Lee-Yang theorem

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May 15, 2014

1 Introduction

In 1952, Lee and Yang published two important papers [1, 2] in statistical mechanics. They gave us a new way of looking at the nature of phase transitions, and suggested that we can regard partition functions as functions of external fields (in the case of Ising model, this would be magnetic fields), whose domains can be extended to the complex plane. In particular, they proved a series of Lee-Yang theorems.

2 Lee-Yang theorems

The Ising model has the Hamiltonian $-\beta\mathcal{H} = K \sum_{<i,j>} \sigma_i\sigma_j + h\sum_{i=1}^{N} \sigma_i$. Here $K > 0$ means ferromagnetic interactions, and $K < 0$ means antiferromagnetic interactions. h is the external magnetic field.

We will formulate the Lee-Yang theorems in terms of Ising model. They also apply to liquid gas systems, if we replace the number of sites N with the volume of the system V, and $z = e^{-2h}$ with $z = e^{\beta\mu}$, the fugacity.

1. The quantity $f(z) = \lim_{N\to\infty} \frac{1}{N} \log Z_N(z)$ exists for all $z > 0$.

2. Let R be a fixed region in the complex z plane, independent of N. R contains part of the real, positive axis. If R does not contain zeroes of $Z_N(z)$, $\forall z \in R$, and $\forall N$, then $f(z)$ is an analytic function for $z \in R$.

$Z_N(z)$ is a polynomial in z, up to some overall z dependence. Since all the coefficients are positive, $Z_N(z)$ cannot have zeroes for $z > 0$. This just means that a system of finite size cannot have phase transitions. However, in the thermodynamic limit $N \to \infty$, $Z(z)$ becomes an infinite series, and could have some zeroes for $z > 0$. What Lee-Yang theorems tell us is that as long as the zeroes (Lee-Yang zeroes) of $Z_N(z)$ stay away from the positive real axis, then $f(z)$ is infinitely differentiable, which means there is no phase transition. If some of the zeroes approach the real z axis, for example z^*, then $f(z)$ is in general not analytic at $z = z^*$. A phase transition at $z = z^*$ is said to be of nth order, if $\frac{d^n f}{dz^n}$ is the lowest derivative that is discontinuous [3].

3. For a finite system of Ising model with ferromagnetic couplings, the zeros of the partition function, when viewed as a function of external magnetic field h, lie at the imaginary axis of h, i.e. on the unit circle of z. This is sometimes call the Lee-Yang circle theorem.

The circle theorem gives a far-reaching result on the nature of phase transitions for Ising model. Since the zeros are at imaginary h, there could be only two possibilities. Either they stay away from $h = 0$, in which case there is no phase transition, or some converge to $h = 0$, in which case there is one phase transition at zero magnetic field and finite temperature, and therefore two phases. The theorem is true regardless of dimension, size, structure, symmetry or periodicity of the lattice system.

The circle theorem was later extended to other models, such as $(\varphi^4)_2$ Euclidean field theory. For other models, although the Lee-Yang zeroes do not have such nice properties, one can still study their distribution to understand the phase transitions. People have also studied zeros in the complex temperature plane (Fisher zeroes), and gained insight into the structure of the free energy [4].

3 Lee-Yang singularity for 1D Ising

We first give an explicit example of how the Lee-Yang singularity theorem manifests in 1D Ising model.

The 1D Ising model can be solved exactly using the method of transfer matrices [5].

Let $< \sigma_i|T|\sigma_j >= \exp[K\sigma_i\sigma_j + \frac{h}{2}(\sigma_i + \sigma_j)]$. Then $T = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix}$.

$Z_N = \sum_{\{\sigma_i=\pm1\}}^{N} \exp[-\beta\mathcal{H}] = \mathrm{Tr}[T^N]$.

The two eigenvalues of T are $\lambda_\pm = e^K \cosh h \pm \sqrt{e^{2K}\sinh^2 h + e^{-2K}}$. Then the partition function has the simple form $Z_N = \lambda_+^N + \lambda_-^N$.

Let's examine the zeros of this partition function. $\lambda_+^N + \lambda_-^N = 0$ implies $\lambda_+ = \exp\frac{i(2n-1)\pi}{N}\lambda_-$, with $n = 1, 2, \cdots N$.

This can be re-written as $\cos\left(\frac{(2n-1)\pi}{2N}\right)\sqrt{e^{-4K} + \sinh^2(h)} = i\sin\left(\frac{(2n-1)\pi}{2N}\right)\cosh h$, which can be further re-written as $\cosh^2 h = \cos^2(\frac{(2n-1)\pi}{2N})(1 - e^{-4K})$.

This has solutions $h_n = i\theta_n$, with $\cos\theta_n = \sqrt{1 - e^{-4K}}\cos\frac{(2n-1)\pi}{2N}$. Indeed, the zeros lie on the imaginary axis of h.

Moreover, as $|\cos\theta_n| \leq \sqrt{1-e^{-4K}} < 1$ at finite temperature, in the limit $N \to \infty$, $\cos\theta \nrightarrow 1$. In other words, $h_n \nrightarrow 0$ as $N \to \infty$. We've just derived the well-known result that there is no phase transition in 1D.

4 A perturbative example of the Lee-Yang circle theorem

We shall now describe a perturbative example of Lee-Yang circle theorem for Ising model on a general d-dimensional square lattice.

