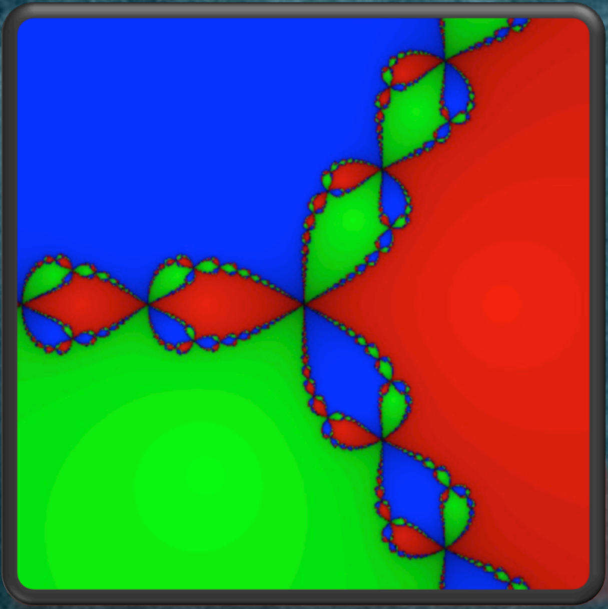
Yang-Lee Zeros of Integrable Field Theories



Giuseppe Mussardo
Sissa-Trieste

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Yang–Lee zeros of the Yang–Lee model

G Mussardo[1,2,4], R Bonsignori[1] and A Trombettoni[1,3]

1 SISSA and INFN, Sezione di Trieste, via Bonomea 265, I-34136, Trieste, Italy
2 International Centre for Theoretical Physics (ICTP), I-34151, Trieste, Italy
3 CNR-IOM DEMOCRITOS Simulation Center, Via Bonomea 265, I-34136 Trieste, Italy

E-mail: mussardo@sissa.it

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Abstract

To understand the distribution of the Yang–Lee zeros in quantum integrable field theories we analyse the simplest of these systems given by the 2D Yang–Lee model. The grand-canonical partition function of this quantum field theory, as a function of the fugacity z and the inverse temperature β, can be computed in terms of the thermodynamics Bethe Ansatz based on its exact S-matrix. We extract the Yang–Lee zeros in the complex plane by using a sequence of polynomials of increasing order N in z which converges to the grand-canonical partition function. We show that these zeros are distributed along curves which are approximate circles as it is also the case of the zeros for purely free theories. There is though an important difference between the interactive theory and the free theories, for the radius of the zeros in the interactive theory goes continuously to zero in the high-temperature limit $\beta \to 0$ while in the free theories it remains close to 1 even for small values of β, jumping to 0 only at $\beta = 0$.

Keywords: integrable quantum field theory, thermodynamics Bethe Ansatz, Yang–Lee zeros

(Some figures may appear in colour only in the online journal)

1. Introduction

Many physical quantities reveal their deeper structure by going to the complex plane. This is the case, for instance, of the analytic properties of the scattering amplitudes where the angular momentum is not longer restricted to be an integer but allowed to take any complex value giving rise in this way to the famous Regge poles [1]. Another famous example is the Yang–Lee theory of equilibrium phase transitions [2, 3] based on the zeros of the grand-canonical partition function in the complex plane of the fugacity: in a nutshell, the main observation of Yang and Lee was that the zeros of the grand-canonical partition functions in the thermodynamic limit usually

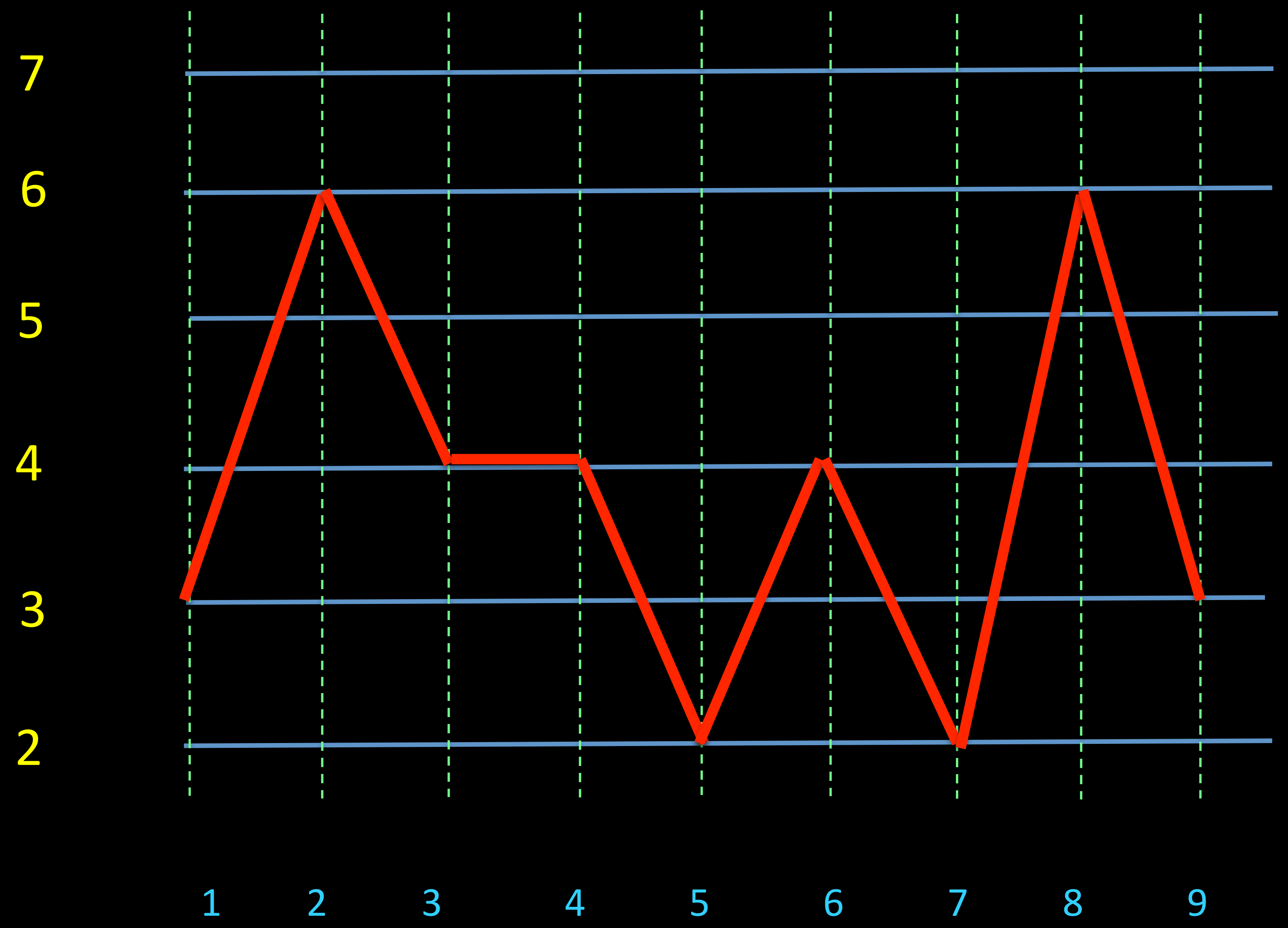
On-going research with Federico Balducci

Danylo Radchenko

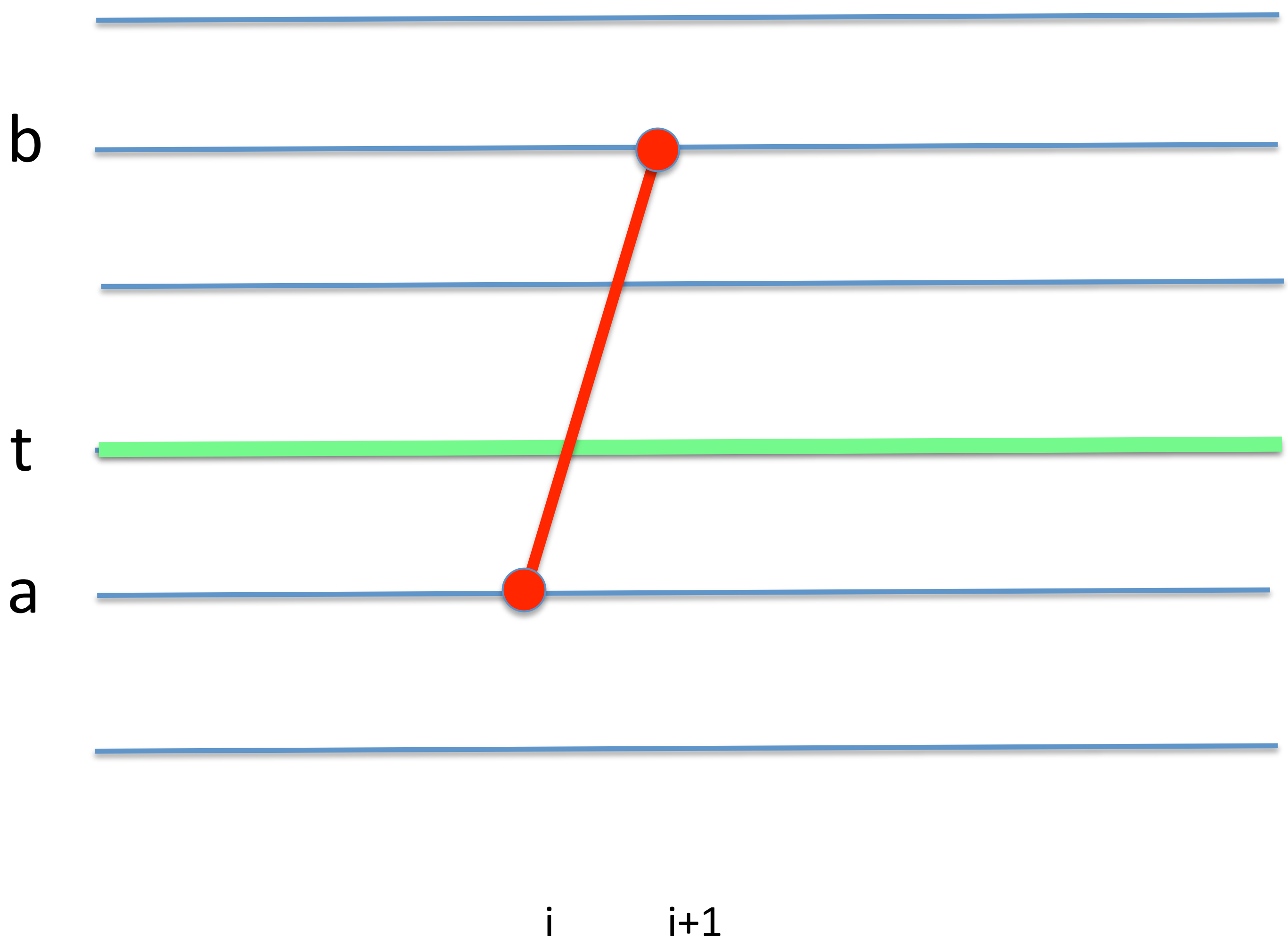
2, 3, 4, 5, 6, …q

Possible states of a fluctuating “spin”

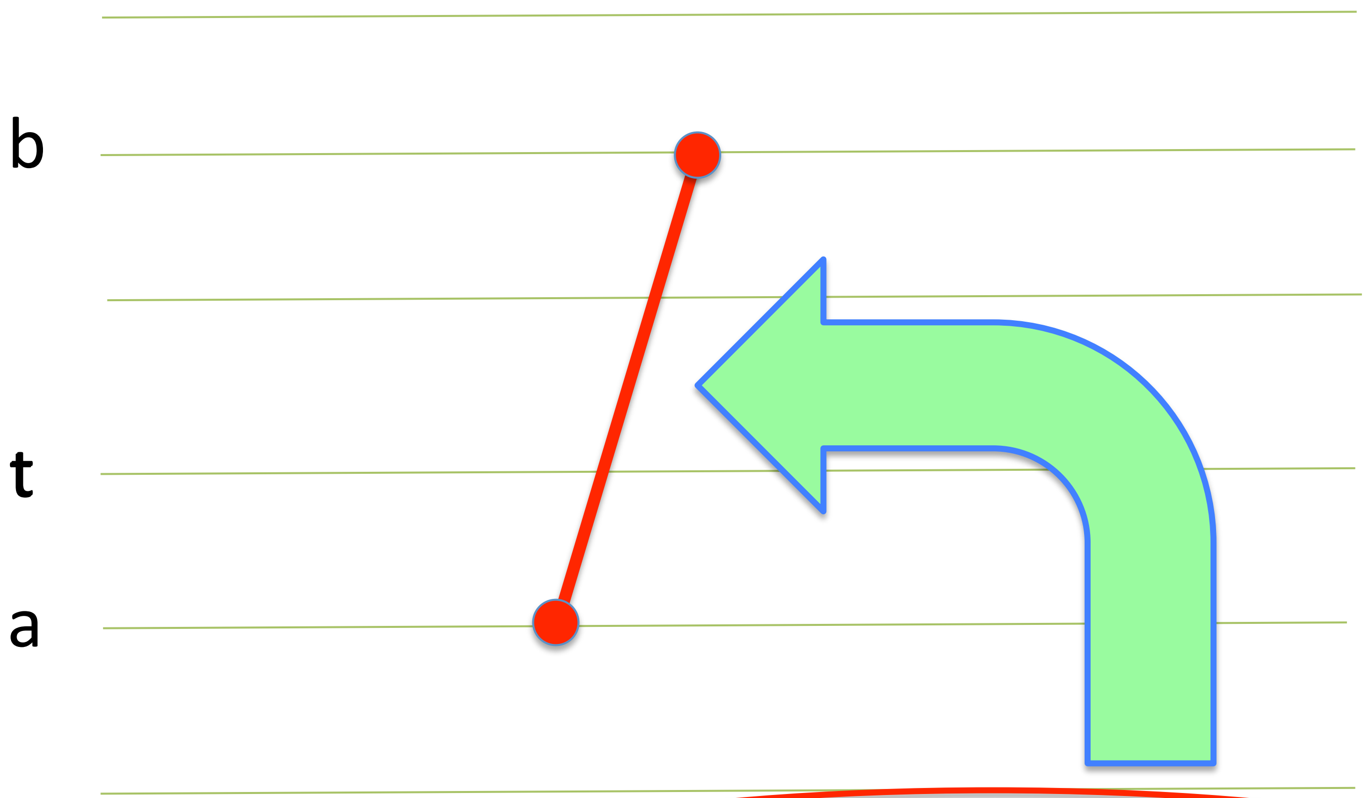
Brattelli diagram



Weight of the elementary jump



Weight of the elementary jump

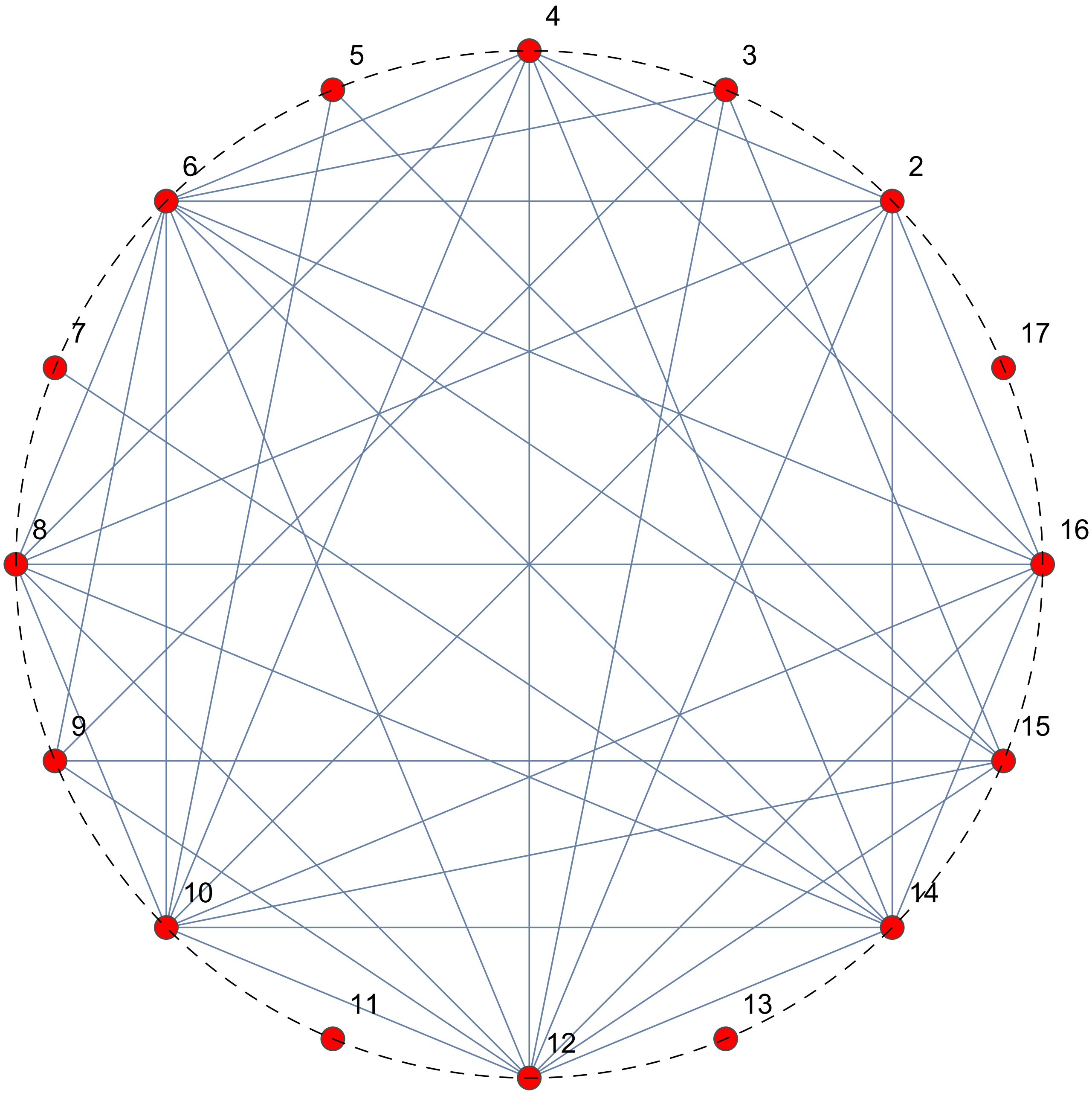


$$w(\beta, z) = e^{-\beta\Phi(a,b)}\ z^{\delta(a,t)}$$

Coprimality matrix

(GM, Giudici, Viti, Zagier 2017)

$$\Phi(a,b) = \begin{cases} 0 & \text{if } \mathrm{gcd(a,b)} \neq 1 \\ 1 & \text{if } \mathrm{gcd(a,b)} = 1 \end{cases}$$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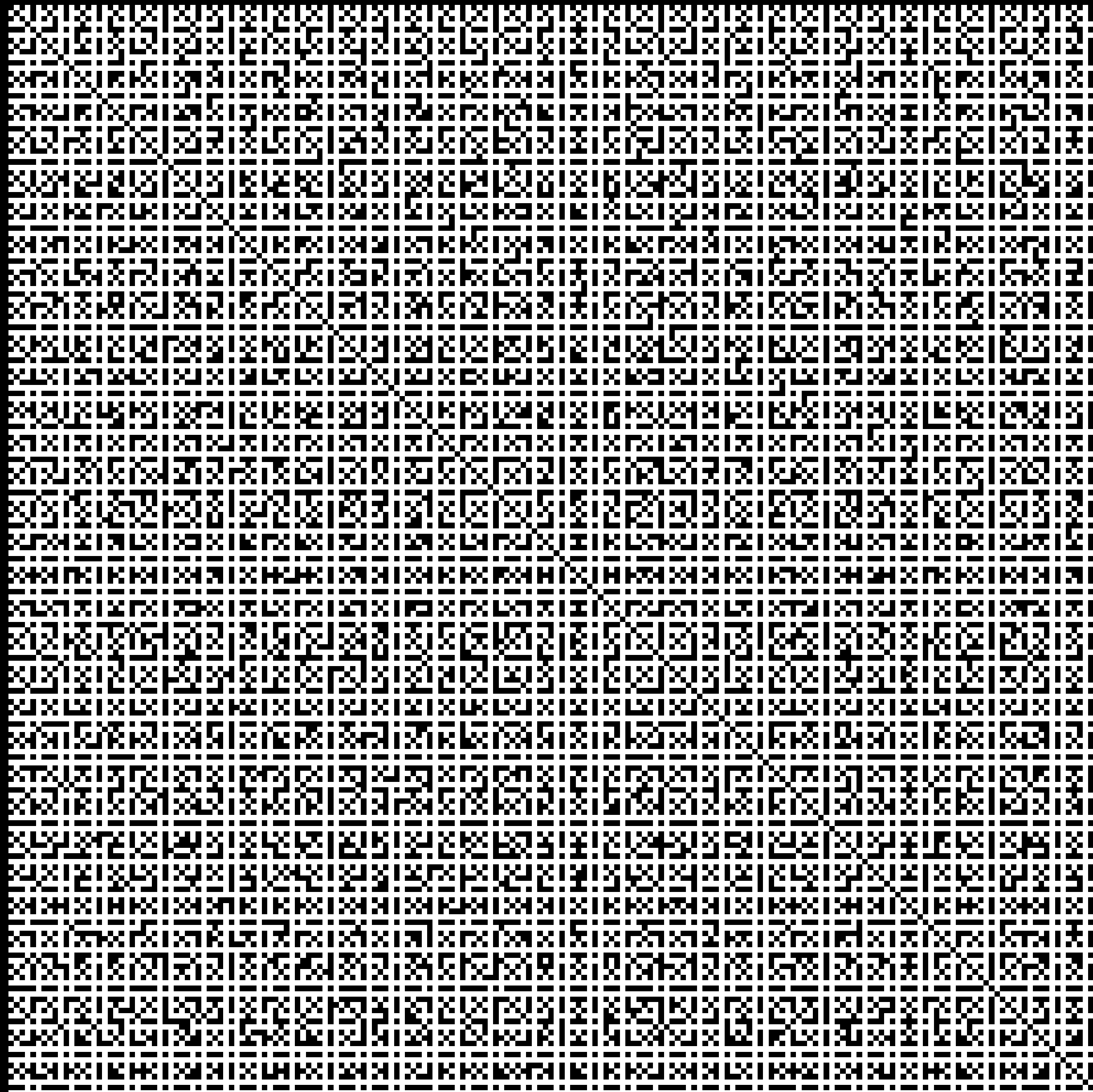
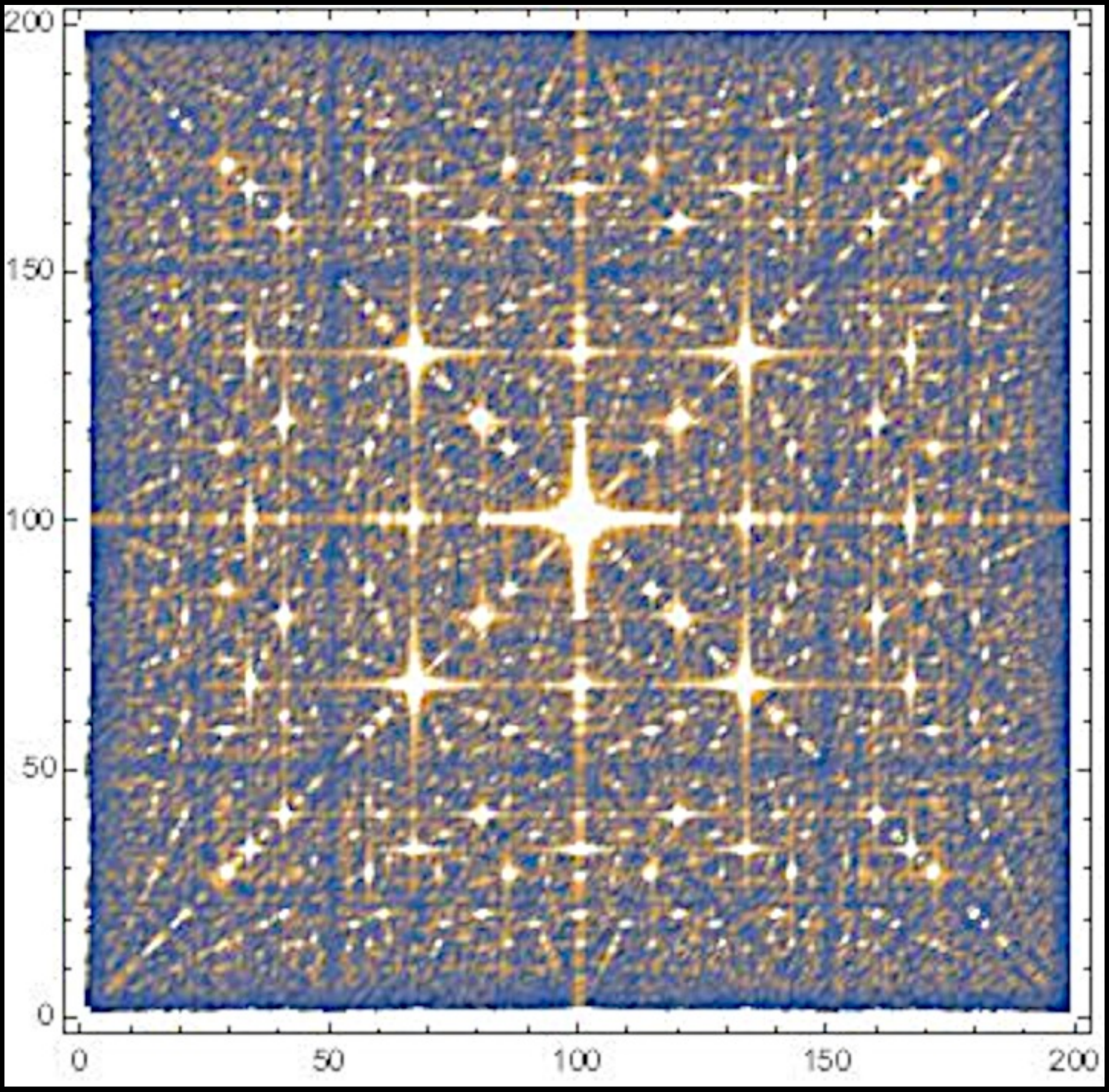
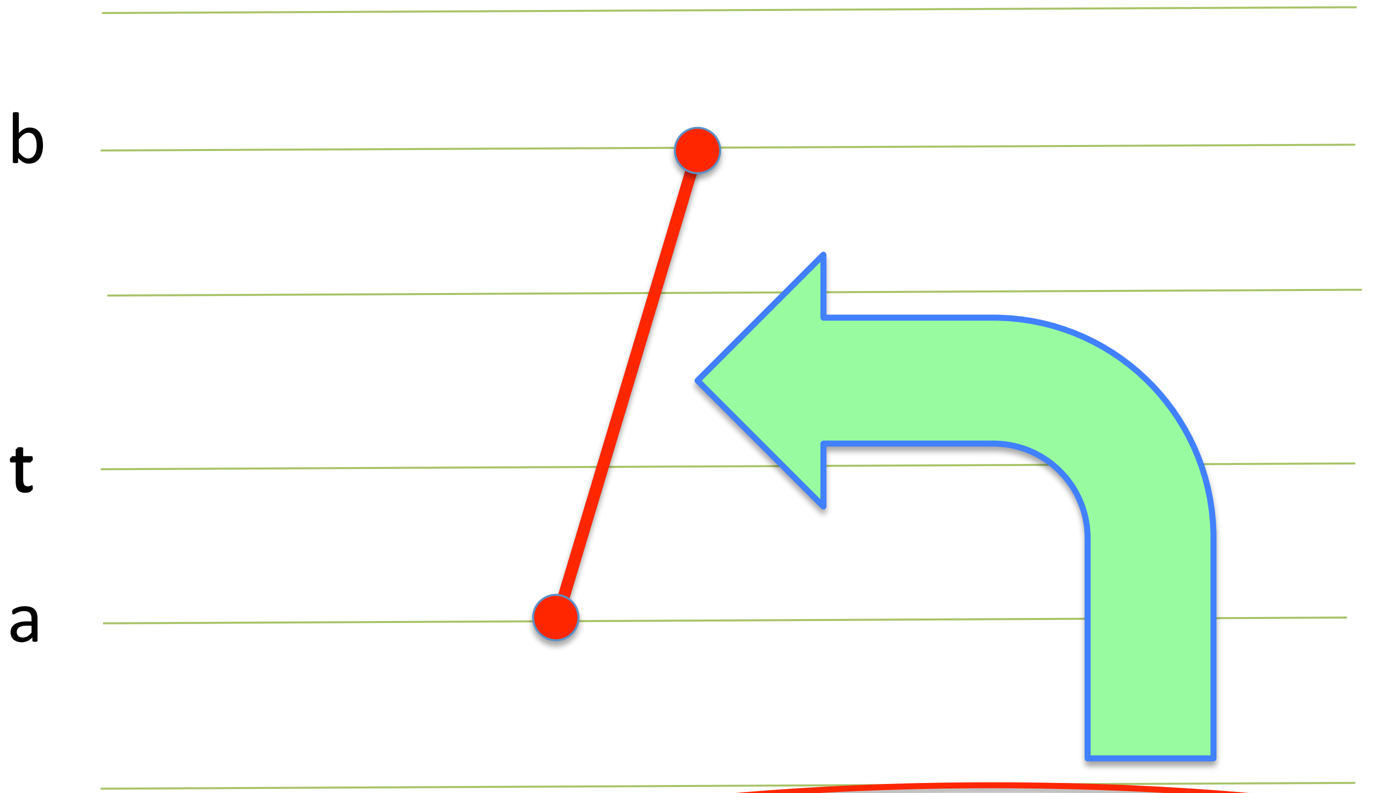
12





