Ex: Lee-Yang theorem

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Introduction:
Consider the Ising model Hamiltonian:

$$(1)\ \mathcal{H} = -\sum_{i,j} J_{i,j} S_i S_j - h \sum_k S_k = \mathcal{H}_{int} + \mathcal{H}_0$$

where S_k are spin variables, h is an external magnetic field and the system is said to be ferromagnetic if all the coefficients $J_{i,j}$ in the interaction term are non-negative. we want to evaluate the partition function for a system of N spins.

$$(2)\ \mathcal{Z}_N \equiv e^{-\beta F} = tr(e^{-\beta \mathcal{H}}) = \sum_i e^{-\beta E_i}$$

where in the last expression we sum over all spin configurations
say we have n spins which are up, this reduced space of configuration has $\begin{pmatrix} N \\ n \end{pmatrix}$ spin configurations instead of 2^N, still the first sum is generally very complex, but the second sum only depends on the number of up spins.

$$(3)\ -h \sum_k S_k = -h(2n - N)$$

we define $z \equiv e^{2\beta h}$, this allows us to write:

$$(4)\ f_N(z) \equiv \mathcal{Z}_N = e^{-\beta N h} \sum_{n=0}^{N} Z_n z^n$$

where Z_n is the partition function for $\mathcal{H}_{int}$ in the subspace of n up spins, so we got that the partition function is a polynomial of degree N in z. we can now state the Lee-Yang theorem for the ferromagnetic Ising model.

Lee-Yang theorem

For the ferromagnetic Ising model of finite size, if one writes the partition function $\mathcal{Z}_N$ as a polynomial $f_N(z)$, of $z \equiv e^{2\beta h}$ where h is the magnetic field. all the roots of the polynomial $f_N(z)$ are on the unit circle in the complex plane.

The theorem can also be stated for a lattice gas, in this case $z \equiv e^{\beta \mu}$, and instead of ferromagnetic interactions, we have attractive interactions.

Importantly the theorem helps us to understand more about phase transitions, a phase transition occurs when there's a discontinuity in the derivatives of the free energy or equivalently the partition function vanishes, so if we find a zero of $f_N(z)$ in the physical axis $0 < z < 1$ we know that there's a phase transition.

The problem:

1. For the 1D Ising closed chain with ferromagnetic interaction $J_{i,j} = \epsilon > 0$, take the solution for the partition function, derived in class.

   (5) $\mathcal{Z}_N = f_N(z) = \lambda_1^N + \lambda_2^N$

   (6) $\lambda_{1,2} \equiv e^{\beta\epsilon} cosh(\beta h) \pm e^{-\beta\epsilon}\sqrt{1 + e^{4\beta\epsilon} sinh^2(\beta h)}$

   Compute **analytically** the roots of $Z_N = f_N(z)$, plot them on the complex plane, show that all the roots lay on the unit circle in the complex plane and that the system exhibits a phase transition in zero temperature.

2. For a set of N spins with ferromagnetic interaction, consider the following simple model, we take all the spins to interact with each other, the interaction is scaled in order to ensure an extensive thermodynamic limit.

   (7) $J_{i,j} = \dfrac{\epsilon}{N} > 0, \quad \forall\ 1 \leq i, j \leq N$

   The physical interpretation for the model is the same as for using MFT or The Bragg Williams formulation on near neighbor ferromagnetic interaction Ising model, but it can be solved exactly. We don't want to use approximations because we dont know how they affect the roots on the unit circle. Write a program to find **numerically** the partition function and plot the roots on the complex plane.

