yang-lee theorem

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Theorem(I): The quantity

$$\Theta = \lim_{V\to\infty}\left(\frac{1}{V}\ln\Xi(z,V,T)\right)$$

exists for all $z > 0$. The result is a continuous, non-decreasing function of z which is independent of the shape of the box (up to some sensible assumptions such as Surface Area$/V \sim V^{-1/3}$ which ensures that the box isn't some stupid fractalshape). Moreover, let R be a fixed, volume independent, region in the complex z plane which contains part of the real, positive axis. If R contains no zero of $\Xi(z,V,T)$ for all $z \in R$ then Θ is a an analytic function of z for all $z \in R$. In particular, all derivatives of Θ are continuous.

$$\Xi(z,V,T)=\sum_N \frac{z^N}{N!\lambda^{3N}}\int\prod_i d^3r_i e^{-\beta\sum_{j<k}U(r_{jk})}$$

Assume: 硬球两体相互作用

$$U(r_{jk})\begin{cases}=\infty, & r\le a,\\ =0, & r>b,\\ \ge u_0, & a<r\le b\end{cases}$$

首先考虑有限体积, 则系统存在粒子数上限 N_0, 此时巨配分函数是 degree=N 的多项式 $\Xi\sim\prod_{j=1}^{N}(z-z_j)$, 但其在实轴上显然没有根, 因此 (1)$z_1\neq$ 正实数;(2) 密度 ρ 和压强 βp 此时都是实的、正的解析函数;(3)define $v^{-1}=\rho$, 则 $p(v,T)$ 是解析函数, 且 $\rho,\left(\frac{\partial\rho}{\partial\ln y}\right)_T,\left(\frac{\partial p}{\partial\rho}\right)_T$ 都是正的, 并有限.

Conclusion: V 有限时, 不会发生相变.

取热力学极限 $N \to \infty, V \to \infty$. Ξ is now defined as an infinite series.

Lemma(I): $z > 0$ 时,

$$\lim_{V\to\infty} \frac{1}{V} \ln \Xi = \beta p$$

存在, 且是 z 的单调连续递增函数.

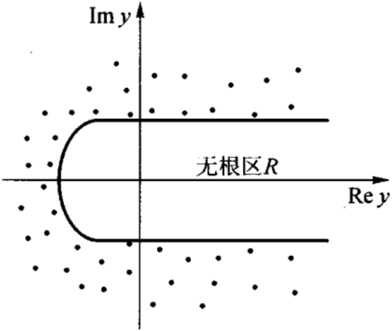
Lemma(II): 设在 z 的复平面上存在区域 R, 其中不包含 Xi 的零点、并且包含了一段正的实 z 轴, 则在 R 内

$$\lim_{V\to\infty} \frac{1}{V} \ln \Xi, \text{ and } \forall\text{正整数}n, \lim_{V\to\infty} \frac{1}{V} \frac{\partial^n}{\partial(\ln z)^n} \ln \Xi$$

都存在, 且是 z 的解析函数. 此外 $\frac{\partial}{\partial(\ln y)}$ 与 $\lim_{V\to\infty}$ 在 R 上对易.

相变

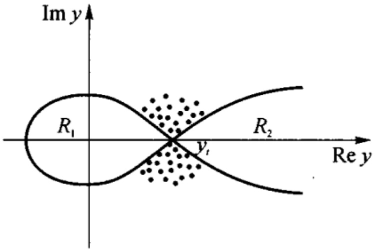
(1) 实轴上无根



density: $\rho = \frac{\partial \Theta}{\partial (\ln z)}$ 存在且大于零 (Lemma(I)).

$p - \rho$: $\frac{\partial p}{\partial \rho} = \frac{\partial p / \partial (\ln z)}{\partial \rho / \partial (\ln z)}$. 而我们知道分母不为零 (见前文有限体积的讨论), 于是无相变.

