

Theorems on Extended Ising Model with Applications to Dilute Ferromagnetism

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It is proved that the zeros of the partition function of an extended Ising model lie on a unit circle in the fugacity plane under certain conditions. Each spin assumes a general value. The key point of the proof is to derive a simple condition sufficient for zeros of polynomials to lie on a unit circle. Conjectured theorems on the Heisenberg model are also discussed.

§ 1. Introduction

The critical behavior of the Ising model with spin $\frac{1}{2}$ has been investigated in terms of Lee-Yang's theorem concerning the distribution of the zeros of the canonical partition function in the fugacity plane.¹⁾⁻⁴⁾ The distribution of the zeros in the complex temperature plane was also used to discuss the nature of critical points.⁵⁾⁻¹¹⁾

In this paper, the Lee-Yang theorem is generalized to an extended Ising model with applications to dilute ferromagnetism.¹²⁾⁻¹⁴⁾ We discuss an idealized annealed system in which the temperature and external parameters are varied infinitely slowly and true thermal equilibrium is realized. This annealed system is formulated by introducing a generating function in the case of Ising spins.^{13),14)} Consider a crystal lattice whose lattice points are named $i=1, 2, \dots, N$. On each lattice point there is either an Ising spin of $S=1/2$ or a nonmagnetic atom. The generating function of this system is given by

$$\mathcal{E}_N = \sum_{s_j = \pm 1, 0} \exp(\sum K_{ij} s_i s_j + \lambda \sum s_j^2 + h \sum s_j), \quad (1.1)$$

where

$$K_{ij} = J_{ij}/kT \quad \text{and} \quad h = mH/kT.$$

In the above Equation (1.1), $s_j=1$ or -1 corresponds to Ising spin (up or down) and $s_j=0$ to a nonmagnetic atom. Since $s_j^2=1$ for spin state and 0 for nonmagnetic atoms, the parameter λ is determined as a function of concentration p of Ising spins from the equation

$$\frac{1}{N} \frac{\partial}{\partial \lambda} \log \mathcal{E}_N = \langle s_j^2 \rangle = p. \quad (1.2)$$

Extending the partition function (1.1) to the form

$$\begin{aligned} \mathcal{E}_N(\{x_{ij}\}; z; \{S_j\}) &= \text{Tr} \exp(\sum K_{ij} s_i s_j + \sum \lambda_j s_j^2 + h \sum s_j); \\ x_{ij} &= e^{-K_{ij}} \quad \text{and} \quad z = e^{-h}, \end{aligned} \tag{1.3}$$

we find the following theorem.

Theorem I-A: In the ferromagnetic system represented by Eq. (1.3), all the roots of the equation

$$\mathcal{E}_N(\{x_{ij}\}; z; \{S_j\}) = 0 \tag{1.4}$$

are on the unit circle in the complex z -plane for $S_j = \frac{1}{2}, 1$ or $\frac{3}{2}$, and for $\lambda_j \geq 0$. S_j indicates a spin quantum number at the j -th lattice site, and s_j is the z component of the spin operator ($s_j = S_j, S_j - 1, \dots, -S_j$).

Since the case $\lambda_j = 0$ corresponds to the usual Ising model, this theorem includes the results obtained in previous papers.¹⁵⁾⁻¹⁷⁾ This theorem can be easily extended to the case of *general spin* in the following way.

Theorem I-B: All the roots of Eq. (1.4) for general spin S_j lie on the unit circle for

$$\lambda_j \geq \lambda^0(S_j), \tag{1.5}$$

where the lower bound $\lambda^0 = \lambda^0(S)$ is given by the largest real root of the equation

$$\begin{aligned} \exp\{\lambda^0 S^2\} &= \exp\{\lambda^0 (S-1)^2\} + \exp\{\lambda^0 (S-2)^2\} + \dots \\ &+ \exp\{\lambda^0 (S-[S]+1)^2\} + (S-[S]+\frac{1}{2}) \exp\{\lambda^0 (S-[S])^2\}, \end{aligned} \tag{1.6}$$

where $[S] = S$ for even half-spin S and $[S] = S - \frac{1}{2}$ for odd half-spin S . The numerical values of $\lambda^0(S)$ are shown in Table.

The above theorem I-B is derived as a special case of the following theorem.

