Wick's theorem, according to which the "intermediate" averages of a product of an even number of Dirac matrices

$$\{\mathbf{P}_{\alpha_1}\mathbf{Q}_{\beta_1}\mathbf{P}_{\alpha_2}\mathbf{Q}_{\beta_2}\ldots\mathbf{P}_{\alpha_k}\mathbf{Q}_{\beta_k}\},$$

are expressed in the limit $n\to\infty$ in terms of pairings by means of the formula

$$(i)^k\{\mathbf{P}_{\alpha_1}\mathbf{Q}_{\beta_1}\ldots\mathbf{P}_{\alpha_k}\mathbf{Q}_{\beta_k}\}$$
$$= \sum_{(P)}(-1)^P\{i\,\mathbf{P}_{\alpha_1}\mathbf{Q}_{\beta_1}\}\{i\,\mathbf{P}_{\alpha_2}\mathbf{Q}_{\beta_2}\}\ldots\{i\mathbf{P}_{\alpha_k}\mathbf{Q}_{\beta_k}\}, \quad (34)$$

where the summation is extended over all the P permutations of the numbers $\beta_1\beta_2\ldots\beta_k$. Since the pairings $\{i\mathbf{P}_\alpha\mathbf{P}_\beta\} = \{i\mathbf{Q}_\alpha\mathbf{Q}_\beta\} = 0$ we see that only those intermediate averages which contain an equal number of $\mathbf{P}_i$ and $\mathbf{Q}_k$ matrices differ from zero. In accordance with formulas (29) and (34) we have

$$\{i\,\mathbf{P}_{\alpha_1}\mathbf{Q}_{\beta_1}\,i\,\mathbf{P}_{\alpha_2}\mathbf{Q}_{\beta_2}\ldots i\,\mathbf{P}_{\alpha_k}\mathbf{Q}_{\beta_k}\}_1$$
$$= \begin{vmatrix} \Sigma'(\alpha_1-\beta_1) & \ldots & \Sigma'(\alpha_1-\beta_k) \\ \Sigma'(\alpha_2-\beta_1) & \ldots & \ldots \\ \ldots & \ldots & \ldots \\ \Sigma'(\alpha_k-\beta_1) & \ldots & \Sigma'(\alpha_k-\beta_k) \end{vmatrix}, \quad (35)$$

$$(-1)^k\{i\mathbf{P}_{\alpha_1}\mathbf{Q}_{\beta_1}\,i\mathbf{P}_{\alpha_2}\mathbf{Q}_{\beta_2}\ldots i\mathbf{P}_{\alpha_k}\mathbf{Q}_{\beta_k}\}_2$$
$$= \begin{vmatrix} \Sigma^*(-\alpha_1+\beta_1+1) & \ldots & \Sigma^*(-\alpha_1-\beta_k+1) \\ \Sigma^*(-\alpha_2-\beta_1+1) & \ldots & \ldots \\ \ldots & \ldots & \ldots \\ \Sigma^*(-\alpha_k+\beta_1+1) & \ldots & \Sigma^*(-\alpha_k+\beta_k+1) \end{vmatrix}. \quad (36)$$

4. CORRELATIONS OF SPINS IN THE SAME ROW

Until now we have been emphasizing that both variants of the calculation of thermodynamic averages are on an equal footing, and that the various expressions obtained are equivalent:

$$\langle\mathbf{F}\rangle = \{\mathbf{V}_1^{-1/2}\mathbf{F}\mathbf{V}_1^{1/2}\}_1 = \{\mathbf{V}_2^{1/2}\mathbf{F}\mathbf{V}_2^{-1/2}\}_2. \quad (37)$$

However, in two cases the true averages $\langle\mathbf{F}\rangle$ coincide with one of the intermediate averages.

In the first case, when **F** depends only on the operators $\mathbf{C}_k = i\mathbf{P}_k\mathbf{Q}_k$, we have [formula (21)]

$$\mathbf{V}_1^{-1/2}\mathbf{F}\mathbf{V}_1^{1/2} = \mathbf{F},$$
$$\langle\mathbf{F}(\ldots\mathbf{C}_k\ldots)\rangle = \{\mathbf{F}(\ldots\mathbf{C}_k\ldots)\}_1. \quad (38)$$

In the second case, when **F** depends only on the operators $\mathbf{S}_k$, we have

$$\mathbf{V}_2^{1/2}\mathbf{F}\mathbf{V}_2^{-1/2} = \mathbf{F};$$
$$\langle\mathbf{F}(\ldots\mathbf{S}_k\ldots)\rangle = \{\mathbf{F}(\ldots\mathbf{S}_k\ldots)\}_2. \quad (39)$$

In carrying out the calculation in accordance with the second variant we have:

$$\langle\mathbf{S}_1\mathbf{S}_{k+1}\rangle = \langle\mathbf{S}_1\mathbf{S}_2\cdot\mathbf{S}_2\mathbf{S}_3\ldots\mathbf{S}_k\mathbf{S}_{k+1}\rangle$$
$$= (-1)^k\{i\mathbf{P}_2\mathbf{Q}_1\cdot i\,\mathbf{P}_3\mathbf{Q}_2\ldots i\mathbf{P}_{k+1}\mathbf{Q}_k\}_2$$
$$= \begin{vmatrix} \Sigma^*(0)\ \Sigma^*(1) & \ldots & \Sigma^*(k-1) \\ \Sigma^*(-1) & \ldots & \Sigma^*(k-2) \\ \ldots & \ldots & \ldots \\ \Sigma^*(1-k) & \ldots & \Sigma^*(0) \end{vmatrix}. \quad (40)$$

