Yang-Lee-Fisher zeros of partition function

References followed:

(1) Blythe & Evans, Braz J Physics, 33, (2003) 464.

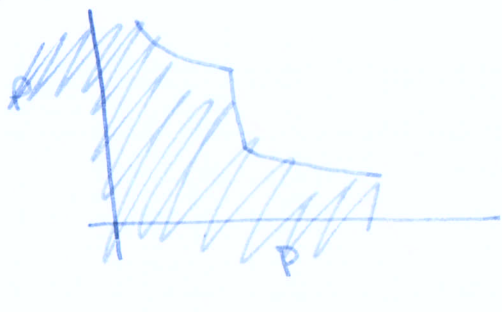
(2) Book of Chowdhury & Stauffer, ch 7.6 and 8.2.3.

(3) Bena, Droz, and Lipowski, Int J mod phys B, 19 (2005), 4269.

(4) Griffiths, ch 1, ~~of a seri~~ vol 1, of Domb & Green & Lebowitz series of books on phase transition and critical phenomena.

At a thermodynamic phase transition, free energy is non-analytic. In the early days of stat mech, it was not universally accepted that free energy density $f = -\frac{1}{V\beta}\log Z$ in stat mech approach could faithfully describe phase transitions. This is partly because the partition function Z is a finite positive degree polynomial in intensive variables (fugacity or e^{β}) for finite system, with positive coefficients, thus analytic. Lee and Yang showed how ~~phase transition or~~ non analytic free energy appear in thermodynamic limit from zeros of partition function on complex plane of intensive variables.

~~An explicit example: a fluid in grand canonical ensemble.~~



Explicit examples:

(1) Canonical ensemble: Consider a spin system with energy $n\cdot\epsilon$ for n^{th} configuration. (fixed energy gap ϵ

Partition function $$Z_{N} = \sum_{n=0}^{m} g(n)\left(e^{-\beta\epsilon}\right)^{n}$$

degeneracy

finite for finite system.

$$= \sum_{n=0}^{m} g(n)\cdot z^{n} \quad \text{with } z = e^{-\beta\epsilon}$$

$$= g(m)\prod_{n=1}^{m}\left(1-\frac{z}{z_n}\right)$$

points where $Z_N = 0$

* Because $g(n)$ are all positive, all roots z_n is complex.

* Free energy density

$$f(z) = -\frac{1}{\beta N}\log Z_N \simeq -\frac{1}{\beta N}\sum_{n=1}^{m}\log\left(1-\frac{z}{z_n}\right)$$

* For finite system, m is finite, and there are no z_n on real z line, so $f(z)$ is analytic.

Only way non analyticity arise is in thermodynamic limit, where z_n's could aproach arbitrarily close to the real z axis.

This was rigorously proven first by Lee & Yang for a fluid system.

(2) Fluid in grand canonical ensemble.

$$Z_G = \sum_{n=0}^{m} \underbrace{\left(e^{\beta\mu}\right)}_{z}^{n} \cdot Z_n(n, V, \beta)$$

canonical partition function.

$$= \prod_{n=1}^{m} \left(1 - \frac{z}{z_n}\right)$$

Pressure

$$p(z) = \frac{1}{V \cdot \beta} \log Z_G$$

density

$$\rho(z) = \beta z \cdot \frac{\partial p}{\partial z}$$

undergoes a first order transition if ρ has jump discontinuity.

Continuous transition, if second derivative $p''(z)$ is discontinuous.

In 1952, Lee-Yang proved that, for a general fluid with interparticle interaction which has a ~~repulsive short distance~~ repulsive hard core and short range attractive part,

(a) thermodynamic limit $p_\infty(z)$ exist for all $z > 0$.

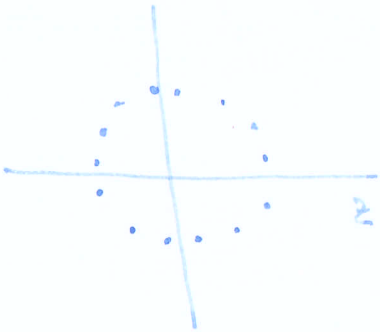
(b) If there are no z_n (roots of Z_G) in a region around a segment of real z line, then the thermodynamic limit $p_\infty(z)$ is analytic in that region.

This implies, non-analyticities in fluid (phase transition) comes from vanishing Z_G.

Lee-Yang also observed that the roots z_n are distributed in a regular fashion rather than spread sporadically or with intricate structure. For Ising systems Lee-Yang showed that roots z_n are distributed along unit circle $|z|=1$, and this is known as Lee-Yang circle theorem.