Theorem I-C: All the zeros of the partition function

$$\begin{aligned} \mathcal{E}_N(\{x_{ij}\}; z; \{S_j\}; \{\lambda_{j,k}\}) \\ = \text{Tr} \exp(\sum K_{ij} s_i s_j + \sum_j \sum_{k=1}^{[S_j]} \lambda_{j,k} s_j^{2k} + h \sum s_j) \end{aligned} \tag{1.7}$$

lie on the unit circle in the complex z -plane for $K_{ij} \geq 0$ if the parameters $\lambda_{j,k} = \lambda_k(S_j)$ (or $\lambda_k(S) = \lambda_k$) satisfy the inequality

$$\begin{aligned} \exp\{\sum_{k=1}^{[S]} \lambda_k S^{2k}\} &\geq \sum_{p=1}^{[S]-1} \exp\{\sum_{k=1}^{[S]} \lambda_k (S-p)^{2k}\} \\ &+ (S-[S]+\frac{1}{2}) \exp\{\sum_{k=1}^{[S]} \lambda_k (S-[S])^{2k}\}. \end{aligned} \tag{1.8}$$

For purposes proving the above theorems, it is convenient to introduce the following function f_n of the variables z_1, \dots, z_n :

$$f_n(\{z_j\}; \{S_j\}; \{\lambda_{j,k}\}) = \sum_{s_1=-S_1}^{S_1} \cdots \sum_{s_n=-S_n}^{S_n} \prod_{i>j} x_{ij}^{-s_i s_j} \prod_j \exp\left(\sum_{k=1}^{[S_j]} \lambda_{j,k} S_j^{2k}\right) \cdot z_j^{s_j}, \quad (1.9)$$

which corresponds to the partition function in an inhomogeneous field with

$$x_{ij} = e^{-K_{ij}} \quad \text{and} \quad z_j = e^{-h_j}.$$

By expanding the above function with respect to the variable z_1 , the following recurrence formula is easily obtained:

$$f_n(\{z_j\}; \{S_j\}; \{\lambda_{j,k}\}) = \sum_{p=-S_1}^{S_1} A_p \left\{ \prod_{k=1}^{[S_1]} \exp(\lambda_{1,k} p^{2k}) \right\} z_1^p, \quad (1.10)$$

where

$$A_p = f_{n-1}(\{z_j x_{1j}^{-p}\}; S_2, \dots, S_n). \quad (1.11)$$

The following simple relations hold in general for real parameters $\{x_{ij}\}$ and $\{\lambda_{j,k}\}$:

$$(i) \quad f_n^*(\{z_j\}; \{S_j\}; \{\lambda_{j,k}\}) = f_n(\{z_j^*\}; \{S_j\}; \{\lambda_{j,k}\}), \quad (1.12)$$

$$(ii) \quad f_n(\{1/z_j\}; \{S_j\}; \{\lambda_{j,k}\}) = f_n(\{z_j\}; \{S_j\}; \{\lambda_{j,k}\}), \quad (1.13)$$

$$(iii) \quad \text{if } |z_2| = \cdots = |z_n| = 1, \text{ then the following symmetry relations}$$

hold:

$$A_{-p} = A_p^* \quad (p = S_1, S_1 - 1, \dots, -S_1). \quad (1.14)$$

It is clear that

$$f_N(z, z, \dots, z; \{S_j\}; \{\lambda_{j,k}\}) = E_N(z; \{S_j\}; \{\lambda_{j,k}\}). \quad (1.15)$$

Therefore, Theorem I-C is an immediate consequence of the following theorem:

Theorem II: If $|z_1| \geq 1, \dots, |z_n| \geq 1$ and

$$f_n(\{z_j\}; \{S_j\}; \{\lambda_{j,k}\}) = 0, \quad (1.16)$$

then

$$|z_1| = |z_2| = \cdots = |z_n| = 1$$

for $0 < x_{ij} \leq 1$, and on the condition (1.8).

In the following sections, we assume that all the x 's are different from 1. The proof can then be easily generalized to include the case when one or more of the x 's are equal to 1. We shall prove Theorem II by mathematical induction in the same way as Lee and Yang.