Calculations according to the first variant proceed in a more complicated fashion. We have

$$\{\mathbf{S}_1\mathbf{S}_{k+1}\}_1 = \{i\mathbf{Q}_1\mathbf{P}_2 i\mathbf{Q}_2\mathbf{P}_3\ldots i\mathbf{Q}_k\mathbf{P}_{k+1}\}_1$$
$$= \{i\mathbf{Q}_1\mathbf{C}_2\ldots\mathbf{C}_k\mathbf{P}_{k+1}\}_1,$$

$$\langle S_1S_{k+1}\rangle = \{(\mathrm{sh}\, H^*P_1 + \mathrm{ch}\, H^* iQ_1)C_2C_3\ldots C_k(\mathrm{ch}\, H^*P_{k+1} + \mathrm{sh}\, H^* iQ_{1+k})\}_1 = \mathrm{ch}^2 H^*\{(iQ_1C_2C_3\ldots C_kP_{k+1})\}_1 + \mathrm{sh}^2 H^*\{(P_1C_2C_3\ldots C_k iQ_{1+k})\}_1. \quad (41)$$

$$(-1)^k\langle S_1S_{k+1}\rangle = \mathrm{ch}^2 H^*\{iP_2Q_1\cdot iP_3Q_2\ldots iP_{k+1}Q_k\}_1 - \mathrm{sh}^2 H^*\{iP_1Q_2\cdot iP_2Q_3\ldots iP_kQ_{k+1}\}_1$$

and, consequently, we obtain finally

$$(-1)^k\langle S_1S_{k+1}\rangle = \mathrm{ch}^2 H^* \begin{vmatrix} \Sigma'(1), & \Sigma'(2) & \ldots & \Sigma'(k) \\ \Sigma'(0) & \Sigma'(1) & \ldots & \Sigma'(k-1) \\ \cdot & \cdot & \cdot & \cdot \\ \Sigma'(2-k) & \ldots & & \Sigma'(1) \end{vmatrix} - \mathrm{sh}^2 H^* \begin{vmatrix} \Sigma'(-1) & \Sigma'(-2) & \ldots & \Sigma'(-k) \\ \Sigma'(0) & \ldots & & \Sigma'(1-k) \\ \cdot & \cdot & \cdot & \cdot \\ \Sigma'(k-2) & \ldots & & \Sigma'(-1) \end{vmatrix}. \quad (42)$$

Formulas (40) and (42) represent two different expressions for $\langle S_k S_{k+1}\rangle$, given in the Introduction.

APPENDIX 1

THE MATRICES V_1 AND V_2

In the papers of Onsager[5] and of Kaufman[2] it is shown that in the limit $n \to \infty$ the matrices $\mathbf{V}_1$ and $\mathbf{V}_2$ are of the form

$$V_1 = (2\,\mathrm{sh}\, 2H)^{n/2} \prod_{k=1}^{n} \exp(H^* C_k), \quad (1.1)$$

$$V_2 = \prod_{k=1}^{n} \exp(H' S_k S_{k+1}), \quad (1.2)$$

where $H = J/kT$ and $H' = J'/kT$ are two dimensionless temperature parameters, J and J' are the energies of interaction between neighbouring spins in the same column and in the same row. The third auxiliary temperature parameter is defined by the formula

$$H^* = \tfrac{1}{2}\ln \mathrm{cth}\, H, \qquad \mathrm{sh}\, 2H^* = 1/\mathrm{sh}\, 2H. \quad (1.3)^*$$

We distinguish between low temperatures $H^* < H'$ and high temperatures $H^* > H'$. At the temperature which satisfies the equation $H^* = H'$ a phase transition takes place.

The matrices $\mathbf{S}_k$ and $\mathbf{C}_k$ are a 2^n-rowed generalization of the Pauli matrices σ_x and σ_z and, consequently, satisfy the conditions

$$S_kC_l - C_lS_k = 0, \qquad S_kC_k + C_kS_k = 0, \qquad l \neq k, \qquad S_k^2 = C_k^2 = 1. \quad (1.4)$$

*cth = coth.

All the matrices $\mathbf{S}_k$, $\mathbf{C}_l$ with different subscripts commute. We always choose such a representation in which all the $\mathbf{C}_k$ are diagonal.

From the system of the 2^n-rowed Pauli matrices $\mathbf{C}_k$, $\mathbf{S}_l$ we go over to the system of the 2n Dirac matrices $\mathbf{P}_k$, $\mathbf{Q}_l$ of dimensionality 2^n by means of the formulas

$$\begin{aligned} P_1 &= S_1, & Q_1 &= iC_1S_1, \\ P_2 &= S_2C_1, & Q_2 &= iC_1C_2S_2, \\ P_3 &= S_3C_1C_2, & Q_3 &= iC_1C_2C_3S_3, \\ &\cdots & &\cdots \\ P_n &= S_nC_1C_2\ldots C_{n-1}; & Q_n &= iC_1C_2\ldots C_nS_n, \end{aligned} \quad (1.5)$$

which satisfy the commutation relations:

$$[P_kP_l]_+ = 2\delta_{kl}, \qquad [Q_kQ_l]_+ = 2\delta_{kl}, \qquad [P_kQ_l]_+ = 0. \quad (1.6)$$

From (4) and (1.5) we obtain

$$S_kS_{k+1} = -iP_{k+1}Q_k, \qquad C_k = iP_kQ_k. \quad (1.7)$$

In the calculation of the averages $\langle \mathbf{F}\rangle$ we can neglect in (1.1) the numerical factor which will in any case cancel out, and we can write the matrices $\mathbf{V}_1$ and $\mathbf{V}_2$ in the form

$$V_1 = \sum_k \exp(iH^* P^k Q_k),$$

$$V_2 = \prod_k \exp(-iH' P_{k+1} Q_k). \quad (1.8)$$

We have for the correlation of two spins situated in the same row

$$\langle S_1S_{1+k}\rangle = \langle (S_1S_2)(S_2S_3)\ldots(S_kS_{k+1})\rangle = (-i)^k\langle P_{k+1}Q_kP_kQ_{k-1}\ldots P_2Q_1\rangle. \quad (1.9)$$

The difference between the limiting values

$$\lim_{k\to\infty}\langle S_1 S_{k+1}\rangle \quad (1.10)$$

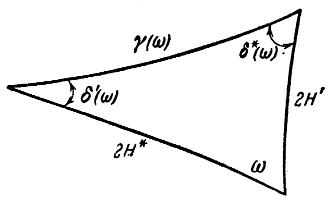
at high and at low temperatures is characteristic. In Appendix 5 is is shown that at high temperatures $H^* > H'$ the correlation of the spins $\langle S_1S_{1+k}\rangle$ as $k \to \infty$ tends in the limit to zero, i.e., at high temperatures there is no long range order in the lattice. At low temperatures the quantity $\langle S_1S_{1+k}\rangle$ tends to a value different from zero as $k \to \infty$, i.e., the lattice does have a long range order. At a temperature $H' = H^*$ a phase transition of the second kind occurs, associated with the disappearance of long range order.