200
150
100
50
0
0
50
100
150
200

Weight of the elementary jump

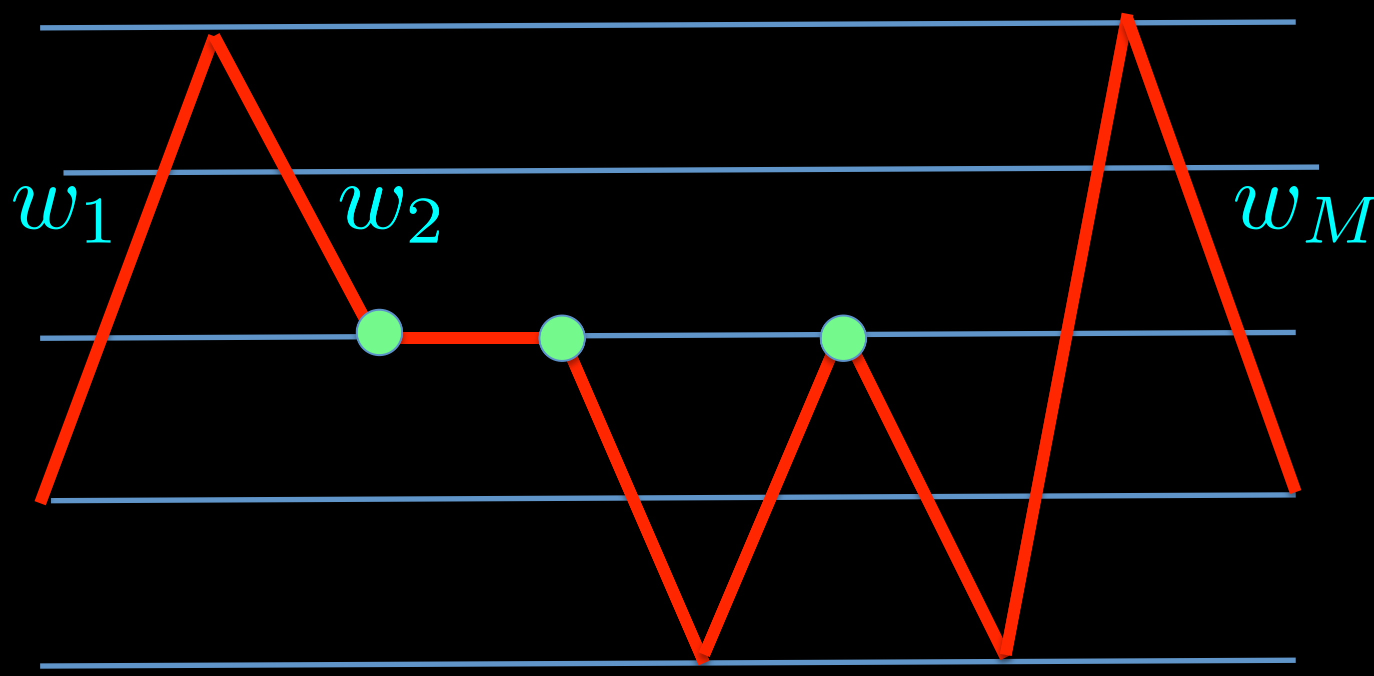


$$w(\beta, z) = e^{-\beta\Phi(a,b)}\, z^{\delta(a,t)}$$

Path Integral

$$\mathcal{P}_t(z) = \sum_{paths} w_1(z)\, w_2(z) \cdots w_M(z)$$

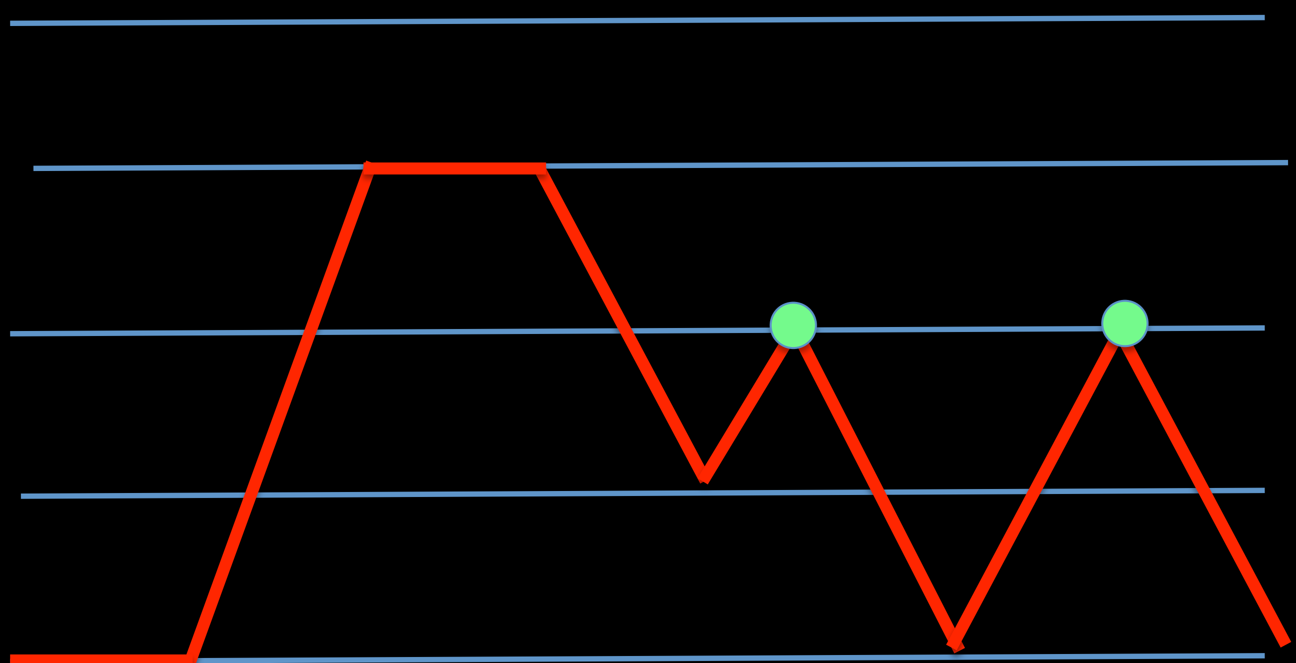
$$= \alpha_0 + \alpha_1\, z + \alpha_2\, z^2 + \cdots + z^M$$



Path Integral

$$\mathcal{P}(z) = \sum_{paths} w_1(z)\, w_2(z) \cdots w_M(z)$$

$$= \alpha_0 + \alpha_1\, z + \alpha_2\, z^2 + \cdots + z^M$$

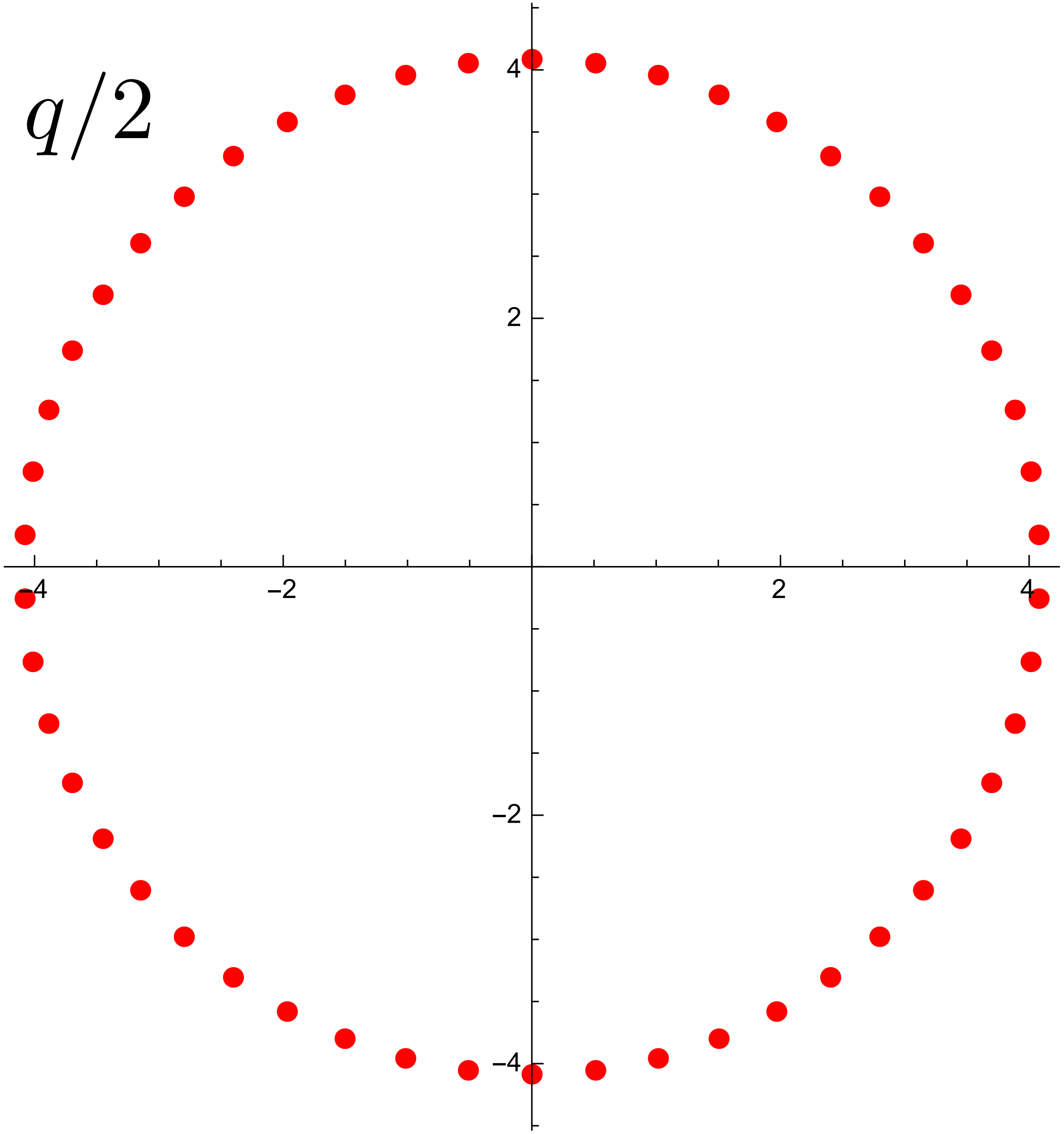


Where are the zeros of these polynomials?

$$q = 8$$

$$t = 5 \quad > q/2$$

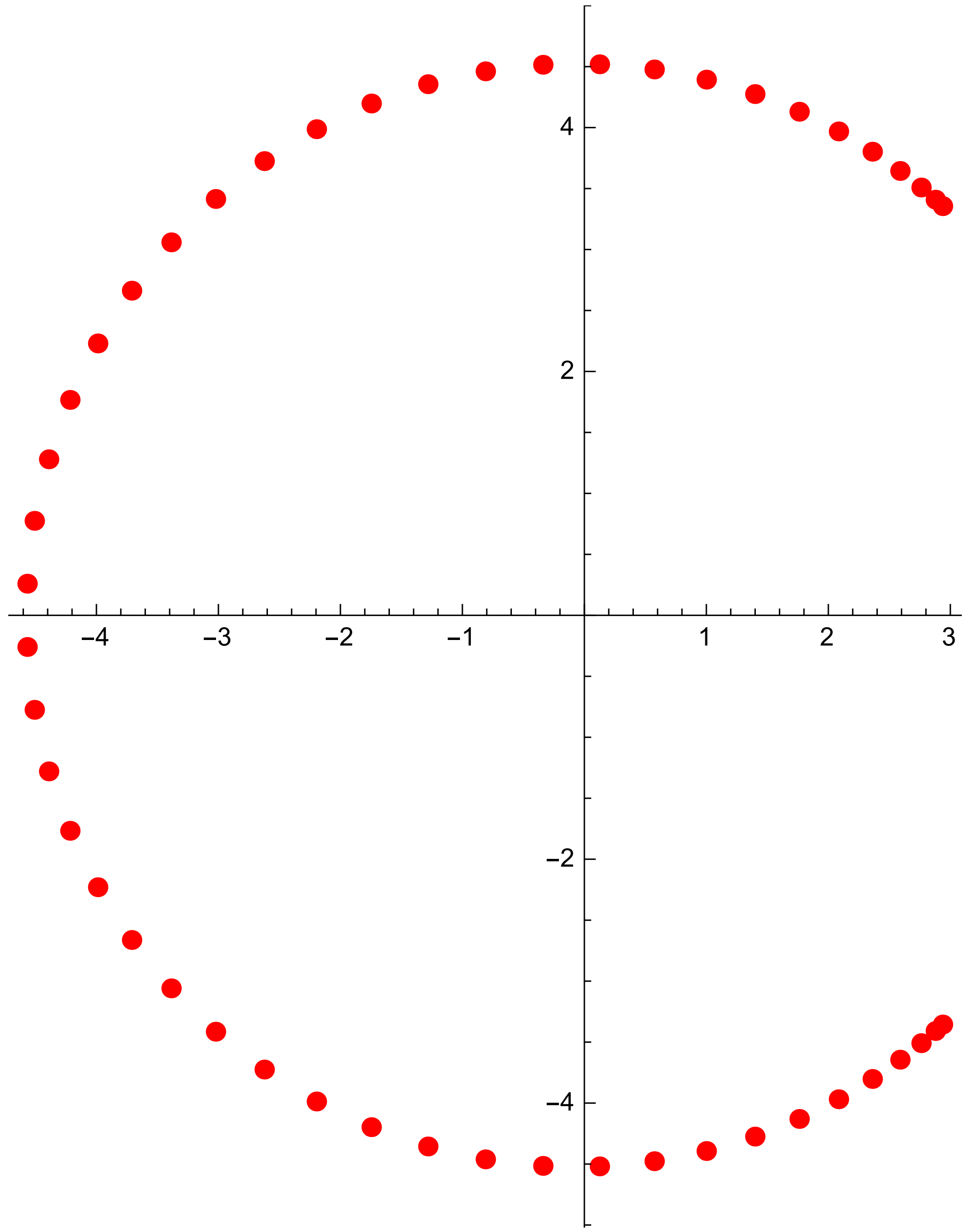
$$\beta = 100$$



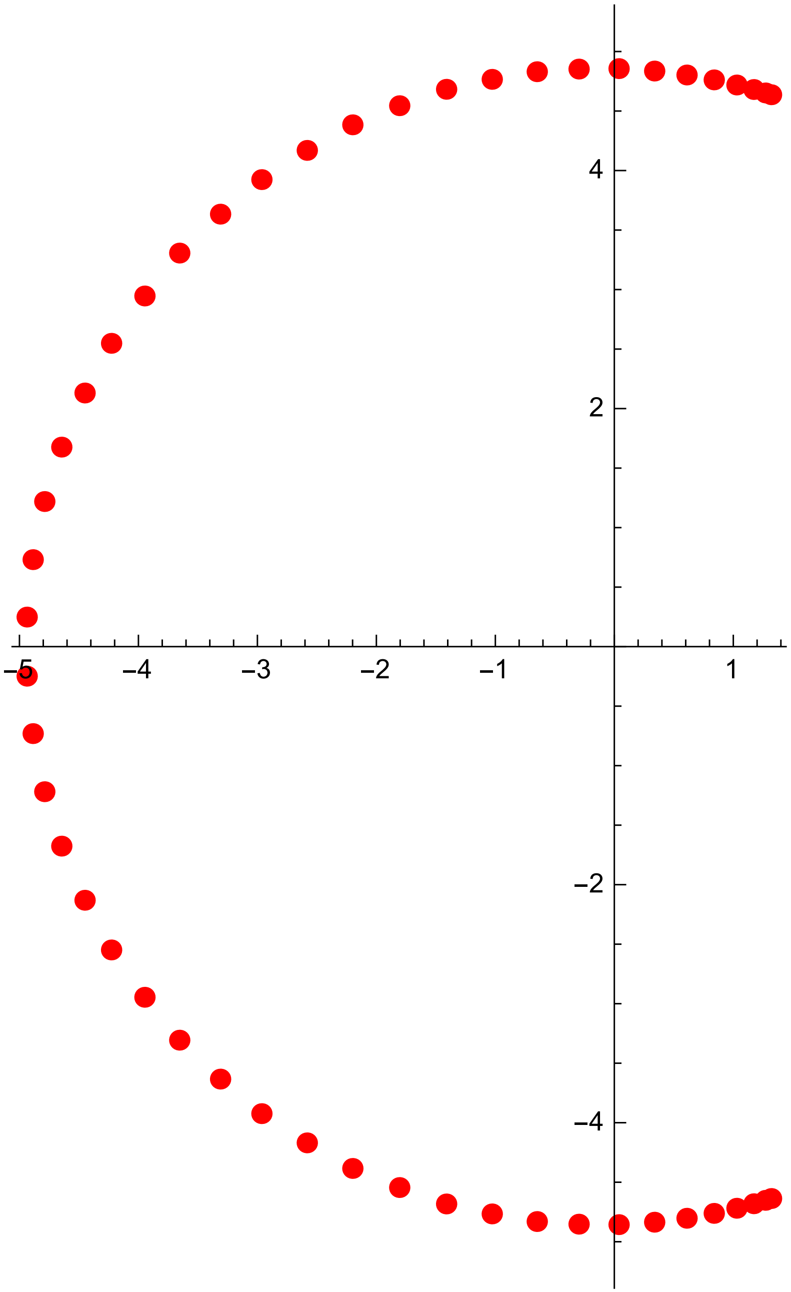
$q = 8$

$t = 5$

$\beta = 10$



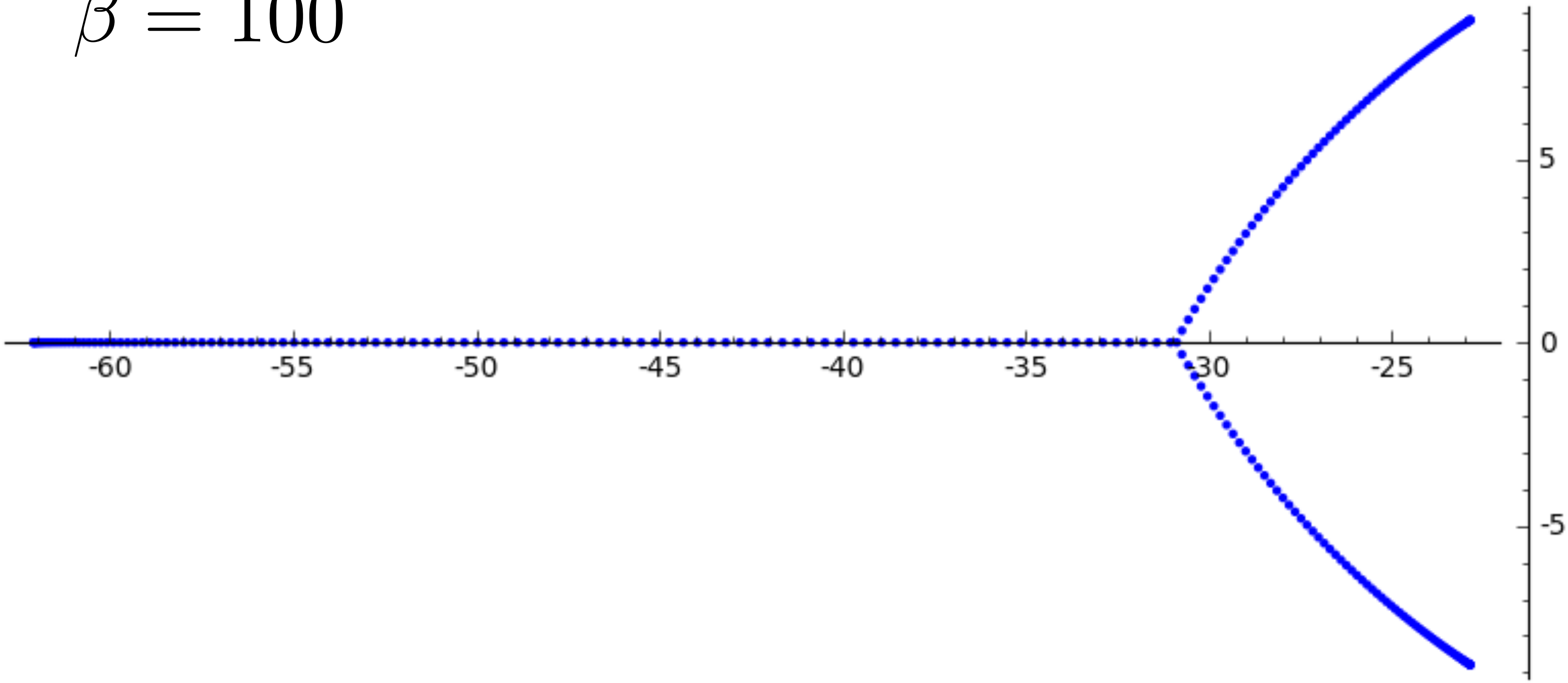
$q = 8$
$t = 5$
$\beta = 1$



$q = 8$

$t = 6$

$\beta = 100$

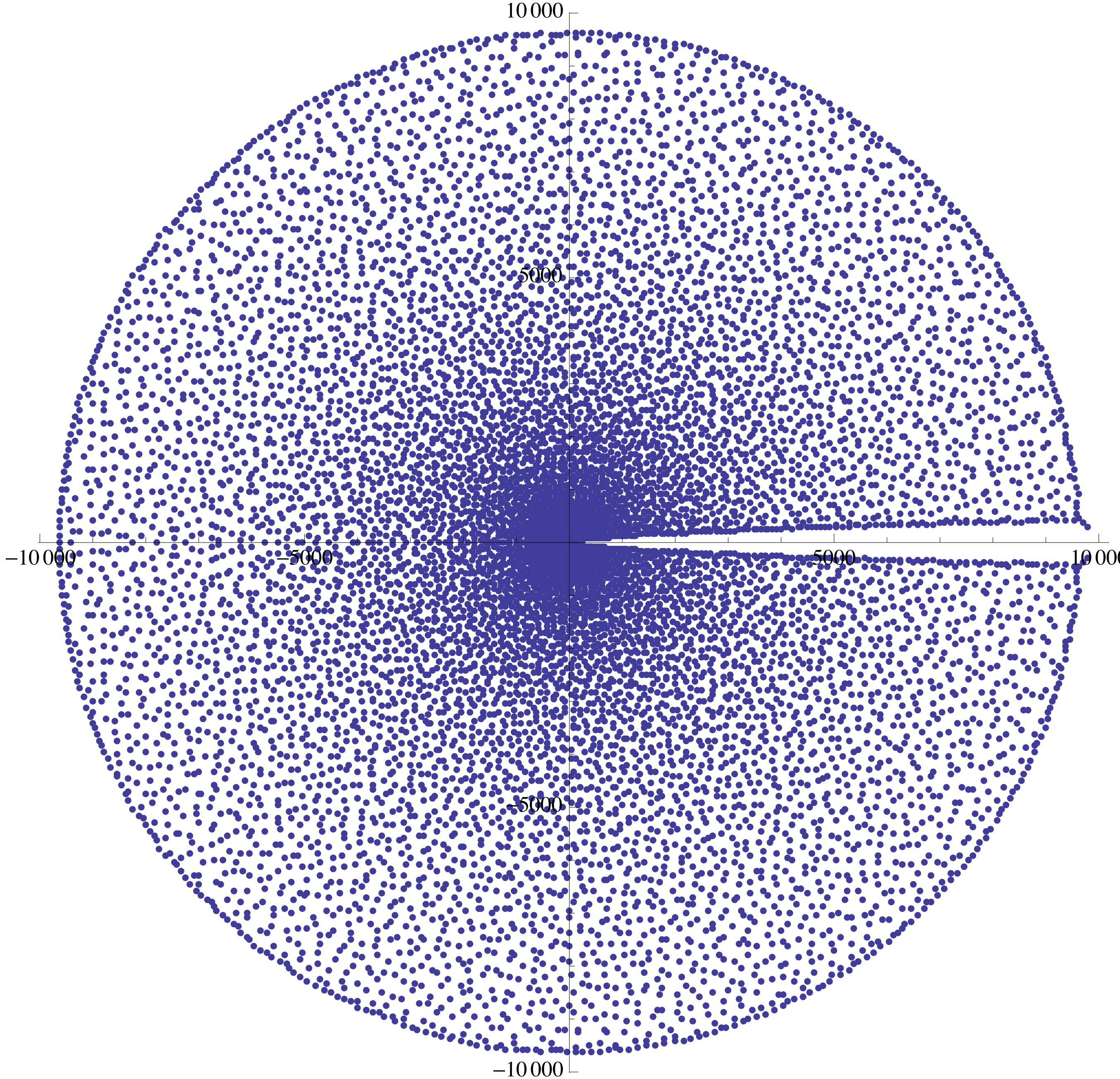


The Prime Polynomial

$$p_n = 2, 3, 5, 7, 11, 13, 17, 19, 23, 31, 37, 41, 43, 47, 53, 59, \ldots$$

$$P(z) = 1 + p_1\, z + \frac{p_2}{2!}\, z^2 + \frac{p_3}{3!}\, z^3 + \cdots \frac{p_n}{n!}\, z^n$$

Where are the zeros of this polynomial?


10 000
5000
−10 000
−5000
5000
10 000
−5000
−10 000

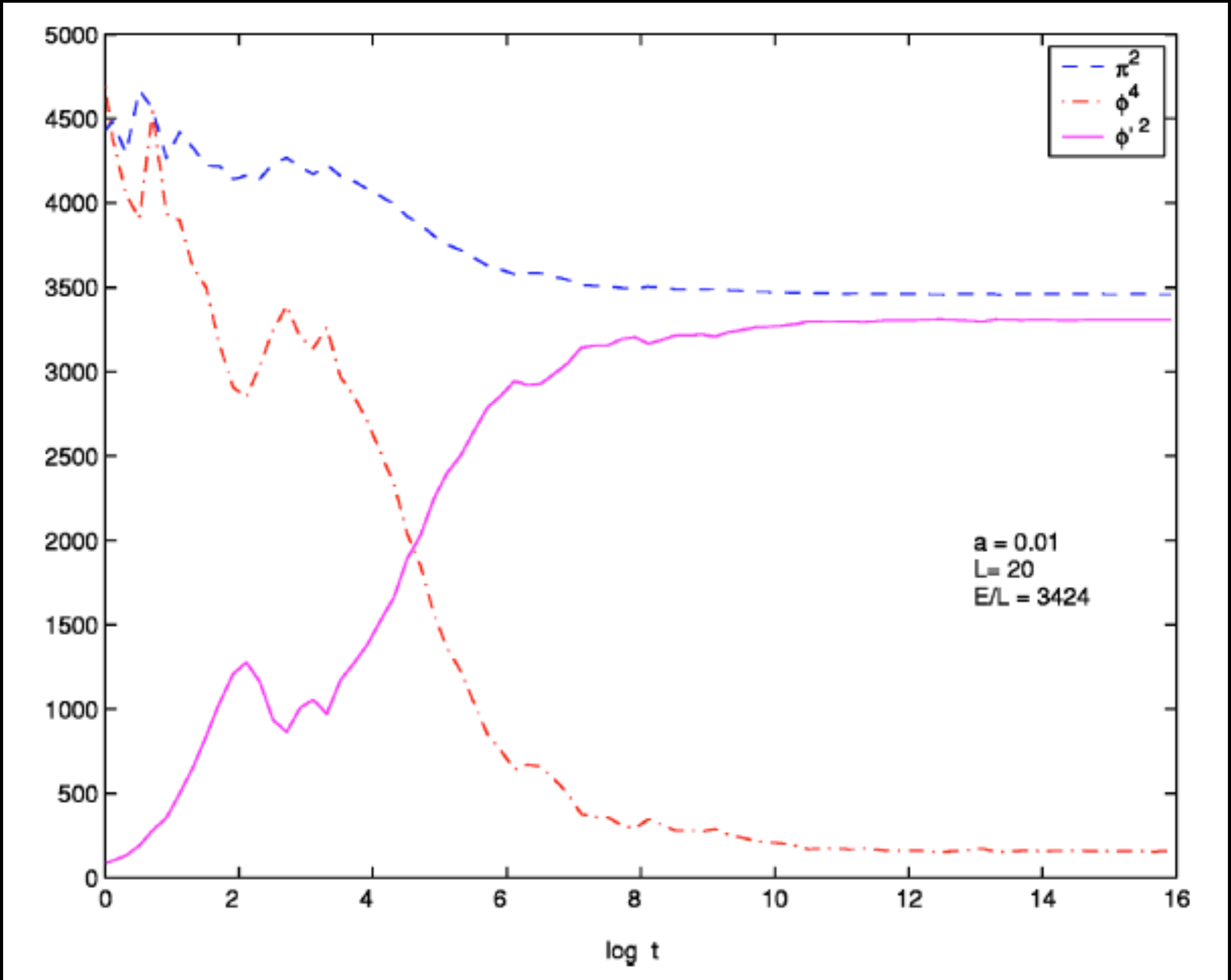
Topics of the seminar

- Yang-Lee theory of phase transitions
- Playing with polynomials
- Circle Theorem and Edge Singularities
- The Yang-Lee model
- Partition function of integrable quantum field theories
- How to experimentally measure the Yang-Lee zeros

Historically but also conceptually

Statistical Physics

has two different faces



π^2
ϕ^4
ϕ'^2
a = 0.01
L= 20
E/L = 3424
log t
0
2
4
6
8
10
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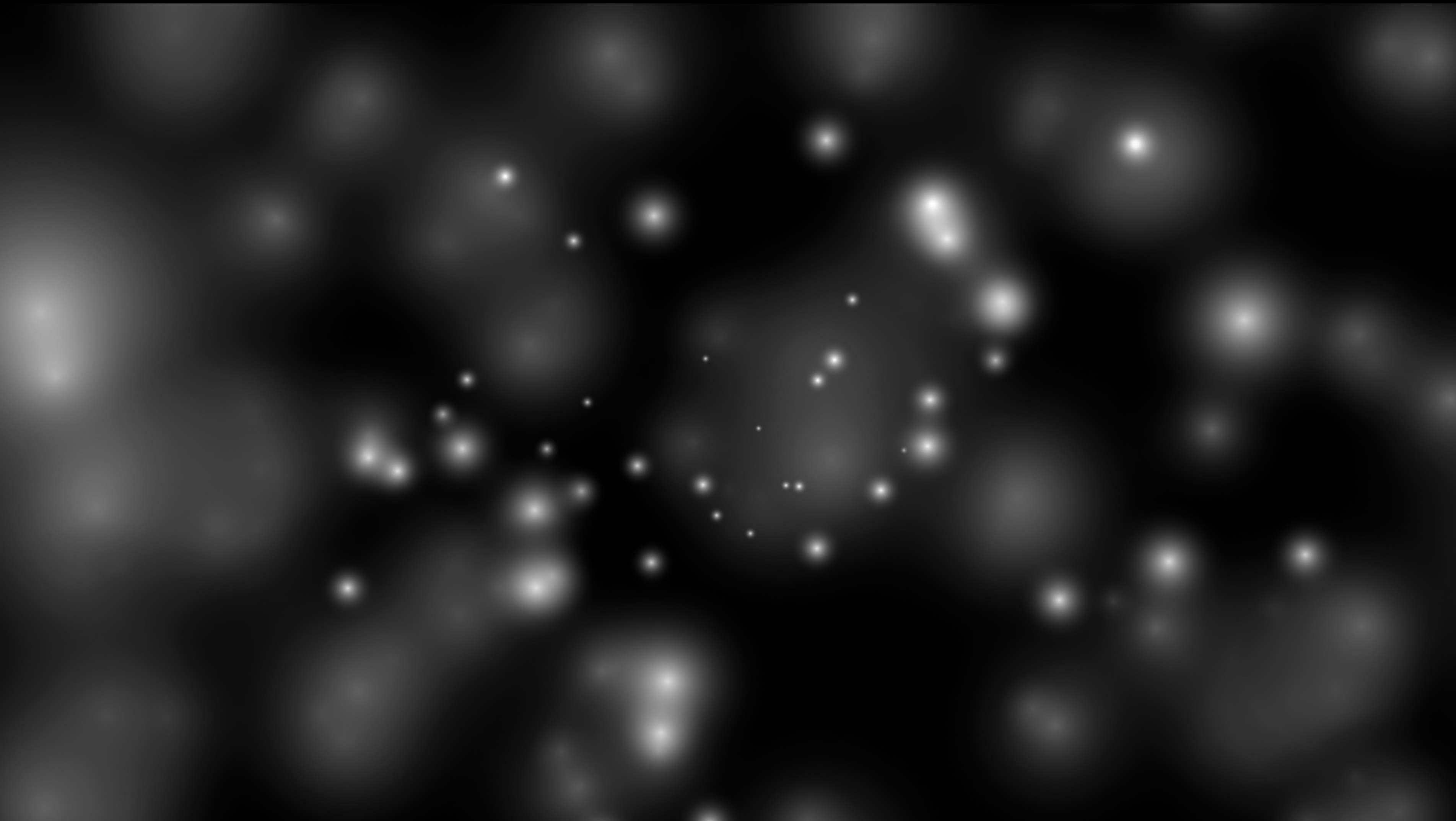
14
16
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000