The solution:

1. We want to solve: $f_N(z) = \lambda_1^N + \lambda_2^N = 0$

$$(8)\ \lambda_1^N = -\lambda_2^N = e^{i(2m-1)\pi}\lambda_2^N,\ m \in \mathbb{Z}$$

$$(9)\ \lambda_1 = e^{\frac{i(2m-1)\pi}{N}}\lambda_2$$

This gives all the roots because we got N different solutions for $1 \leq m \leq N$.
The next step is to multiply both sides by $e^{-\frac{i(2m-1)\pi}{2N}}$:

$$(10)\ \lambda_1 e^{-\frac{i(2m-1)\pi}{2N}} = \lambda_2 e^{\frac{i(2m-1)\pi}{2N}}$$

$$(11)\ cos\left(\frac{(2m-1)\pi}{2N}\right)(\lambda_1 - \lambda_2) = isin\left(\frac{(2m-1)\pi}{2N}\right)(\lambda_1 + \lambda_2)$$

We take the square of both sides:

$$(12)\ (e^{-4\beta\epsilon} + sinh^2(\beta h))cos^2\left(\frac{(2m-1)\pi}{2N}\right) = -sin^2\left(\frac{(2m-1)\pi}{2N}\right)cosh^2(\beta h)$$

After rearranging:

$$(13)\ cosh^2(\beta h) = (1 - e^{-4\beta\epsilon})cos^2\left(\frac{(2m-1)\pi}{2N}\right) \leq 1$$

The right side is always smaller than or equal to 1, therefore this has solutions only for pure imaginary βh, so we define $e^{i\theta} \equiv z \equiv e^{2\beta h}$, where $\theta \in \mathbb{R}$ is the angle of the unit circle in the complex plane. Remarkably we see that alll the roots in z are on the unit circle, as stated by the Lee-Yang theorem.
Now with the use of some trigonometric identities:

$$(14)\ cos(\theta) = 2cos^2\left(\frac{\theta}{2}\right) - 1 = 2cosh^2(\beta h) - 1 = -e^{-4\beta\epsilon} + (1 - e^{-4\beta\epsilon})cos\left(\frac{(2m-1)\pi}{N}\right)$$

And similarly:

$$(15)\ sin(\theta) = \pm 2\sqrt{1 - (1 - e^{-4\beta\epsilon})cos^2\left(\frac{(2m-1)\pi}{2N}\right)}\sqrt{(1 - e^{-4\beta\epsilon})cos^2\left(\frac{(2m-1)\pi}{2N}\right)}$$

All of the N roots are on the unit circle and to the left of the 2 points:

$$(16)\ z = (1 - 2e^{-4\beta\epsilon}) \pm 2ie^{-2\beta\epsilon}\sqrt{(1 - e^{-4\beta\epsilon})}$$

So for any finite $\beta\epsilon$, the roots can't reach the real axis, this confirms the well-established fact that the 1D Ising chain is ferromagnetic only at zero temperature.

Fig.1,Fig.2 and Fig.3 below are for the same number of spins $N = 60$, but for different values of $\beta\epsilon$, we can see that for larger values of $\beta\epsilon$ the roots start to distribute more equally and are getting closer to the real axis.

Fig 1. roots of the 1D Ising chain partition function, $N = 60, \beta\epsilon = 0.8$

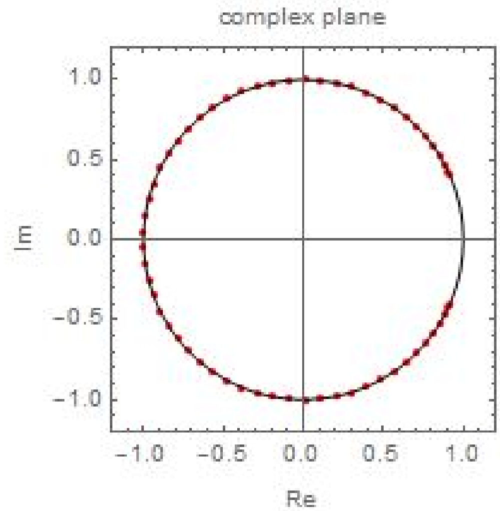


Fig 1. roots of the 1D Ising chain partition function, $N = 60, \beta\epsilon = 1$