(2) 极限下根向实轴逼近



If we look at points z where zeros appear on the positive real axis, then Θ will generally not be analytic. If $\partial\Theta/\partial z$ is discontinuous, then the system is said to undergo a first order phase transition. More generally, if $\partial^m\Theta/\partial z^m$ is discontinuous for $m = n$, but continuous for all $m < n$, then the system undergoes an n^{th} order phase transition.($\sim$ 点的密度)

Theorem(II): The zeroes of the $\Xi(z)$ all lie on the unit circle $|z| = 1$, where $z = e^{\beta\mu}$.

- Ising model in a random field
- lattice gas in a random medium
- 有序-无序转变

I 的详细证明见李政道的《统计力学》3.1 和 3.2, 下面介绍 II 的证明.

There are at least two different lines of approach, algebraic or analytic. We choose the latter(simple).

Suppose we have a finite graph G with vertices labelled by i = 1, . . . , N and edges by (jk) with j < k. At each vertex i there is an Ising spin si taking the values ± 1. The partition function of the classical ising model is

$$Z(h) = \sum_{\{s_i\}} \exp \beta \left(\sum_{jk} V_{jk} s_i s_j + \sum_{j} h_j s_j \right), \tag{1}$$

and can be mapped to a lattice gas by $n_j = \frac{1}{2}(s_j + 1)$ taking 0 or 1. Restricting $n \leq 1 \to$ fermions. Taking $V_{jk} \leq 0 \to$ attractive.

Then considering the grand partition function

$$\Xi(z) = \sum_{n_j=0,1} \prod_j z_j^{n_j} \exp\left(-4\beta \sum_{jk} V_{jk}(n_j - n_k)^2\right), \tag{2}$$

where $z_j = e^{2\beta h_j}$ is the local activity.
Under the Ising symmetry($s_j \to -s_j, h_j \to -h_j$), which translates into ($n_j \to 1 - n_j, z_j \to z_j^{-1}$), the grand partition function is invariant,

$$\Xi(z) = (\prod_{j=1}^{N} z_j)\Xi(z^{-1}). \tag{3}$$

V_{jk} is real $\to \Xi(z) = \overline{\Xi}(\overline{z})$

We can state that $\Xi(z)$ is non-zero in $\bigcap_{j=1}^{N}\{|z_j|<1\}$.(对 N 做数学归纳法)
The case $N=1$ is trivial, where $\Xi(z_1)=1+z_1$.
For $N=2$, $\Xi(z_1,z_2)=1+a_{12}(z_1+z_2)+z_1z_2$, which vanishes when $z_2=-\frac{1+a_{12}z_1}{a_{12}+z_1}$. This maps $|z_1|<1$ into $|z_2|>1$, in other words there is no way to take the $|z_1|<1$ and $|z_2|<1$ at the same time.
Suppose it is true for all graphs of degree $\leq N-1$. Considering the sum over n_1 in (2), the term with $n_1=0$ just gives the partition function without site 1($\mathcal{G}\backslash\{1\}$), while that with $n_1=1$ modifies the activities at the remaining vertices of $\mathcal{G}\backslash\{1\}$.

Setting $a_{jk} = e^{-\beta V_{jk}} \leq 1$, then

$$\begin{aligned}\Xi^{\mathcal{G}}(z_1,\ldots,z_n) = \quad & \Xi^{\mathcal{G}\backslash 1}(a_{12}z_1,\ldots,a_{1n}z_n) \\ & + z_1 a_{12}\ldots a_{1n}\Xi^{\mathcal{G}\backslash 1}(z_2/a_{12},\ldots,z_n/a_{1n}). \end{aligned} \tag{4}$$