APPENDIX 2

FORMULAS OF HYPERBOLIC TRIGONOMETRY

1. The cosine formula:

$$\mathrm{ch}\,\gamma(\omega) = \mathrm{ch}\, 2H^*\,\mathrm{ch}\, 2H' - \mathrm{sh}\, 2H^*\,\mathrm{sh}\, 2H' \cos\omega. \quad (2.1)$$



2. The sine formula:

$$\frac{\sin \delta'(\omega)}{\operatorname{sh} 2H'} = \frac{\sin \delta^*(\omega)}{\operatorname{sh} 2H^*} = \frac{\sin \omega}{\operatorname{sh} \gamma(\omega)}. \quad (2.2)$$

3. The five element formula:

$$\operatorname{sh}\gamma(\omega)\cos\delta'(\omega) = \operatorname{sh} 2H^* \operatorname{ch} 2H' - \operatorname{ch} 2H^* \operatorname{sh} 2H' \cos\omega,$$

$$\operatorname{sh}\gamma(\omega)\cos\delta^*(\omega) = \operatorname{sh} 2H' \operatorname{ch} 2H^* - \operatorname{ch} 2H' \operatorname{sh} 2H^* \cos\omega. \quad (2.3)$$

4. The four element formula:

$$\sin\omega \operatorname{ctg}\delta'(\omega) = \operatorname{sh} 2H^* \operatorname{cth} 2H' - \operatorname{ch} 2H^* \cos\omega,$$
$$\sin\omega \operatorname{ctg}\delta^*(\omega) = \operatorname{sh} 2H' \operatorname{cth} 2H^* - \operatorname{ch} 2H' \cos\omega. \quad (2.4)^*$$

From formula (2.4), taking into account the fact that

$$e^{2ix} = (\operatorname{ctg} x + i) / (\operatorname{ctg} x - i),$$

it follows that

$$\delta'(\omega) = \frac{1}{2i}\ln\frac{\operatorname{sh} 2H^* \operatorname{cth} 2H' - \operatorname{ch} 2H^* \cos\omega + i\sin\omega}{\operatorname{sh} 2H^* \operatorname{cth} 2H' - \operatorname{ch} 2H^* \cos\omega - i\sin\omega},$$

$$\delta^*(\omega) = \frac{1}{2i}\ln\frac{\operatorname{sh} 2H' \operatorname{cth} 2H^* - \operatorname{ch} 2H' \cos\omega + i\sin\omega}{\operatorname{sh} 2H' \operatorname{cth} 2H^* - \operatorname{ch} 2H' \cos\omega - \sin\omega}, \quad (2.5)$$

from which we obtain:

$$\delta'(H', H^* | \omega) = \delta^*(H^*, H' | \omega),$$
$$\delta'(-\omega) = -\delta'(\omega), \qquad \delta^*(-\omega) = -\delta^*(\omega). \quad (2.6)$$

APPENDIX 3

FERMI OPERATORS AND THE BOGOLYUBOV TRANSFORMATION

Instead of the Dirac operators P_k and Q_k we introduce the Fermi operators

$$A_k = {}^1\!/_2(P_k + iQ_k), \qquad A_k^+ = {}^1\!/_2(P_k - iQ_k),$$
$$P_k = A_k + A_k^+, \qquad iQ_k = A_k - A_k^+, \quad (3.1)$$

for which the following commutation relations hold:

$$[A_k, A_l]_+ = 0, \quad [A_k^+, A_l^+]_+ = 0, \quad [A_k, A_l^+] = \delta_{kl}. \quad (3.2)$$

The canonical transformation of Bogolyubov[6]

$$A'_k = \sum_\alpha (u_{k\alpha} A_\alpha + v_{k\alpha} A^+_\alpha),$$

$$A^+{}_k' = \sum_\alpha (u^*_{k\alpha} A^+_\alpha + v^*_{k\alpha} A_\alpha), \quad (3.3)$$

where

$$\sum_{(\alpha)} (u_{k\alpha} u^*_{l\alpha} + v_{k\alpha} v^*_{l\alpha}) = \delta_{kl},$$

$$\sum_{(\alpha)} (u_{k\alpha} v_{l\alpha} + u_{l\alpha} v_{k\alpha}) = 0 \quad (3.4)$$

corresponds, in accordance with formulas (3.1), to the canonical transformation of the Dirac operators

$$P_k' = \sum_{(\alpha)} (\alpha_{k\alpha} P_\alpha + \beta_{k\alpha} Q_\alpha), \qquad Q_k' = \sum_{(\alpha)} (\alpha_{k\alpha}' P_\alpha + \beta_{k\alpha}' Q_\alpha),$$

$$\alpha_{k\alpha} = \frac{1}{2}[(u_{k\alpha} + u_{k\alpha}^*) + (v_{k\alpha} + v_{k\alpha}^*)],$$

$$\beta_{k\alpha} = \frac{i}{2}[(u_{k\alpha} - u_{k\alpha}^*) - (v_{k\alpha} - v_{k\alpha}^*)];$$

$$\alpha_{k\alpha}' = -\frac{i}{2}[(u_{k\alpha} - u_{k\alpha}^*) + (v_{k\alpha} - v_{k\alpha}^*)],$$

$$\beta_{k\alpha}' = \frac{1}{2}[(u_{k\alpha} + u_{k\alpha}^*) - (v_{k\alpha} + v_{k\alpha}^*)]. \quad (3.5a)$$