Physics encoded

in

the Ensembles

Grand-Canonical Partition Function and its Zeros

$$\Omega_N(z) = \sum_{k=0}^{N} \frac{1}{k!} Z_k(V,T) z^k$$

This is a real polynomial

- Positive coefficients, for classical statistical physics
- Alternaning sign coefficients, for quantum fermionic systems

Grand-Canonical Partition Function and its Zeros

$$\Omega_N(z) = \sum_{k=0}^{N} \frac{1}{k!} Z_k(V,T) z^k = \prod_{l=1}^{N} \left(1 - \frac{z}{z_l}\right)$$

This is a real polynomial

Its zeros are either (negative) real numbers or complex conjugated

Playing with Polynomials

- Moments of zeros

$$s_k = \sum_{l=1}^{N} z_l^k$$

$$\Omega_N = 1 + \gamma_1 z + \gamma_2 z^2 + \ldots + \gamma_k z^k + \ldots +$$

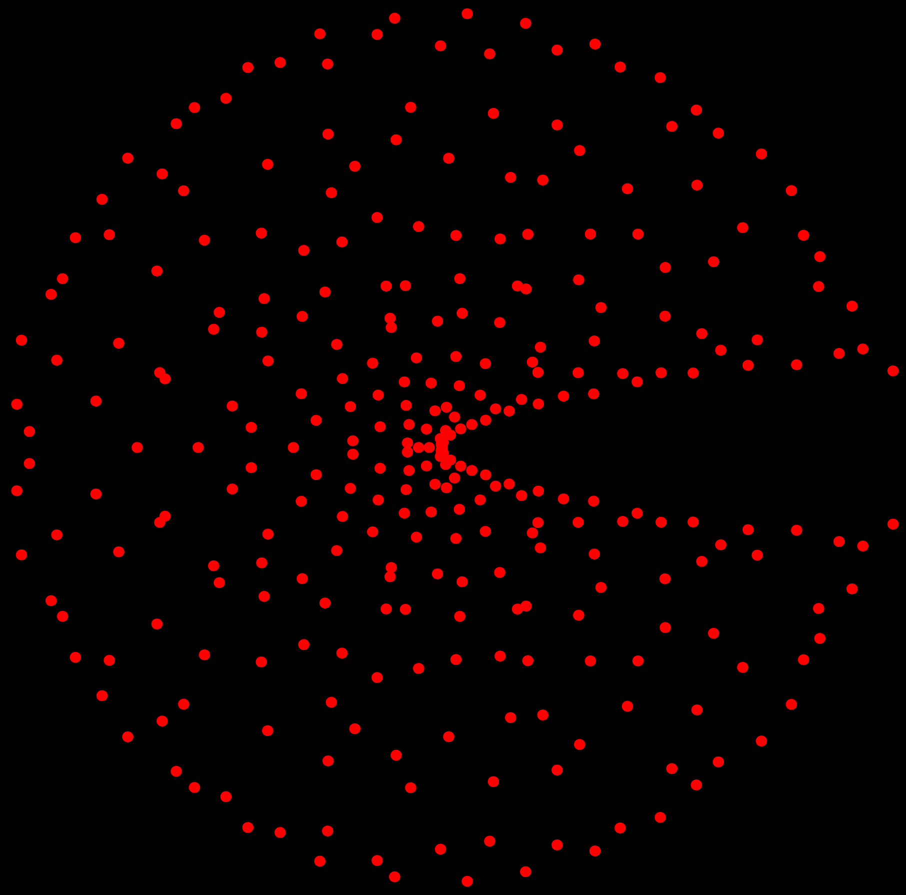
$$+ \gamma_{N-l} z^{N-l} + \gamma_{N-l+1} z^{N-l+1} + \ldots + \gamma_N z^N .$$

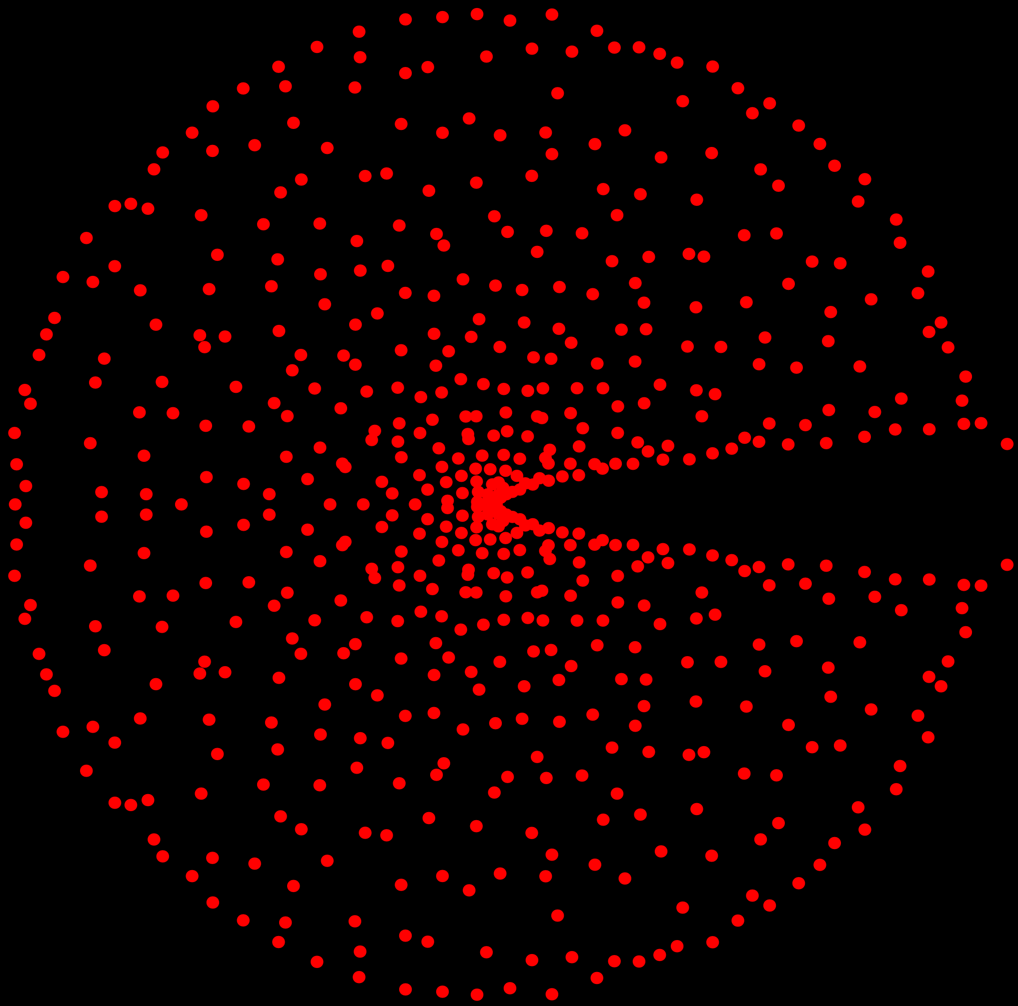
Playing with Polynomials

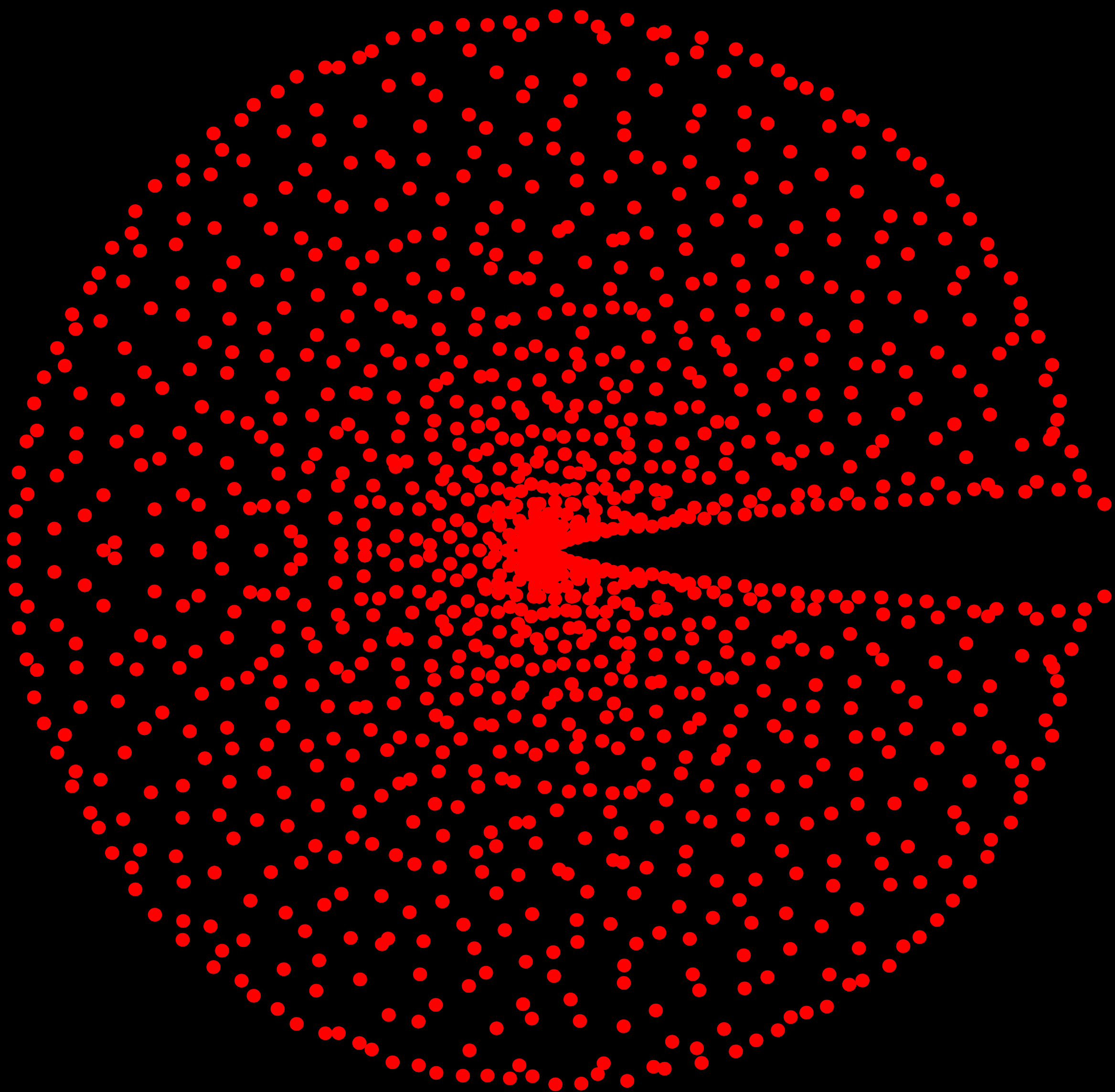
- Moments of zeros $$s_k = \sum_{l=1}^{N} z_l^k$$

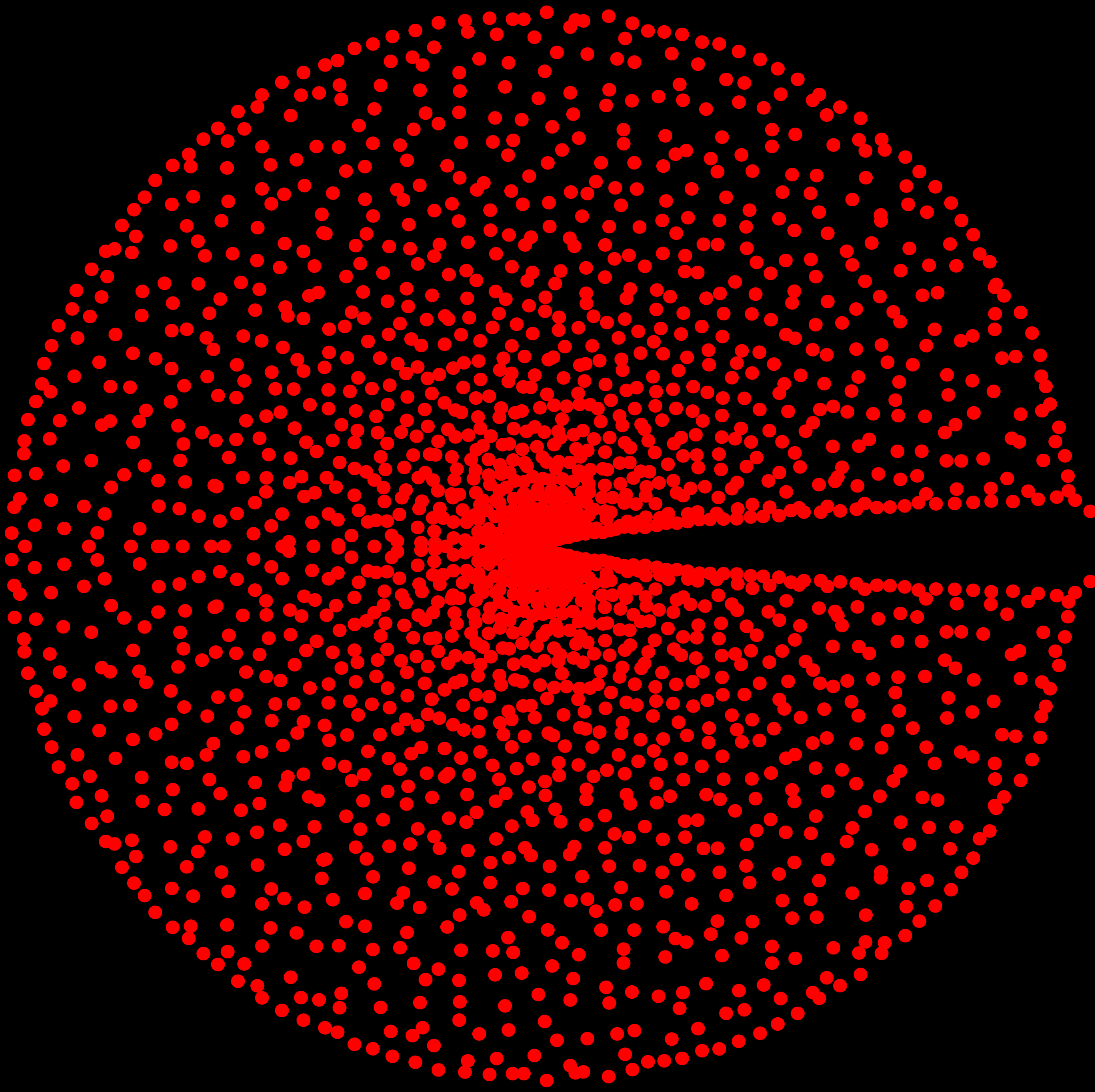
$$\Omega_N = \underbrace{1 + \gamma_1 z + \gamma_2 z^2 + \ldots + \gamma_k z^k}_{\hat{s}_k = s_{-k}} + \ldots +$$

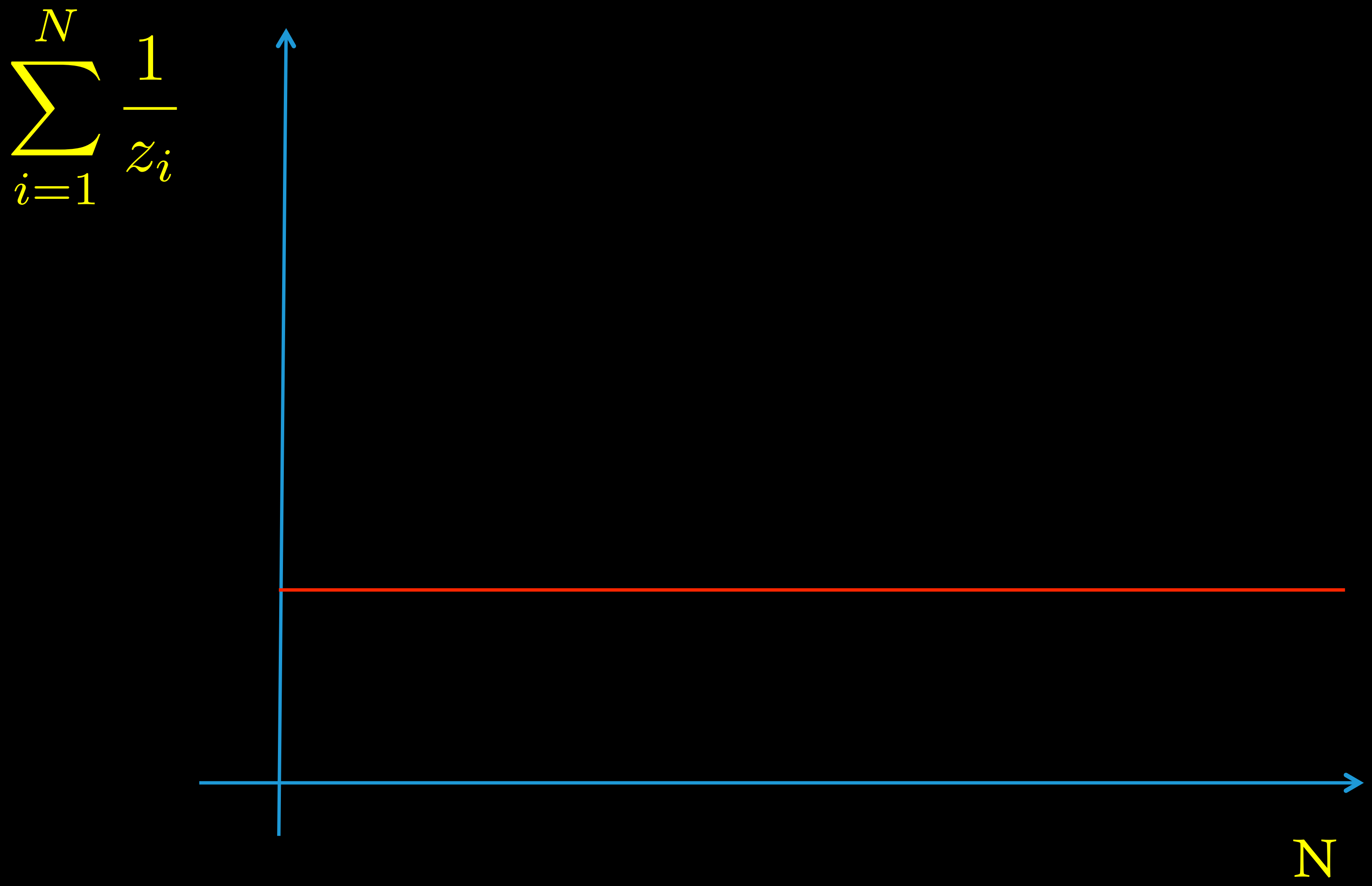
$$+ \underbrace{\gamma_{N-l} z^{N-l} + \gamma_{N-l+1} z^{N-l+1} + \ldots + \gamma_N z^N}_{s_l} .$$

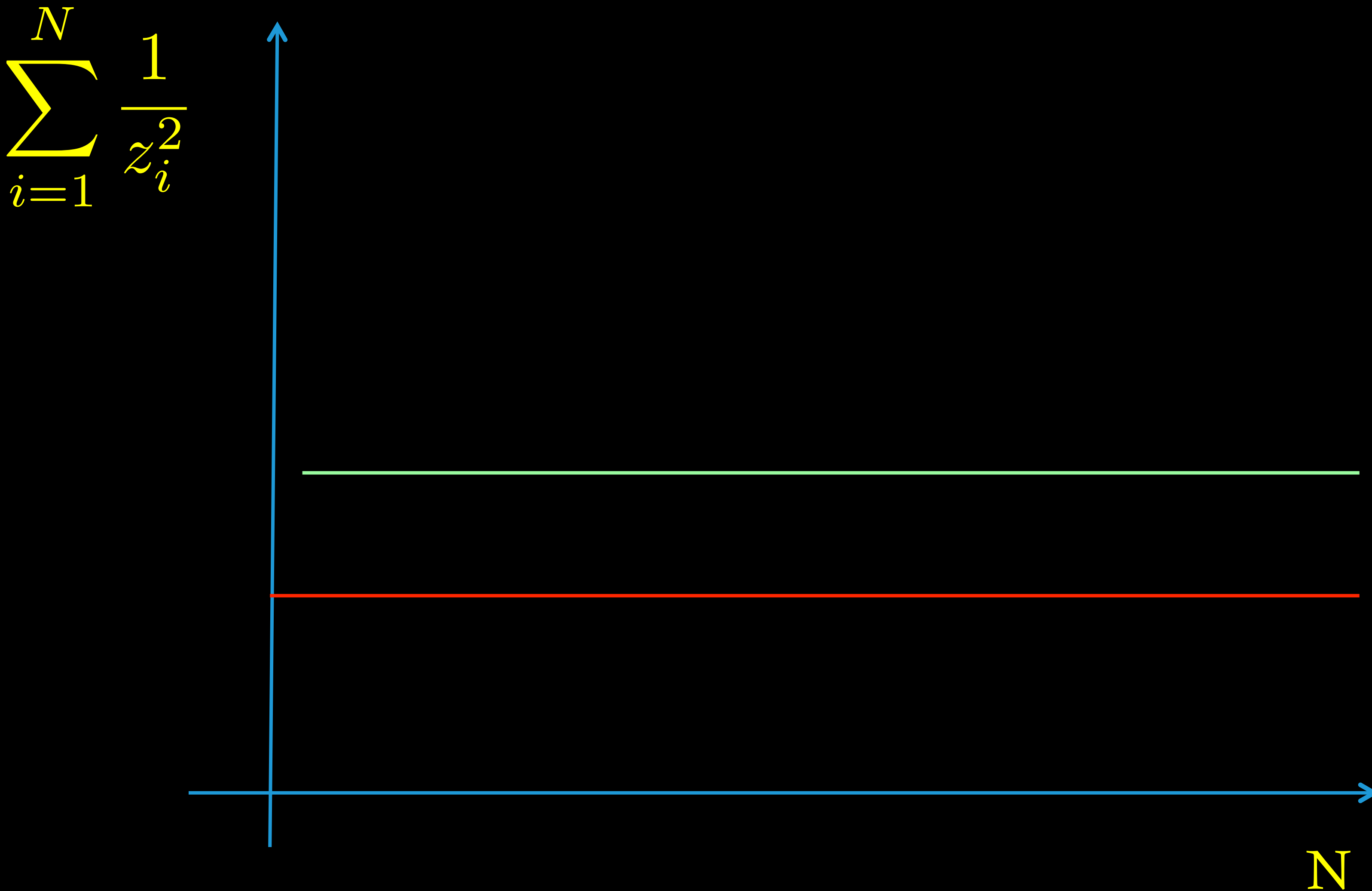




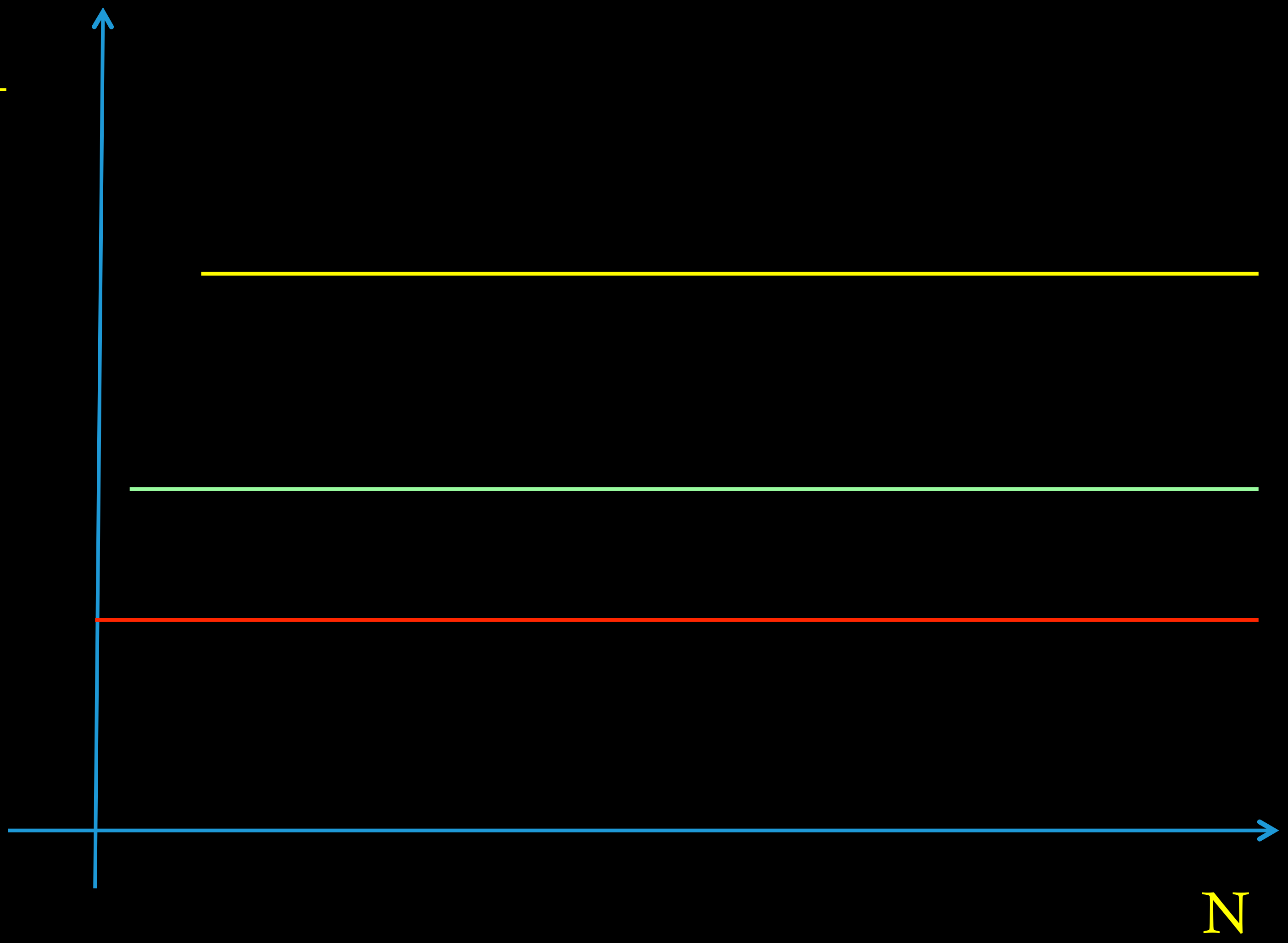





$\sum_{i=1}^{N} \frac{1}{z_i}$
N


$\sum_{i=1}^{N} \frac{1}{z_i^2}$
N

$$\sum_{i=1}^{N} \frac{1}{z_i^3}$$



Playing with Polynomials

- Moments of zeros

$$s_k = \sum_{l=1}^{N} z_l^k$$

$$\Omega_N = \prod_{l=1}^{N} \left(1 - \frac{z}{z_l}\right)$$

Playing with Polynomials

- Moments of zeros $$s_k = \sum_{l=1}^{N} z_l^k$$

$$\mathcal{F}_N(z) = \log \Omega_N(z) = \sum_{l=1}^{N} \log\left(1 - \frac{z}{z_l}\right) =$$

$$-\sum_{l=1}^{N} \sum_{m=1}^{\infty} \frac{1}{m}\left(\frac{z}{z_l}\right)^m \equiv \sum_{m=1}^{\infty} b_m z^m$$

$$b_m = -\frac{1}{m} \sum_{l=1}^{N} \frac{1}{z_l^m} = -\frac{1}{m} s_{-m}$$

Playing with Polynomials

- Moments of zeros $$s_k = \sum_{l=1}^{N} z_l^k$$

$$b_1 = \gamma_1$$

$$2!b_2 = 2\,\gamma_2 - \gamma_1$$

$$3!b_3 = 3!\,\gamma_3 - 6\,\gamma_2\gamma_1 + 2\,\gamma_1^3$$

$$\vdots \qquad\qquad \vdots$$

Playing with Polynomials

- Moments of zeros $$s_k = \sum_{l=1}^{N} z_l^k$$

$$\Omega_N = \underbrace{1 + \gamma_1 z + \gamma_2 z^2 + \ldots + \gamma_k z^k}_{\hat{s}_k = s_{-k}} + \ldots +$$

$$+ \underbrace{\gamma_{N-l} z^{N-l} + \gamma_{N-l+1} z^{N-l+1} + \ldots + \gamma_N z^N}_{s_l} .$$

Playing with Polynomials

- Moments of zeros

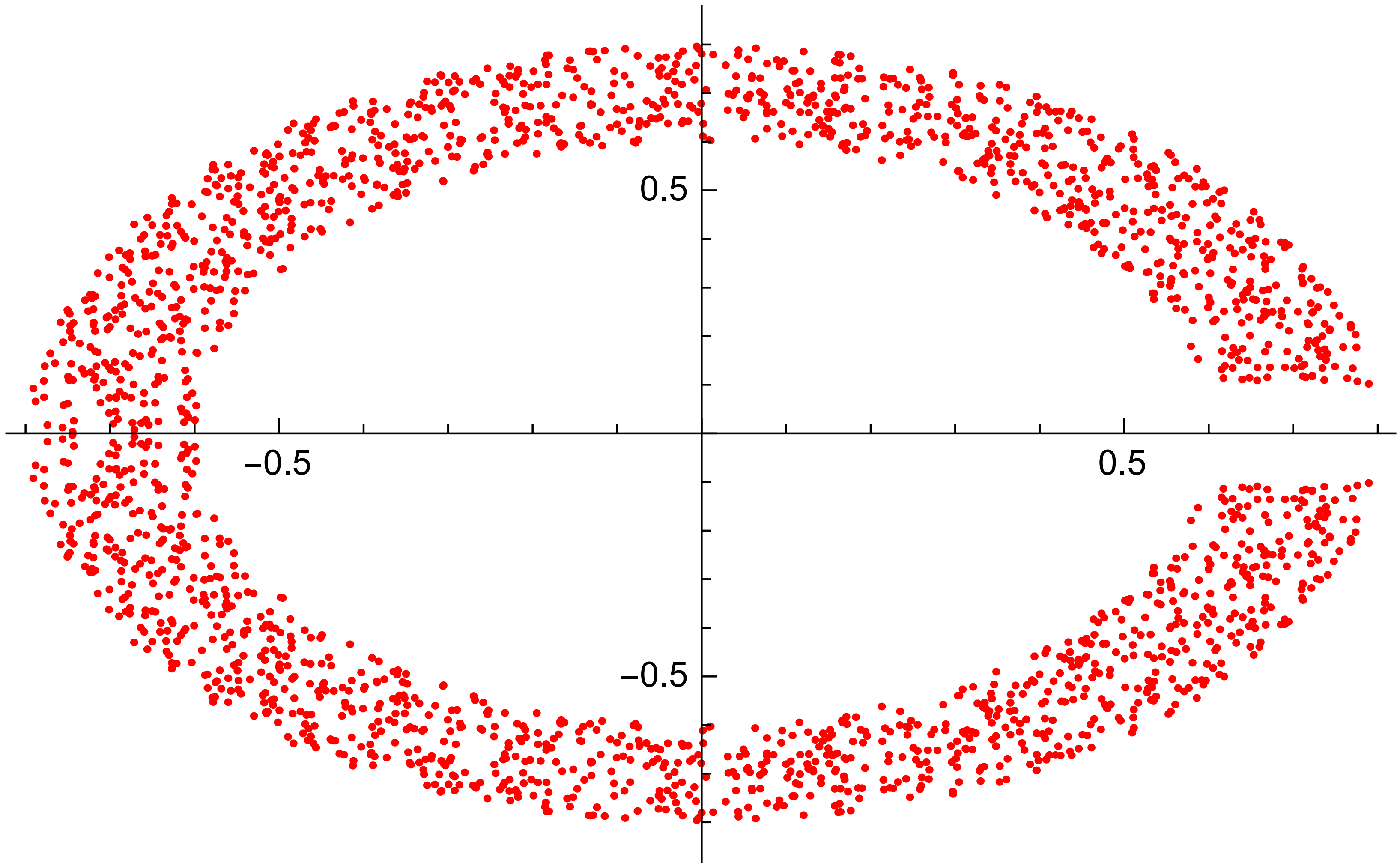
$$s_k = \sum_{l=1}^{N} z_l^k$$

- Bounds on the module of the zeros

$$R_d \leq |z_i| \leq R_u$$

For instance, Enestrom-Kakeya

$$R_d = \min\left\{\frac{\gamma_k}{\gamma_{k+1}}\right\} \quad , \quad R_u = \max\left\{\frac{\gamma_k}{\gamma_{k+1}}\right\}$$



