The Lee-Yang Theorem and applications

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Abstract: We present the Lee-Yang theory that links the study of phase transitions to the localization of zeros in the complex fugacity plane. We prove the Lee-Yang theorem using Asano's contraction method and we apply it for the one and two dimensional Ising model. We also show that the Lee-Yang formalism can shed some light on the difficult task of counting the number of ground states in supersymmetric theories.

I. INTRODUCTION

The birth of statistical mechanics provided us with a mechanical explanation to many thermodynamical phenomena. It established a relation between the microscopic and macroscopic worlds, hence it is of primary importance to Physics. The Ising model is the simplest model in which we can study the theory of phase transitions. In 1924, Ising himself proved in his thesis that the one dimensional case undergoes no phase transition at $T \neq 0$. The two dimensional model was far more challenging and it was not until 1944 that Onsager showed that the square lattice Ising ferromagnet undergoes a phase transition at a critical temperature when no magnetic field is applied. Nowadays, the two dimensional Ising model in a nonzero magnetic field remains unsolved.

In 1952 Yang and Lee published two articles [3] and [4] in which a new perspective on the understanding of phase transitions was presented. The first article corresponds to our first section, in which we establish a relation between phase transitions and the distribution of the roots of the grand canonical partition function. In the second section, we focus on the Ising model, we prove the Lee-Yang theorem presented in the second article using the Asano's contraction method introduced in [5] for the Heisenberg model. This adaptation is due to [2]. We also compute the explicit distribution of roots in the complex fugacity plane. For the one dimensional case, we verify the Ising result that there is no phase transition. In the two dimensional case, we are able to confirm that the two dimensional Ising model has only one phase transition, which was not proved in Onsager original paper.

Finally, we explore further applications to the Lee-Yang theory showing that the study of the distribution of roots can also play an interesting role in counting the number of ground states for a supersymmetric quantum theory.

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II. ZEROS OF THE PARTITION FUNCTION

Consider a system of N particles with a Hamiltonian $\mathcal{H}$ that has energy eigenvalues E_r. The probability of the system being in some particular state with energy E_r at a temperature T is given by $p_r = \frac{e^{-\beta E_r}}{Z_N(T,V)}$, where $\beta = 1/k_B T$ and $Z_N(T,V)$ is known as the **canonical partition function** defined as

$$Z_N(T,V) = \sum_r e^{-\beta E_r},$$

where the sum extends over all possible states. $Z_N(T,V)$ depends on T explicitly and on V and N through the energy $E_r(V,N)$.

If we do not fix the number of particles in the system, it is useful to work in the grand canonical ensemble, the partition function of which is the **grand canonical partition function**, that allows us to describe the system through the chemical potential μ, V and T. It is convenient to introduce the fugacity $z = e^{\beta\mu}$. The grand canonical partition function is therefore expressed as

$$\mathcal{Q}_M(z,V,T) = \sum_{n=0}^{M} Z_n(V,T) z^n, \tag{1}$$

where M is the maximum number of particles that can be put in the volume V.

We need to establish a connection between statistical mechanics and thermodynamics. To that end, let us recall the grand potential defined as $\Xi = U - TS - \mu N$. We hypothesize that the grand canonical partition function and the grand potential are related through

$$\Xi(\mu,V,T) = -k_B T \ln \mathcal{Q}(\mu,V,T). \tag{2}$$

However, the distinct ensembles only describe the same macroscopic properties in the thermodynamic limit, that is, $N \to \infty$ and $V \to \infty$ with $N/V =$ constant. The pressure p and density ρ are accordingly given by

$$\frac{p}{k_B T} = \lim_{V\to\infty} \left(\frac{1}{V} \ln \mathcal{Q} \right), \tag{3}$$

$$\rho = \lim_{V\to\infty} \left(\frac{\partial}{\partial \ln z} \frac{1}{V} \ln \mathcal{Q} \right). \tag{4}$$

The formal existence of this limit is not clear. Nevertheless, Lee and Yang proved two theorems which ensure that in the thermodynamic limit we recover the expected behavior.