As can be easily verified, from (3.3) follow the formulas for the inverse transformation of Bogolyubov:

$$A_\alpha = \sum_{(k)} (u_{k\alpha}^* A_k' + v_{k\alpha} A_k'^+),$$

$$A_\alpha^+ = \sum_{(k)} (u_{k\alpha} A_k'^+ + v_{k\alpha}^* A_k'), \quad (3.6)$$

and, consequently, from (3.5a) by means of the replacements $u_{k\alpha} \to u_{k\alpha}^*$, $u_{k\alpha}^* \to u_{k\alpha}$ one obtains the inverse transformations for the Dirac matrices:

$$P_\alpha = \sum_k (\alpha_{k\alpha} P_k' + \alpha_{k\alpha}' Q_k'),$$

$$Q_\alpha = \sum_{(k)} (\beta_{k\alpha} P_k' + \beta_{k\alpha}' Q_k'). \quad (3.5b)$$

Imposing on the operators P_k and Q_k the periodicity conditions

$$P_{k+n} = P_k, \qquad Q_{k+n} = Q_k \quad (3.7)$$

and choosing for the functions $u_{k\alpha}$ and $v_{k\alpha}$ the functions

$$u_{k\alpha} = n^{-1/2}\exp(2\pi i k\alpha/n), \qquad v_{k\alpha} = 0, \quad (3.8)$$

we obtain the Fourier expansions for the operators A_k, A_k^+:

$$A_k = n^{-1/2}\sum_{(\alpha)} a(\alpha)\exp(2\pi i k\alpha/n),$$

$$A_k^+ = n^{-1/2}\sum_{(\alpha)} a^+(-\alpha)\exp(2\pi i k\alpha/n), \quad (3.9)$$

*ctg = cot.

and the inverse formulas:

$$a(\alpha) = n^{-1/2}\sum_k \mathbf{A}_k \exp(-2\pi i\alpha k/n),$$

$$a^+(-\alpha) = n^{-1/2}\sum_k \mathbf{A}_k^+ \exp(-2\pi i\alpha k/n). \quad (3.10)$$

We write in terms of its components the Fourier transformation

$$\mathbf{P}'_k = \mathbf{P}_k \operatorname{ch} x + i\mathbf{Q}_k \operatorname{sh} x,$$

$$i\mathbf{Q}'_k = \mathbf{P}_k \operatorname{sh} x + i\mathbf{Q}_k \operatorname{ch} x. \quad (3.11)$$

In terms of the Fermi operators we have

$$\mathbf{A}'_k = e^x\mathbf{A}_k, \qquad \mathbf{A}_k^{+\prime} = e^{-x}\mathbf{A}_k^+ \quad (3.12)$$

and in terms of Fourier components we have

$$a'(\alpha) = e^x a(\alpha), \quad a^{+\prime}(-\alpha) = e^{-x}a^+(-\alpha). \quad (3.13)$$

Further, we consider the transformation

$$\mathbf{P}'_k = \mathbf{P}_k \operatorname{ch} y + i\mathbf{Q}_{k-1} \operatorname{sh} y,$$

$$i\mathbf{Q}'_k = \mathbf{P}_{k+1} \operatorname{sh} y + i\mathbf{Q}_k \operatorname{ch} y. \quad (3.14)$$

In terms of the Fermi operators we have

$$\mathbf{A}'_k = \mathbf{A}_k \operatorname{ch} y + \tfrac{1}{2}(\mathbf{A}_{k-1} + \mathbf{A}_{k+1} - \mathbf{A}^+_{k+1} + \mathbf{A}^+_{k+1}) \operatorname{sh} y,$$

$$\mathbf{A}_k^+ = \mathbf{A}_k \,\mathbf{ch}\, y + \tfrac{1}{2}(\mathbf{A}_{k-1} - \mathbf{A}^+_{k-1} - \mathbf{A}_{k+1} - \mathbf{A}^+_{k+1}) \,\mathbf{sh}\, y. \quad (3.15)$$

In accordance with formulas (3.9) we obtain in terms of the Fourier components

$$a'(\alpha) = \left(\operatorname{ch} y + \cos\frac{2\pi\alpha}{n}\operatorname{sh} y\right) a(\alpha) + \left(i \operatorname{sh} y \cdot \sin\frac{2\pi\alpha}{n}\right) a^+(-\alpha),$$

$$a^+(-\alpha) = -\left(i \operatorname{sh} y \cdot \sin\frac{2\pi\alpha}{n}\right) a(\alpha) + \left(\operatorname{ch} y - \cos\frac{2\pi\alpha}{n}\operatorname{sh} y\right) a^+(-\alpha). \quad (3.16)$$

APPENDIX 4

REDUCTION OF THE MATRICES T_1 AND T_2 TO DIAGONAL FORM

We utilize the Bogolyubov transformation[6] in order to find the canonical transformations $(P_k, Q_l) \to (\overline{P}_k, \overline{Q}_l)$, $(P_k, Q_l) \to (\overline{\overline{P}}_k, \overline{\overline{Q}}_l)$, which bring the matrices $\mathbf{T}_1$ and $\mathbf{T}_2$ into diagonal form.