0.5
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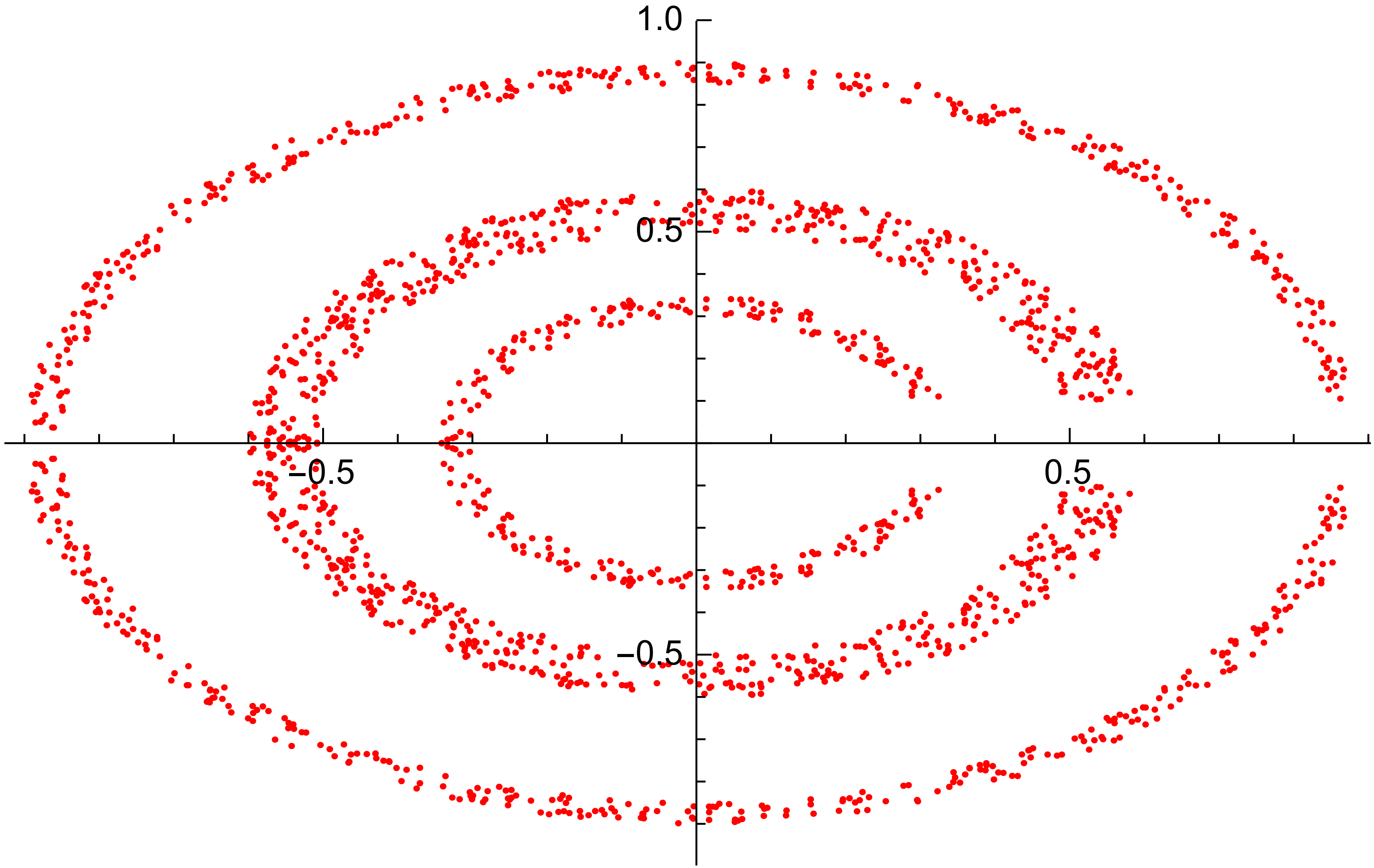
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0.5
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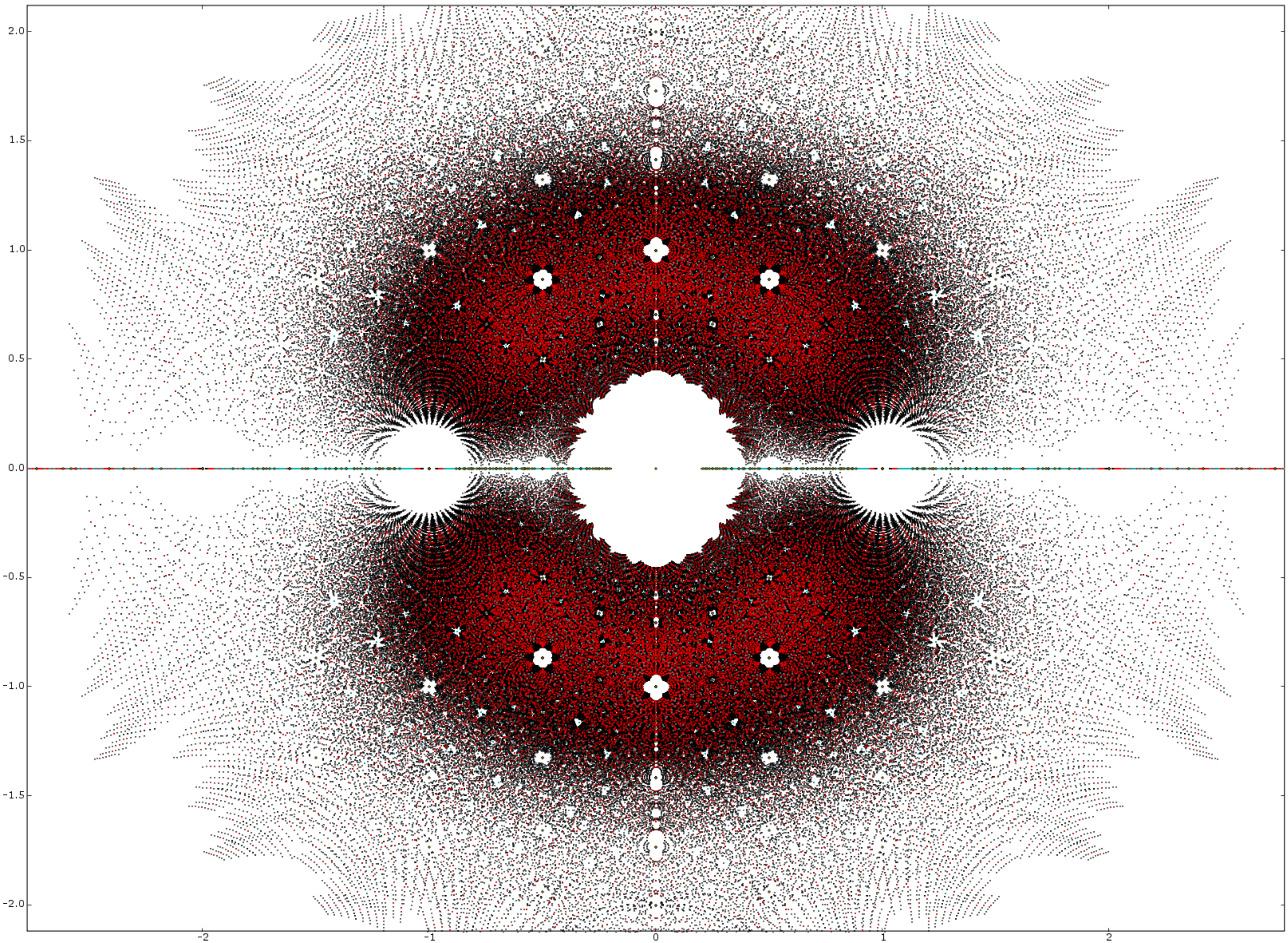
0.5
−0.5



2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2
-1
0
1
2

Can any distribution of complex conjugate zeros

be eligible

for defining a possible physical statistical system?

PHYSICAL REVIEW VOLUME 87, NUMBER 3 AUGUST 1, 1952

Statistical Theory of Equations of State and Phase Transitions. I. Theory of Condensation

C. N. Yang and T. D. Lee
Institute for Advanced Study, Princeton, New Jersey
(Received March 31, 1952)

A theory of equations of state and phase transitions is developed that describes the condensed as well as the gas phases and the transition regions. The thermodynamic properties of an infinite sample are studied rigorously and Mayer's theory is re-examined.

I. INTRODUCTION

THIS and a subsequent paper will be concerned with the problem of a statistical theory of equations of state and phase transitions. This problem has always interested physicists both from the practical viewpoint of seeking for a workable theory of properties of matter (such as a theory of liquids) and also from the more academic viewpoint of understanding the occurrence of the discontinuities associated with phase transitions in the thermodynamic functions.

The work reported in this paper is quite general and fairly abstract. We are returning in a subsequent paper to the illustration and application of the methods here outlined. In order to present the work of this present paper in its proper perspective, it may be helpful if we outline briefly the history of our own thinking on the subject.

About a year ago one of us was able to make progress[1] with the problem of the spontaneous magnetization of the Ising model, taking advantage of some special properties of this problem when treated by the Onsager-Kaufman method.[2] We then noted that the solution there obtained was also the solution of another, physically quite different, but formally identical, problem. This is the problem of a lattice gas with attractive interaction between nearest neighbors. We were thus able to follow in detail the behavior of such a lattice gas, which in many ways should reveal the features of an actual gas. In particular, we were able to study and characterize the condensation phenonenon, and to identify the liquid, gas, and transition regions in the $p-v$ diagram. The isotherms thus obtained are flat in the transition region and rise very rapidly with increasing density in the liquid phase. At this point, we were led to compare the specific solution with the well-known work[3] of Mayer on the theory of condensation of gases. In particular we were led to inquire as to why, in Mayer's theory, the isotherms stay flat beyond the condensation point and do not give the equation of state for the liquid phase. It soon became apparent that this difference lay, not in the difference of the models, but in the inadequacy of Mayer's method for dealing with a condensed phase. This led to a study of the analytical behavior of the grand partition function of an assembly of interacting atoms, and we were able, as in the special case mentioned above, to identify and characterize quite generally the condensation phenomena. These general conclusions will be presented in the present paper.

The problem is approached by allowing the fugacity to take on complex values. Although only real values c the fugacity are of any physical interest, the analytic behavior of the thermodynamic functions can only completely revealed by going into the complex pl whereby one is able to obtain a description of the densed phases as well as the gas phase and the tra regions. This approach is of a very general nat can be applied to other problems of phase tr such as ferromagnetism, order disorder transi It will be emphasized that also this approac to practical approximation methods for the of systems undergoing transitions. These p discussed in paper II.

The physical conclusions of this paper de mathematical results which we shall st of two theorems. Due to the nature (which involves a double limiting p perative to have mathematical rigor out. The proofs are necessarily of a m and will be given in the appendix.

II. INTERACT

We consider a monatomic ga

$$U=\sum u$$

where r_{ij} is the distance bet The following assumptions of these interactions:

(1) The atoms have diameter a, so that $u(r$

(2) The interaction

$$u(r$$

(3) $u(r)$ is nowh

The theory can body forces and

[1] C. N. Yang, Phys. Rev. 85, 808 (1952).
[2] L. Onsager, Phys. Rev. 65, 117 (1944); B. Kaufman, Phys. Rev. 76, 1232 (1949).
[3] J. E. Mayer, J. Chem. Phys. 5, 67 (1937); J. E. Mayer and Ph. G. Ackermann, J. Chem. Phys. 5, 74 (1937); J. E. Mayer and S. F. Harrison, J. Chem. Phys. 6, 87, 101 (1938); B. Kahn and G. E. Uhlenbeck, Physica 5, 399 (1938). M. Born and K. Fuchs, Proc. Roy. Soc. (London) A166, 391 (1938).

PHYSICAL REVIEW VOLUME 87, NUMBER 3 AUGUST 1, 1952

Statistical Theory of Equations of State and Phase Transitions. II. Lattice Gas and Ising Model

T. D. Lee and C. N. Yang
Institute for Advanced Study, Princeton, New Jersey
(Received March 31, 1952)

The problems of an Ising model in a magnetic field and a lattice gas are proved mathematically equivalent. From this equivalence an example of a two-dimensional lattice gas is given for which the phase transition regions in the $p-v$ diagram is exactly calculated.

A theorem is proved which states that under a class of general conditions the roots of the grand partition function always lie on a circle. Consequences of this theorem and its relation with practical approximation methods are discussed. All the known exact results about the two-dimensional square Ising lattice are summarized, and some new results are quoted.

INTRODUCTION

IN paper I[1] we have seen that the problem of a statistical theory of phase transitions and equations of state is closely connected with the distribution of roots of the grand partition function. It was shown there that the distribution of roots determines completely the equation of state, and in particular its behavior near the positive real axis prescribes the properties of the system in relation to phase transitions. It was also shown there that the equation of state of the condensed phases as well as the gas phase can be correctly obtained from a knowledge of the distribution of roots. While this general and abstract theory clarifies the problems underlying the statistical theory of phase transitions and condensed phases, it is natural to ask whether it also provides us with a means of obtaining practical approximation methods for calculating properties pertaining to phase transitions and condensed phases.

The problem is clearly that of seeking for the properties of the distribution of roots of the grand partition function. At first sight this appears to be a formidable problem, as the roots are in general complex and would naturally be expected to spread themselves for an infinite sample in the entire complex plane, or at least regions of the complex plane, and make it very difficult to calculate their distribution. We were quite surprised, therefore, to find that for a large class of problems of practical interest, the roots behave remarkably well in that they distribute themselves not all over the complex plane, but only on a fixed circle. This fact will be stated as a theorem in Sec. IV of the present paper and proved in the appendix. Implications of the theorem are discussed in Sec. V.

Also in this paper we shall give a proof (Sec. II) that the problem of an Ising model with a magnetic field is mathematically identical with that of a "lattice gas." From this identification we were able to trace exactly the transition region in the $p-v$ diagram of a two-dimensional lattice gas in detail. This will be presented in Sec. III and forms a clear illustration of the discussions of paper I and of Sec. V of the present paper.

At the end of Sec. V we give a summary of all the exact knowledge known to us about the two-dimensional Ising model in a magnetic field and its relationship with the distribution of roots of the partition function.

II. ISING MODEL AND LATTICE GAS

We shall in this section show that the problems of an Ising model in a magnetic field and of a lattice gas are mathematically equivalent. In the former problem one considers a lattice of interacting spins each of which can assume two possible positions: ↑ and ↓. In the latter, one considers a corresponding lattice with each lattice point either vacant or occupied by an atom.[2] To each configuration of the lattice of spins there corresponds a configuration of the lattice gas in which a lattice point is vacant or occupied according as whether the corresponding spin is ↑ or ↓. Using this geometrical correspondence, one could establish the mathematical equivalence of the two problems.

For clarity of presentation we shall take as an example a simple cubic lattice and consider first the Ising model problem with nearest neighbor interaction. The same treatment can be applied to any lattice with arbitrary interaction between the spins. Denote by [↑↑], [↓↓], and [↑↓] the total number of nearest neighboring spins that are respectively parallel and upward, parallel and downward, and antiparallel to each other. Also denote by [↑] and [↓] the total numbers of upward and downward spins in the lattice.

Table I. Identification of corresponding quantities in Ising model and lattice gas.[a]

Ising model		Lattice gas
No. of spins	=	volume
No. of ↓ spins	=	No. of atoms
$2/(1-I)$	=	specific volume v
$-F-H$	=	pressure p

[a] I, H, and F are respectively the intensity of magnetization, the magnetic field, and the free energy per spin in the Ising model problem.

[1] C. N. Yang and T. D. Lee, Phys. Rev. 87, 404 (1952).

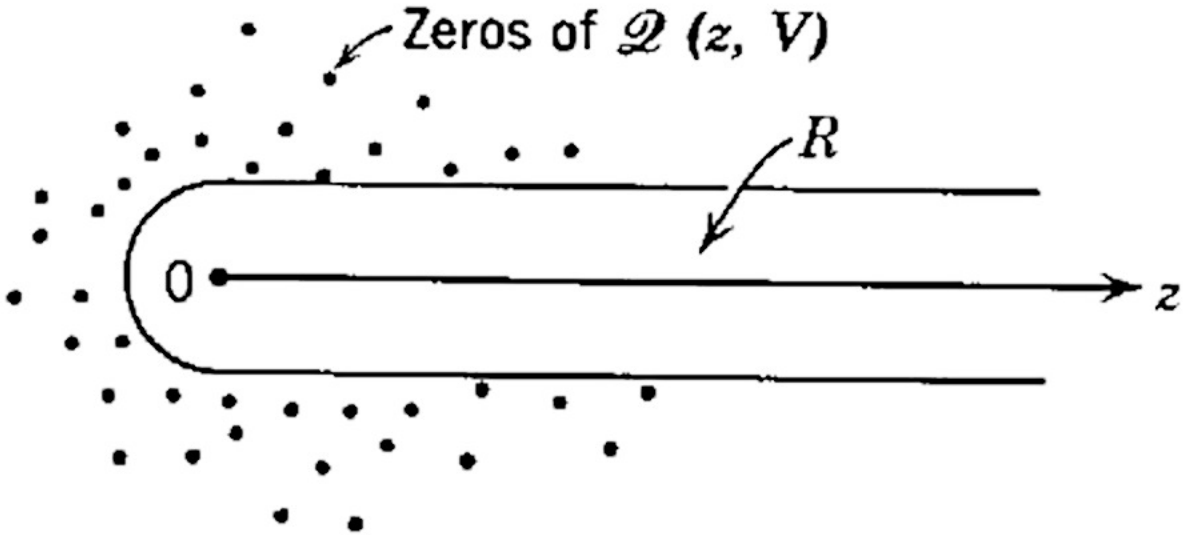
[2] Similar ideas have been used in the "hole theory of liquids." See, e.g., J. E. Lennard-Jones and A. F. Devonshire, Proc. Roy. Soc. (London) A169, 317 (1939); A170, 464 (1939). F. Cernuschi and H. Eyring, J. Chem. Phys. 7, 547 (1939).

Grand-Canonical Partition Function and its Zeros

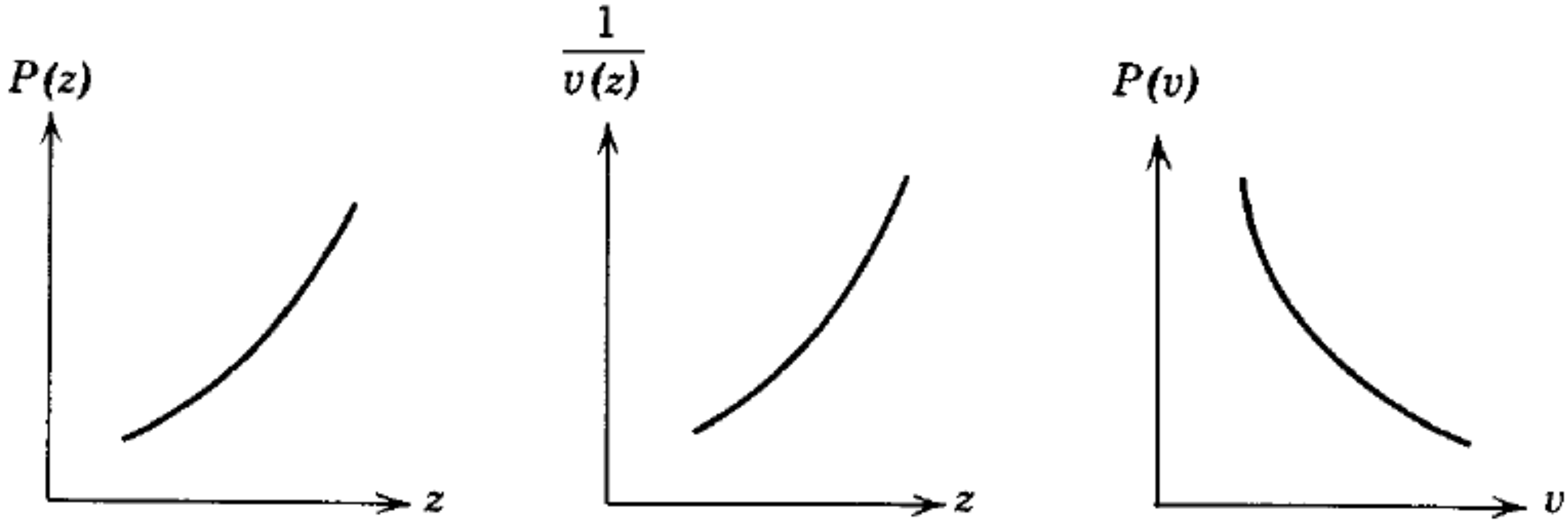
$$\Omega_N(z) = \sum_{k=0}^{N} \frac{1}{k!} Z_k(V,T) z^k = \prod_{l=1}^{N} \left(1 - \frac{z}{z_l}\right)$$

$$\frac{p(z)}{kT} \equiv \hat{f}(z) = \frac{1}{V} \sum_{l=1}^{N} \log\left(1 - \frac{z}{z_l}\right)$$

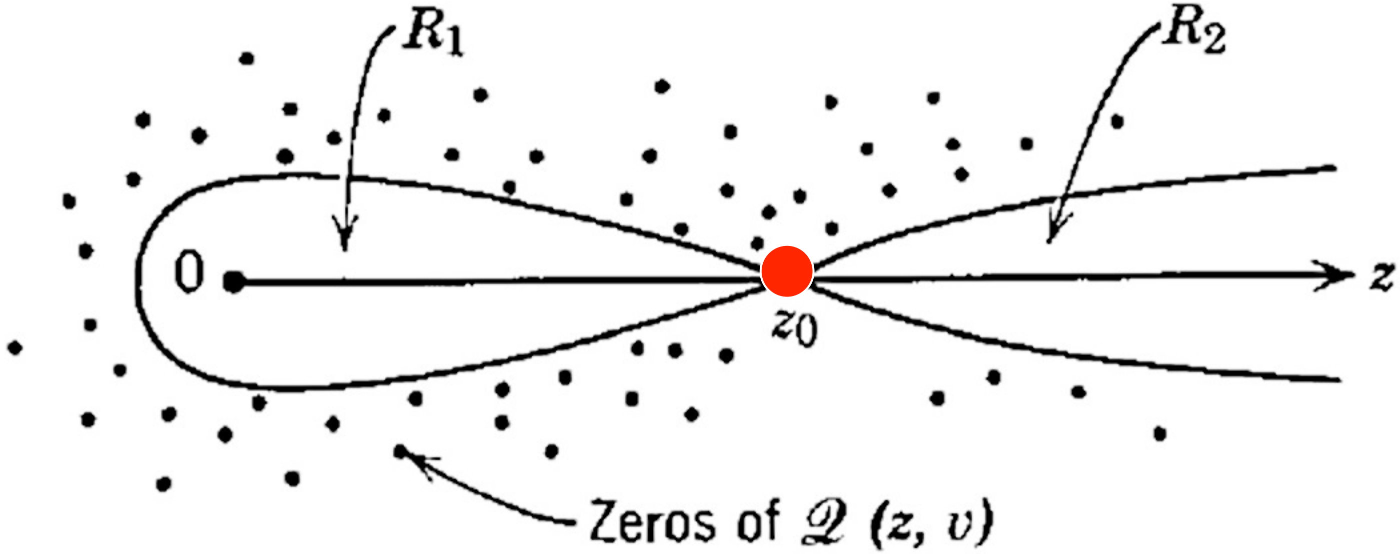
$$\rho(z) \equiv z\hat{f}'(z) = \frac{1}{V} \sum_{l=1}^{N} \frac{z}{z - z_l}$$



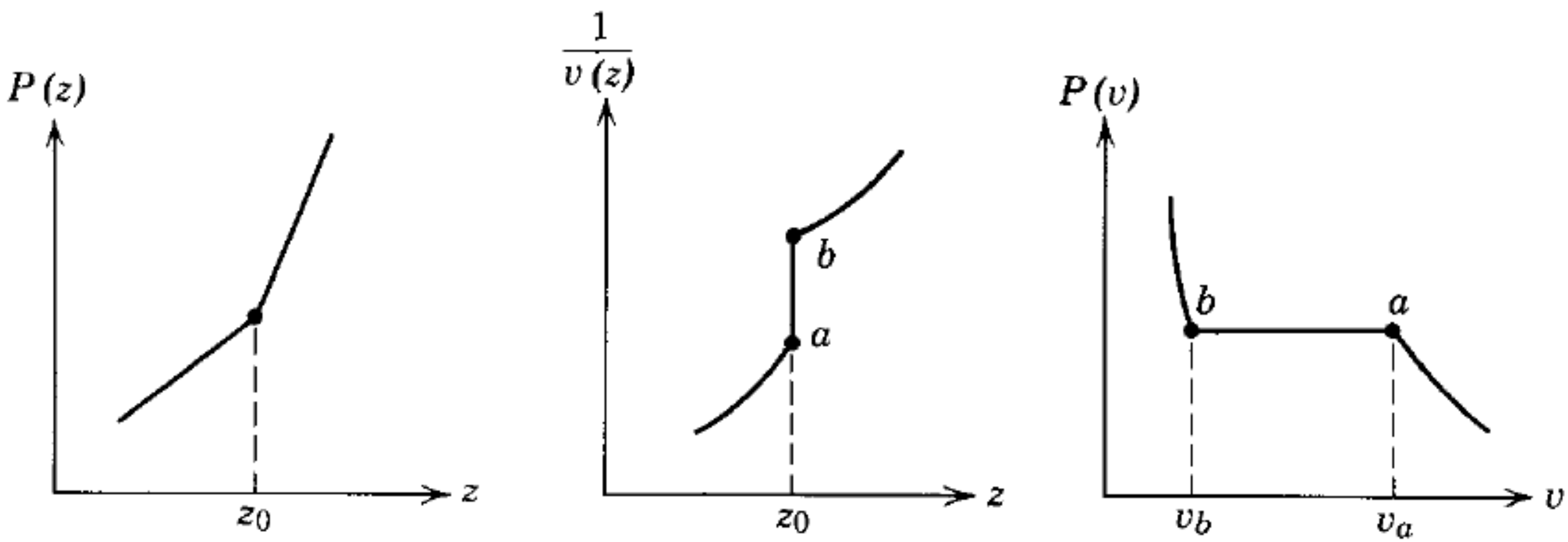
Zeros of $\mathscr{Q}(z, V)$
R
0
z



P(z)
z
$\frac{1}{v(z)}$
z
P(v)
v



R_1
R_2
0
z
z_0
Zeros of $\mathscr{Q}(z, v)$



$P(z)$
z
z_0
$\frac{1}{v(z)}$
a
b
z
z_0
$P(v)$
b
a
v
v_b
v_a

Yang-Lee Zeros and two-dimensional Electrostatics

Imagine the zeros condensate in an area *A* or a curve *C* in the complex plane with a local positive density η(z)

$$\frac{p(z)}{kT} = \int_{A} d\xi \, \eta(\xi) \, \log\left(1 - \frac{z}{\xi}\right)$$

$$= \varphi(z) + i\psi(z)$$

Yang-Lee Zeros and two-dimensional Electrostatics

Imagine the zeros condensate in an area *A* or a curve *C* in the complex plane with a local positive density η(z)

$$\varphi(z) = \int_{\mathcal{A}} d\xi \, \eta(\xi) \, \log \left| 1 - \frac{z}{\xi} \right|$$

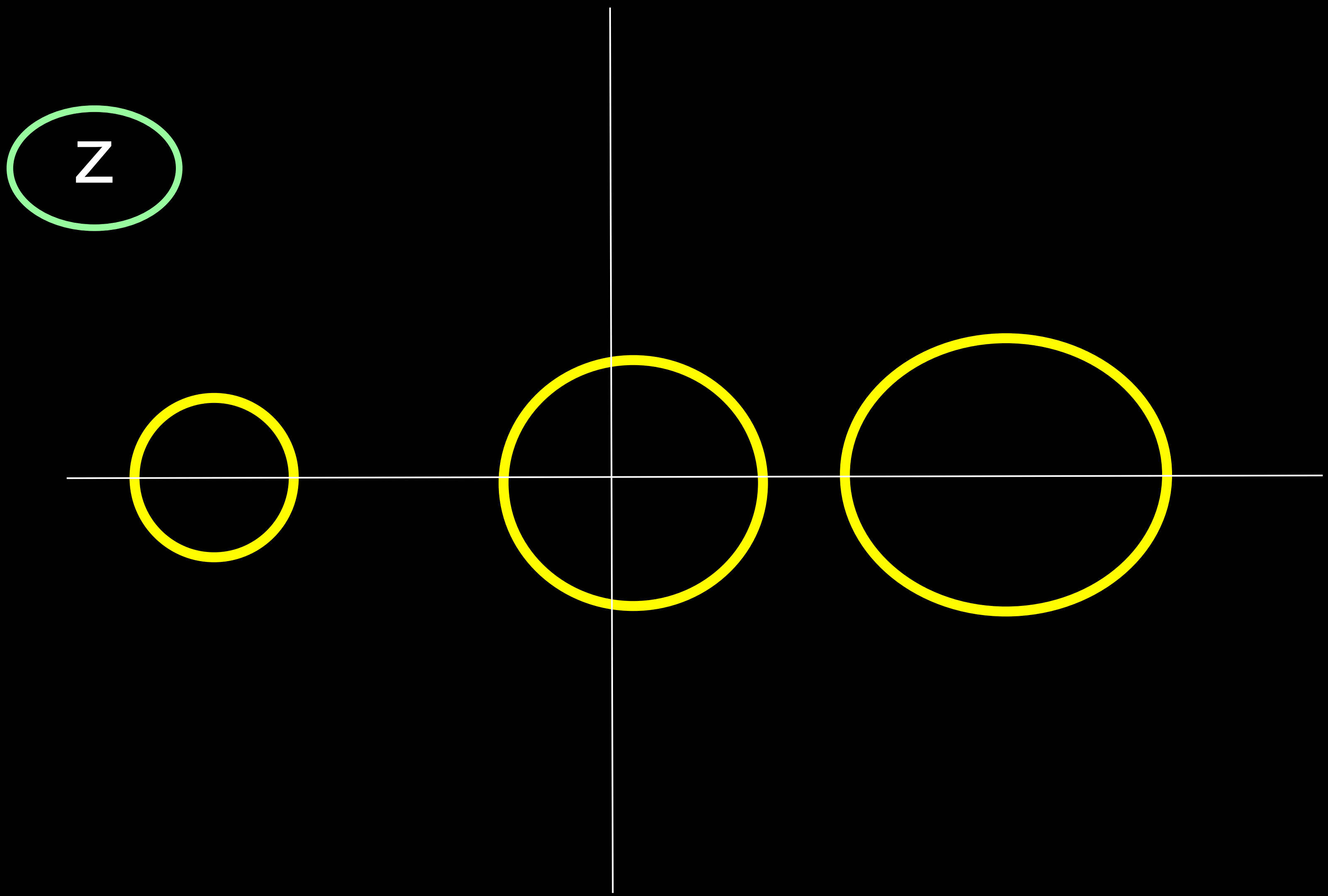
Green function of two-dimensional electrostatics