We note that the partition function has a 2^N-fold symmetry, corresponding to flipping each individual spin. The Hamiltonian is invariant if we perform the operation $\sigma_i \to -\sigma_i$ for all spins and $h \to -h$ simultaneously. Hence, the partition function is also invariant under $h \to -h$.

Write $Z_N(h) = \exp(-\beta f_+ N)$, and $Z_N(-h) = \exp(-\beta f_- N)$, where f is the free-energy per site. Then $Z_N = \frac{1}{2}(\exp(-\beta f_+ N) + \exp(-\beta f_- N))$. We can redefine the free energy and then $Z_N = \exp(-\beta f_+)^N + \exp(-\beta f_-)^N$, which is analogous to the 1D Ising model.

If we treat the magnetic field as complex, then it's unclear what defines the ground state . However, we can at least do a formal expansion around the state with all spins up, which is really the low temperature expansion for positive magnetic field.

The first few terms in the expansion looks like $Z_N(h) = e^{dNK+Nh}(1 + Ne^{-4dK-2h} + dNe^{-4(2d-1)K-4h} + \frac{N(N-2d-1)}{2}e^{-8dK-4h} + \cdots)$ and the free energy is of the form $\beta f_+ = -(dK+h) - e^{-4dK-2h} - de^{-4(2d-1)K-4h} - \frac{2d+1}{2}e^{-8dK-4h} + \cdots$. That of $Z_N(-h)$ and βf_- are similar, with h replaced by $-h$.

The condition $Z_N = 0$ translates into $\mathrm{Re}(f_+ - f_-) = 0$ and $\mathrm{Im}(f_+ - f_-) = \frac{(2n-1)\pi}{\beta N}$. $\beta(f_+ - f_-) = -2h + 2e^{-4dK}\sinh(2h) + 2de^{-4(2d-1)K}\sinh(4h) + (2d+1)e^{-8dK}\sinh(4h) + \cdots$. So we see that $\mathrm{Re}(h) = 0$ is a solution, and then $\mathrm{Re}(\beta(f_+ - f_-)) = 0$ to all orders. The zeros are at $\theta_n = \frac{(2n-1)\pi}{2N} + e^{-4dK}\sin(\frac{(2n-1)\pi}{N}) + \cdots$ [6].

5 Renormalization of 1D Ising model, and Lee-Yang zeroes

If we use a renormalization scheme in which we eliminate every other spin, we get the following recursion relations

$e^{2h'} = e^{2h}\frac{\cosh(2K+h)}{\cosh(2K-h)}$

$e^{4K'} = \frac{\cosh(4K)+\cosh(2K)}{2\cosh^2(h)}$

It is obvious that $m = 1+e^{4K}\sinh^2(h)$ is renormalization invariant. Use it to eliminate h, and introduce the variable $x = -\frac{m}{e^{4K}-1}$, we can transform the recursion relations into $x' = 4x(1-x)$, which is the logistic map. This will exhibit chaos for almost all $0 < x < 1$, i.e. $1 - e^{4K} < m < 0$. The first inequality constrains h to be imaginary, i.e. $h = i\theta$. The second one implies $\sin^2(\theta) > e^{-4K}$ [7].

In essence, the boundary of chaos is precisely the lowest Lee-Yang zero in the thermodynamic limit.

It is unclear to the author if these chaotic behaviour means anything physical. Also, it is observed that all the Lee-Yang zeroes fall into the chaotic region. Since the above logistic map contains cycles of arbitrary length. do the Lee-Yang zeros correspond to genuine chaos or just cycles?

Recall that, for a 1D Ising model of N sites, the Lee-Yang zeroes are of the form $\cos(\theta) = \sqrt{1-e^{-4K}}\cos\frac{(2n-1)\pi}{2N}$, the corresponding new variable is $x = \sin^2\frac{(2n-1)\pi}{2N}$. Then $x' = \sin^2(\frac{(2n-1)\pi}{N})$.[1] It is obvious that the form of expression is essentially unchanged, and the Lee-Yang zeroes are eventually mapped into cycles! However, the map never gets back to a zero in the same system, since $2(2n-1)$ is even.

If N is even, the recursion relation maps the Lee-Yang zeroes for a system of size N to the zeroes of a system of size $\frac{N}{2}$. If $N = 2^n$, each iteration gives back the Lee-Yang zeroes for a system of half the size, until we hit $N = 1$, at which $x = 0$, and will stay at 0 forever.

6 Conclusion

The Lee-Yang theorems concerning phase transitions were discussed, and the circle property of the Lee-Yang zeroes of 1D Ising model is explicitly presented, with those of higher dimensions obtained perturbatively. While the renormalization relation for 1D Ising model only have trivial fixed points, it reduces to $r = 4$ logistic map in a restricted region of imaginary magnetic field, which is in general chaotic for $0 < x < 1$. Although the Lee-Yang zeroes fall into the chaotic region, they do not correspond to chaotic behaviour, but can be mapped into cycles after a few iterations. In [7] it was observed that the Lee-Yang zeroes for 1D Potts model also have a boundary which is the boundary of the logistic map, but it is unclear what is the behaviour of the zeroes under such map, since we do not have the analytic form of the zeroes for finite N. It will be interesting to study the recursion maps of the Lee-Yang zeroes of a model if we have a well-defined renormalization scheme, to see if such chaotic and cycle behaviour is universal.

[1] The general solution of the logistic map $x_n = 4x_{n-1}(1-x_{n-1})$ is $x_n = \sin^2(2^n\theta\pi)$.

References

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