Note: Proof of Lee-Yang Theorem [a]

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I. THE SETUP AND LEMMAS

We will be dealing with the following grand partition function in this document.

$$\Xi^G(\{z_j\}) = \sum_{\{n_j=0,1\}} \prod_j (z_j)^{n_j} e^{-4\beta \sum_{(j<k)} V_{jk}(n_j-n_k)^2} \quad \text{(grand partition function)} \tag{1}$$

This grand partition function is for Ising model or lattice gas model.

In order to facilitate the discussion in the next section, let us first introduce two identities and a theorem.

Lemma. The grand partition function (5) satisfies the following identity.

$$\Xi^G(\{z_j\}) = z_1 z_2 \cdots z_N \Xi^G(\{1/z_j\}) \tag{2}$$

Proof. By simply calculating the right-hand side,

$$\begin{aligned} z_1 z_2 \cdots z_N \Xi^G(\{1/z_j\}) &= z_1 z_2 \cdots z_N \sum_{\{n_j=0,1\}} \prod_{j=1}^N \left(\frac{1}{z_j}\right)^{n_j} e^{-4\beta \sum_{(j<k)} V_{jk}(n_j-n_k)^2} \\ &= \sum_{\{n_j=0,1\}} \prod_{j=1}^N z_j^{1-n_j} e^{-4\beta \sum_{(j<k)} V_{jk}(n_j-n_k)^2} \\ &= \sum_{\{m_j=1,0\}} \prod_{j=1}^N z_j^{m_j} e^{-4\beta \sum_{(j<k)} V_{jk}(m_j-m_k)^2} \quad (m_j := 1 - m_j) \end{aligned} \tag{3}$$

Here, nj and m_j are dummy index, then we are done. ∎

Lemma. The grand partition function (5) satisfies the following identity.

$$\Xi^G(\{z_j\}) = \left\{\Xi^G(\{z_j^*\})\right\}^* \tag{4}$$

Proof. Obivous.

[a] See: `https://github.com/hironaoy/notes/LeeYangTheorem`

II. GENERALISED PROPOSITION AND ITS PROOF

Proposition. Let

$$\Xi^G(\{z_j\}) = \sum_{\{n_j=0,1\}} \prod_j (z_j)^{n_j} e^{-4\beta \sum_{(j<k)} V_{jk}(n_j-n_k)^2} \quad \text{(grand partition function).} \tag{5}$$

Then the grand partition function $\Xi^G(\{z_j\})$ is non-zero in $\bigcap_{j=1}^{N}\{|z_j|<1\}$.

Proof. This proposition can be proven by induction on N, which is the number of sites of the system under consideration. **Suppose this proposition is true for the situation which the number of sites are less than or equal to $N-1$.** The grand partition function can be written in the following form by calculating the sum over n_N in (5):

$$\begin{aligned}\Xi^G(\{z_j\}) &= \sum_{n_N=0,1} (z_N)^{n_N} \sum_{\{n_j;\, j<N\}} \prod_{j<N} (z_j)^{n_j} e^{-4\beta\sum_{k<N} V_{1k}(n_j-n_k)^2} e^{-4\beta\sum_{(j<k<N)}(n_j-n_k)^2} \\ &= \sum_{\{n_j;\, j<N\}} \prod_{j<N} (z_j)^{n_j} e^{-4\beta\sum_{k<N} V_{1k}n_k^2} e^{-4\beta\sum_{(j<k<N)}(n_j-n_k)^2} \\ &\quad + z_N \sum_{\{n_j;\, j<N\}} \prod_{j<N} (z_j)^{n_j} e^{-4\beta\sum_{k<N} V_{1k}(1-n_k)^2} e^{-4\beta\sum_{(j<k<N)}(n_j-n_k)^2}.\end{aligned} \tag{6}$$

Since n_k only takes 0 or 1,

$$e^{-4\beta\sum_{k<N} V_{1k}n_k^2} = e^{-4\beta\sum_{k<N} V_{1k}n_k^2}, \quad e^{-4\beta\sum_{k<N} V_{1k}(1-n_k)^2} = e^{4\beta\sum_{k<N} V_{1k}n_k - 4\beta\sum_{k<N} V_{1k}}. \tag{7}$$

Then, setting $a_{jk} := e^{-\beta V_{jk}} \leq 1$,

$$\Xi^G(\{z_j\}) = \Xi^{G\backslash\{N\}}(a_{12}z_2, a_{13}z_3, \dots) + z_1 a_{12}a_{13}\cdots a_{1N}\Xi^{G\backslash\{N\}}(z_2/a_{12}, z_2/a_{13}, \cdots). \tag{8}$$

where $\Xi^{G\backslash\{N\}}(\{z_j\})$ is the grand partition function for a system with $N-1$ sites. In other words, $\Xi^{G\backslash\{N\}}(\{z_j\})$ is the grand partition function for the system that the Nth site is removed. Then using (**??**) and (**??**), we can write

$$\Xi^G(\{z_j\}) = \Xi^{G\backslash\{N\}}(a_{12}z_2, a_{13}z_3, \dots) + z_1 z_2\cdots z_N\Xi^{G\backslash\{N\}}(a_{12}/z_2^*, a_{13}/z_2^*, \cdots). \tag{9}$$