Theorem 1. *[3] Assume that the shape of V is such that its surface area does not increase faster than $V^{2/3}$. Then for all positive real values of z, $V^{-1}\ln\mathcal{Q}$ approaches, as $V\to\infty$, a limit which is independent of the shape of V. Furthermore, this limit is a continuous, monotonically increasing function of z.*

Theorem 2. *[3] If in the complex z plane a region R containing a segment of the positive real axis does not contain any roots of (1), then, in this region, as $V\to\infty$, all the quantities*

$$\left(\frac{\partial}{\partial\ln z}\right)^k \frac{1}{V}\ln\mathcal{Q} \text{ with } k=0,1,\ldots$$

approach limits which are analytic with respect to z. Furthermore the operators $(\partial/\partial\ln z)$ and $\lim_{V\to\infty}$ commute in R.

As we can see from equation (1), $\mathcal{Q}_M$ is a polynomial on z and, since the coefficients are positive, $\mathcal{Q}_M$ cannot have positive roots. We conclude that the grand potential will be a well behaved function and therefore we do not expect any singularities or discontinuities in any of the functions derived from it. For this reason, no phase transition takes place in a finite system. A non-analytic behavior is only possible in the thermodynamic limit. The roots of (1) are functions of the parameters V, T and the nature of the interaction between the particles of the system. As we increase the volume (and therefore the maximum number of particles that can be fit in) it is possible that a succession of zeros close in to a point of the real positive axis, say t. Any neighborhood of t is not a region R free of roots, so t is a candidate for a phase transition and divides the complex z plane into two distinct regions as we can see in figure 1.

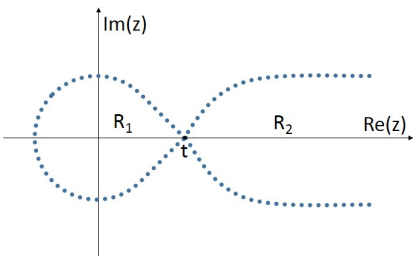

FIG. 1: The two regions separated by the limit point

In the point $z=t$, the pressure p is continuous by theorem 1, but the analyticity of its derivative is not guaranteed by theorem 2. In the case that its derivative presents a discontinuity at point t corresponding to p_0, we have that ρ undergoes a discontinuity jump at point t between the corresponding densities of the two phases, ρ_1 and ρ_2. This situation reflects a first order transition between two phases represented by regions 1 and 2 as noted in figure 2.

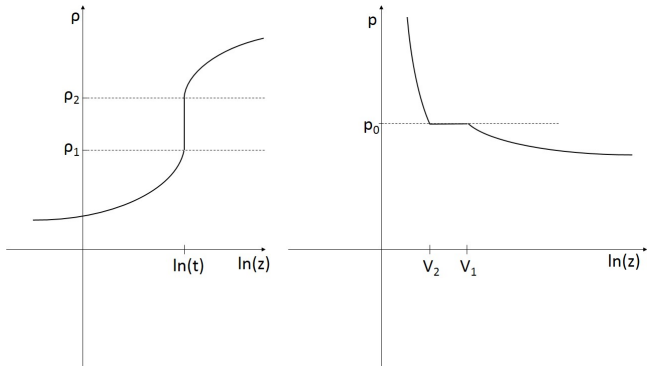

FIG. 2: Diagrams $\rho-\ln(z)$ and $p-\ln(z)$

Suppose now that the roots of $\mathcal{Q}_M(z)=0$ close in to the real axis at two points $z=t_1,t_2$. By the same reasoning as in the previous case, we expect three distinct phases of the system separated by t_1 and t_2. As the temperature varies, the points t_1 and t_2 will in general move along the real z axis. If at a certain temperature T_c one of the points, say t_1, it is not longer a limit point of the distribution of zeros, then T_c corresponds to the critical temperature for the transition between phase 1 and phase 2. On the other hand, if t_1 and t_2 merge together at a particular temperature T_0, we would have a triple point at that temperature.