§ 2. Theorems on the zeros of polynomials

In this section, we describe some theorems useful for proving Theorem II or its extension (if possible). The lemma about conditions sufficient for zeros

of polynomials to lie on a unit circle, which has been obtained in previous papers,^{15),16)} can be generalized in the following form

Theorem III: Consider the following equation:

$$f(z) = a_0 z^m + a_1 z^{m-1} + \dots + a_m = 0. \tag{2.1}$$

If $a_0 a_k^* = a_{m-k} a_m^*$ and

$$|a_0| \geq |a_1| + \dots + |a_{q-1}| + \left(\frac{m+1}{2} - q\right) |a_q|; \quad q = [m/2],$$

then all the roots of Eq. (2.1) have the absolute value equal to 1.

This is easily derived from the following two theorems.

*The Schur-Kohn-Yamamoto theorem:*¹⁸⁾ The condition necessary and sufficient for all the roots of Eq. (2.1) to have the absolute value equal to 1 is that

(i) $a_0 a_k^* = a_{m-k} a_m^*$ and that (ii) all the roots of the equation $f'(z) = 0$ satisfy the inequality $|z| \leq 1$.

Since $|a_{m-k}| = |a_k|$ on the condition (i), Theorem III can be derived by application of the following theorem to the above condition (ii).

*Theorem:*¹⁹⁾ If the coefficients in Eq. (2.1) satisfy the inequality

$$|a_0| \geq |a_1| + |a_2| + \dots + |a_m|, \tag{2.2}$$

then none of the roots of Eq. (2.1) has an absolute value larger than 1 ($|z| \leq 1$).

This is easily proved from Rouché's theorem and the continuity of the roots with respect to the coefficients.

The following theorem will be useful in extending theorem II, for example, to the region $\lambda_{j,k} \geq 0$, including the usual Ising model with general spin.

Theorem IV: The condition necessary and sufficient for all the roots of Eq. (2.1) to have an absolute value equal to 1 is that (i) $a_0 a_k^* = a_{m-k} a_m^*$ and (ii) the following hermite matrix S_m is semi-positive definite:

$$S_m \geq 0, \tag{2.3}$$

where

$$S_m = (S_{ij}); \quad (i, j = 0, \dots, m-2),$$

$$S_{ii} = \begin{cases} \sum_{k=0}^i \{(m-k)^2 |a_k|^2 - (k+1)^2 |a_{m-k-1}|^2\} & \text{for } i \leq [m/2 - 1], \\ S_{m-i-2, m-i-2} & \text{for } i > [m/2 - 1], \end{cases}$$

and

$$S_{ij} = \begin{cases} m(m+i-j) a_0^* a_{j-1} - (j-i+1) a_{m+i-j-1}^* a_{m-1} & \text{for } j > i, \\ S_{ji}^* & \text{for } i > j. \end{cases} \tag{2.4}$$

Some examples of the matrix S_m and their principal minor determinants are shown in Appendix A,

Theorem IV is a simple version of the Schur-Kohn-Yamamoto theorem using the following Schur-Kohn theorem.

The Schur-Kohn theorem: The condition necessary and sufficient for none of the roots of Eq. (2.1) to have the absolute value larger than 1 is that Bézout's matrix for Eq. (2.1) is semi-positive definite.¹⁹⁾

The following theorem is also useful for proof of Theorem II extended to a wider region in the case $n=1$ (see Appendix B).

The Eneström-Kakeya theorem: If the coefficients of Eq. (2.1) satisfy the relation,

$$a_0 \geq a_1 \geq \dots \geq a_m \geq 0, \quad (2.5)$$

then none of the roots of Eq. (2.1) has the absolute value larger than 1 ($|z| \leq 1$).

§ 3. Proof of Theorem II

For the purpose of proving Theorem II by mathematical induction, it is convenient to set up the following assertion:

Assertion A: There exist roots of Eq. (1.16) with respect to the variable z_k for $|z_1| \geq 1, \dots, |z_{k-1}| \geq 1, |z_{k+1}| \geq 1, \dots, |z_n| \geq 1$.