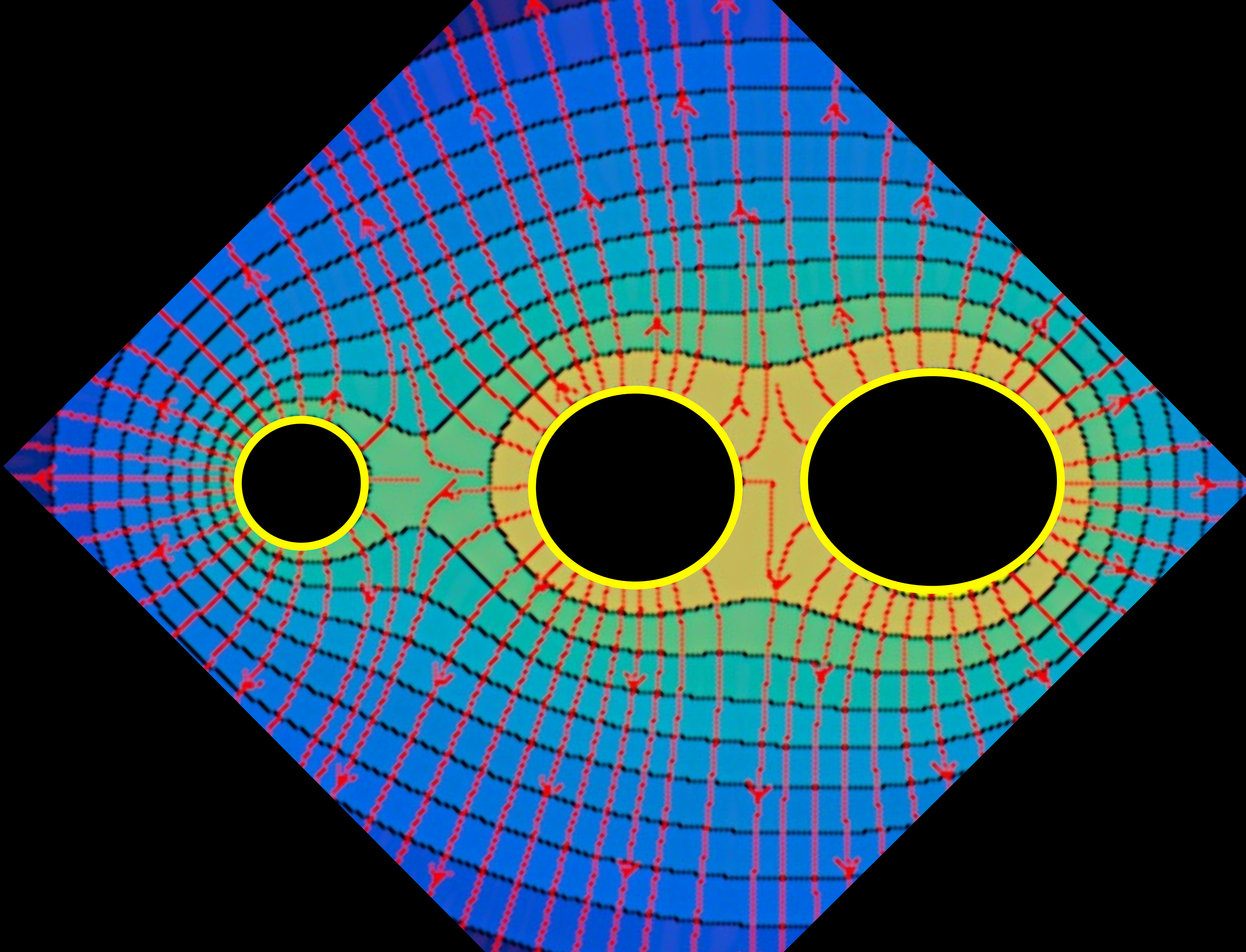
Yang-Lee Zeros and two-dimensional Electrostatics

Imagine the zeros condensate in an area *A* or a curve *C* in the complex plane with a local positive density η(z)

$$\Delta\varphi(z) = 2\pi\,\eta(z)$$

Wherever η(z) =0, the pressure should be a harmonic function


Z



Equation of State and Yang-Lee Zeros

$$\frac{p(z)}{kT} \equiv f(z) = \int_C \eta(\xi) \log\left(1 - \frac{z}{\xi}\right)$$

$$\rho(z) = z\,\frac{df(z)}{dz} = z \int_C \frac{\eta(\xi)}{z - \xi}$$

Is it possible to determine $\eta(\xi)$?

Equation of State and Yang-Lee Zeros

$$\frac{p(z)}{kT} \equiv f(z) \quad ; \quad \rho(z) = z\,\frac{df(z)}{dz}$$

$$f(z) = \int_C \eta(\xi)\,\log\left(1 - \frac{z}{\xi}\right)$$

Is it possible to determine $\eta(\xi)$?

In general, this is an extremely difficult task

1. Eliminate z between the two expressions and find the explicit equation of state $p(\rho, T)$

2. Use the previous parameterizations to find a non-linear first order diff. eq. for the function f(z)

3. By integration, we have a functional equation

$$\mathcal{F}(f, z) = 0$$

whose solution in general is not unique and it may have also several Riemann surfaces

4. The branching points belong to the contour $\mathcal{C}$

Example. YL zeros for van der Waals gases

(Hemmer and Hauge)

$$\frac{p(z)}{kT} = f(z) = \frac{\rho}{1-\rho} - \nu\rho^2$$

$$\rho(z) = z\,\frac{df(z)}{dz}$$

$$\nu = \frac{a}{kT}$$ depends on temperature

Example. YL zeros for van der Waals gases

(Hemmer and Hauge)

$$\frac{p(z)}{kT} = f(z) = \frac{\rho}{1-\rho} - \nu\rho^2$$

$$\rho(z) = z\,\frac{df(z)}{dz}$$

$$z\left(\frac{dz}{d\rho}\right) = z\left[(1-\rho)^{-2} - 2\nu\rho\right]$$

Example. YL zeros for van der Waals gases

$$z = \frac{\rho}{1-\rho} \exp\left[\frac{\rho}{1-\rho} - 2\nu\rho\right]$$

The inverse function ρ is multivalued and so the function $f(z)$

$$f(z) = f[\rho(z)] = \frac{\rho(z)}{1-\rho(z)} - \nu\rho^2(z)$$

Example. YL zeros for van der Waals gases

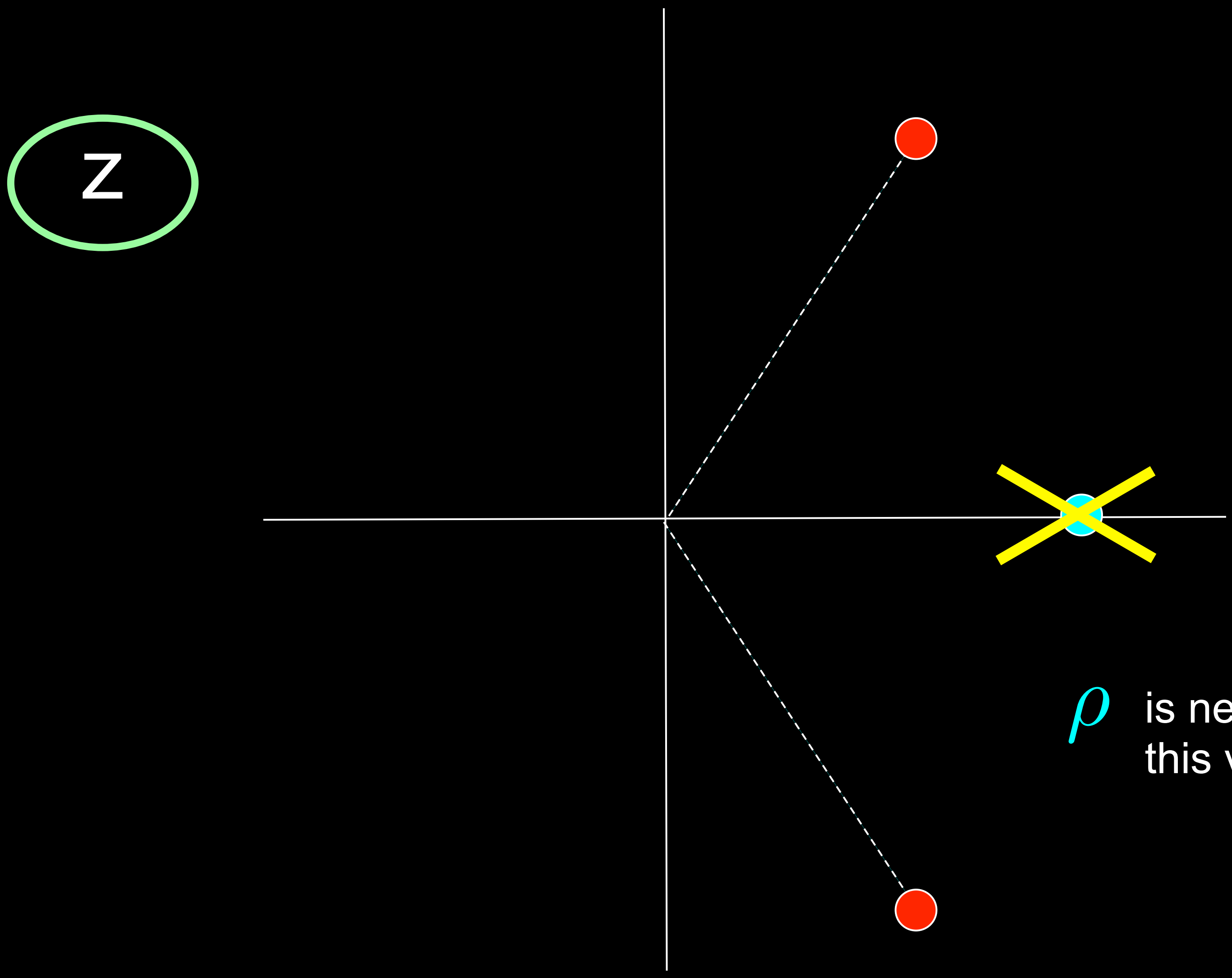
$$z = \frac{\rho}{1-\rho}\,\exp\left[\frac{\rho}{1-\rho} - 2\nu\rho\right]$$

Singularities

$$z\left(\frac{dz}{d\rho}\right) = z\left[(1-\rho)^{-2} - 2\nu\rho\right] = 0$$

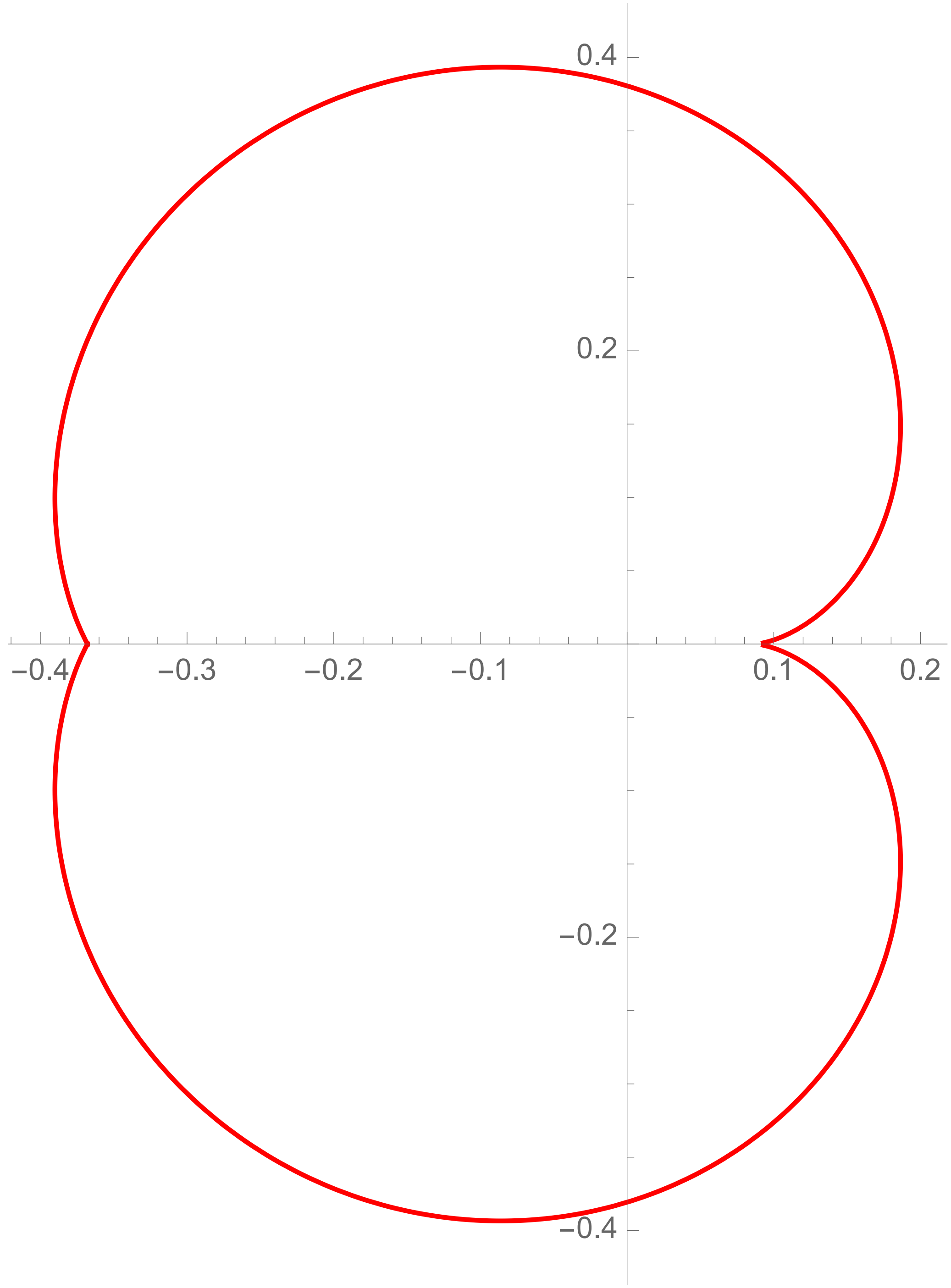
$$2\nu\rho(1-\rho)^2 = 1$$

$T \geq T_c$

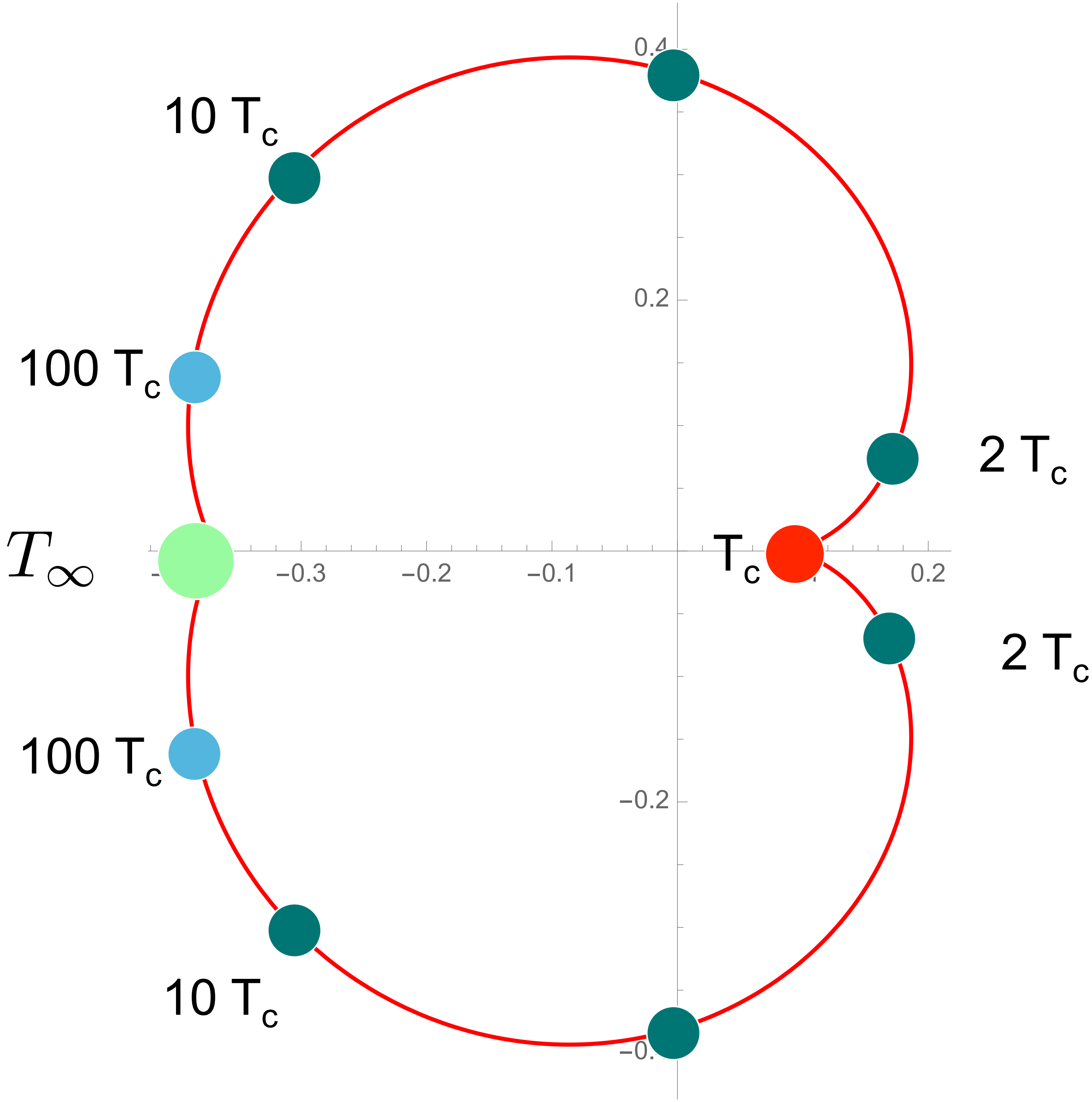


ρ is negative at this value of z

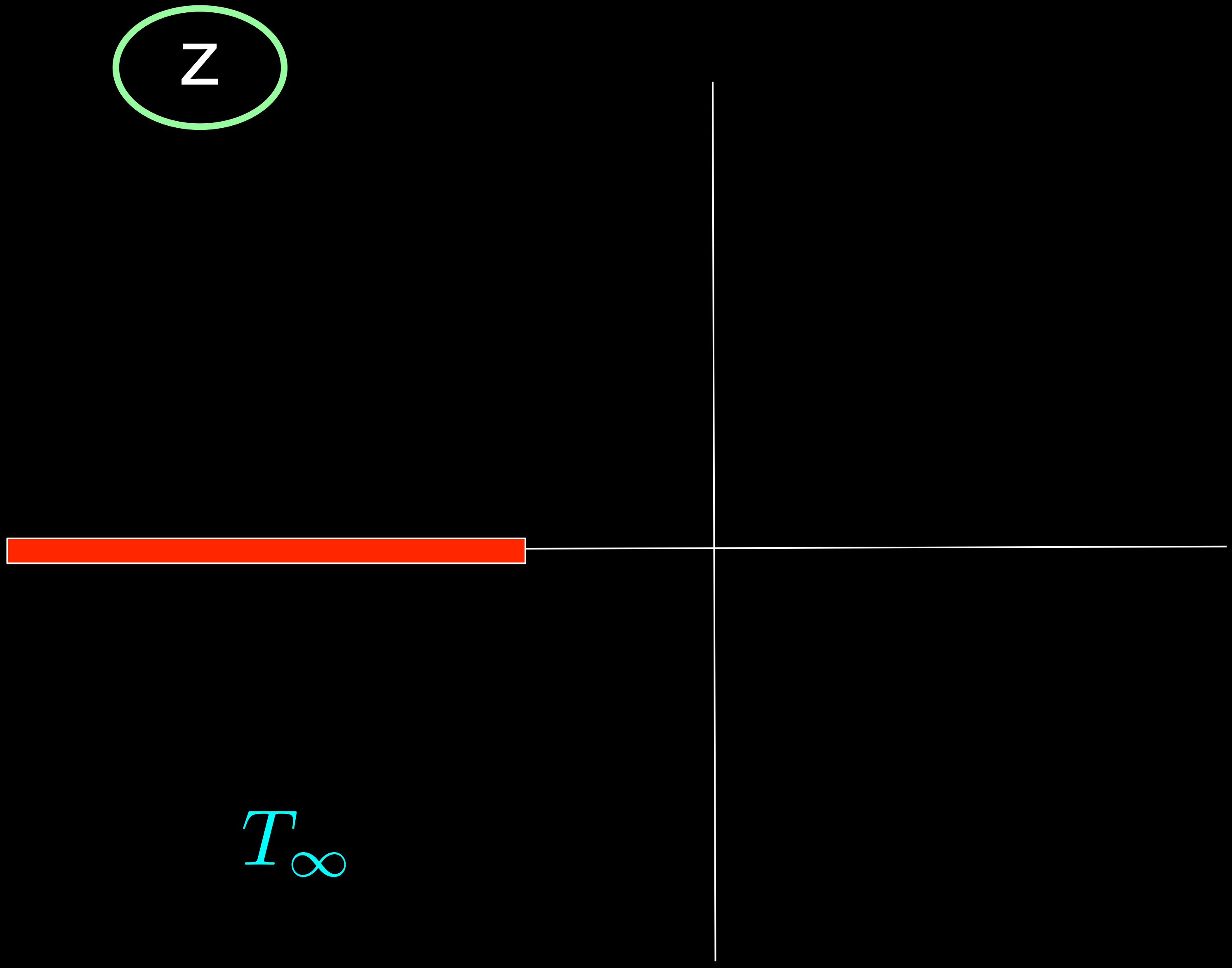
How these branch points move with temperature?

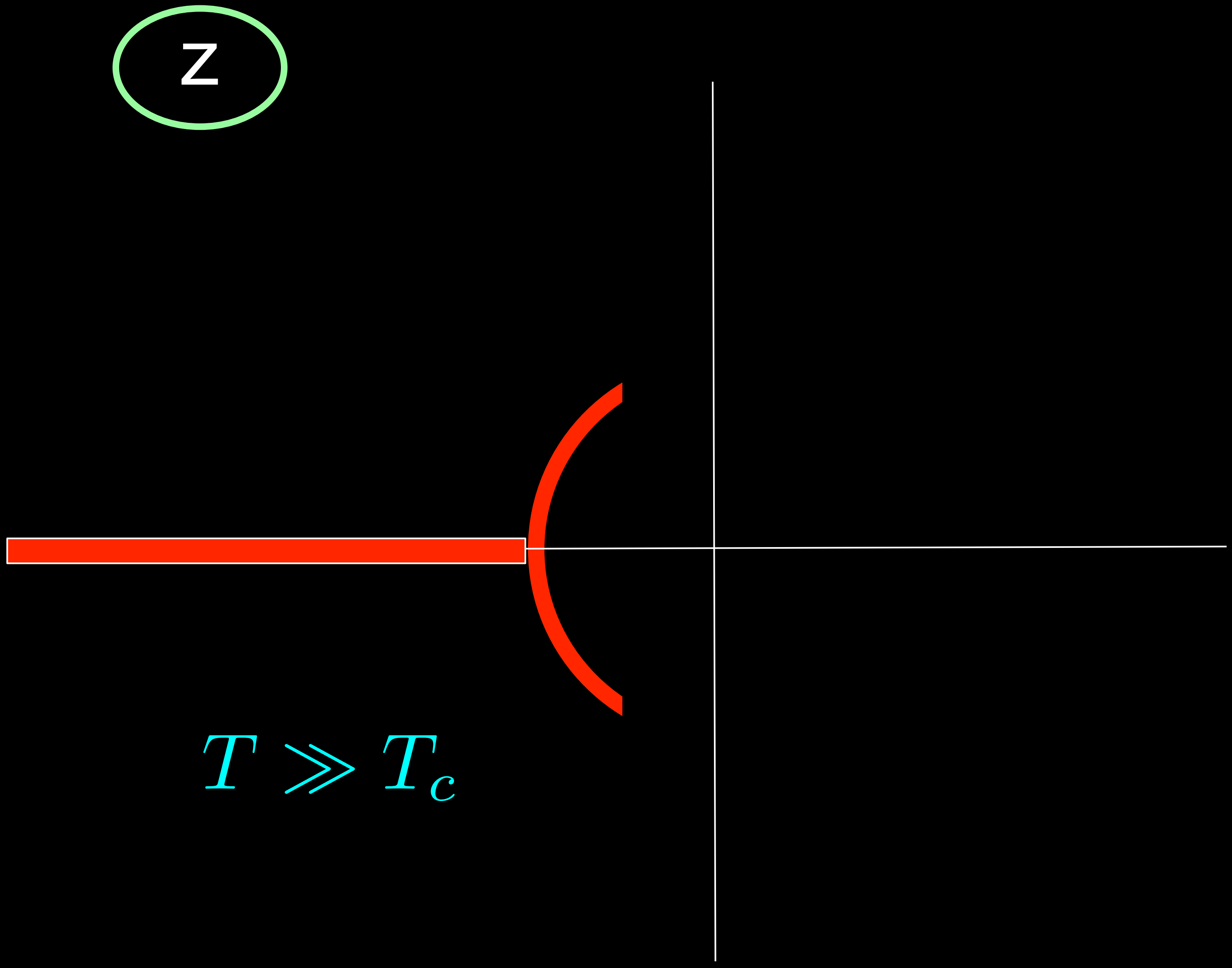


0.4
0.2
−0.2
−0.4
−0.4
−0.3
−0.2
−0.1
0.1
0.2

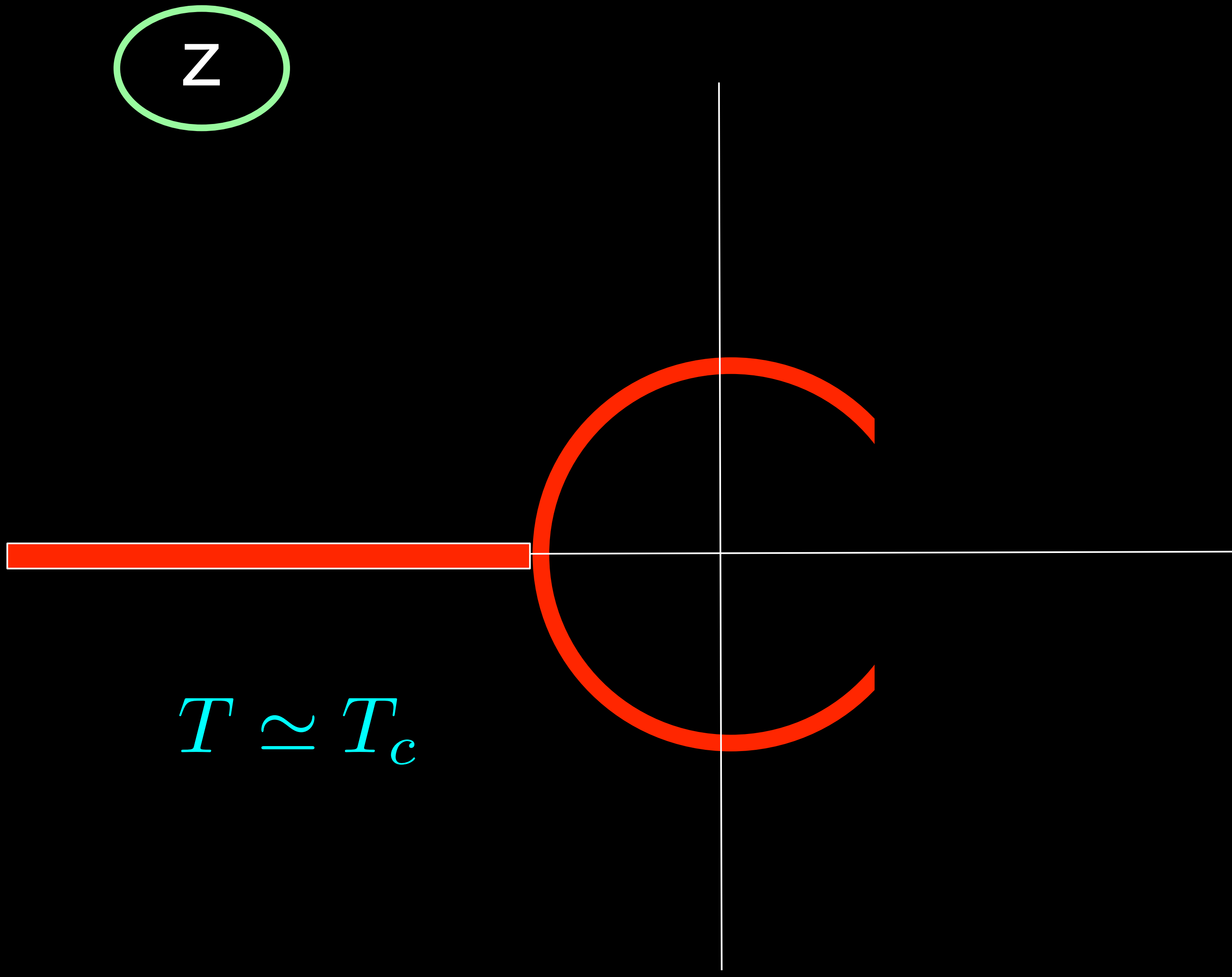


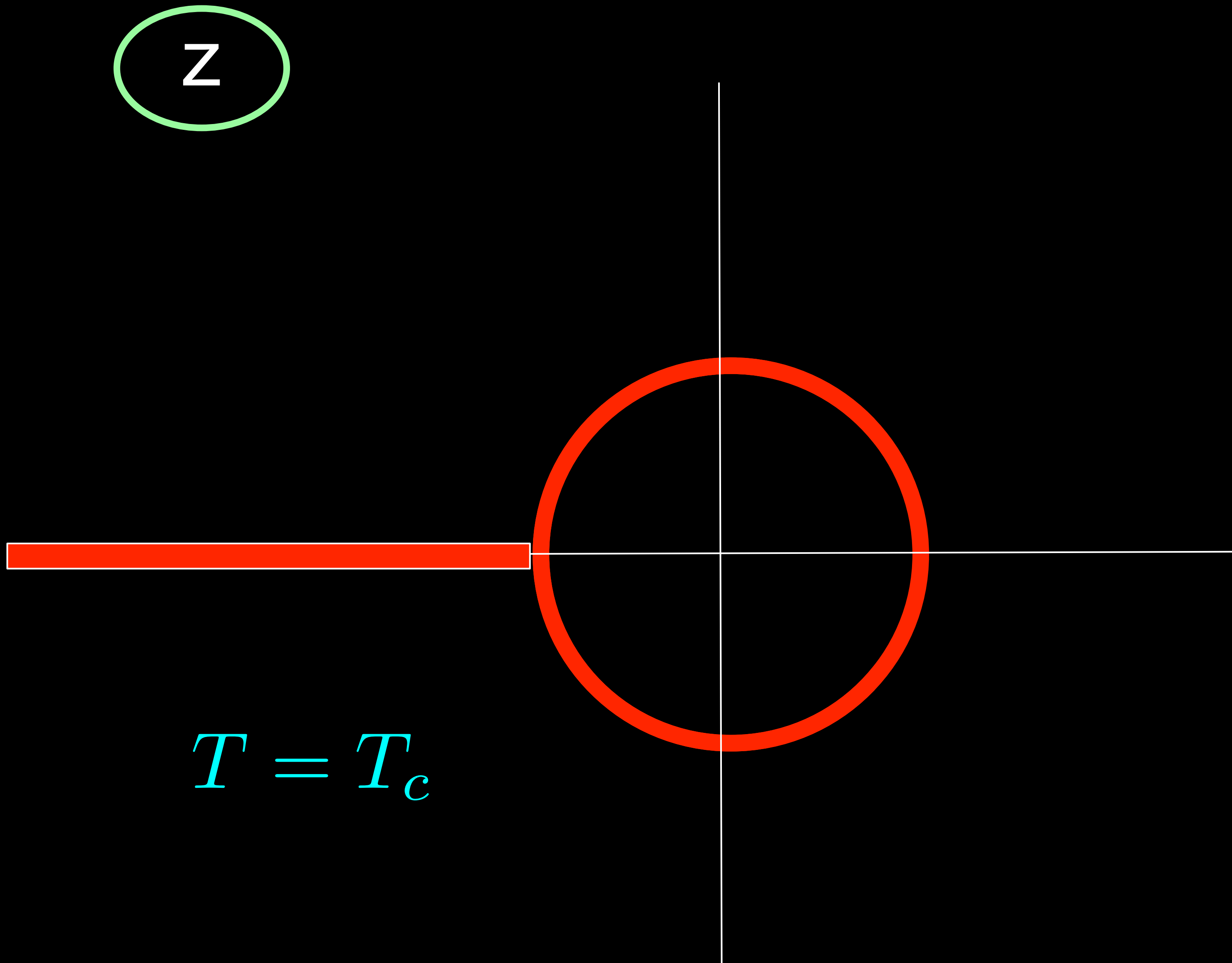
10 T_c
100 T_c
T_∞
100 T_c
10 T_c
2 T_c
T_c
2 T_c
0.4
0.2
−0.2
−0.3
−0.2
−0.1
0.2