The theory of Lee and Yang establishes a connection between the study of phase transitions and the distribution of zeros of the grand partition function in the fugacity complex plane. However, the study of these distributions is still a very complicated problem. In the following section we discuss the nature of the distribution of zeros for the one and two dimensional Ising model, which happens to be particularly simple.

III. ISING MODEL AND LATTICE GAS

Consider an arbitrary n-dimensional lattice with N sites. At each site of the lattice we assign a variable $\sigma_i\in\{-1,+1\}$ representing the site's spin (up or down). Each site i interacts with each nearest neighbor j with energy $-J\sigma_i\sigma_j$. We will restrict our study to the ferromagnetic case, that is, $J>0$. We also consider an external constant magnetic field H acting over all the sites. This system is known as the **Ising model** and its Hamiltonian is given by

$$\mathcal{H}=-J\sum_{(ij)}\sigma_i\sigma_j-\mu H\sum_i\sigma_i. \tag{5}$$

Let q be the number of nearest neighbors at each site and N_-, N_+ the number of spins facing down and up

respectively and finally let N_{++} be the number of nearest neighbor pairs with both spins facing up. It can be shown that the partition function of this system can be written as (see [1])

$$Z_N(H,T) = e^{\beta N\left(\frac{1}{2}qJ-\mu H\right)} \sum_{N_+=0}^{N} e^{-2\beta(qJ-\mu H)N_+} \sum_{N_{++}} \Omega_N(N_+,N_{++}) e^{4\beta J N_{++}}, \tag{6}$$

where $\Omega_N(N_+,N_{++})$ is the degeneracy of a given energy, that is, the number of different lattice configurations that macroscopically have the same energy.

We have the expression for the Ising model partition function, however, the Lee-Yang theorems apply to the grand canonical partition functions. We will now relate the canonical and grand canonical partition functions of the Ising model and the **lattice gas**. A lattice gas is a collection of A atoms distributed through a n-dimensional lattice of size N (which it will play the role of the volume). Each lattice site can be occupied by at most one atom and we associate an energy $-\varepsilon$ ($\varepsilon > 0$) to each pair of atoms that are nearest neighbors. Thus the total energy will be $E = -\varepsilon L$, where L is the total number of nearest-neighbor pairs of atoms. Let $\Omega_N(A,L)$ denote the degeneracy of the state with energy $-\varepsilon L$, that is, the number of distinct ways in which we can distribute A atoms through the N sites of the lattice such that the total energy of interaction is $-\varepsilon L$. The partition function of this system is then given by

$$Z_A(T,V) = \sum_L \Omega_N(A,L) e^{\beta\varepsilon L},$$

and the corresponding grand canonical partition function will be

$$\mathcal{Q}(z,N,T) = \sum_{A=0}^{N} z^A Z_A(N,T). \tag{7}$$

We can establish a formal correspondence between the lattice gas and the Ising model as noted in [1]. The canonical partition function of the Ising model (6) corresponds to the grand canonical partition function of the lattice gas (7), with $z = \exp -2\beta(qJ-\mu H)$, $L = N_{++}$, $\varepsilon = 4J$ and $A = N_+$. Therefore the study of the two systems is equivalent. We will now proceed to apply the theory of Lee-Yang to the Ising model. Accordingly, the zeros of the grand canonical partition function of the lattice gas will correspond to the zeros of the canonical partition function of the Ising model. In that regard, it is convenient to work with expression (5) to get an alternative expression for the Ising model partition function (this one expressed as a sum over all the sites). It will be useful to let the magnetic field have different values at each site, therefore we consider that at site i the magnetic field is h_i. Thus we have that

$$Z_N = \frac{1}{2^N} \exp\left(\beta J\gamma + \beta\mu \sum_i h_i\right) P(\beta, h_i),$$

where γ is the total number of interacting pairs and P is given by

$$P = \sum_{\sigma_i=\pm 1} \exp\left[\beta J \sum_{(ij)} (\sigma_i\sigma_j - 1) + \beta\mu \sum_i h_i(\sigma_i - 1)\right].$$