What we need to show is that $\Xi^G(\{z_j\})$ is non-zero. Suppose (9) be zero, then at least the following condition must be met.

$$\left|\Xi^{G\backslash\{N\}}(a_{12}z_2, a_{13}z_3, \dots)\right| = \left|z_1 z_2\cdots z_N\Xi^{G\backslash\{N\}}(a_{12}/z_2^*, a_{13}/z_2^*, \cdots)\right| \tag{10}$$

Since $\Xi^{G\backslash\{N\}}(a_{12}z_2, a_{13}z_3, \dots)$ is non-zero by hypothesis, this condition can be rewritten in the following form.

$$\left|\frac{z_1 z_2\cdots z_N\Xi^{G\backslash\{N\}}(a_{12}/z_2^*, a_{13}/z_2^*, \cdots)}{\Xi^{G\backslash\{N\}}(a_{12}z_2, a_{13}z_3, \dots)}\right| = 1 \tag{11}$$

Now, let us prove that this condition is not met by proving the sufficient condition:

$$\sup_{|a_{1j}|\leq 1}\sup_{|z_j|<1}\left|\frac{z_1z_2\cdots z_N\Xi^{G\backslash\{N\}}(a_{12}/z_2^*,a_{13}/z_2^*,\cdots)}{\Xi^{G\backslash\{N\}}(a_{12}z_2,a_{13}z_3,\dots)}\right|<1. \tag{12}$$

By the maximum modulas principle, which was introduced in the last section, we only need to consider the boundary with respect to z_j.

$$\begin{aligned}\sup_{|a_{1j}|\leq 1}\sup_{|z_j|<1}\left|\frac{z_1z_2\cdots z_N\Xi^{G\backslash\{N\}}(a_{12}/z_2^*,a_{13}/z_2^*,\cdots)}{\Xi^{G\backslash\{N\}}(a_{12}z_2,a_{13}z_3,\dots)}\right| &< \sup_{|a_{1j}|\leq 1}\sup_{|z_j|=1}\left|\frac{z_1z_2\cdots z_N\Xi^{G\backslash\{N\}}(a_{12}/z_2^*,a_{13}/z_2^*,\cdots)}{\Xi^{G\backslash\{N\}}(a_{12}z_2,a_{13}z_3,\dots)}\right| \\ &= \sup_{|a_{1j}|\leq 1}\sup_{|z_j|<1}\left|\frac{\Xi^{G\backslash\{N\}}(a_{12}/z_2^*,a_{13}/z_2^*,\cdots)}{\Xi^{G\backslash\{N\}}(a_{12}z_2,a_{13}z_3,\dots)}\right|\end{aligned} \tag{13}$$

Also, since $|z_j|=1$, we can replace $1/z_j^*$ with z_j. Then we get

$$\sup_{|a_{1j}|\leq 1}\sup_{|z_j|<1}\left|\frac{z_1z_2\cdots z_N\Xi^{G\backslash\{N\}}(a_{12}/z_2^*,a_{13}/z_2^*,\cdots)}{\Xi^{G\backslash\{N\}}(a_{12}z_2,a_{13}z_3,\dots)}\right| < \sup_{|a_{1j}|\leq 1}\sup_{|z_j|=1}\left|\frac{\Xi^{G\backslash\{N\}}(a_{12}/z_2^*,a_{13}/z_2^*,\cdots)}{\Xi^{G\backslash\{N\}}(a_{12}z_2,a_{13}z_3,\dots)}\right|=1. \tag{14}$$

Here, we proved (12) which proves the negation of (11) which proves that the grand partition function for a system with N sites is non-zero under the hypothesis that grand partition function for a system with $N-1$ sites is non-zero. Then, we are done. ∎

III. LEE-YANG THEOREM

Now, we specialise to the case when all the z_j are z, and $\Xi^G(z)$ is a polynomial of degree N.

Theorem. The zeros of $\Xi^G(z)$ all lie on the unit circle $\{z;\,|z|=1\}$ if exist.

Proof. From the proposition we proved in the last section, the interior of the unit circle is free of zeros. From (**??**), which with the proposition leads to

$$\Xi^G(z)=z^N\Xi^G(1/z)\neq 0 \quad \text{in} \quad \{z;\,|z|<1\}, \tag{15}$$

it is also non-zero in the exterior. In order to check that we can subsititute $1/z$ with some other variable w:

$$\frac{\Xi^G(w)}{w^N}\neq 0 \quad \text{in} \quad \{w;\,|w|>1\} \tag{16}$$

We are done. ∎