z
T_∞

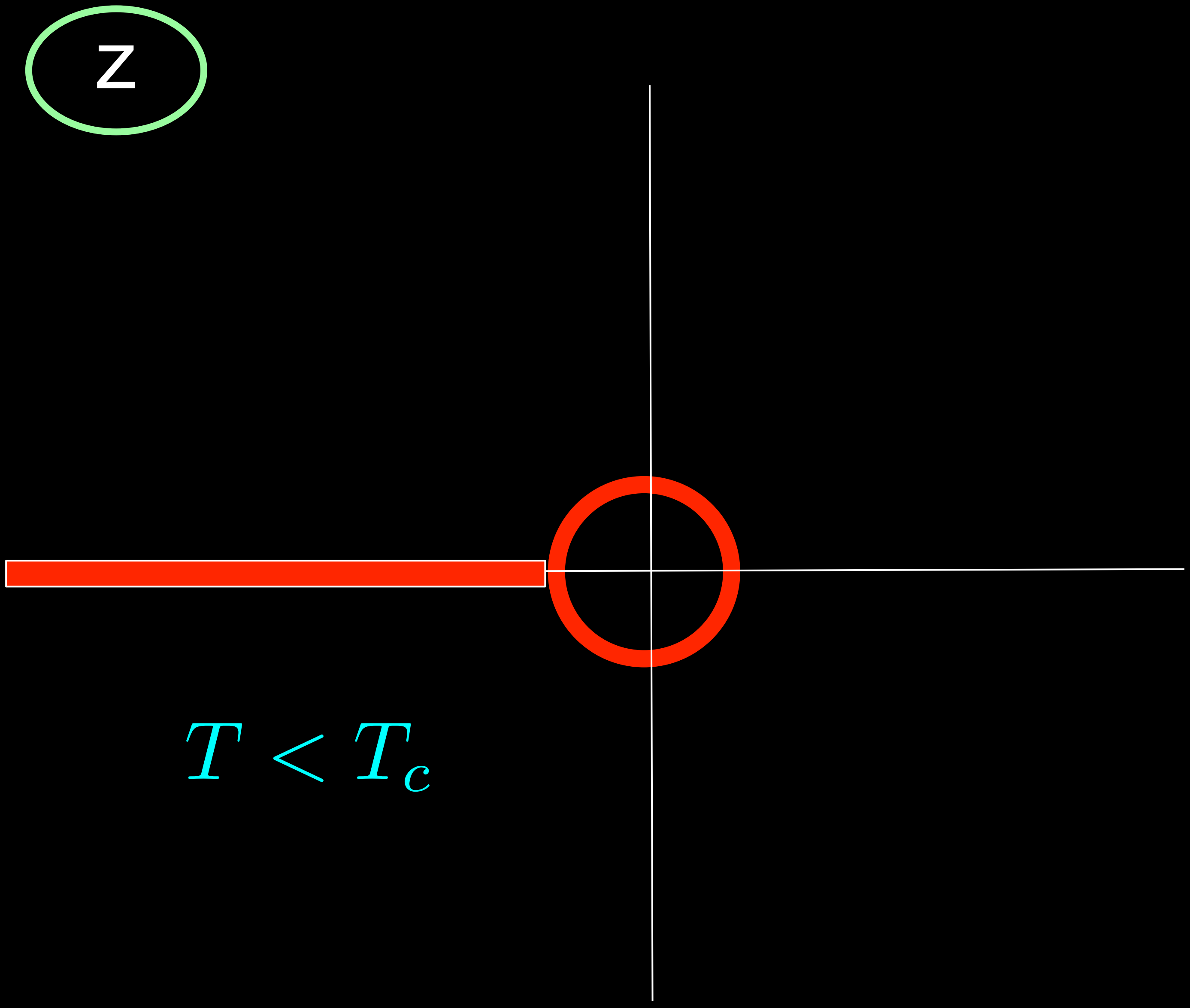


z
$T \gg T_c$

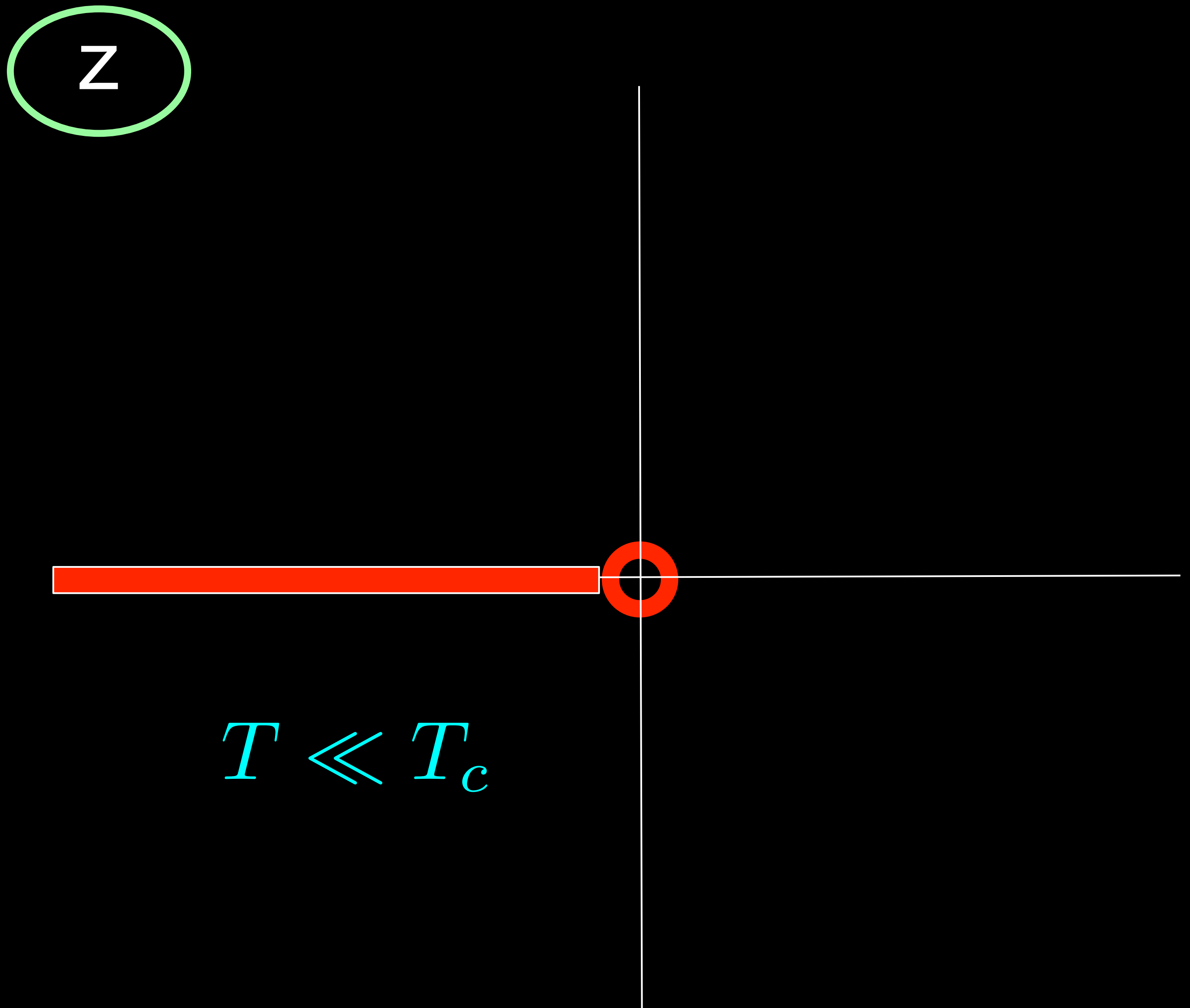

z
$T \simeq T_c$



$$T = T_c$$



$T < T_c$

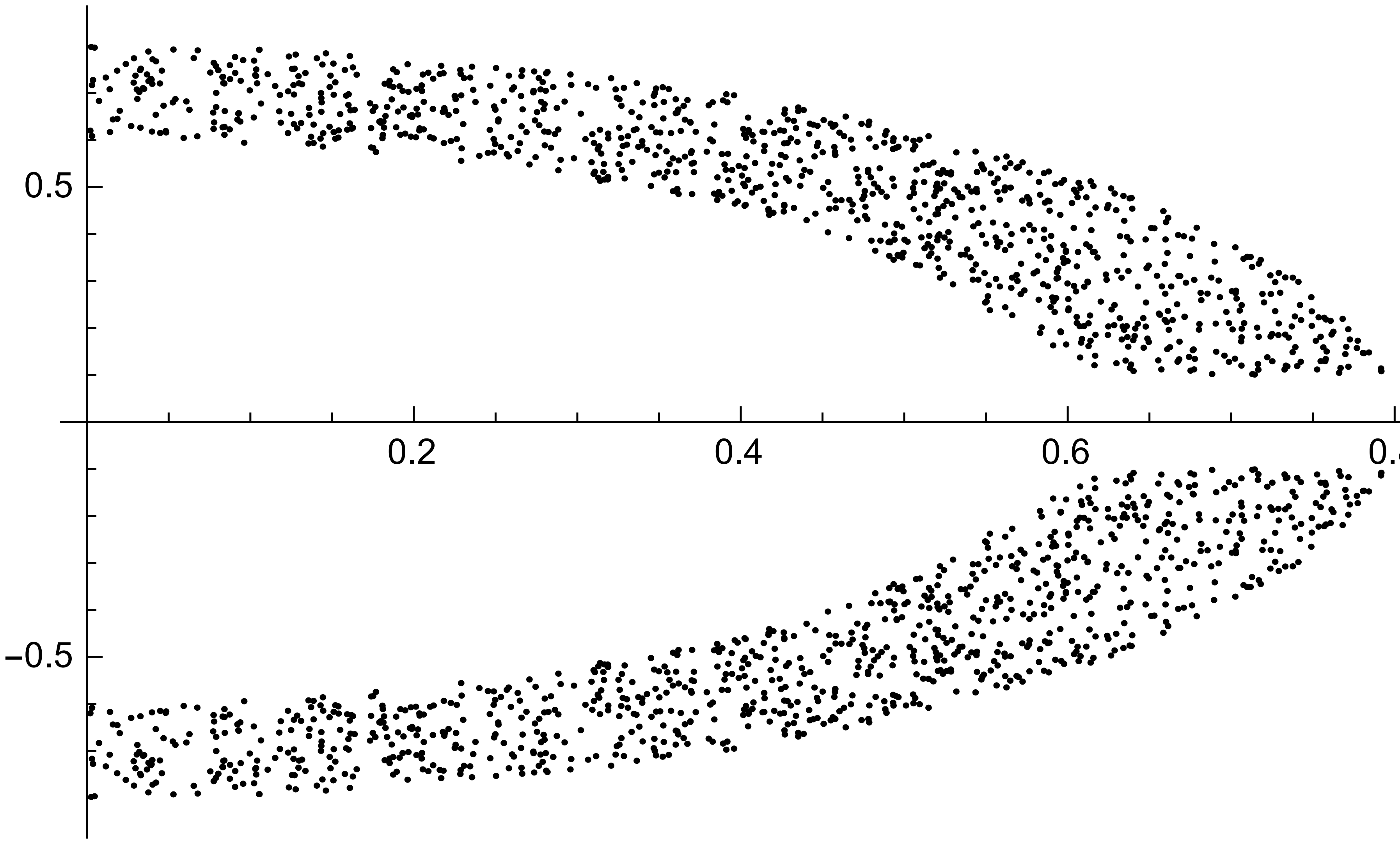

Z
$T \ll T_c$

Yang-Lee zeros are associated to positive charge distribution of electrostatics

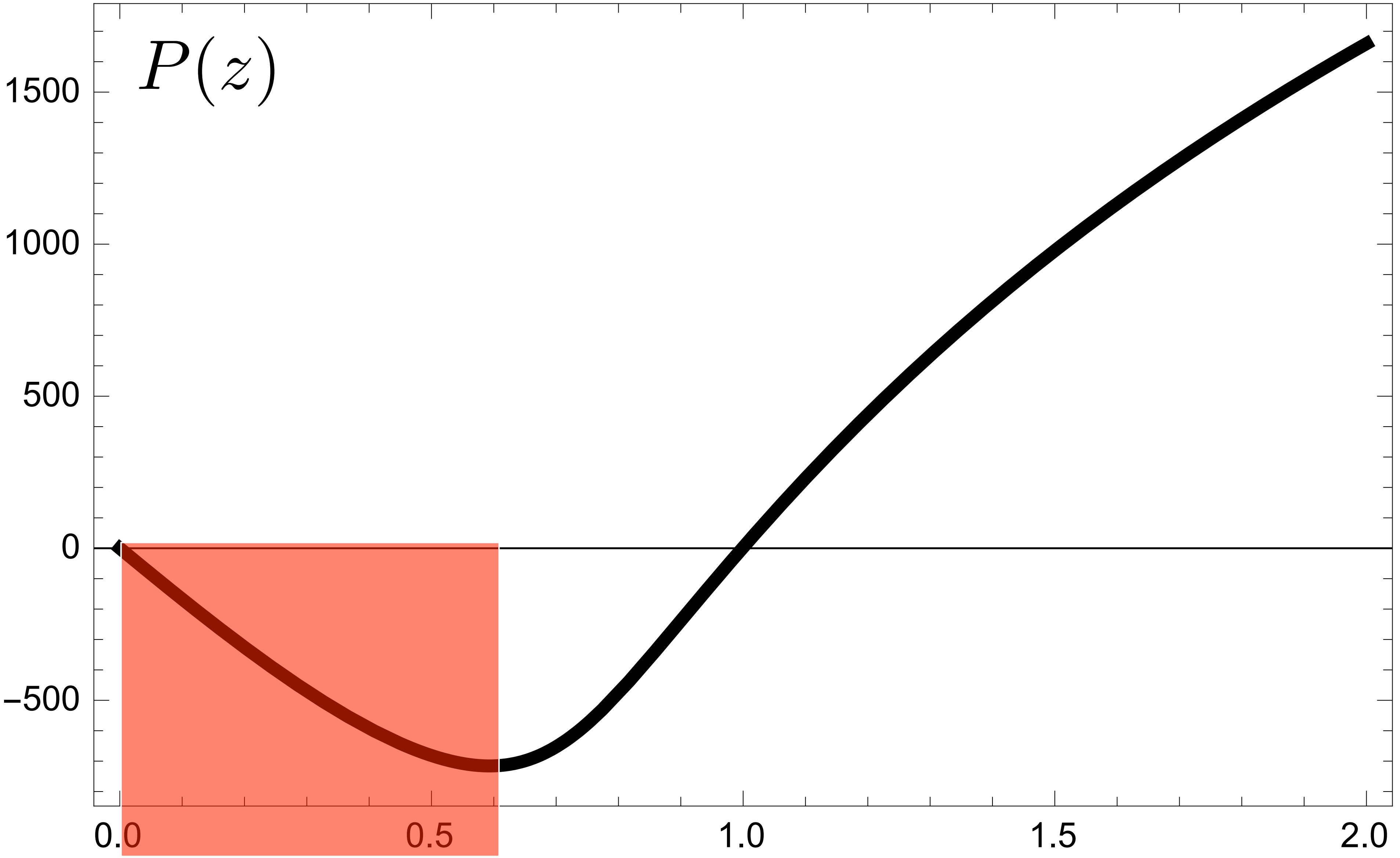
But, is any (positive) charge distribution of electrostatics

good

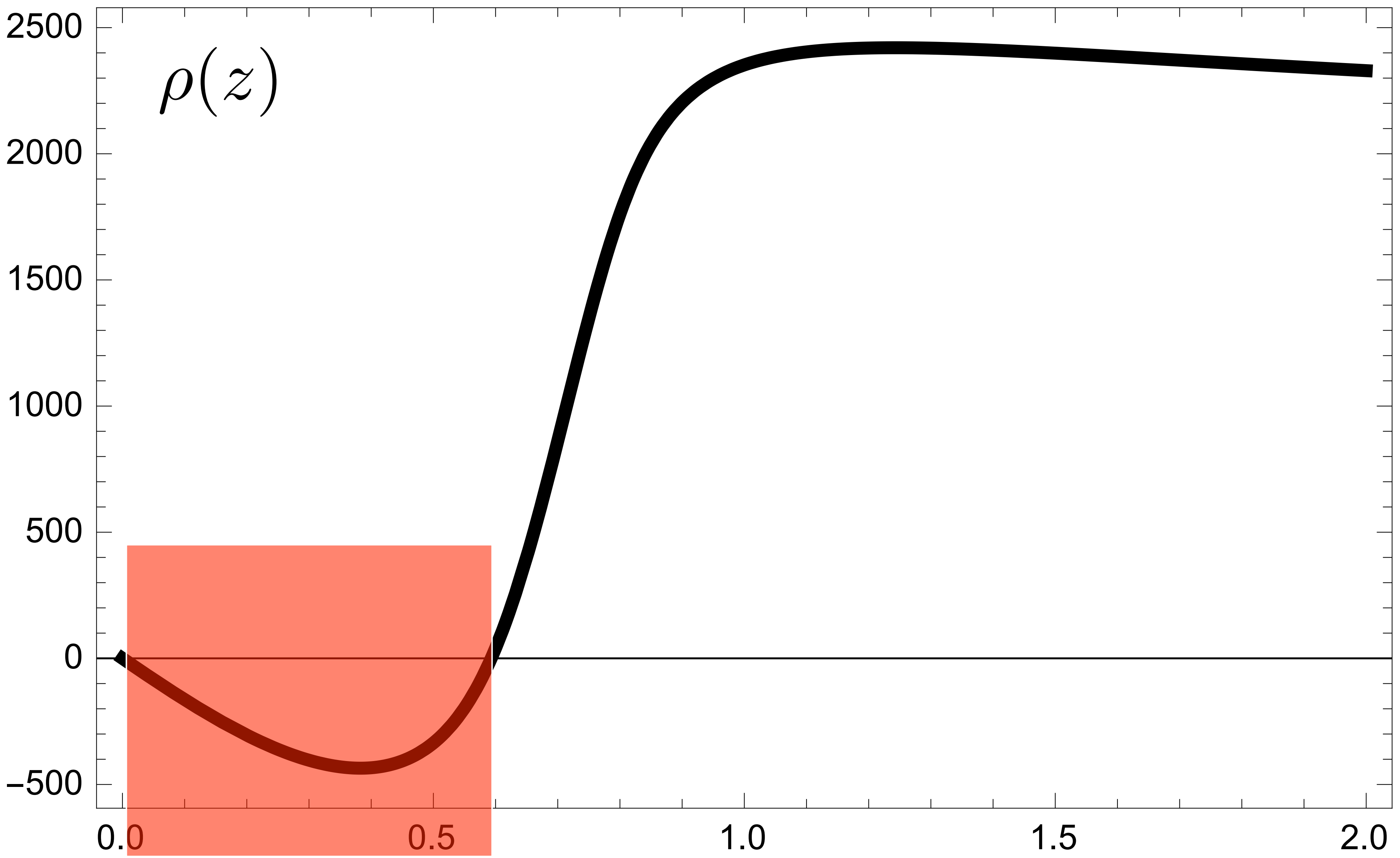
for a statistical physics interpretation?



0.5
0.2
0.4
0.6
0.8
−0.5



$P(z)$
1500
1000
500
0
−500
0.0
0.5
1.0
1.5
2.0



ρ(z)
2500
2000
1500
1000
500
0
−500
0.0
0.5
1.0
1.5
2.0

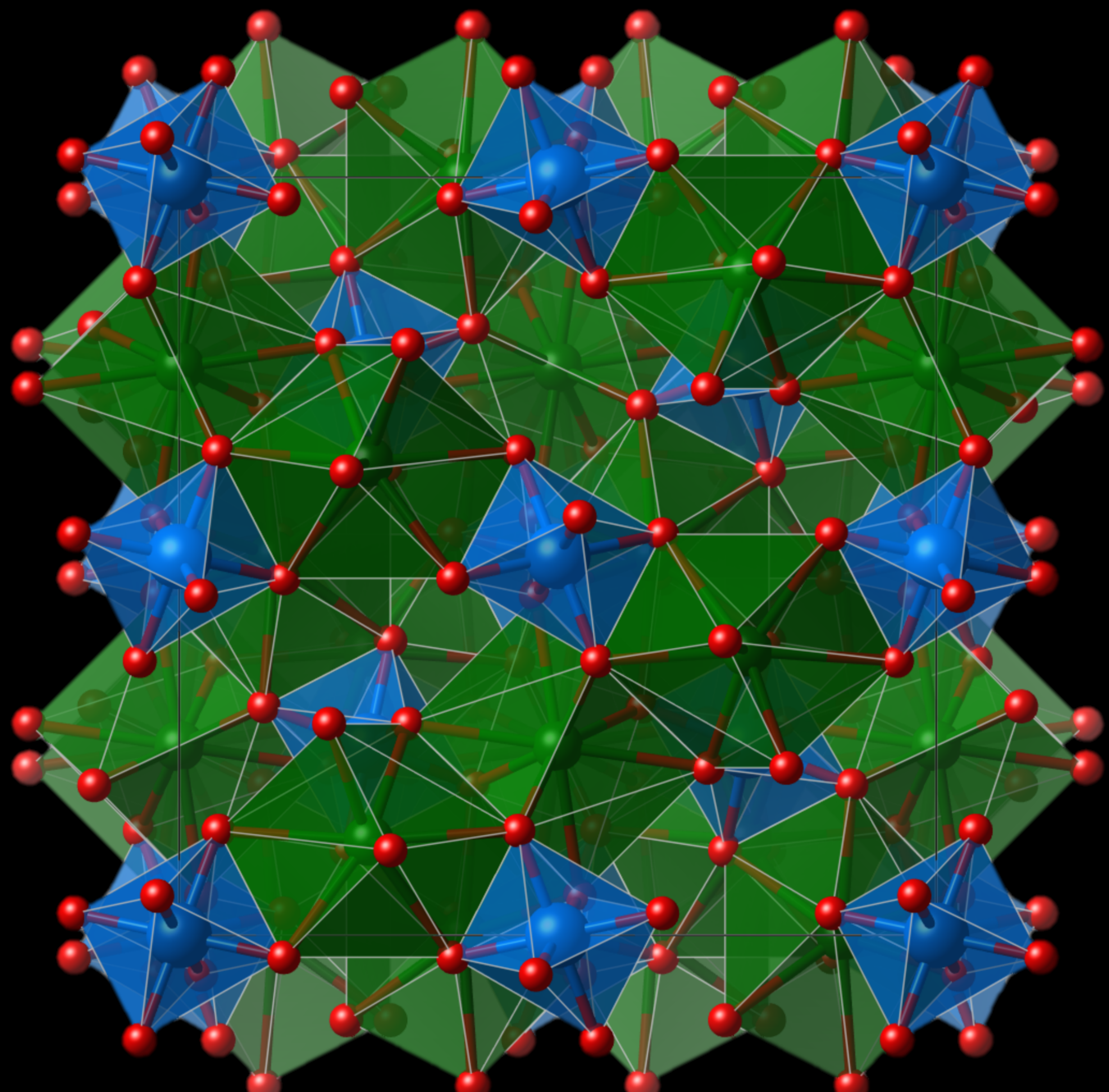
“Yang-Lee Inverse Problem”

Find which are the distributions of zeros which lead to physical statistical models

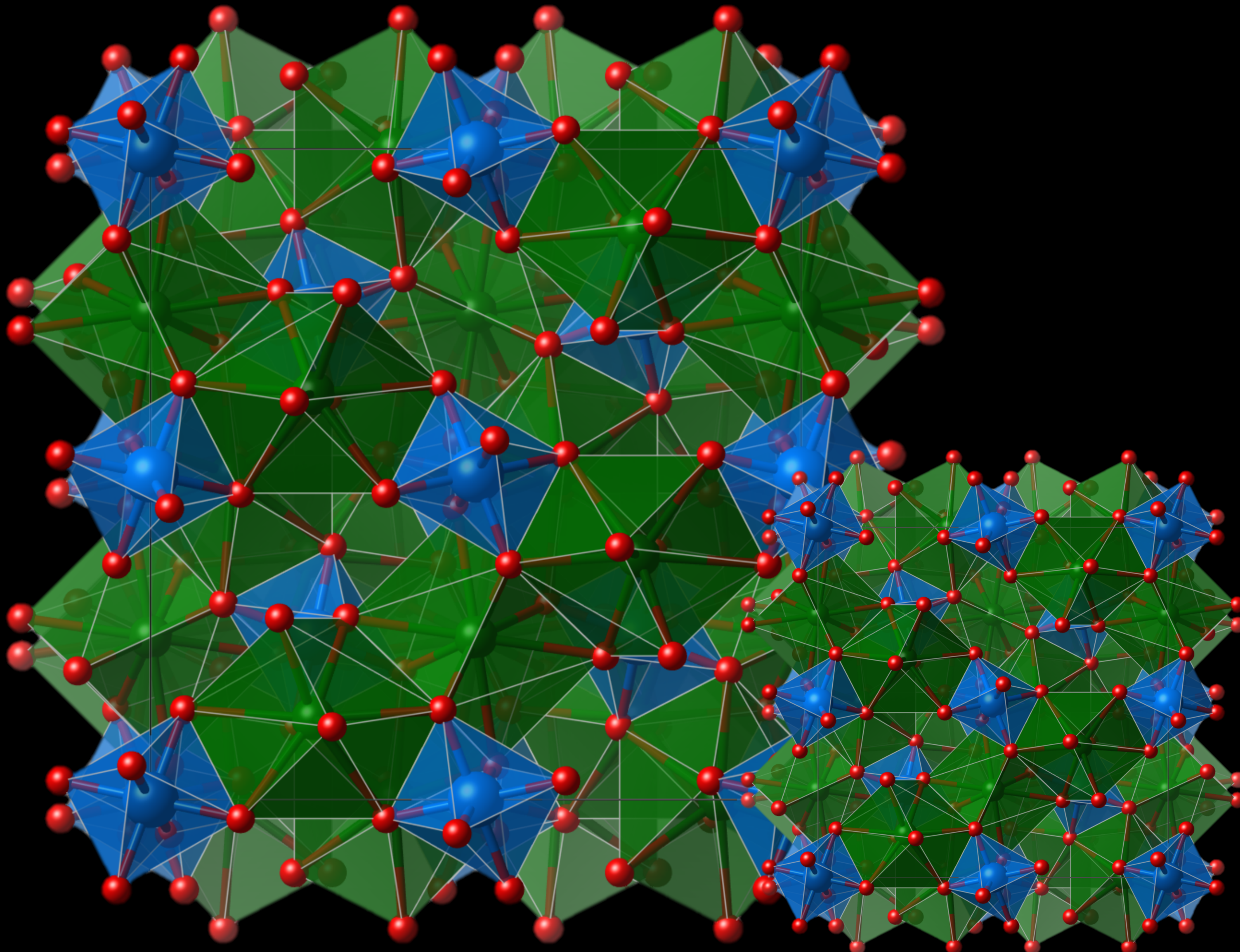
So far, the only case where we can pin down such distributions of zeros is when the zeros are located

on a CIRCLE

Yang-Lee Zeros of the Ising model



Yang-Lee Zeros of the Ising model



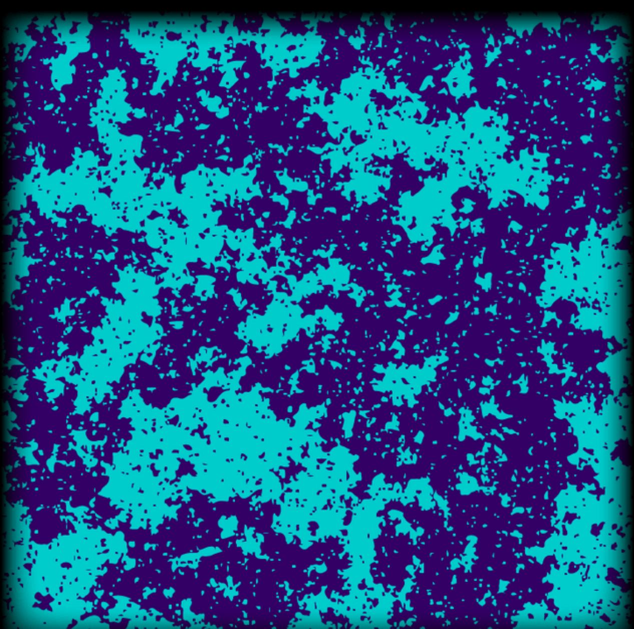
Yang-Lee Zeros of the Ising model

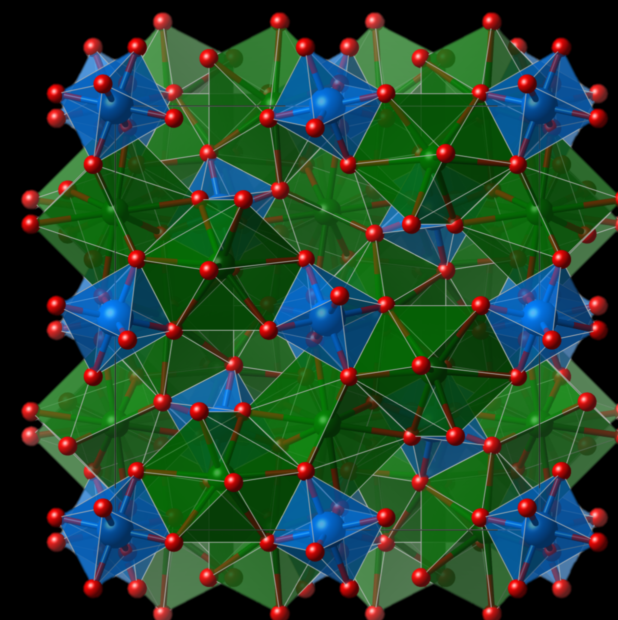
$$H = -\sum_{i,j} \sigma_i \sigma_j - B \sum_i \sigma_i$$

$$\Omega_N(\beta, B) = \sum_{\{\sigma_i\}} e^{-\beta H}$$

$$= \sum_{k=0}^{N} P_k \, z^k$$

$$z = e^{-2\beta B}$$





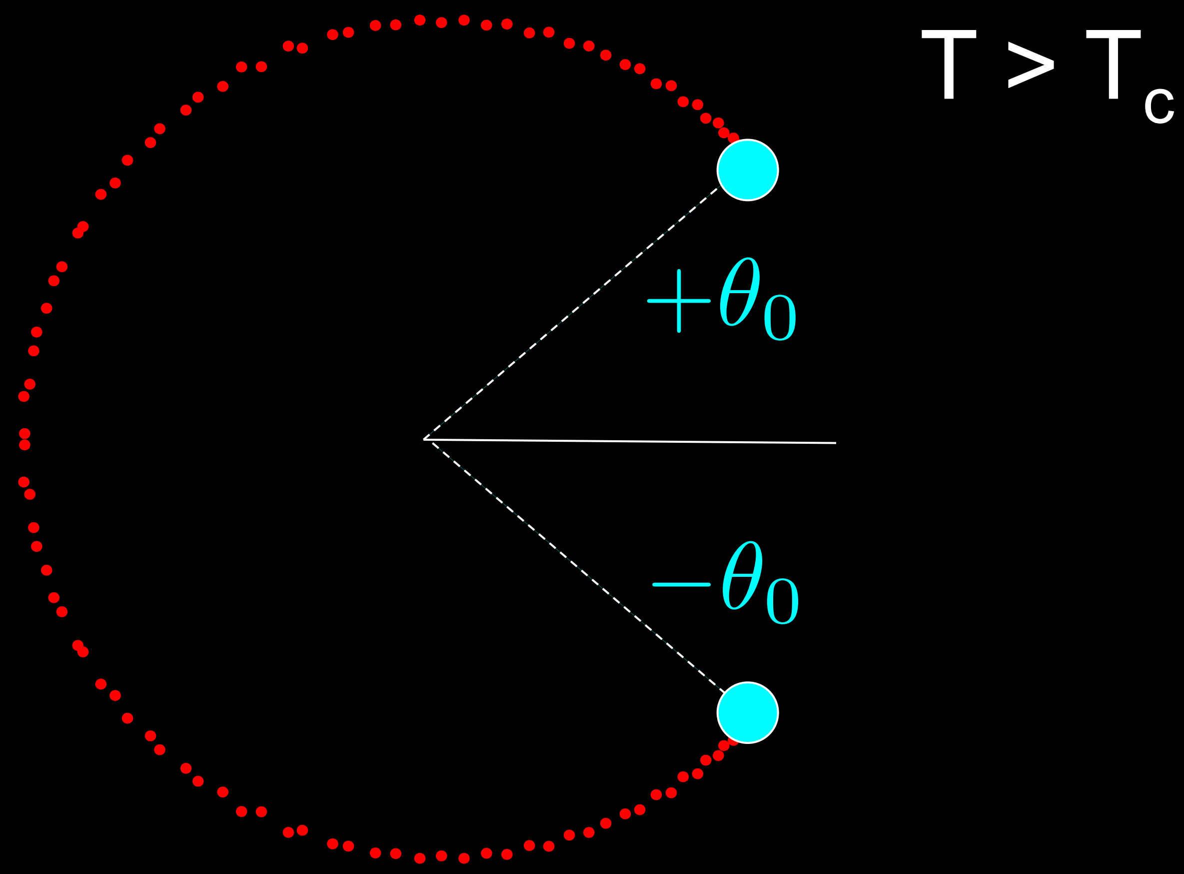
Palindrome polynomial

$$\Omega_N(z) = 1 + P_1\, z + P_2 z^2 + \cdots + P_2\, z^{N-2} + P_1\, z^{N-1} + z^N$$