It is handy to define the variables $\rho_i = e^{-2\beta\mu h_i}$ and $\tau = e^{-2J\beta}$. In this way P is a polynomial of degree one in each of the ρ_i and of degree L in τ. The roots of this polynomial are distributed in the unit circle in the ρ complex plane as stated by the following theorem.

Theorem 3 (Lee-Yang circle theorem)**.** *For a finite Ising model system with ferromagnetic couplings, the zeros of the canonical partition function lie on the unit circle in the complex ρ-plane.*

Proof. We first consider P a polynomial of degree one in each of the ρ_i and then set all $\rho_i = \rho$. The expression for the simplest graph of two vertices linked is $P = 1 + \tau(\rho_1+\rho_2) + \rho_1\rho_2$. It is clear that any simple graph can be constructed joining simple graphs of two vertices and identifying the sites of the union as we can see in the following figure.

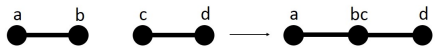

FIG. 3: Construction of a three vertex graph from the elementary one.

We now look how can we build the polynomial P of the new graph from its components which we will refer as P_1 and P_2. We notice that P_i is affine in ρ_i, hence we can write $P_1 = B_+ + \rho_b B_-$ where B_+ refers to the contribution with $\sigma_b = +1$ and B_- refers to the one with $\sigma_b = -1$. Analogously, we have $P_2 = C_+ + \rho_c C_-$. When b and c are identified, we have a new variable ρ_{bc} that is assigned to the site bc. The total polynomial before the union is

$$P_{12} = B_+C_+ + \rho_b B_-C_+ + \rho_c B_+C_- + \rho_b\rho_c B_-C_-,$$

and the polynomial after the identification is given by

$$P_{bc} \equiv B_+C_+ + \rho_{bc} B_-C_- \equiv A_{++} + \rho_{bc} A_{--}.$$

This contraction process allows us to obtain the polynomial P for an arbitrary graph starting from the most elemental one. We will now prove that the theorem is true for the 2 vertex graph, then we will see that this property survives the contraction process and therefore it is also true for an arbitrary graph. The polynomial $P = 1 + \tau(\rho_1+\rho_2) + \rho_1\rho_2$ vanishes if

$$\rho_1 = \frac{1+\tau\rho_2}{\tau+\rho_2}.$$

It is easy to check that if $|\rho_2| > 1$ then $|\rho_1| < 1$ and the other way around, so the polynomial cannot vanish

if both ρ_1 and ρ_2 have modulus smaller or greater than one. When we set $\rho_1 = \rho_2 = \rho$, this proves the theorem for $n = 2$. We now need to check that this property indeed survives the contraction process. We take $\rho_b = \rho_c = \rho$ and keep all other ρ_i constant, thus we have that before the vertex identification $P_{12} = A_{++} + \rho(A_{-+} + A_{+-}) + \rho^2 A_{--}$. Assume $P_{12}(a) \neq 0$ when $|\rho_i| < 1$ for all i, this implies that $|A_{++}| > |A_{--}|$, in which case the polynomial after the identification $P_{bc} = A_{++} + \rho A_{--}$ does not vanish for $|\rho| < 1$. If now we set all $\rho_i = \rho$, the polynomial P_{bc} is a palindromic polynomial due to the spin reversal symmetry. If a is a root of the polynomial, then $1/a$ is also a root of it. Then P_{bc} cannot vanish for $|\rho| < 1$ and $|\rho| > 1$. This completes the proof. □

Following [1], the partition function of the Ising model is given by the trace of the matrix

$$M = \begin{pmatrix} e^{\beta(J+\mu h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-\mu h)} \end{pmatrix}.$$