Clearly, Assertion A holds for $n=1$. Theorem II is also easily proved for $n=1$ from the application of Theorem III to the equation

$$f_1(z; S; \lambda_k) = \sum_{p=-S}^S z^p \exp\left(\sum_{k=1}^{[S]} \lambda_k p^{2k}\right) = 0. \quad (3.1)$$

Assume that Theorem II and Assertion A are true for $n=m-1$. Then, it is shown that Assertion A holds for $n=m$. The coefficient of the highest order in Eq. (1.16) with respect to the variable z_k is given by

$$f_{m-1}(\{z_j x_{kj}^{-S_k}\}) \exp\left(\sum_j \lambda_{k,j} S_k^{2j}\right) \quad (3.2)$$

and

$$|z_j x_{kj}^{-S_k}| \geq x_{kj}^{-S_k} > 1.$$

Consequently, the coefficient (3.2) does not vanish from the assumption that Theorem II is valid for $n=m-1$. This means that Assertion A holds for $n=m$.

We show that it leads to contradiction to assume that Theorem II is not true for $n=m$.

Under the above assumption that Theorem II is not true for $n=m$, there exists a set of z 's equal to z_1, \dots, z_m such that

$$f_m(z_1, \dots, z_m; \{S_j\}; \{\lambda_{j,k}\}) = 0, \quad (3.3)$$

and

$$|z_1| > 1 \quad \text{and} \quad |z_2|, |z_3|, \dots, |z_m| \quad \text{all} \quad \geq 1. \quad (3.4)$$

We can repeat the Lee-Yang procedure in a generalized form as follows. Keeping z_3, \dots, z_m fixed and regarding z_2 as a function of z_1 defined by (3.3), one obtains a limit \mathcal{Z}_2 for z_2 as $z_1 \rightarrow \infty$, which is given by the equation,

$$f_{m-1}(\mathcal{Z}_2 x_{12}^{-S_1}, z_3 x_{13}^{-S_1}, \dots, z_m x_{1m}^{-S_1}; \{S_j\}) = 0, \tag{3.5}$$

from Assertion A for $n = m - 1$. Under the assumption that Theorem II is true for $n = m - 1$, one obtains

$$|\mathcal{Z}_2| < |\mathcal{Z}_2 x_{12}^{-S_1}| < 1.$$

Therefore, keeping z_3, \dots, z_m fixed one can increase $|z_1|$ and define z_2 as a continuous function of z_1 . Since by (3.4), z_2 starts to be ≥ 1 in absolute magnitude and tends to a limit < 1 in absolute magnitude as $z_1 \rightarrow \infty$, there must be a value equal to z_1' so that z_2 assumes a value z_2' equal to 1 in absolute magnitude, i.e.

$$f_m(z_1', z_2', z_3, \dots, z_m; \{S_j\}; \{\lambda_{j,k}\}) = 0,$$

and

$$|z_1'| > 1, \quad |z_2'| = 1, \quad |z_3| \geq 1, \dots, |z_m| \geq 1. \tag{3.6}$$

We can fix z_2', z_4, \dots, z_m and regard z_3 as a function of z_1' and follow the same procedure as mentioned above. Continuing this way we finally get a set of values z_1'', \dots, z_m'' such that

$$f_m(z_1'', \dots, z_m''; \{S_j\}; \{\lambda_{j,k}\}) = 0,$$

and

$$|z_1''| > 1, \quad |z_2''| = \dots = |z_m''| = 1. \tag{3.7}$$

On the other hand, we prove that if

$$|z_2| = \dots = |z_m| = 1 \text{ and } f_m(\{z_j\}; \{S_j\}; \{\lambda_{j,k}\}) = 0, \tag{3.8}$$

then $|z_1| = 1$ under the condition (1.8). In the same way as in the previous papers,^{15),16)} we find that a function

$$|f_{m-1}(t_2 z_2, \dots, t_m z_m; \{S_j\}; \{\lambda_{j,k}\})|^2$$

is a monotonously increasing function of all t_k for $t_k > 1$ and $|z_2| = \dots = |z_m| = 1$. Therefore, the following inequality is obtained:

$$|f_{m-1}(\{x_{1j}^{-k} z_j\}; \{S_j\})| \geq |f_{m-1}(\{x_{1j}^{-k'} z_j\}; \{S_j\})| \tag{3.9}$$

for $|z_j| = 1$ and $k \geq k' \geq 0$.

Consequently, in terms of Theorem III and the recurrence formula (1.10), one finds that if $|z_2| = \dots = |z_m| = 1$ and Eq. (3.8) holds, then $|z_1| = 1$ under the condition (1.8).