Original result (1952): for d-dim ferromagnetic Ising spin, with magnetic field h, and

$$H = -\sum_{i<j} J_{ij}\,\sigma_i\sigma_j - h\sum_i \sigma_i$$



zeros of canonical partition function Z on complex $z = e^{-2\beta h}$ plane (with $h \geq 0$), lie on unit circle $|z| = 1$.

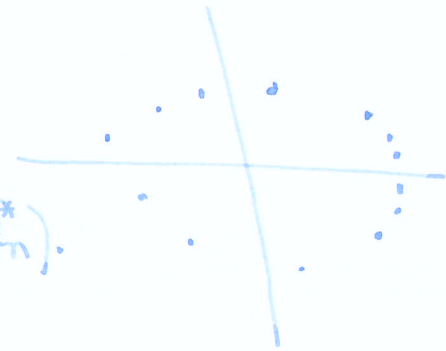
An immediate consequence of this result is that, there are no transition for non-zero magnetic field ($z < 1$), at a finite non-zero temp, irrespective of dimension, lattice, interaction J_{ij} (as long as thermodynamic limit exist).

Since then, the result has been extended for other systems as well [see Bena et al for a list of systems], such as ϕ^4 euclidean field theory.

* Of course, there are models for which roots may not lie on a line, in fact they can even be fractals [Itzykson & Luck, 1985]

Nature of transition: Phase transitions happen when roots z_n converge arbitrarily close to a point/region on real z-line.

This can be intuitively seen by an electrostatic correspondence, as follows:



Because Z is real, the roots z_n comes in complex conjugate pairs (z_n, z_n^*).

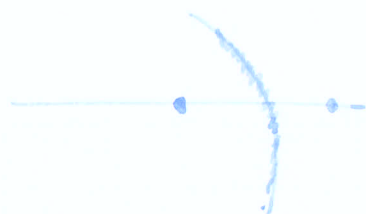
Then, free energy along real z-line

$$f(z) = -\frac{1}{\beta V}\sum_{n=1}^{m/2} g(n) \log\left[\left(1-\frac{z}{z_n}\right)\left(1-\frac{z}{z_n^*}\right)\right]$$

$$= -\frac{1}{\beta V}\sum_{n=1}^{m/2} g(n)\cdot \log\frac{(z-z_n)(z-z_n^*)}{|z_n|^2}$$

$$= -\frac{1}{\beta V}\sum_{n=1}^{m} g(n)\log\left|1-\frac{z}{z_n}\right|$$

Notice that $\log\left|1-\frac{z}{z_n}\right|$ is the potential in 2d at z due to a point charge at z_n. Then $f(z)$ is the potential due to charges at roots z_n. In the thermodynamic limit, if the roots are ~~to~~ compactly distributed along a line, that $f(z)$ is the potential due to a line-charge of charge density $\frac{1}{\beta V} g(n) \to \frac{1}{\beta V}\lambda(z_n)$.



Potential across the line charge is ~~discontinuous~~. non-analytic.

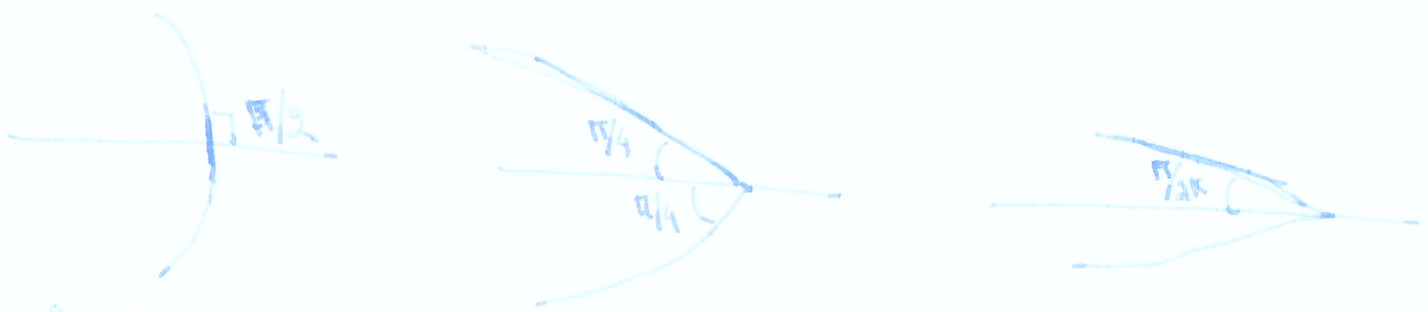
More precisely,

① If the ~~[illegible]~~ density of roots (line charge density) is non-zero on the real line ~~[illegible]~~ at a point $z = z_c$, ie $\lambda(z_c) \neq 0$, then first derivative of $f(z)$ is discontinuous (electric field). This means a first ~~[illegible]~~ order phase transition at z_c.