We consider first the transformation of the matrix $\mathbf{T}_1 = \mathbf{V}_1^{1/2}\mathbf{V}_2\mathbf{V}_1^{1/2}$ and write out the sequence of rotations which realize in the 2n-dimensional space the rotation $R(\mathbf{T}_1)$:

$$\mathbf{P}'_k = \mathbf{P}_k \operatorname{ch} H^* + i\mathbf{Q}_k \operatorname{sh} H^*,$$

$$\mathbf{P}_k'' = \mathbf{P}'_k \operatorname{ch} 2H' - i\mathbf{Q}'_{k-1} \operatorname{sh} 2H',$$

$$\mathbf{P}_k''' = \mathbf{P}_k'' \operatorname{ch} H^* + i\mathbf{Q}_k'' \operatorname{sh} H^*,$$

$$i\mathbf{Q}'_k = \mathbf{P}_k \operatorname{sh} H^* + i\mathbf{Q}_k \operatorname{ch} H^*,$$

$$i\mathbf{Q}_k'' = \mathbf{P}'_{k+1} \operatorname{sh} 2H' + i\mathbf{Q}'_k \operatorname{ch} 2H',$$

$$i\mathbf{Q}_k''' = \mathbf{P}_k'' \operatorname{sh} H^* + i\mathbf{Q}_k'' \operatorname{ch} H^*. \quad (4.1)$$

Utilizing formulas (3.13) and (3.16) we rewrite them in terms of Fourier components ($x = H^*$, $y = -2H'$):

$$a'(\alpha) = e^{H^*}a(\alpha), \qquad a^+(-\alpha) = e^{-H^*}a^+(-\alpha),$$

$$a''(\alpha) = \left(\operatorname{ch} 2H' - \cos\frac{2\pi\alpha}{n}\operatorname{sh} 2H'\right) \times a'(\alpha) - i \operatorname{sh} 2H' \sin\frac{2\pi\alpha}{n} a^{+\prime}(-\alpha),$$

$$a^{+\prime\prime}(-\alpha)\left(\operatorname{ch} 2H' + \cos\frac{2\pi\alpha}{n}\operatorname{sh} 2H'\right) \times a^{+\prime}(-\alpha) + i \operatorname{sh} 2H' \sin\frac{2\pi\alpha}{n} a'(\alpha),$$

$$a'''(\alpha) = e^{H^*}a''(\alpha), \qquad a^{+\prime\prime\prime}(-\alpha) = e^{-H^*}a^{+\prime\prime}(-\alpha). \quad (4.2)$$

For the resulting transformation $R(\mathbf{T}_1)$ we obtain

$$a'''(\alpha) = e^{2H^*}\left(\operatorname{ch} 2H' - \cos\frac{2\pi\alpha}{n}\operatorname{sh} 2H'\right) \times a(\alpha) - i\sin\frac{2\pi\alpha}{n}\operatorname{sh} 2H' a^+(-\alpha), \quad (4.3)$$

$$a^{+\prime\prime\prime}(-\alpha) = i\sin\frac{2\pi\alpha}{n}\operatorname{sh} 2H' a(\alpha) + e^{-2H^*}\left(\operatorname{ch} 2H' + \cos\frac{2\pi\alpha}{n}\operatorname{sh} 2H'\right) a^+(-\alpha),$$

or, utilizing formulas (2.1), (2.2) and (2.3) of Appendix 2, we obtain

$$a'''(\alpha) = [\operatorname{ch}\gamma(\alpha) + \operatorname{sh}\gamma(\alpha)\cos\delta'(\alpha)]a(\alpha) - i \operatorname{sh}\gamma(\alpha)\sin\delta'(\alpha) a^+(-\alpha),$$

$$a^{+\prime\prime\prime}(-\alpha) = i \operatorname{sh}\gamma(\alpha)\sin\delta'(\alpha) a(\alpha) + [\operatorname{ch}\gamma(\alpha) - \operatorname{sh}\gamma(\alpha)\cos\delta'(\alpha)]a^+(-\alpha). \quad (4.4)$$

It can be easily verified that the matrix of this transformation is unimodular, and its trace is equal to $2\cosh\gamma(\alpha)$. Consequently, its eigenvalues will be $\exp[\gamma(\alpha)]$ and $\exp[-\gamma(\alpha)]$. The unitary transformation

$$\bar{b}(\alpha) = a(\alpha)\cos\frac{\delta'(\alpha)}{2} - ia^+(-\alpha)\sin\frac{\delta'(\alpha)}{2},$$

$$\bar{b}^+(-\alpha) = -ia(\alpha)\sin\frac{\delta'(\alpha)}{2} + a^+(-\alpha)\cos\frac{\delta'(\alpha)}{2} \quad (4.5)$$

brings it to diagonal form

$$\bar{b}'''(\alpha) = e^{\gamma(\alpha)}\bar{b}(\alpha), \quad \bar{b}^{+'''}(-\alpha) = e^{-\gamma(\alpha)}\bar{b}^{+}(-\alpha). \quad (4.6)$$

Going over in accordance with formulas (3.10) from the Fourier components $a(\alpha)$, $a^{+}(-\alpha)$ to the Fermi operators A_k, A_k^{+}, we obtain from (4.5)

$$\bar{b}(\alpha) = \frac{1}{n^{1/2}}\sum_k\left\{A_k\cos\frac{\delta'(\alpha)}{2} - iA_k^{+}\sin\frac{\delta'(\alpha)}{2}\right\} \times \exp\left(-\frac{2\pi i\alpha k}{n}\right),$$

$$\bar{b}^{+}(-\alpha) = \frac{1}{n^{1/2}}\sum_k\left\{-iA_k\sin\frac{\delta'(\alpha)}{2} + A_k^{+}\cos\frac{\delta'(\alpha)}{2}\right\} \times \exp\left(-\frac{2\pi i\alpha k}{n}\right), \quad (4.7)$$

or

$$\bar{b}(\alpha) = \frac{1}{n^{1/2}}\sum_k\left\{A_k\cos\frac{\delta'(\alpha)}{2} - iA_k\sin\frac{\delta'(\alpha)}{2}\right\} \times \exp\left(-\frac{2\pi i\alpha k}{n}\right),$$

$$\bar{b}^{+}(\alpha) = \frac{1}{n^{1/2}}\sum_k\left\{iA_k\sin\frac{\delta'(\alpha)}{2} + A_k^{+}\cos\frac{\delta'(\alpha)}{2}\right\} \times \exp\left(\frac{2\pi i\alpha k}{n}\right). \quad (4.8)$$