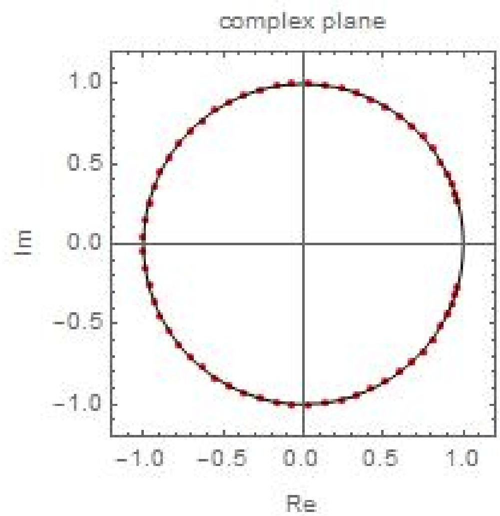
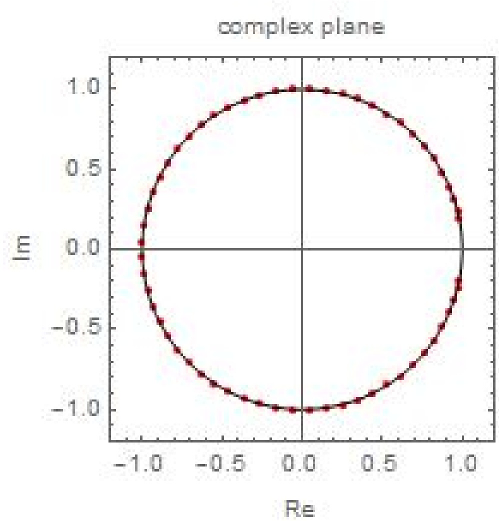


Fig 1. roots of the 1D Ising chain partition function, $N = 60, \beta\epsilon = 1.2$



2. All the spins in the system interact with each other, so the interaction term now is really simple, it now depends only on the number of up spins n and we can write it exactly.

$$(17)\ -\sum_{i,j} J_{i,j} S_i S_j = -\frac{\epsilon}{N}\sum_{i,j} S_i S_j$$

$$(18)\ -\frac{\epsilon}{N}\sum_{i,j} S_i S_j = -\frac{\epsilon}{N}\left(\binom{n}{2} + \binom{N-n}{2} - n(N-n)\right) = -\frac{\epsilon}{2N}((N-2n)^2 - N)$$

The second term we already have, so now we can write the energy, for a system with n up spins:

$$(19)\ E_n = -\frac{\epsilon}{2N}((2n-N)^2 - N) - h(2n-N) = -\frac{\epsilon}{2N}(M^2 - N) - hM$$

The energy can be written using the magnetization of the system $M \equiv \sum_i S_i = 2n - N$.
The exact partition function for the system is:

$$(20)\ \mathcal{Z}_N = f_N(z) = \sum_{n=0}^{N} \binom{N}{n} e^{-\beta E_n} = e^{-\frac{\beta N h}{2} - \frac{\beta\epsilon}{2}} \sum_{n=0}^{N} \binom{N}{n} e^{\frac{\beta\epsilon}{2N}(2n-N)^2} z^n$$

This can be solved approximately by taking a Gaussian approximation:

$$(21)\ \binom{N}{n} \approx const * e^{-\frac{1}{2N}(M^2 + \frac{M^4}{6N^2})}$$

$$(22)\ \mathcal{Z}_N \approx \sum_{n=0}^{N} e^{\frac{1}{2N}((\beta\epsilon - 1)M^2 - \frac{M^4}{6N^2})} z^n$$

From the theory of phase transition we know that a phase transition exists for a positive coefficient of M^2, so the critical value is $\beta_c = \frac{1}{\epsilon}$. there are also two simple limits one can take to solve in exact.
In the limit of no interaction or high temperature $\beta\epsilon$, we have the simple non interacting N spins in a magnetic field.