② If $\lambda(z)$ vanishes linearly as it approaches z_c, ie $\lambda(z) \simeq |z - z_c|$, then $f'(z)$ is continuous, but $f''(z_c)$ not. Means a second order transition.

③ In general, $\lambda(z) \simeq |z - z_c|^K$ with $K \geq 1$, then it is K-th order transition.

Typically these are related to how the line of z_n's approach the real line.

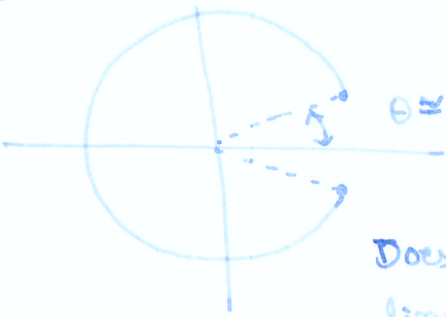


first order — second order — Kth order.

Ref: Blyth & Evans.

Remark: For historical reasons, zeros ~~of~~ in complex fugacity plane ($e^{\beta\mu}$) are referred as Lee-Yang zeros, and those in complex temperature plane ($e^{-\beta}$) ~~are~~ as Fisher zeros.

Remark: for 1-d Ising model



$\theta \cong \arccos(1-2e^{-4\beta J})$

Does not touch real z line for any non zero temp.

Remark: Besides mathematical explanation of phase transition, zeros of partition function is a useful numerical ~~app~~ method of determining phase transition points and the nature of transition.

Remark: the idea can be extended for non-equilibrium phase transitions as well.

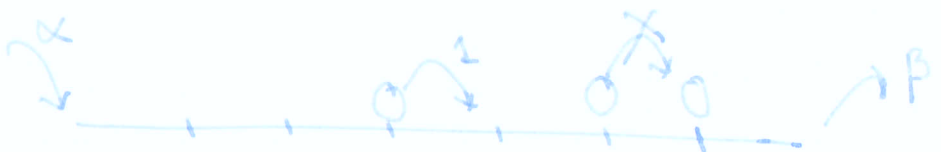
It is not immediate what plays the role of partion function Z. One candidate is the product of eigenvalues of the associated Markov Matrix, except the $\lambda=0$. [Ref: Blyth & Evans]

For a Markov process, $\partial_t P = \mathcal{W} P$, the largest eigenvalue $\lambda_0 = 0$, and rest of the eigenvalues $\lambda_i \le 0$. Typically, a phase transition (as a function of external parameters), corresponds to non-analytic change in stationary probability, and this happen when the gap $\lambda_0 - \lambda_n$ vanishes. Then one may consider

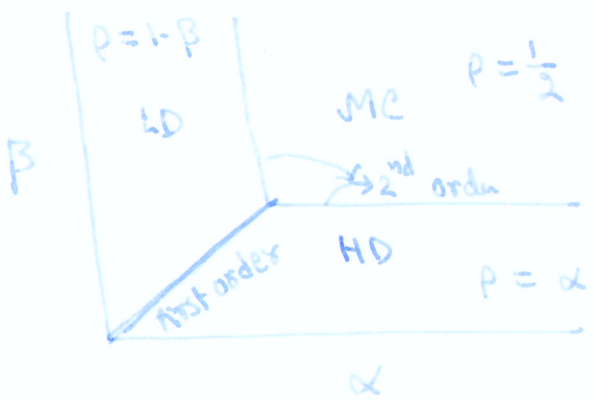
$$Z_m = \prod_{n=1}^{m} (-\lambda_n)$$

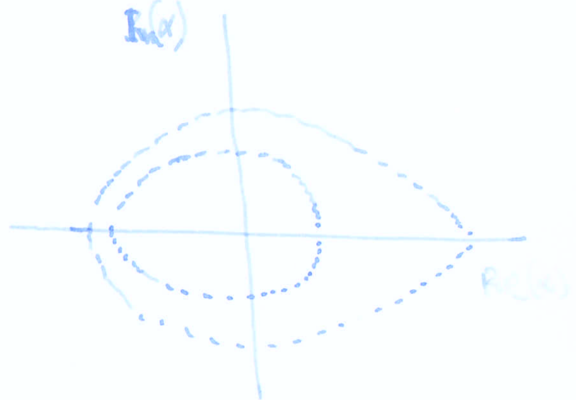
as quantity equivalent of partition function, such that zeros of Z on complex control parameter (z) space indicate phase transition. Just as in equilibrium, these roots approach real z-line in the thermodynamic limit.