We now show that the transformation (4.8) is the inverse Bogolyubov transformation (3.6) with the coefficients

$$u_{k\alpha}^{*} = \frac{1}{n^{1/2}}\cos\frac{\delta'(\alpha)}{2}\exp\left(-\frac{2\pi i\alpha k}{n}\right),$$

$$v_{k\alpha} = -\frac{i}{n^{1/2}}\sin\frac{\delta'(\alpha)}{2}\exp\left(-\frac{2\pi i\alpha k}{n}\right). \quad (4.9)$$

Indeed, in accordance with formulas (3.4) we have, taking into account the fact that $\delta'(\alpha) = -\delta'(-\alpha)$,

$$\sum_{(\alpha)}(u_{k\alpha}u_{l\alpha}^{*} + v_{k\alpha}v_{l\alpha}^{*}) = \frac{1}{n}\sum_{(\alpha)}\left\{\cos^2\frac{\delta'(\alpha)}{2}\exp\left(\frac{2\pi i\alpha(k-l)}{n}\right) + \sin^2\frac{\delta'(\alpha)}{2}\exp\left(\frac{2\pi i\alpha(l-k)}{n}\right)\right\}$$

$$= \frac{1}{n}\sum_{(\alpha)}\left\{\cos\frac{2\pi\alpha}{n}(k-l) + i\cos\delta(\alpha)\sin\frac{2\pi\alpha}{n}(k-l)\right\} = \delta_{kl}, \quad (4.10)$$

$$\sum_{(\alpha)}(u_{k\alpha}v_{l\alpha} + u_{l\alpha}v_{k\alpha}) = \frac{-i}{n}\sum_{\alpha}\sin\delta'(\alpha)\cos\frac{2\pi\alpha}{n}(k-l) = 0.$$

Formula (4.8) is the desired canonical transformation of the initial matrices $A_k = \frac{1}{2}(P_k + iQ_k)$ into the new matrices $\bar{b}_\alpha = \frac{1}{2}(\bar{P}_\alpha + i\bar{Q}_\alpha)$, in terms of which T_1 is diagonal.

From (4.8) and (4.9) we obtain in accordance with formulas (3.5a), (3.5b) and (4.9)

$$\bar{P}_\alpha = \sum_{(k)}(\sigma_{k\alpha}\bar{P}_k + \sigma'_{k\alpha}\bar{Q}_k),$$

$$\bar{Q}_\alpha = \sum_{(k)}(\tau_{k\alpha}\bar{P}_k + \tau'_{k\alpha}\bar{Q}_k), \quad (4.11)$$

$$P_k = \sum_{(\alpha)}(\sigma_{k\alpha}\bar{P}_\alpha + \tau_{k\alpha}\bar{Q}_\alpha),$$

$$Q_k = \sum_{(\alpha)}(\sigma'_{k\alpha}\bar{P}_\alpha + \tau'_{k\alpha}\bar{Q}_\alpha), \quad (4.12)$$

where

$$\sigma_{k\alpha} = \frac{1}{n^{1/2}}\cos\left(\frac{2\pi\alpha k}{n} + \frac{\delta'(\alpha)}{2}\right),$$

$$\tau_{k\alpha} = -\frac{1}{n^{1/2}}\sin\left(\frac{2\pi\alpha k}{n} + \frac{\delta'(\alpha)}{2}\right),$$

$$\sigma'_{k\alpha} = \frac{1}{n^{1/2}}\sin\left(\frac{2\pi\alpha k}{n} - \frac{\delta'(\alpha)}{2}\right),$$

$$\tau'_{k\alpha} = \frac{1}{n^{1/2}}\cos\left(\frac{2\pi\alpha k}{n} - \frac{\delta'(\alpha)}{2}\right). \quad (4.13)$$

The calculation in the case of the matrix $T_2 = V_2^{1/2}V_1V_2^{1/2}$ is carried out analogously. We write out in terms of the Fourier components the sequence of rotations which realize in the 2n-dimensional space the rotation

$$R(T_2) = R(V_2^{1/2})R(V_1)R(V_2^{1/2}),$$

$$a'(\alpha) = \left(\operatorname{ch}H' + \cos\frac{2\pi\alpha}{n}\operatorname{sh}H'\right) \times a(\alpha) - \left(i\operatorname{sh}H'\sin\frac{2\pi\alpha}{n}\right)a^{+}(-\alpha),$$

$$a^{+'}(-\alpha) = \left(i\operatorname{sh}H'\sin\frac{2\pi\alpha}{n}\right)a(\alpha) + \left(\operatorname{ch}H' - \operatorname{sh}H'\cos\frac{2\pi\alpha}{n}\right)a^{+}(-\alpha),$$

$$a''(\alpha) = e^{-2H^{*}}a'(\alpha),$$

$$a^{+''}(-\alpha) = e^{2H^{*}}a^{+'}(-\alpha),$$

$$a'''(\alpha) = \left(\operatorname{ch}H' + \cos\frac{2\pi\alpha}{n}\operatorname{sh}H'\right) \times a''(\alpha) - \left(i\operatorname{sh}H'\sin\frac{2\pi\alpha}{n}\right)a^{+''}(-\alpha),$$

$$a^{+'''}(-\alpha) = \left(i\operatorname{sh}H'\sin\frac{2\pi\alpha}{n}\right)a''(\alpha) + \left(\operatorname{ch}H' - \cos\frac{2\pi\alpha}{n}\operatorname{sh}H'\right)a^{+}(-\alpha). \quad (4.14)$$

For the resultant transformation $R(T_2)$ we obtain

$$a'''(\alpha) = \left\{\operatorname{ch}\gamma(\alpha) + \operatorname{sh}\gamma(\alpha)\cos\left[\frac{2\pi\alpha}{n} + \delta^*(\alpha)\right]\right\} a(\alpha)$$
$$-\left\{i\operatorname{sh}\gamma(\alpha)\sin\left[\frac{2\pi\alpha}{n} + \delta^*(\alpha)\right]\right\} a^+(-\alpha),$$
$$a^{+'''}(-\alpha) = \left\{i\operatorname{sh}\gamma(\alpha)\sin\left[\frac{2\pi\alpha}{n} + \delta^*(\alpha)\right]\right\} a(\alpha)$$
$$+\left\{\operatorname{ch}\gamma(\alpha) - \operatorname{sh}\gamma(\alpha)\cos\left[\frac{2\pi\alpha}{n} + \delta^*(\alpha)\right]\right\} a^+(-\alpha). \tag{4.15}$$