$$(23)\ f_N(z) \sim (1+z)^N$$

In this limit all the roots are at $Z = -1$, and there won't be a phase transition in the thermodynamic limit.
The second limit one can take is infinite interaction or zero temperature $\beta\epsilon \to \infty$, here we have that only two terms in the expansion are important, $n = 0$, N:

$$(24)\ f_N(z) \sim 1 + z^N$$

In this limit the roots are $z_m = e^{i\frac{2m-1}{N}\pi}, 1 \le m \le N$, in the thermodynamic the roots will be equally distributed on the unit circle, including zero and therefore we will have a phase transition.
In Fig.4, Fig.5 and Fig.6 the plots are for the same number of spins N, but for different values of $\beta\epsilon$ around the critical value $\beta_c\epsilon = 1$. The red points are for exact solution, the blue points are for the Gaussian approximation, we can see significant deviations of the blue points from the red ones. Remarkably again all the roots are on the unit circle, as stated by the Yang-Lee theorem. We can see that the roots are becoming equally distributed when $\beta\epsilon$ becomes larger, and when $\beta\epsilon$ becomes smaller we see that the roots approach $z = -1$, in agreement with the limits we took.

Fig 1. roots of the partition function, $N = 60$,$\beta\epsilon = 0.8$

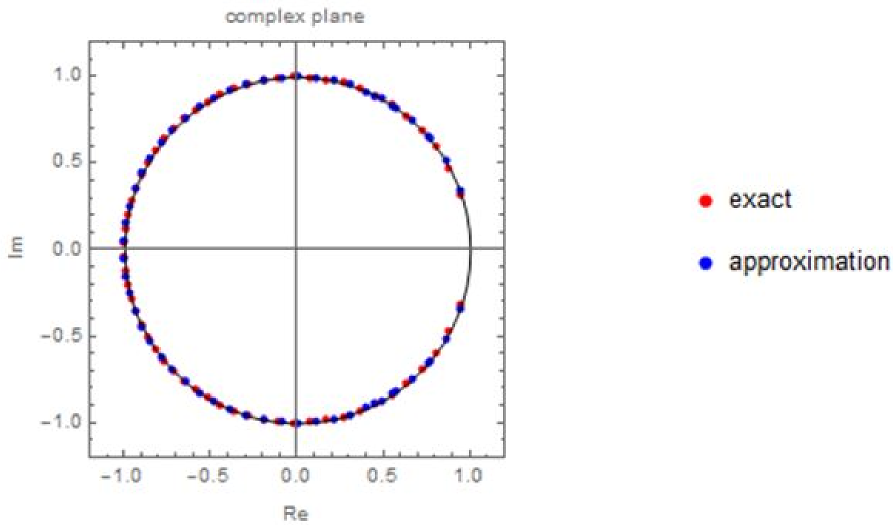


Fig 1. roots of the partition function, $N = 60$,$\beta\epsilon = 1$

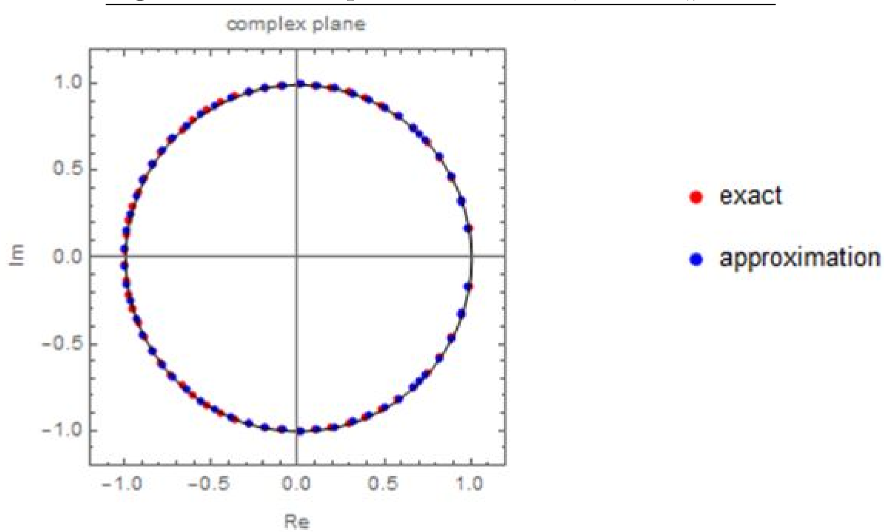


Fig 1. roots of the partition function, $N = 60$,$\beta\epsilon = 1.2$