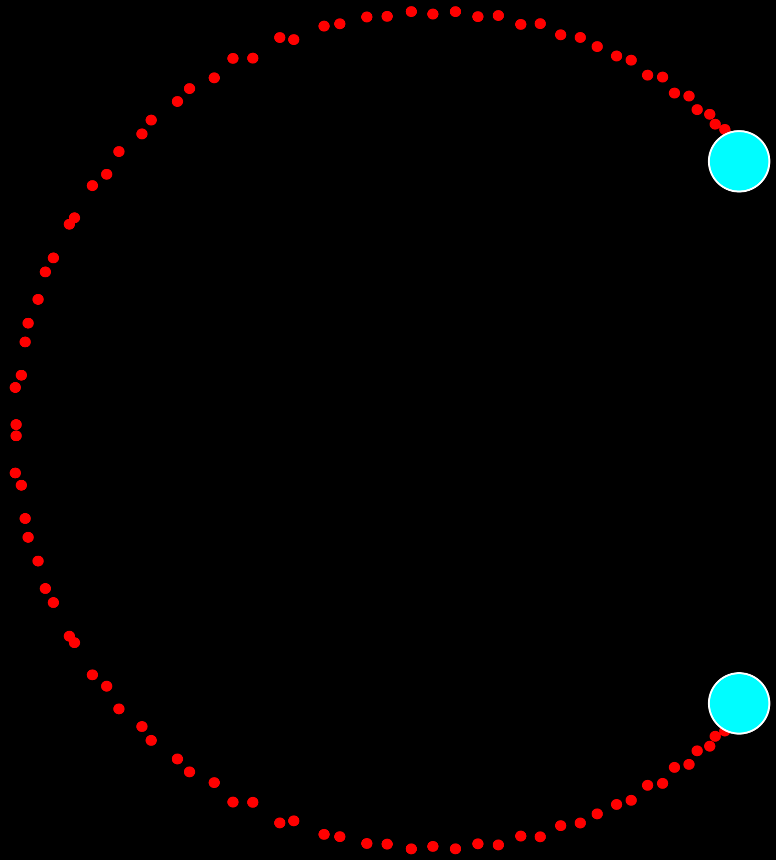
$$P_k = P_{N-k}$$

If z_a is a root, also $1/z_a$ is also a root !

Lee-Yang Zeros of the Ising model

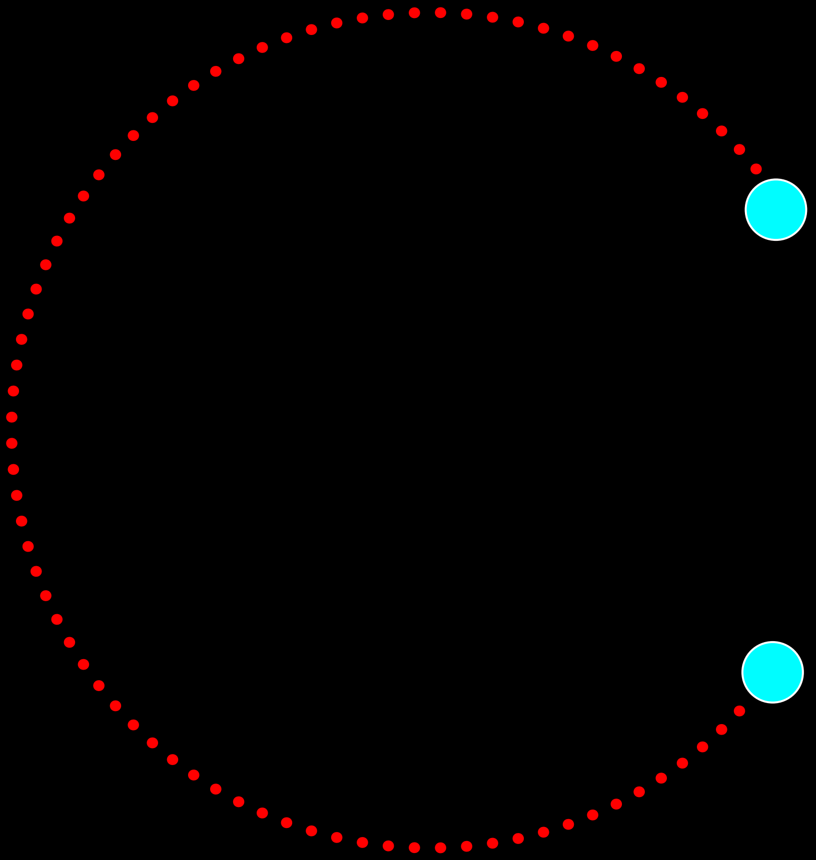


Lee-Yang Zeros of the Ising model

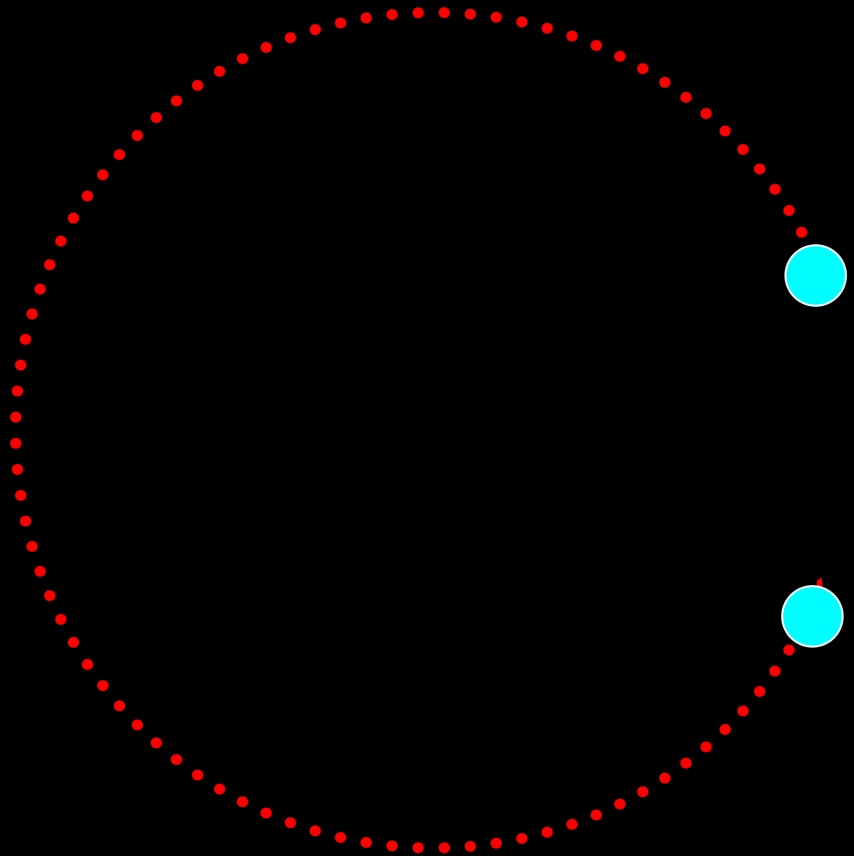


$T > T_c$

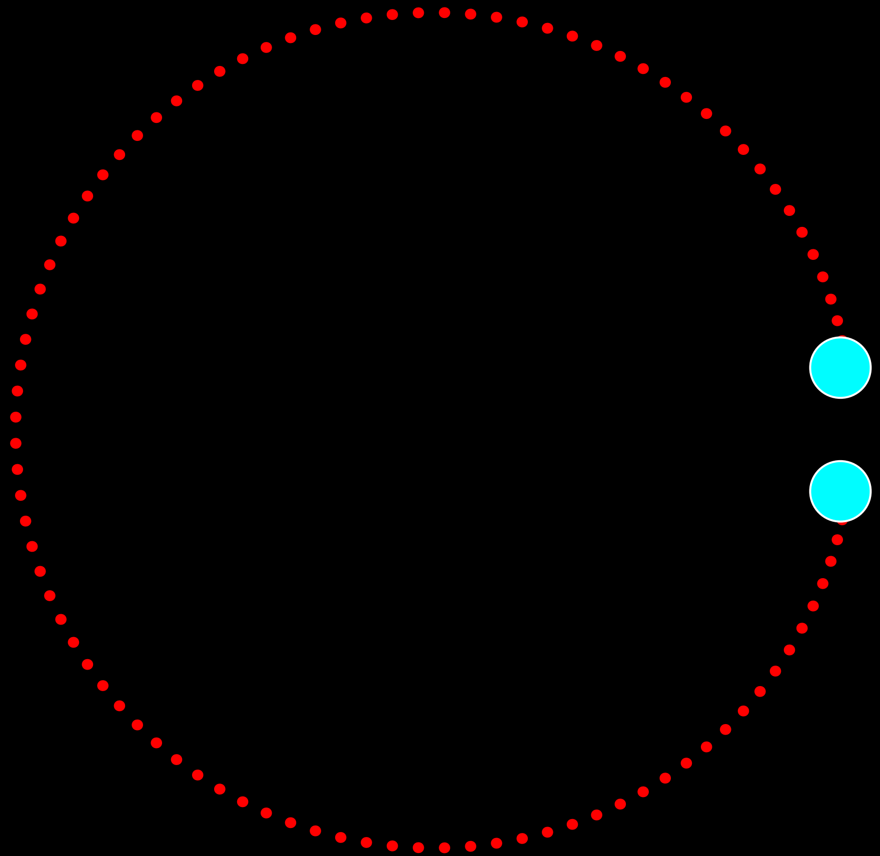
Lee-Yang Zeros of the Ising model



Lee-Yang Zeros of the Ising model

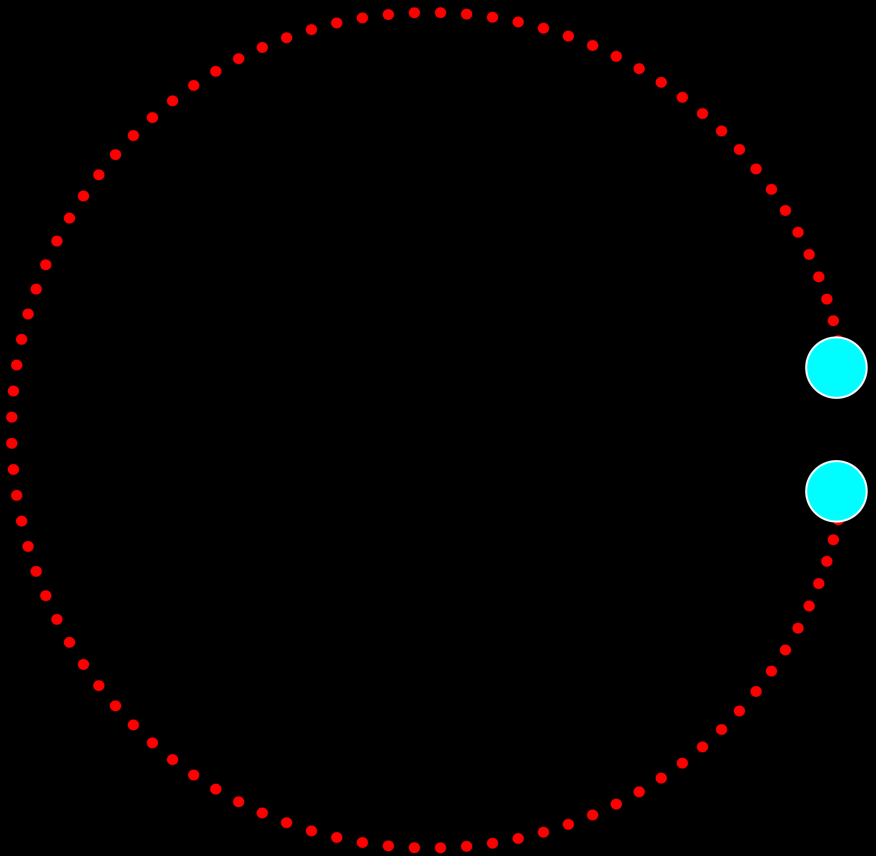


Lee-Yang Zeros of the Ising model

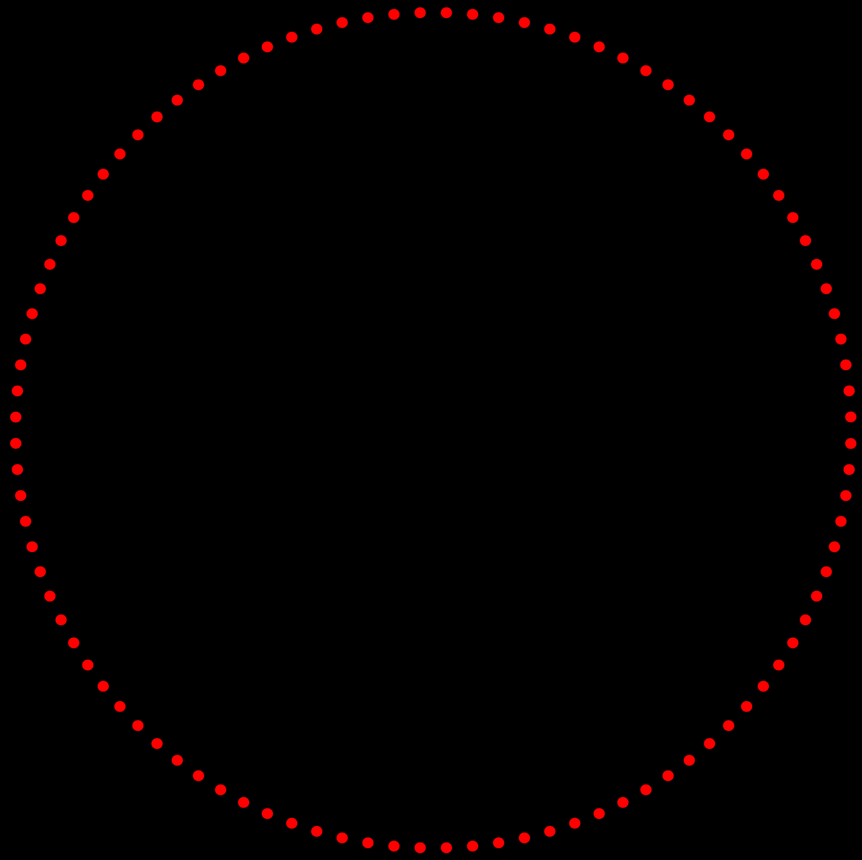


$T \approx T_c$

Yang-Lee Zeros of the Ising model



Lee-Yang Zeros of the Ising model



$T < T_c$

General features

- This pattern emerges only for ferromagnetic couplings
- The spreading of the zeros is due to interaction

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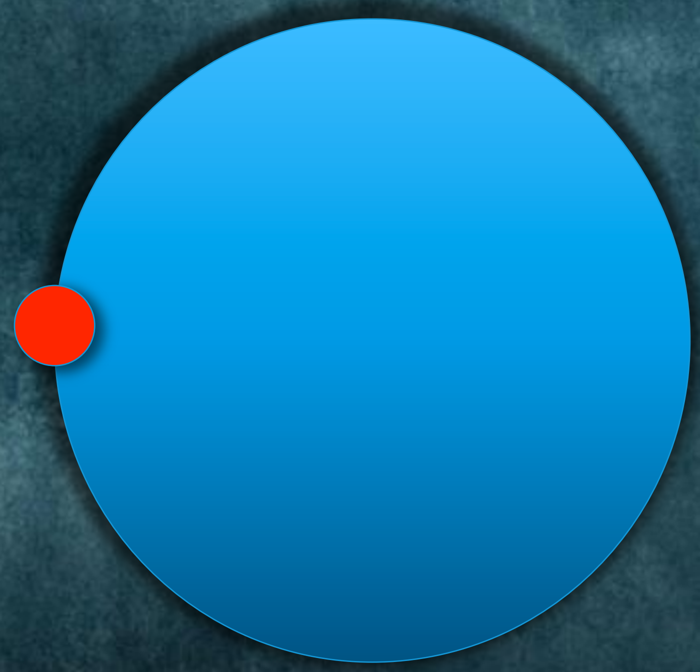

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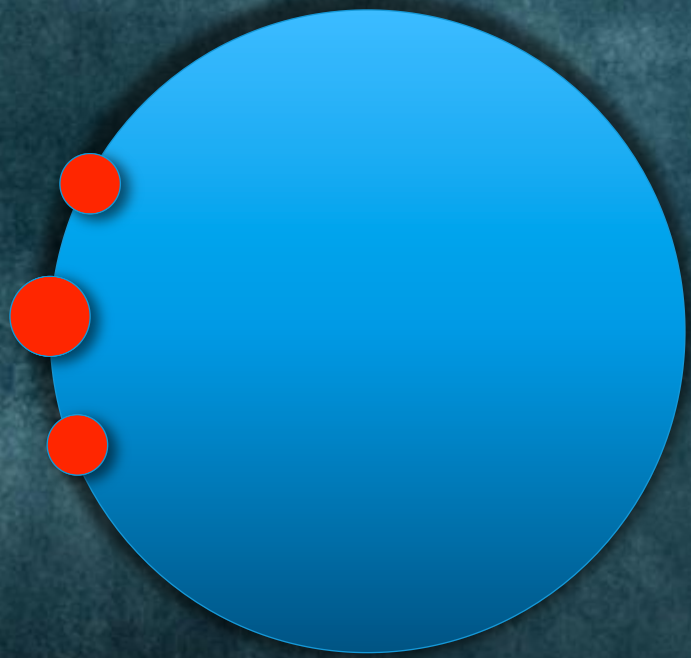

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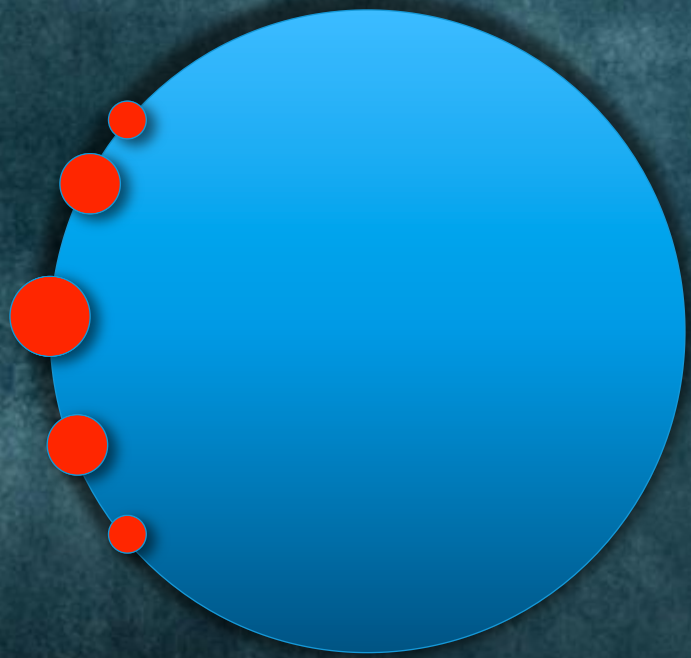

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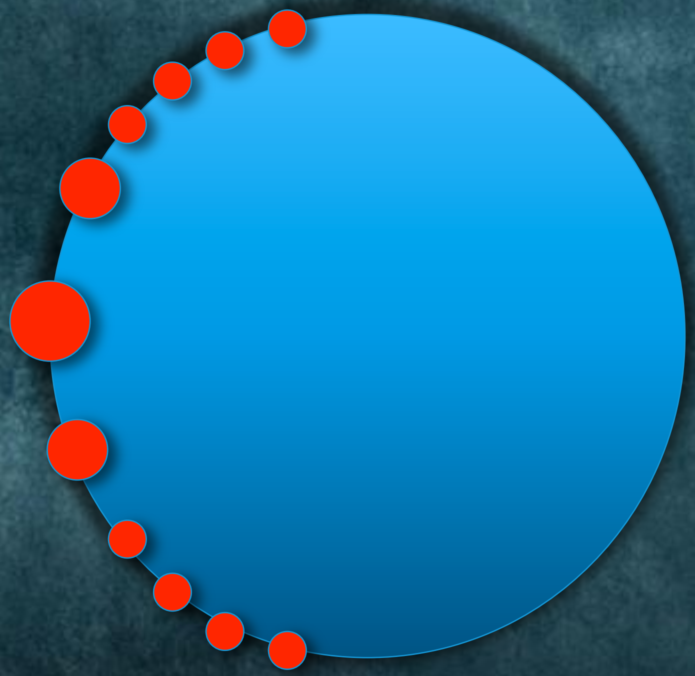


General features

- This pattern emerges only for ferromagnetic couplings
- The spreading of the zeros is due to interaction
- The only known analytic distribution of zeros: in 1-d!

$$\eta(\theta) = \frac{1}{2\pi} \frac{\sin\frac{\theta}{2}}{\sqrt{\sin^2\frac{\theta}{2} - \sin^2\frac{\theta_0}{2}}}$$

$$\theta_0 = \arccos\left(1 - 2e^{-2\beta J}\right)$$

General features

- This pattern emerges only for ferromagnetic couplings
- The spreading of the zeros is due to interaction
- The only known analytic distribution of zeros: in 1-d!
- Knowing $\eta(\theta)$, we will get the magnetization at finite temperature and in a magnetic field

$$M = 1 - 4z \int_0^{\pi} \eta(\theta) \, \frac{z - \cos\theta}{z^2 - 2z\cos\theta + 1} \, d\theta$$

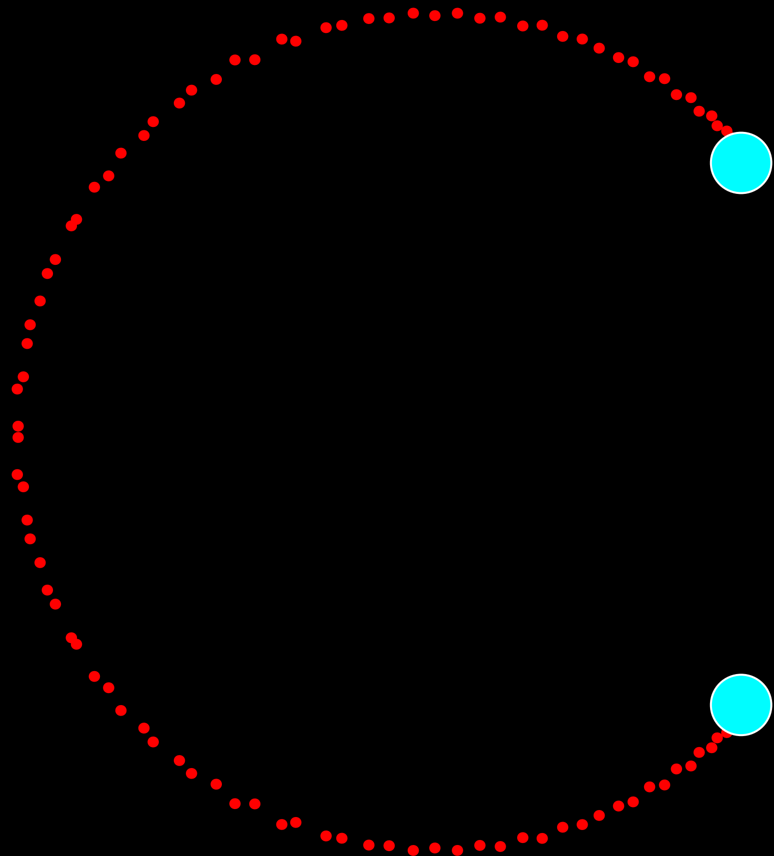
General features

- It is possible to prove that any η(θ), with η'(θ) >0, may lead to a new physical statistical system!

$$\frac{d\rho}{dz} = \int_0^{\pi} \frac{\xi\, \eta'(2\arctan\xi)}{(1+\xi)^2((z+1)^2\xi^2+(z-1)^2} d\xi \quad > 0$$

- Edge singularities and Yang-Lee model

Edge Singularities



$T > T_c$

The density of zeros is anomalous nearby the edge singularities

$$\eta(\theta) \simeq |\theta - \theta_0|^\sigma$$

Edge Singularities

For all purposes, this anomalous behaviour

$$\eta(\theta) \simeq |\theta - \theta_0|^\sigma$$

can be seen as a critical phenomena

P.J. Kortman and R.B. Griffiths, Phys. Rev. Lett. 27, 1439 (1971).

What is then the Landau-Ginzburg theory which describes it?

Yang-Lee Model

M. E. Fisher, Phys. Rev. Lett. 40, 1610 (1978).

$$\mathcal{A} = \int d^d x \left[\frac{1}{2}(\partial\phi)^2 + i(h - h_0)\phi + ig\,\phi^3 \right]$$

- Such a QFT is NOT hermitian
- However it is a CP invariant theory
- The spectrum is then real

$$(CP)\,\phi\,(CP) = -\phi \qquad (CP)\,\mathcal{A}\,(CP) = \mathcal{A}^\dagger$$

- Upper critical dimension d = 6

Yang-Lee Model

Exact solution in d=2

- At criticality ($h = h_0$), it is described by the simplest CFT

J.Cardy, Phys. Rev. Lett. 54, 1354 (1985).