Diagonalizing the matrix M we obtain the two eigenvalues $\lambda_+ > \lambda_-$. Therefore the partition function will be $Z_N(T,h) = \lambda_+^N + \lambda_-^N$. It can be seen that

$$\lambda_\pm = \cos\left(\frac{\theta}{2}\right) \pm \left(\tau^2 - \sin^2\left(\frac{\theta}{2}\right)\right)^{1/2}$$

where $\theta = \frac{-i\beta\mu H}{2}$. The solutions of the equation $Z_N(\theta,\tau) = 0$ are given by $\cos\theta = -\tau^2 + (1-\tau^2)\cos[(2k-1)\pi/N]$ with $k \in \mathbb{N}$. As N increases the distribution becomes continuous. We plotted this solutions in figure 4 for decreasing values of τ. What we see is that as τ decreases, the distribution of roots tend to close to the real axis. The circle is closed at the limit $\tau \to 0$ ($\cos\theta = 1$), which corresponds to $T = 0$. This proves that the one dimensional Ising model has no phase transition for $T > 0$.

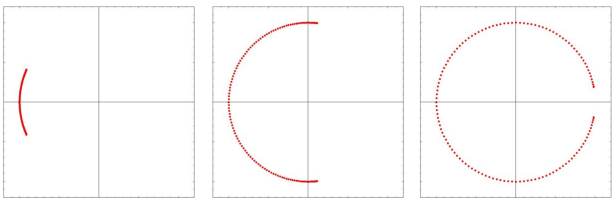

FIG. 4: Roots of the one dimensional Ising model partition function.

A more challenging system is the two dimensional Ising model. A general analytic solution for $H \neq 0$ is still unknown, however, Kramers and Wannier showed in [6] that, for the case of a simple quadratic lattice with no magnetic field, the partition at temperature T, $Z(0,T)$ and the one at temperature T^* are connected by

$$Z(0,T^*) = \left[\frac{\cosh(2\gamma^*)}{\cosh(2\gamma)}\right]^N Z(0,T), \tag{8}$$

where $\gamma = J/kT$ and T^* and T are connected as $\tanh\gamma^* = \exp(-2\gamma)$. Note that as $T \to \infty$, we have that $T^* \to 0$, hence this equation establishes a connection between low and high values of the temperature of the partition function. If there exists a point T_0 where the zeros of the partition function close in to the positive real axis, then due to (8) this is also true for T_0^*. However, according to Lee-Yang circle theorem, it can be only one singularity in this system, because the distribution of zeros along the circle can close onto the positive real axis at no more than one point. Accordingly, if there is a singularity of any kind, it must occur at a temperature T_c (called the Curie temperature) , such that $T_c = T_c^*$, that is,

$$\tanh(\gamma_c) = \exp(-2\gamma_c) \to \gamma_c = \frac{1}{2}\ln(\sqrt{2}+1).$$

In [7] it is proved that indeed this temperature corresponds to a phase transition between the ferromagnetic and paramagnetic phases. We simulated the 2 dimensional Ising model for rectangular lattices from 3×3 to 5×6. In contrast to the one dimensional case, the gap around the positive real axis does depend on the size of the lattice. In our computed range, the gap closes as the size increases as we expect from the known fact that at the thermodynamic limit the distribution of zeros close in to the real axis. The angle α of the closest zero to the positive real axis as a function of the dimension of the lattice ($n \times m$) is shown in the following table for the case $\tau = \frac{1}{\sqrt{2}+1}$ which is where we expect the phase transition.