Example:



Totally asymmetric exclusion process





Example: Directed percolation.

Some well known solvable models in stat mech:

Ref: Stat field theory, by Giuseppe Mussardo.

1-d Ising model and transfer matrix:

$$H = -J\sum_i \sigma_i \sigma_{i+1} - h\sum_i \sigma_i \qquad \text{with } \sigma_i = \pm 1$$

Partition function

$$Z_N = \sum_{\{\sigma_i\}} e^{+\beta J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} + \beta h \sum_{i=1}^{N} \sigma_i}$$

Let's define

$$Z_N(\sigma_N) = \sum_{\sigma_1} \cdots \sum_{\sigma_{N-1}} e^{-\beta H}$$

$:=$ the partion function with the N-th spin σ_N fixed.

Then,

$$Z_{N+1}(\sigma_{N+1}) = \sum_{\sigma_N} \cdots \sum_{\sigma_1} e^{+\beta J \sigma_{N+1}\sigma_N + \beta h \sigma_{N+1}} \times e^{+\beta J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} + \beta h \sum_{i=1}^{N} \sigma_i}$$

$$= \sum_{\sigma_N} \underbrace{e^{\beta J \sigma_{N+1}\sigma_N + \beta h \sigma_{N+1}}}_{T(\sigma_{N+1},\sigma_N)} \times Z_N(\sigma_N).$$

$$\Rightarrow \boxed{Z_{N+1}(\sigma_{N+1}) = \sum_{\sigma_N} T(\sigma_{N+1}, \sigma_N) \cdot Z_N(\sigma_N)}$$

Here $T(\sigma', \sigma)$ is the transfer matrix.

~~This~~ Note, σ_i are dummy variables, and summed over. Therefore, recursively writing we get

$$Z_{N+1}(\sigma_{N+1}) = \sum_{\sigma_N,\cdots,\sigma_1} T(\sigma_{N+1},\sigma_N)\,T(\sigma_N,\sigma_{N-1})\cdots T(\sigma_2,\sigma_1)\cdot Z_1(\sigma_1)$$

$$\Rightarrow \boxed{Z_{N+1}(\sigma') = \sum_{\sigma} T^N(\sigma',\sigma)\cdot e^{\beta h\sigma}}$$

$$\Rightarrow \boxed{Z_{N+1} = \sum_{\sigma'}\sum_{\sigma} T^N(\sigma',\sigma)\, e^{\beta h\sigma}}$$ For open Ising chain.

For periodic boundary:

$$Z_N = \sum_{\sigma'}\sum_{\sigma} T^N(\sigma',\sigma) = \operatorname{Tr} T^N$$

Here

$$T(\sigma',\sigma) = \left(e^{\beta J\sigma'\sigma + \beta h\sigma'} \right) \equiv \begin{array}{c|cc} & |+\rangle & |-\rangle \\ \hline \langle +| & e^{\beta J+\beta h} & e^{-\beta J+\beta h} \\ \langle -| & e^{-\beta J-\beta h} & e^{\beta J-\beta h} \end{array}$$

~~A simplification:~~

For the 2x2 matrix, there are two eigenvalues,

$$\lambda_\pm = e^{\beta J}\cosh(\beta h) \pm \sqrt{e^{2\beta J}\cosh^2(\beta h) - 2\sinh(2\beta J)}$$

Then,

$$Z_N = \operatorname{Tr} T^N = \lambda_+^N + \lambda_-^N$$

$\Rightarrow$ free energy density

$$f(J,h) = -\frac{1}{N\beta}\ln Z_N = -\frac{1}{\beta}\left(\ln\lambda_+ + \frac{1}{N}\ln\left(1+\frac{\lambda_-^N}{\lambda_+^N}\right)\right)$$

For large N,

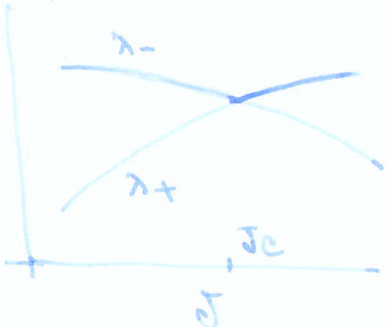
$$f(J,h) \simeq -\frac{1}{\beta} \ln \lambda_+$$

The subleading term is negligible when $\lambda_- < \lambda_+$. This is the case for $h>0$. Only for $h=0$, ~~and $\beta \to \infty$ (temp $=0$)~~

$$\cancel{\lambda_+ = \lambda_- =} \quad \lambda_\pm = e^{\beta J} \pm e^{-\beta J}$$

and $\lambda_+ = \lambda_-$ for $\beta \to \infty$, therefore free energy could show phase transition.