The first term is non-zero by hypothesis, and the second may be written $z_1\ldots z_n\overline{\Xi^{\mathcal{G}\backslash 1}}(a_{12}/\bar{z_2},\ldots,a_{1n}/\bar{z_n})$,
Beside we can say that the second term is smaller than the first,

$$\sup_{|a_{1j}|\leq 1}\ \sup_{|z_j|<1}\left|\frac{z_1\ldots z_n\overline{\Xi^{\mathcal{G}\backslash 1}}(a_{12}/\bar{z_2},\ldots,a_{1n}/\bar{z_n})}{\Xi^{\mathcal{G}\backslash 1}(a_{12}z_1,\ldots,a_{1n}z_n)}\right| \leq 1, \tag{5}$$

because
Continuity: the left-hand side does not change if we go with $|a_{1j}| \leq 1 \to |a_{1j}| < 1$.
Maximum modulus principle: the supremum is attained on the boundary, so we need to consider the bound $|z_j| = 1$, where the left-hand side become 1.

$$\Xi^{\mathcal{G}}(z_1,\ldots,z_n) = \Xi^{\mathcal{G}\backslash 1}(a_{12}z_1,\ldots,a_{1n}z_n) + z_1\ldots z_n\overline{\Xi^{\mathcal{G}\backslash 1}}(a_{12}/\bar{z_2},\ldots,a_{1n}/\bar{z_n}). \quad (6)$$

We can see the first term is largger than the second, so it is impossible to find a point making $\Xi^{\mathcal{G}}(z_1,\ldots,z_n)$ vanishes.
However for the present we specialize to the case when all the z_j are equal to z, and Ξ is a polynomial of degree N in z.
Proof:From the our statement before, the interior of the unit circle is free of zeroes. But from (3) the exterior of the unit circle is also zero-free. That's all.

Example:

$$\Xi = \frac{(1+z)^V(1-z)^V}{1-z}, V \in \mathbb{Z}$$

根 $z=-1, e^{2\pi ik/V}$ 分布在单位圆上，极限下根的密度增加，有些根将接近 $z=1$. 通过 Θ 计算 p,ρ，得到状态方程，

$$\beta p = \begin{cases} \ln\frac{V}{V-1}, & V>2; \\ \ln 2, & \frac{2}{3}\le V\le 2; \\ \ln\frac{V(1-V)}{(2V-1)^2}, & \frac{1}{2}<V<\frac{2}{3}. \end{cases}$$

具体步骤见李政道的《统计力学》3.3

others：静电模拟

$$\frac{1}{V}\ln \Xi = \sum_{l=0}^{\infty} \alpha_l(V) z^l$$

迈耶的猜想和其猜想的错误证明源于 $l \to \infty$ 和 $V \to \infty$ 两个极限过程的不合理的对调. 他们先取 $V \to \infty$ 就无法得到割线和实轴相交的位置. 应该先让 V 有限并使 $l \to \infty$, 得到根向实轴逼近的趋势, 再取 $V \to \infty$ 定出相变点.

在 yang 和 lee 的第二篇文献中，他们利用了外部磁场 h 下的铁磁 Ising 模型与具有 activity $z = e^{\beta h}$ 的晶格气体之间的等价性，证明了：在任何 degree$= N$ 的有限图上，配分函数仅在单位圆上有零点，此时这对应于纯虚数的 h.
此外，由于对于实数 h，Ξ 是正项的和，因此这些零点离实轴有一定距离. 这种情况应在适当规则的晶格上和热力学极限下，在足够高的温度下持续存在，并且当 $|Imh|$ 大于某个临界值 h_c 时，零点应在虚轴上变得密集. 这个极限点被称为杨-李边界 (Yang-Lee edge). 在零磁场 $h = 0$ 下，free energy per site 的极限 $\lim_{N\to\infty}\left(-\frac{1}{N}\right)\log Z$ 随着温度 T 从上方接近临界温度 T_c 时出现奇异性.yang 和 lee 认为其来源于杨-李边界接近实轴，即 $h_c \to 0$.

References I

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2. 《统计力学》李政道
3. 《Statistical Physics》David tong