Thus, the above two results contradict one another, which means that

Theorem II must hold for $n=m$. This completes the proof of Theorem II by induction.

§ 4. Conjectured theorems on the Heisenberg model

As pointed out in the case of small lattices,^{2),20),21)} the extension of the Lee-Yang theorem to Heisenberg ferromagnets seems to be possible in the following way.

Conjectured Theorem A: In the ferromagnetic Heisenberg model ($J_{ij} \geq 0$), all the roots of the equation

$$\mathcal{E}_N(z; \{S_j\}) = \text{Tr} \exp(\sum K_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + h \sum S_j^z) = 0 \quad (4.1)$$

are on the unit circle in the complex z -plane.

Remark that it is possible to define the function f_n of the variables z_1, \dots, z_n as in the Ising model:

$$f_n(\{z_j\}; \{S_j\}) = \text{Tr} \{ \exp(\sum K_{ij} \mathbf{S}_i \cdot \mathbf{S}_j) \prod_j z_j^{-S_j^z} \}. \quad (4.2)$$

Since the Zeeman term $\sum S_j^z$ commutes the exchange interaction $\sum K_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$, we obtain the relation

$$\mathcal{E}_N(z; \{S_j\}) = f_N(z, \dots, z; \{S_j\}). \quad (4.3)$$

The function (4.2) can be rewritten as

$$f_n(\{z_j\}; \{S_j\}) = \sum_{k=-S_1}^{S_1} z_1^{-k} g_{n-1}(k; z_2, \dots, z_n; \{S_j\}), \quad (4.4)$$

where

$$\begin{aligned} g_{n-1}(k; z_2, \dots, z_n; \{S_j\}) \\ = \text{Tr}' \{ \langle k | \exp(\sum K_{ij} \mathbf{S}_i \cdot \mathbf{S}_j) | k \rangle \prod_{j=2}^n z_j^{-S_j^z} \} \end{aligned} \quad (4.5)$$

and $|k\rangle$ is an eigenstate of S_1^z :

$$S_1^z |k\rangle = k |k\rangle.$$

From the inversion symmetry of the Hamiltonian in the spin space, the following relations hold in general for real parameters $\{K_{ij}\}$:

$$(i) \quad f_n^*(\{z_j\}; \{S_j\}) = f_n(\{z_j^*\}; \{S_j\}), \quad (4.6)$$

$$(ii) \quad f_n(\{1/z_j\}; \{S_j\}) = f_n(\{z_j\}; \{S_j\}), \quad (4.7)$$

$$(iii) \quad g_n^*(k; \{z_j\}; \{S_j\}) = g_n(k; \{z_j^*\}; \{S_j\}), \quad (4.8)$$

$$(iv) \quad g_n(k; \{1/z_j\}; \{S_j\}) = g_n(-k; \{z_j\}; \{S_j\}), \quad (4.9)$$

$$(v) \quad \text{if } |z_2| = \dots = |z_n| = 1, \text{ then the following symmetry rela-}$$

tions hold:

$$g_{n-1}(-k; \{z_j\}) = g_{n-1}^*(k; \{z_j\});$$

$$(k = S_1, S_1 - 1, \dots, -S_1). \quad (4.10)$$

Therefore, instead of proving conjectured Theorem A, we may verify the following theorem:

Conjectured Theorem B: If $f_n(\{z_j\}; \{S_j\}) = 0$ and $|z_1| \geq 1, \dots, |z_n| \geq 1$, then $|z_1| = |z_2| = \dots = |z_n| = 1$ for $K_{ij} \geq 0$.

For simplicity, we discuss the case of all $S_j = \frac{1}{2}$. In terms of the symmetry relation,

$$g_{n-1}(-\frac{1}{2}; \{z_j\}) = g_{n-1}^*(\frac{1}{2}; \{z_j\})$$

for $|z_2| = 1, \dots, |z_n| = 1$, one finds that if $|z_2| = 1, \dots, |z_n| = 1$, and if $f_{n-1}(\{z_j\}) = 0$, then $|z_1| = 1$. It is shown that conjectured Theorem B holds in the cases $n=1$ (trivial) and $n=2$ (Appendix C). As a result of the above discussions, the proof of conjectured Theorem B by mathematical induction as in the Ising model reduces to the verification of the following assertion:

Assertion B: If $g_{m-1}(S_1; z_2, \dots, z_m) = 0$ and $|z_2| \geq 1, \dots, |z_m| \geq 1$, then

$$|z_2| = |z_3| = \dots = |z_m| = 1$$

under the assumption that Theorem B is valid for $n = m - 1$.