The matrix of this transformation is unimodular, and its trace is equal to $2\cosh\gamma(\alpha)$. Consequently, its eigenvalues will be $\exp[\gamma(\alpha)]$ and $\exp[-\gamma(\alpha)]$. The unitary transformation

$$\overline{\overline{b}}(\alpha) = -ia^+(-\alpha)\sin\left[\frac{\pi\alpha}{n} + \frac{\delta^*(\alpha)}{2}\right]$$
$$+ a(\alpha)\cos\left[\frac{\pi\alpha}{n} + \frac{\delta^*(\alpha)}{2}\right],$$
$$\overline{\overline{b}}^+(-\alpha) = a^+(-\alpha)\cos\left[\frac{\pi\alpha}{n} + \frac{\delta^*(\alpha)}{2}\right]$$
$$-ia(\alpha)\sin\left[\frac{\pi\alpha}{n} + \frac{\delta^*(\alpha)}{2}\right] \tag{4.16}$$

brings it into diagonal form

$$\overline{\overline{b}}'''(\alpha) = e^{\gamma(\alpha)}\overline{\overline{b}}(\alpha),$$
$$\overline{\overline{b}}^{+'''}(-\alpha) = e^{-\gamma(\alpha)}\overline{\overline{b}}^+(-\alpha). \tag{4.17}$$

Going over from the Fourier components to the Fermi operators we obtain

$$\overline{\overline{b}}(\alpha) = \frac{1}{n^{1/2}}\sum_k\left\{-i\sin\left[\frac{\pi\alpha}{n} + \frac{\delta^*(\alpha)}{2}\right]\mathbf{A}_k\right.$$
$$\left.+\cos\left[\frac{\pi\alpha}{n} + \frac{\delta^*(\alpha)}{2}\right]\mathbf{A}_k^+\right\}\exp\left(\frac{2\pi i\alpha k}{n}\right). \tag{4.18}$$

The transformation (4.18) is the inverse Bogolyubov transformation with the coefficients

$$u^*_{k\alpha} = \frac{-i}{n^{1/2}}\sin\left[\frac{\pi\alpha}{n} + \frac{\delta^*(\alpha)}{2}\right]\exp\left(\frac{2\pi i\alpha k}{n}\right),$$
$$v_{k\alpha} = \frac{1}{n^{1/2}}\cos\left[\frac{\pi\alpha}{n} + \frac{\delta^*(\alpha)}{2}\right]\exp\left(\frac{2\pi i\alpha k}{n}\right). \tag{4.19}$$

In accordance with formulas (3.5a), (3.5b), and (4.19) we obtain

$$\mathbf{P}_k = \sum_{(\alpha)}(\lambda_{k\alpha}\overline{\overline{\mathbf{P}}}_\alpha + \mu_{k\alpha}\overline{\overline{\mathbf{Q}}}_\alpha),$$
$$\mathbf{Q}_k = \sum_{(\alpha)}(\lambda'_{k\alpha}\overline{\overline{\mathbf{P}}}_\alpha + \mu'_{k\alpha}\overline{\overline{\mathbf{Q}}}_\alpha), \tag{4.20}$$
$$\overline{\overline{\mathbf{P}}}_\alpha = \sum_{(k)}(\lambda_{k\alpha}\mathbf{P}_k + \lambda'_{k\alpha}\mathbf{Q}_k),$$
$$\overline{\overline{\mathbf{Q}}}_\alpha = \sum_{(k)}(\lambda_{k\alpha}\mathbf{P}_k + \mu'_{k\alpha}\mathbf{Q}_k), \tag{4.21}$$

where

$$\lambda_{k\alpha} = \frac{1}{n^{1/2}}\cos\left[\frac{2\pi\alpha}{n}\left(k-\frac{1}{2}\right) - \frac{\delta^*(\alpha)}{2}\right],$$
$$\mu_{k\alpha} = \frac{1}{n^{1/2}}\sin\left[\frac{2\pi\alpha}{n}\left(k-\frac{1}{2}\right) - \frac{\delta^*(\alpha)}{2}\right],$$
$$\lambda'_{k\alpha} = \frac{1}{n^{1/2}}\sin\left[\frac{2\pi\alpha}{n}\left(k+\frac{1}{2}\right) + \frac{\delta^*(\alpha)}{2}\right],$$
$$\mu'_{k\alpha} = \frac{-1}{n^{1/2}}\cos\left[\frac{2\pi\alpha}{n}\left(k+\frac{1}{2}\right) + \frac{\delta^*(\alpha)}{2}\right]. \tag{4.22}$$

APPENDIX 5

DERIVATION OF THE ONSAGER FORMULA

In the theory of Toeplitz matrices [4,7] a formula is derived for the limiting value of the determinant

$$T^*(n) = \begin{vmatrix} \Sigma^*(0) & \Sigma^*(1) & \ldots & \Sigma^*(n-1) \\ \Sigma^*(-1) & \Sigma^*(0) & \ldots & \Sigma^*(n-2) \\ \cdots & \cdots & \cdots & \cdots \\ \Sigma^*(1-n) & \ldots & \ldots & \Sigma^*(0) \end{vmatrix} = \langle S_1 S_{n+1}\rangle$$

for $n \to \infty$. In accordance with this formula

$$\lim_{n\to\infty} T^*(n) = \lim_{n\to\infty} e^{(n+1)h_0}\prod_{k=1}^{k=n}\exp(-kh_k^2), \tag{5.1}$$
$$h_k = \frac{1}{2\pi}\int_0^{2\pi} i\delta^*(\omega)e^{i\omega k}\,d\omega. \tag{5.2}$$