$n \times m$	α
3×3	0.471998
3×4	0.370325
4×4	0.281611
4×5	0.234112
5×5	0.188399
5×6	0.162265

IV. THE WITTEN INDEX

Supersymmetry field theories have been studied both for phenomenological reasons and as a toy model where theoretical problems are simplified and can be solved analytically. In that regard, it is crucial to understand under which conditions supersymmetry is spontaneously broken because we do not live in a supersymmetric world. The fundamental requirement for supersymmetry to be broken is that the ground state energy of the field theory is non zero (see [8]). It will be useful to work with the operator $(-1)^F = \exp(2\pi i J_z)$ where J_z is the z component of the angular momentum. Let's assume that for a given supersymmetric theory there are n_F^0 fermionic states and n_B^0 bosonic states with zero energy. When we vary the parameters of this theory such as the mass, the volume and the coupling constant, one pair of bosonic

and fermionic states that had $E \neq 0$ can move down to $E = 0$ in which case both n_F^0 and n_B^0 would increase by one. Similarly, a pair of states with $E = 0$ can move to $E \neq 0$ and both n_F^0 and n_B^0 would decrease by one. Note that these situations are not possible for a single state because as soon as it has $E \neq 0$ it must have a supersymmetric partner. So we can conclude that the difference $I = n_B^0 - n_F^0$ remains invariant as we vary the parameters of the theory. This difference I is known as the **Witten index**. Therefore, if $I \neq 0$, then supersymmetry is unbroken because either $n_B^0 \neq 0$ or $n_F^0 \neq 0$. On the other hand, if $I = 0$ we cannot distinguish between the cases $n_B^0 = n_F^0 = 0$ in which supersymmetry would be broken and $n_B^0 = n_F^0 \neq 0$ in which it be unbroken. We observe that

$$I = n_b^0 - n_F^0 = Tr(-1)^F,$$

since states of non zero energy do not contribute to the trace because they appear in pairs with opposite sign.

It is possible to define a more refined index (see [9]) which gives complete information about the ground states because it contains the angular momentum introduced as a fugacity z as $\mathrm{Tr}(-1)^F z^{J_z}$. Setting $z = 1$ we recover the original Witten index. In many frequent cases, the refined index gives a polynomial in z that is palindromic. If this polynomial has all the roots distributed in the unit circle, then we can express it as $P = \prod_{i=1}^{N}(z - e^{i\theta_i})(z - e^{-i\theta_i})$. Since the factors of the product are just $z^2 - 2\cos\theta_i z + 1$, we have that $|P(z = 1)| \leq 2^N$. A concrete example can be found when we study those situations where no fermionic ground states exist. In this case the index reduces to the number of ground states. We consider a quantum mechanical system composed of one superparticle of one type and M superparticles of a different type. The number of ground states is

$$\Omega(M, k, z) = \begin{cases} \frac{z^{M(M-k)} \prod_{i=1}^{k}(1-z^{2i})}{\prod_{i=1}^{M}(1-z^{2i}) \prod_{i=1}^{k-M}(1-z^{2i})} & \text{if } k \geq M, \\ 0, & \text{if } k < M, \end{cases}$$

where k is a constant called the Dirac pairing. It is clear that if $\Omega = 0$, then $\prod_{i=1}^{k}(1 - z^{2i}) = 0$ and so $|z| = 1$. The number of ground states is then less than 2^N, where $N = M(k - M)$ is the number of root pairs of Ω. All in all, we have been able to link the Lee-Yang theory to the study of the number of ground states in a supersymmetric theory. However, we still not know under which conditions the index satisfies the Lee-Yang theorem, which we leave as an interesting approach to explore in the future.

V. CONCLUSIONS

- The theory Lee-Yang reduces the study of phase transitions to the study of the location of zeros of the grand canonical partition function. However, in general, the procedure is still complicated.
- For the one and two dimensional Ising model, the Lee-Yang theorem provides meaningful and elegant results that shed light on the still unresolved aspects of the problem. For instance, it helps us prove that the two dimensional Ising model has only one phase transition.
- The lattice gas and the Ising model are mathematically equivalent.
- The formalism of Lee-Yang theory can also be used in some supersymmetric quantum problems to obtain information about the number of ground states of a supersymmetric theory.

Acknowledgments

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