It seems difficult to prove Assertion B in general, because the relation between the functions f_n and g_n is not so simple as in the Ising model.

§ 5. Discussion

If we apply the same argument to dilute ferromagnetism in terms of Theorem I as in previous papers,²⁾⁻⁴⁾ we find that the results predicted by the scaling law²²⁾ are valid even in the case of dilute ferromagnetism.

Extension of Theorem I is expected to be possible to the region $\lambda_{j,k} \geq 0$, including the usual Ising model with general spin. According to Theorem IV, the above problem reduces to the verification of the following assertion:

Assertion C: If Theorem II is valid in the case of $n = m - 1$ for $\lambda_{j,k} \geq 0$, then the hermite matrix \mathbf{S} is semi-positive definite for $|z_2| = \dots = |z_m| = 1$.

The relevant theorem of the usual Ising model with general spin ($S = \frac{1}{2}, 1, \frac{3}{2}$ and 2) has been confirmed by a high-speed computer.^{10), 23)}

In the ferromagnetic Heisenberg model, Theorems A and B are intuitively expected to hold from the consideration that the interaction $-J_{1j} \mathbf{S}_1 \cdot \mathbf{S}_j$ in the function g_{n-1} after tracing in the spin space S_1 will play a role of a positive effective field as was shown in the case $n=2$ (see Appendix C).

It should be noticed that Theorem I holds in the case when values of Bohr magneton differ at each lattice point, including non-magnetic atoms. This is easily confirmed from Theorem II, putting $z_1 = z^{p_1}, \dots, z_n = z^{p_n}$ (Bohr magneton $m_j = p_j m$; all $p_j \geq 0$, and $|z_j| \geq 1$ corresponds to $|z| \geq 1$, respectively).

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Appendix A

Hermite matrix S_m

Matrix $S_2 \geq 0$ corresponds to the inequality $|a_1| \leq 2|a_0|$. S_3 is given by

$$S_3 = \begin{pmatrix} 9|a_0|^2 - |a_2|^2 & 6a_0^*a_1 - 2a_1^*a_2 \\ 6a_0a_1^* - 2a_1a_2^* & 9|a_0|^2 - |a_2|^2 \end{pmatrix}. \quad (\text{A} \cdot 1)$$

Therefore, the condition $S_3 \geq 0$ is represented by

$$3|a_0| \geq |a_1| \quad (\text{A} \cdot 2)$$

and

$$9|a_0|^2 \geq |a_1|^2 + 2|3a_0^*a_1 - a_1^{*2}|, \quad (\text{A} \cdot 3)$$

where we have used $a_2 = a_1^*$ and $a_3 = a_0^*$. In the case $n=4$, the matrix S_4 is given by

$$S_4 = \begin{pmatrix} 16|a_0|^2 - |a_1|^2 & 2(6a_0^*a_1 - a_2^*a_1^*) & 8a_0^*a_2 - 3a_1^{*2} \\ (*) & 4(4|a_0|^2 + 2|a_1|^2 - a_2^2) & 2(6a_0^*a_1 - a_2^*a_1^*) \\ (**) & (*) & 16|a_0|^2 - |a_1|^2 \end{pmatrix}, \quad (\text{A} \cdot 4)$$

where we have used $a_4 = a_0^*$, $a_3 = a_1^*$ and $a_2 = a_2^*$.

Appendix B

Extension of Theorem II in the case $n=1$

For brevity, we discuss the case of $\lambda_{1,1} = \lambda$ and $\lambda_{1,2} = \dots = 0$, which corresponds to Theorem I-B. Since

$$f(z) = z^S f_1(z; S; \lambda) = a_0 z^{2S} + a_1 z^{2S-1} + \dots + a_{2S} \quad (\text{B} \cdot 1)$$

with

$$a_k = \exp \{ \lambda (S - k)^2 \},$$

we obtain the following inequality:

$$2Sa_0 \geq (2S-1)a_1 \geq \dots \geq a_{2S-1} > 0 \quad (\text{B} \cdot 2)$$

under the condition

$$\lambda' \geq \lambda \geq -\lambda'' ; \lambda'' = \frac{1}{2S-1} \ln \left(\frac{2S}{2S-1} \right)$$

and

$$\lambda' = \min \left\{ \frac{\ln(2/1)}{2S-3}, \frac{\ln(3/2)}{2S-5}, \dots, \left(S - \left[S - \frac{1}{2} \right] \right) \ln \frac{[S]}{[S]-1} \right\}. \quad (B.3)$$