Since $\delta^*(\omega)$ is an odd function of ω, then $h_0 = 0$ and

$$\lim_{n\to\infty} T^*(n) = \prod_{k=1}^{\infty}\exp(-kh_k^2). \tag{5.3}$$

For the evaluation of the Fourier components h_k of the function $i\delta^*(\omega)$ we turn to formula (2.5), and expand the numerator and the denominator into the product of two factors ($Z = e^{i\omega}$, $\overline{Z} = e^{-i\omega}$):

$$i\delta^*(\omega) = \frac{1}{2}\ln\frac{(\operatorname{cth}H' - \operatorname{th}H^*Z)(\operatorname{th}H' - \operatorname{th}H^*\overline{Z})}{(\operatorname{cth}H' - \operatorname{th}H^*\overline{Z})(\operatorname{th}H' - \operatorname{th}H^*Z)}. \tag{5.4}$$ *

We consider separately the two cases:

I. $0 < \operatorname{th}H^* < \operatorname{th}H' < 1$ (low temperatures):

$$i\delta^*(\omega) = \frac{1}{2}$$
$$\times\ln\frac{(1-\operatorname{th}H'\operatorname{th}H^*Z)(\operatorname{th}H' - \operatorname{th}H^*\overline{Z})}{(1-\operatorname{th}H'\operatorname{th}H^*\overline{Z})(\operatorname{th}H' - \operatorname{th}H^*\overline{Z})}; \tag{5.5}$$

*th = tanh.

II. $0 < \text{th}\, H' < \text{th}\, H^* < 1$ (high temperatures):

$$i\delta^*(\omega) = \frac{1}{2} \times \ln \frac{\bar{Z}(1 - \text{th}\, H' \,\text{th}\, H^* Z)(\text{th}\, H^* - \text{th}\, H' Z)}{Z(1 - \text{th}\, H' \,\text{th}\, H^* \bar{Z})(\text{th}\, H^* - \text{th}\, H' \bar{Z})}. \quad (5.6)$$

Utilizing the formula $-\ln(1-x) = (x^n/n)$ we obtain in case I

$$i\delta^*(\omega) = \frac{1}{2}\sum_{n=1}^{\infty}\frac{1}{n}\left\{-(\text{th}\, H^*\,\text{th}\, H')^n Z^n - \left(\frac{\text{th}\, H^*}{\text{th}\, H'}\right)^n \bar{Z}^n + \left(\frac{\text{th}\, H^*}{\text{th}\, H'}\right)^n Z^n + (\text{th}\, H^*\,\text{th}\, H')^n \bar{Z}^n\right\}, \quad (5.7)$$

and in case II

$$i(\delta^*(\omega) + \omega) = \frac{1}{2}\sum_{n=1}^{\infty}\frac{1}{n}\left\{-(\text{th}\, H^*\,\text{th}\, H')^n Z^n - \left(\frac{\text{th}\, H'}{\text{th}\, H^*}\right)^n Z^n + (\text{th}\, H^*\,\text{th}\, H')^n \bar{Z}^n + \left(\frac{\text{th}\, H'}{\text{th}\, H^*}\right)^n \bar{Z}^n\right\}. \quad (5.8)$$

Expanding the function $i\omega$ in a Fourier series we obtain

$$i\omega = -\sum \frac{(-1)^k}{k}(Z^k - \bar{Z}^k). \quad (5.9)$$

Thus, the Fourier coefficients h_k of the function $i\delta^*(\omega)$ have the form

I. $H' > H^*$:

$$h_k = \frac{1}{2k}\left\{\left(\frac{\text{th}\, H^*}{\text{th}\, H'}\right)^k - (\text{th}\, H^*\,\text{th}\, H')^k\right\}; \quad (5.10)$$

II. $H' < H^*$:

$$h_k = \frac{1}{2k}\left\{2(-1)^k - \left(\frac{\text{th}\, H'}{\text{th}\, H^*}\right)^k - (\text{th}\, H^*\,\text{th}\, H')^k\right\}. \quad (5.11)$$

We now calculate $\sum_1^\infty k h_k^2$. At low temperatures:

$$\sum_1^\infty k h_k^2 = \frac{1}{4}\sum_1^\infty \frac{1}{k}\left\{(\text{th}\, H^*)^{2k}\left[\left(\frac{1}{\text{th}\, H'}\right)^{2k} + (\text{th}\, H')^{2k} - 2\right]\right\}$$
$$= -\frac{1}{4}\left\{\ln\left(1 - \left(\frac{\text{th}\, H^*}{\text{th}\, H'}\right)^2\right) + \ln\left[1 - (\text{th}\, H^*\,\text{th}\, H')^2\right] - 2\ln(1 - \text{th}^2 H^*)\right\}$$
$$= -\frac{1}{4}\ln\frac{(1-\text{th}^2 H^*)^2 - \text{th}^2 H^*(\text{cth}^2 H' + \text{th}^2 H' - 2)}{(1-\text{th}^2 H^*)^2}$$
$$= -\frac{1}{4}\ln\left\{1 - \frac{\text{sh}^2 2H^*}{\text{sh}^2 2H'}\right\} \quad (5.12)$$

at high temperatures:

$$\sum_1^\infty k h_k^2 = \frac{1}{4}\sum_1^\infty \frac{1}{k}\{4 + (\ldots\ldots)\} \to \infty, \quad (5.13)$$

since the series diverges. In accordance with formula (5.1):

low temperatures:

$$\lim_{k\to\infty} |\langle S_1 S_{k+1}\rangle| = (1 - \text{sh}^2 2H^* / \text{sh}^2 2H')^{1/4} = (1 - \text{sh}^{-2} 2H\, \text{sh}^{-2} 2H')^{1/4},$$

at high temperatures:

$$\lim_{k\to\infty} |\langle S_1 S_{k+1}\rangle| = 0. \quad (5.14)$$

From this follows the Onsager formula given in the text.

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