Remark: Within transfer matrix approach, a phase transition corresponds to degenerate largest eigenvalue.



In 1-d Ising model, Perron-Frobenius theorem says that there are no phase transition. In 2-d, we shall see, that transfer matrix become infinite (in thermodynamic limit), and perron Frobenius does not hold, therefore the model can ~~under~~ (does) undergo a phase transition.

For 1-d classical systems, there are ~~many~~ ~~to~~ examples where associated transfer matrix ~~is not~~ does not ~~belong~~ follow the criterias for Perron-Frobenius theorem (e.g, reducible matrix, or infinite size), and there could be phase transitions.

Therefore, ~~inspite of a~~ contrary to a common misconception, there are indeed, examples of 1-d classical systems which undergo phase transition at a finite temperature.

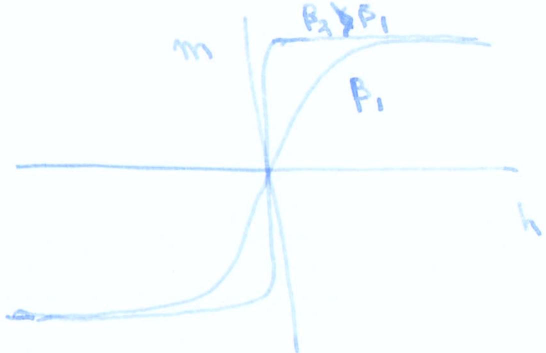
Ref : ① Cuesta & Sánchez, J. stat. Phys, 115, 869 (2004).

② Saryal, Klamser, Sadhu, Dhar, PRL, 121, 240601 (2018).

~~Correlat~~

Average magnetization :

$$m = \frac{\partial f}{\partial h} = \frac{e^{\beta J} \sinh \beta h}{\sqrt{e^{2\beta J}\cosh^2 \beta h - 2\sinh 2\beta J}}$$



Correlation :

$$\langle \sigma_i \sigma_j \rangle = \frac{1}{Z_N} \sum_{\sigma_i, \sigma_j} \sigma_i \, T^{|i-j|}(\sigma_i, \sigma_j) \, \sigma_j \, T^{N-|i-j|}(\sigma_j, \sigma_i)$$

$$= \frac{1}{Z_N} \mathrm{Tr}\left(S\, T^{|i-j|} \, S \, T^{N-|i-j|} \right)$$

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

A way to explicitely compute this is by ~~unitary~~ similarity transformation

$$U^{-1} T U = \mathrm{diag}(\lambda_+, \lambda_-) \qquad \text{with } U^{-1} U = \mathbb{1}$$

Gives

$$\mathrm{Tr}\left(S\, T^{r}\, S\, T^{N-r}\right) = \mathrm{Tr}\left(\underbrace{U^{-1} S U}_{R}\, U^{-1} T^{r} U\, \underbrace{U^{-1} S U}_{R}\, U^{-1} T^{N-r} U\right)$$

$$= \mathrm{Tr}\left(R \cdot \mathrm{diag}(\lambda_+^{r}, \lambda_-^{r}) \cdot R \cdot \mathrm{diag}(\lambda_+^{N-r}, \lambda_-^{N-r})\right)$$

This will give

$$\langle \sigma_i \sigma_{i+r} \rangle \simeq R_1^2 + R_2 R_3 \left(\frac{\lambda_-}{\lambda_+}\right)^{r}$$

and similarly $\langle \sigma_i \rangle^2 \simeq R_1^2$

here $R = \begin{pmatrix} R_1 & R_2 \\ R_3 & R_4 \end{pmatrix}$

Giving, correlation

$$\langle \sigma_i \sigma_{i+r} \rangle_c \simeq R_1 \cdot R_3 \cdot \left(\frac{\lambda_-}{\lambda_+}\right)^{r} \sim e^{-r/\xi}$$

$$\text{with } \xi = \frac{1}{\log \frac{\lambda_+}{\lambda_-}}$$

Therefore correlation length diverges when $\lambda_+ = \lambda_-$, ie, at phase transition.

For details of calculation, and for open boundary condition see ch 2, book by Giuseppe Mussardo, statistical field theory.