Then, none of the roots of the equation $f'(z) = 0$ have an absolute value larger than 1 on the condition (B.3) in terms of the Eneström-Kekeya theorem. Therefore, all the roots of Eq. (B.1) have the absolute value equal to 1 for $\lambda' \geq \lambda \geq \lambda''$ in terms of the Schur-Kohn-Yamamoto theorem. On the other hand, it is easily confirmed (see Table) that

$$\lambda' > \lambda^0(S) \quad \text{for } 2 \leq S \leq 9/2. \quad (B.4)$$

Table. $\lambda^0(S)$ is a lower bound in Theorems I and II. λ_{eff}^0 is an effective lower bound. $\lambda'(S)$ is an upper bound appearing in Appendix B, which should be compared with $\lambda^0(S)$.

S	$\lambda^0(S)$	$\lambda_{\text{eff}}^0 = S^2 \lambda^0$	$\lambda'(S)$
1/2	$-\infty$	$-\infty$	—
1	$-\ln 2$	$-\ln 2$	—
3/2	0	0	—
2	.1221	0.49	$\ln 2 = .6932$
5/2	.1406	0.88	$(\ln 2)/2 = .3466$
3	.1346	1.21	$(\ln 2)/3 = .2311$
7/2	.1229	1.51	$(\ln 2)/4 = .1733$
4	.1108	1.77	$(\ln 3/2)/3 = .1352$
9/2	.0997	2.02	$(\ln 3/2)/4 = .1014$
5	.0900	2.25	$(\ln 3/2)/5 = .08109$
11/2	.0817	2.47	$(\ln 3/2)/6 = .06758$
6	.0745	2.68	$(\ln 4/3)/5 = .05754$
13/2	.0683	2.88	$(\ln 4/3)/6 = .04791$
7	.0629	3.08	$(\ln 4/3)/7 = .04110$
15/2	.0582	3.27	$(\ln 4/3)/8 = .03596$
8	.0540	3.46	$(\ln 5/4)/7 = .03188$
17/2	.0504	3.64	$(\ln 5/4)/8 = .02789$
9	.0472	3.82	$(\ln 5/4)/9 = .02479$
19/2	.0443	4.00	$(\ln 5/4)/10 = .02232$
10	.0418	4.18	$(\ln 6/5)/9 = .02026$
...
∞	0	∞	0

Consequently, Theorem I-B holds for $\lambda \geq -\lambda''$ and $S \leq 9/2$ in the case $n = 1$.

Appendix C

Proof of Theorem B for $n = 2$

The function $g_1(k; z_2)$ is given by

$$g_1(k; z_2) = \text{Tr}' \langle k | \exp(KS_1 \cdot S_2) | k \rangle_{z_2^{-S_2^z}}. \quad (\text{C} \cdot 1)$$

By a simple manipulation, we obtain

$$\langle \frac{1}{2} | \exp(KS_1 \cdot S_2) | \frac{1}{2} \rangle = A \exp(h' S_2^z), \quad (\text{C} \cdot 2)$$

where

$$A = a(1 - x^2/16)^{1/2}, \quad h' = 2 \tanh^{-1}(x/4),$$

$$a = e^{-K/4} \left(\cosh \frac{K}{2} + \frac{1}{2} \sinh \frac{K}{2} \right) \quad \text{and} \quad x = \left(\tanh \frac{K}{2} \right) / \left(2 + \tanh \frac{K}{2} \right). \quad (\text{C} \cdot 3)$$

Therefore, $J > 0$ (or $K > 0$) corresponds to $h' > 0$. Moreover, the relation between the functions g_1 and f_1 is represented by

$$g_1(k; z) = A f_1(e^{-h'/2} z^k). \quad (\text{C} \cdot 4)$$

This means that Theorem B holds for $n=2$.

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