1	Φ	Φ	1
0	$-1/5$	$-1/5$	0

$$\Phi * \Phi = 1 + \Phi \qquad C = -\frac{22}{5}$$

Yang-Lee Model

Exact solution in d=2

- At criticality ($h = h_0$), it is described by the simplest CFT

- Away from criticality, the simplest integrable QFT

G. Mussardo, J.Cardy, Phys. Lett. 225, 275 (1989).

Integrable QFT: infinite conserved charges

(A.B. Zamolololodchikov)

$$\partial_\mu T^{\mu\nu\rho\cdots} = 0 \qquad Q^s = \int dx\, T^{0\nu\rho\cdots}$$

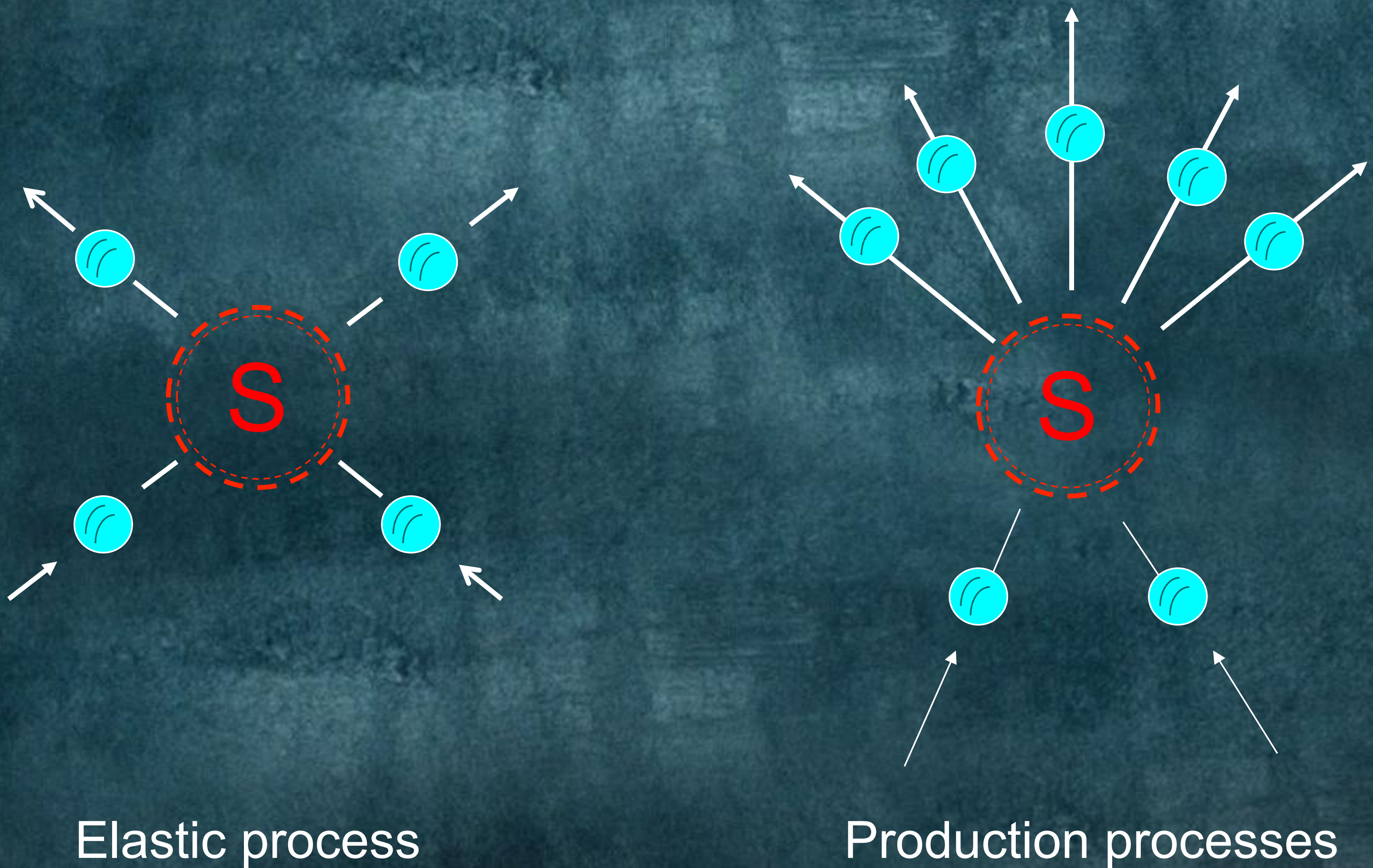
$$[H, Q^s] = 0$$

$$Q^s\, |p_1, p_2, \cdots p_N > = \sum_{k=1}^{N} p_k^s\, |p_1, p_2, \cdots p_N >$$

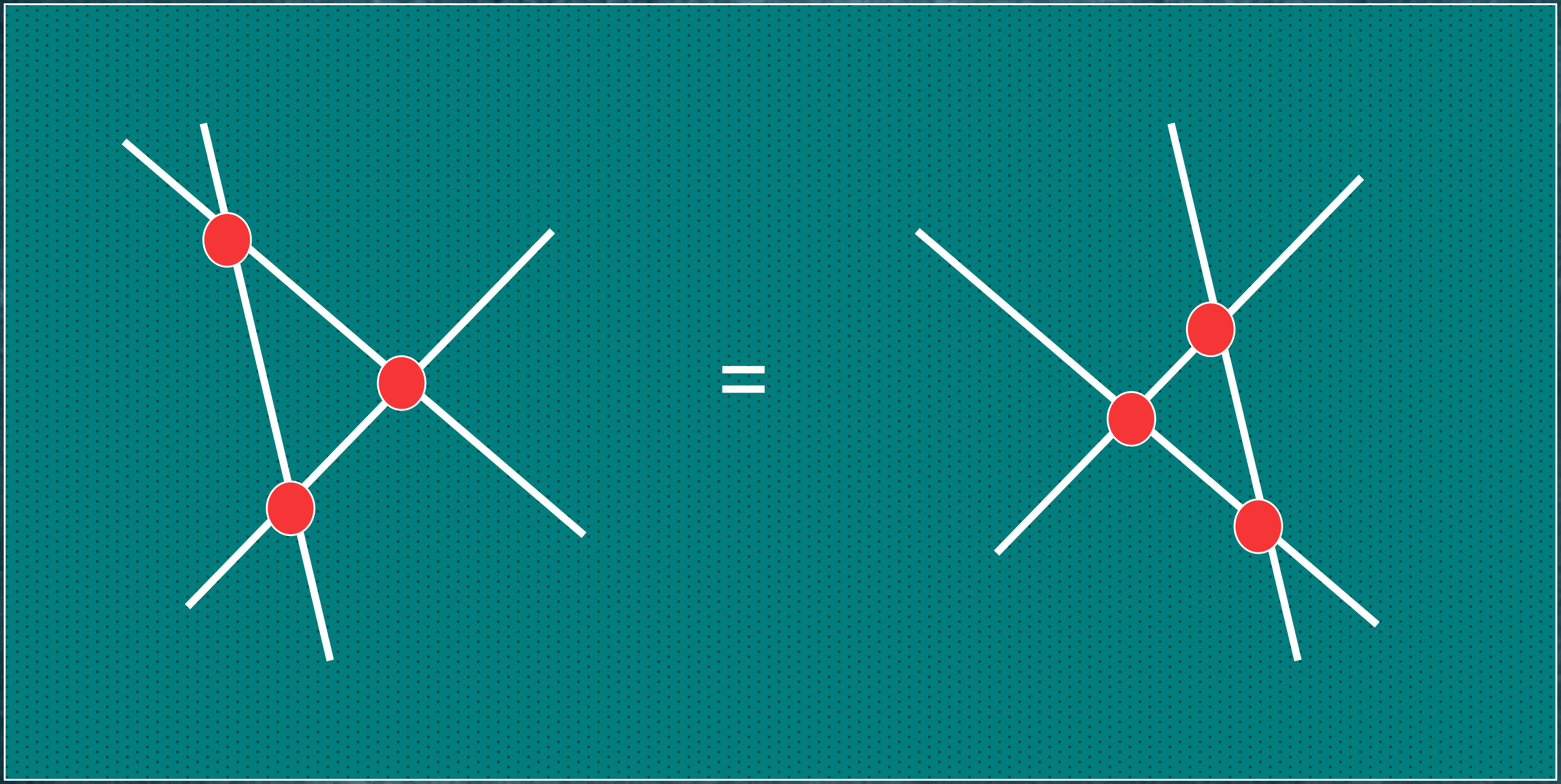
Since these charges are conserved, we have infinite constraints

$$\sum_{in} p_i^s = \sum_{out} p_l^s$$

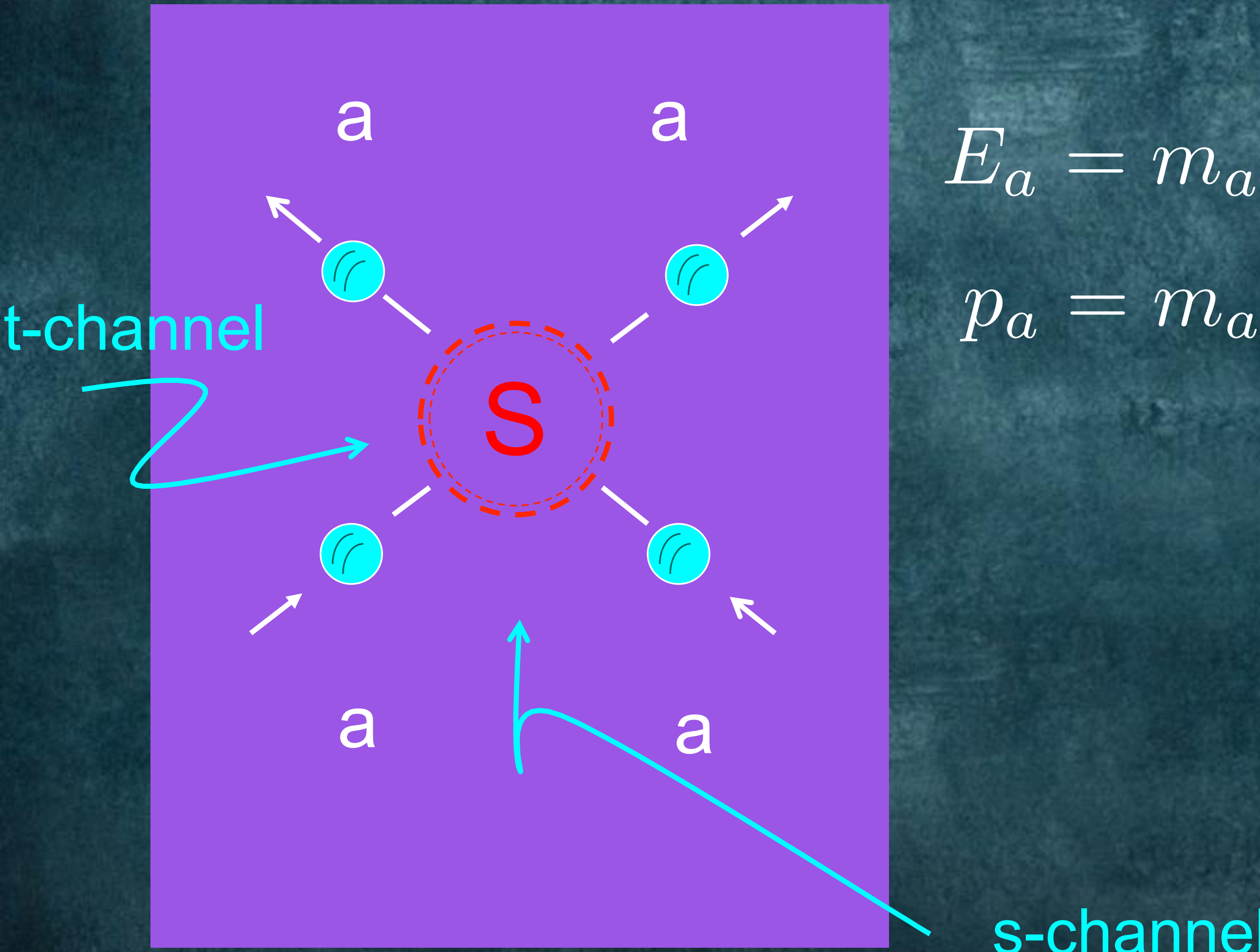
Integrable vs NonIntegrable QFT



Factorization and Yang-Baxter Equations



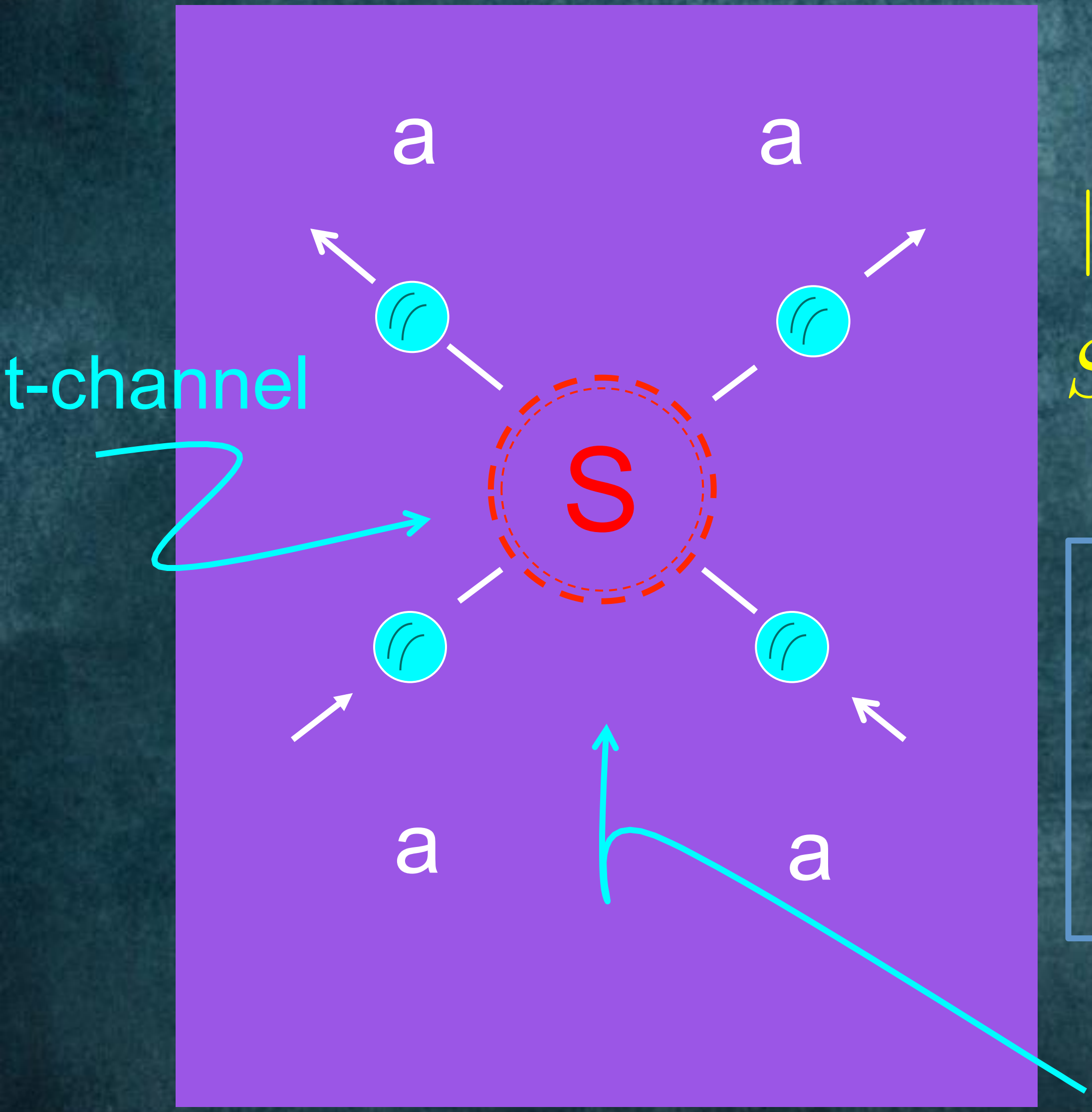
Two-body S-matrix



$$E_a = m_a \cosh \theta_a$$

$$p_a = m_a \sinh \theta_a$$

Two-body S-matrix



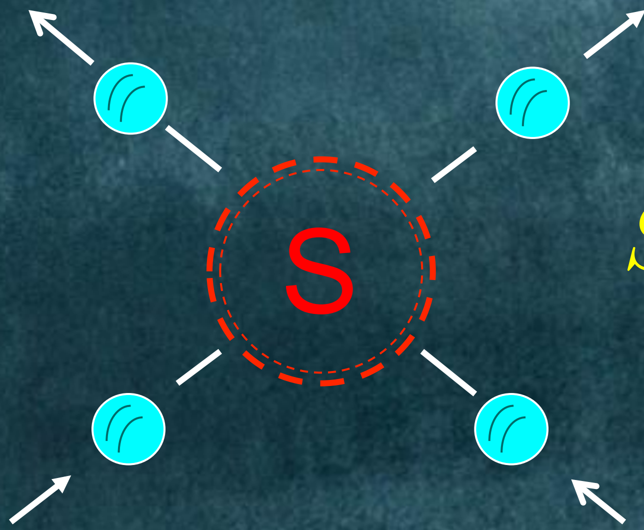
$$|A(\theta_1)\,A(\theta_2)\rangle \;=\; S(\theta_1-\theta_2)\,|A(\theta_2)\,A(\theta_1)\rangle$$

$$S(\theta)\,S(-\theta) \;=\; 1$$

$$S(\theta) \;=\; S(i\pi-\theta)$$

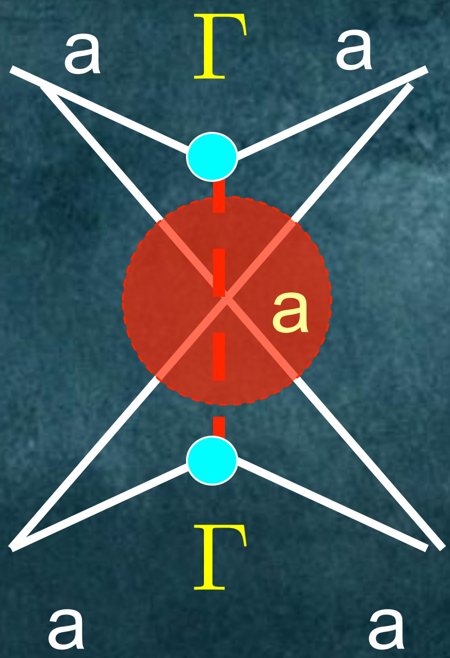
Exact S-matrix of the Yang-Lee model

G. Mussardo, J.Cardy, Phys. Lett. 225, 275 (1989).



$$S_{YL}(\theta) = \frac{\tanh\frac{1}{2}\left(\theta + \frac{2\pi i}{3}\right)}{\tanh\frac{1}{2}\left(\theta - \frac{2\pi i}{3}\right)}$$

The particle A is bound state of itself



$$S(\theta) \;=\; i\,\frac{\Gamma^2}{\theta - i\frac{2\pi}{3}}$$

$$m_b^2 = s\left(\frac{2\pi i}{3}\right) = 4m^2\cos^2\left(\frac{\pi}{3}\right) = m_a^2$$

$$\Gamma^2 = (ih)^2 \;< 0$$

So, we would like to compute and study the pattern of Yang-Lee zeros in an integrable QFT such as the Yang-Lee model

(YL)^2 problem

Important Remark for QFT

The Grand Canonical Partition Function is a "weighted" counting

$$\Omega(z) = \sum_{N=0}^{\infty} \frac{1}{N!} Z_N \, z^N$$

But, for this reason, the variable N must have a "definite" meaning!

The corresponding operator must commute with the Hamiltonian

Example:

N= Number of particles or solitons (which must be conserved)

Important Remark for QFT

The Grand Canonical Partition Function is a "weighted" counting

$$\Omega(z) = \sum_{N=0}^{\infty} \frac{1}{N!} Z_N \, z^N$$

In the context of QFT, this remarks essentially points to

Integrable QFT

Let's go back to the problem of computing and studying

the pattern of Yang-Lee zeros

in the simplest integrable QFT given by the

Yang-Lee model

How to do it?

Exact Partition Function

This is given by Thermodynamics Bethe Ansatz

(Yang-Yang; Al.B. Zamolodchikov)

$$\Omega(z) \;=\; \exp\left[mL \int_{-\infty}^{+\infty} \cosh\theta \log\left(1 + z\, e^{-\epsilon(\theta,z)}\right) \frac{d\theta}{2\pi} \right]$$

$$\epsilon(\theta,z) \;=\; m\beta\, \cosh\theta - \int_{-\infty}^{\infty} \frac{d\theta'}{2\pi}\, \varphi(\theta-\theta')\, \log\left(1 + z\, e^{-\epsilon(\theta',z)}\right)$$

$$\varphi(\theta) \;=\; -i\, \frac{1}{S}\, \frac{dS}{d\theta}$$

Exact Partition Function

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(Al.B. Zamolodchikov)

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$$\varphi(\theta) \;=\; -i\,\frac{1}{S}\,\frac{dS}{d\theta}$$

Free Theories

$$\Omega(z) \;=\; e^{\pm \sum_p \log\left(1 \pm z\, e^{-\beta \epsilon_p}\right)} \equiv e^{F_\pm(z,\beta)}$$

$$F_\pm(z,\beta) = \pm \int d\epsilon\, g(\epsilon)\, \log\left(1 \pm z\, e^{-\beta\epsilon}\right)$$

$$= \frac{V}{\lambda_T^d} \sum_{k=1}^{\infty} (\mp 1)^{k+1} \frac{z^k}{k^{\frac{d}{2}+1}}$$

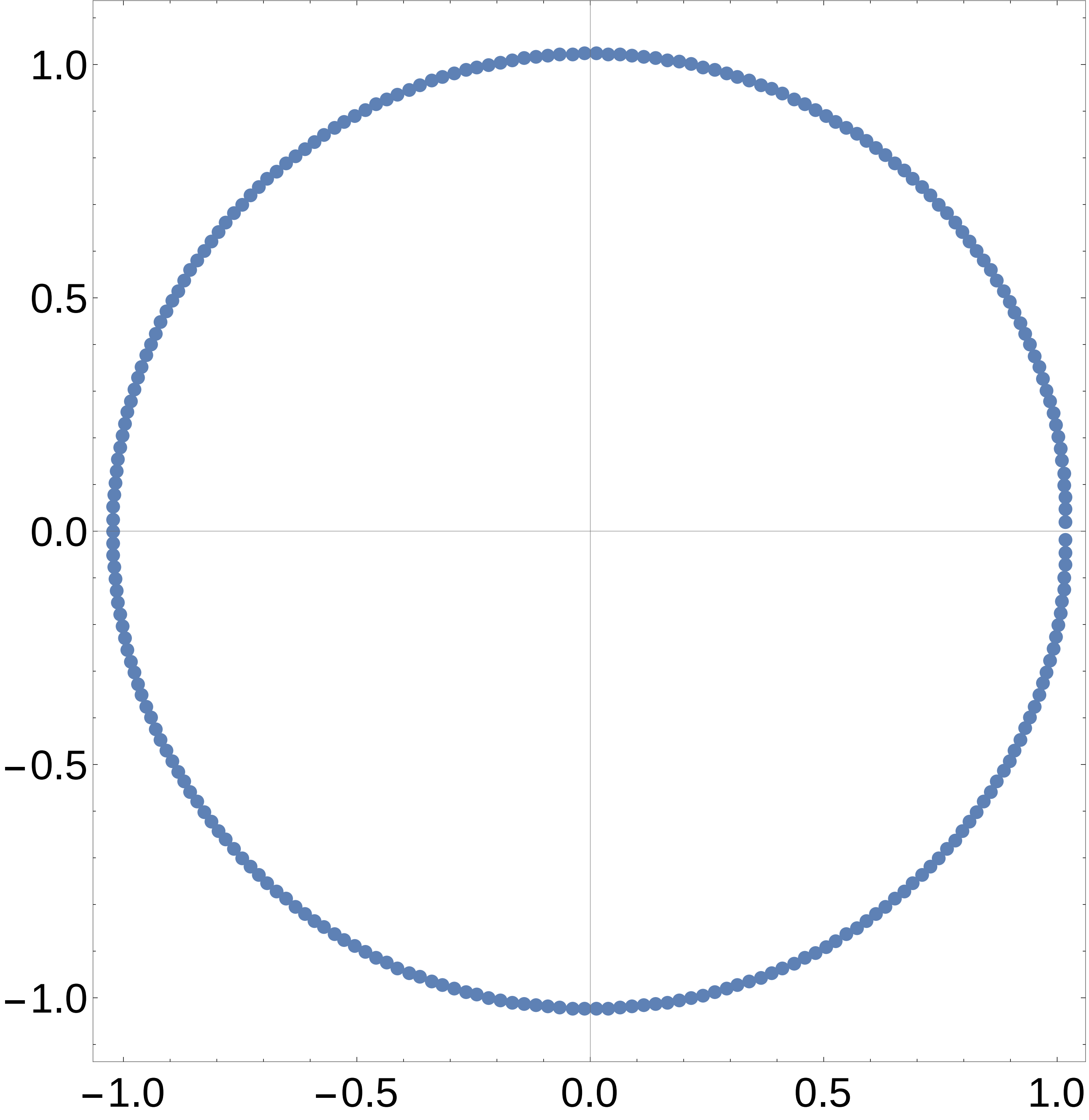
Poly-logarithm

Free Theories

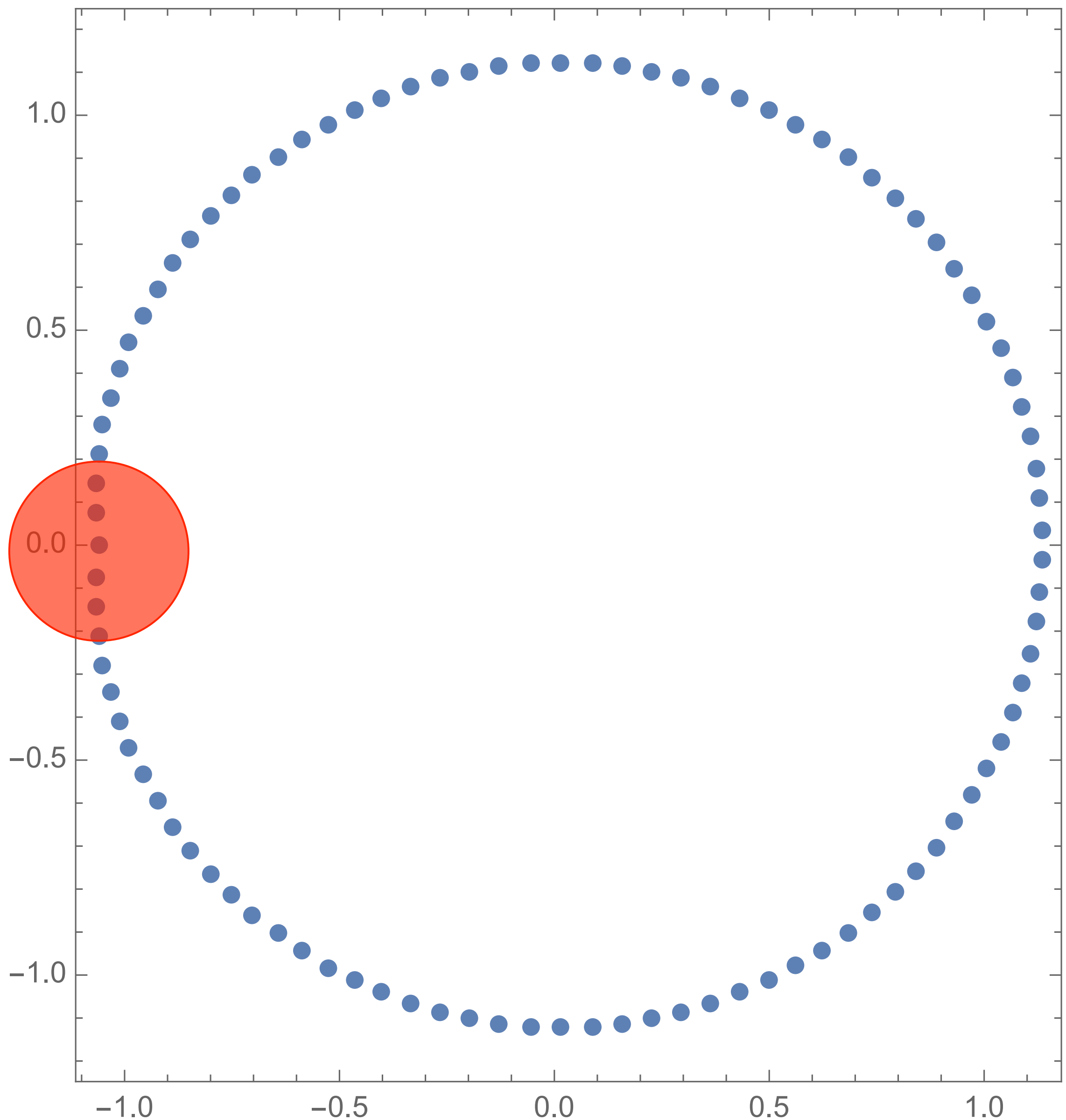
$$\Omega(z) \;=\; e^{\pm \sum_p \log\left(1 \pm z\, e^{-\beta \epsilon_p}\right)} \equiv e^{F_{\pm}(z,\beta)}$$

$$= 1 + \alpha_1 z + \alpha_2 z^2 + \alpha_3 z^3 + \cdots + \alpha_N z^N + \cdots$$

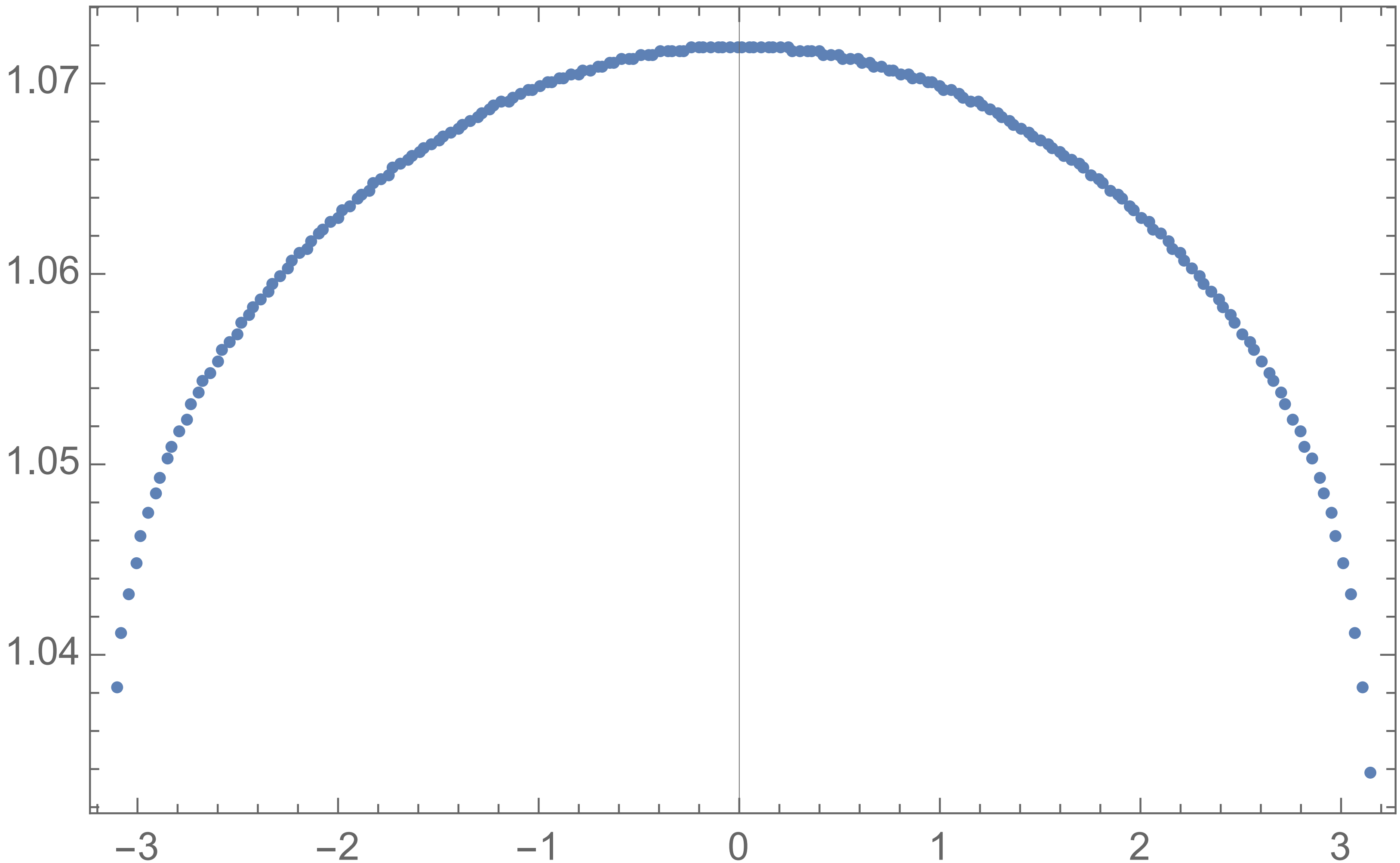
Let’s truncate it at level N and compute the zeros



1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0



1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0



1.07
1.06
1.05
1.04
−3
−2
−1
0
1
2
3

A nice proof based on Fourier Series

$$\left(\frac{\lambda_T}{V}\right) \log \Omega = \sum_{n=1}^{\infty} b_n z^n$$

$$b_n = -\frac{1}{n} \sum_{l=1}^{N} \left(\frac{1}{z_l}\right)^n = -\frac{1}{n} \int_{-\pi}^{\pi} \eta(\theta) \cos(n\theta)\, d\theta$$

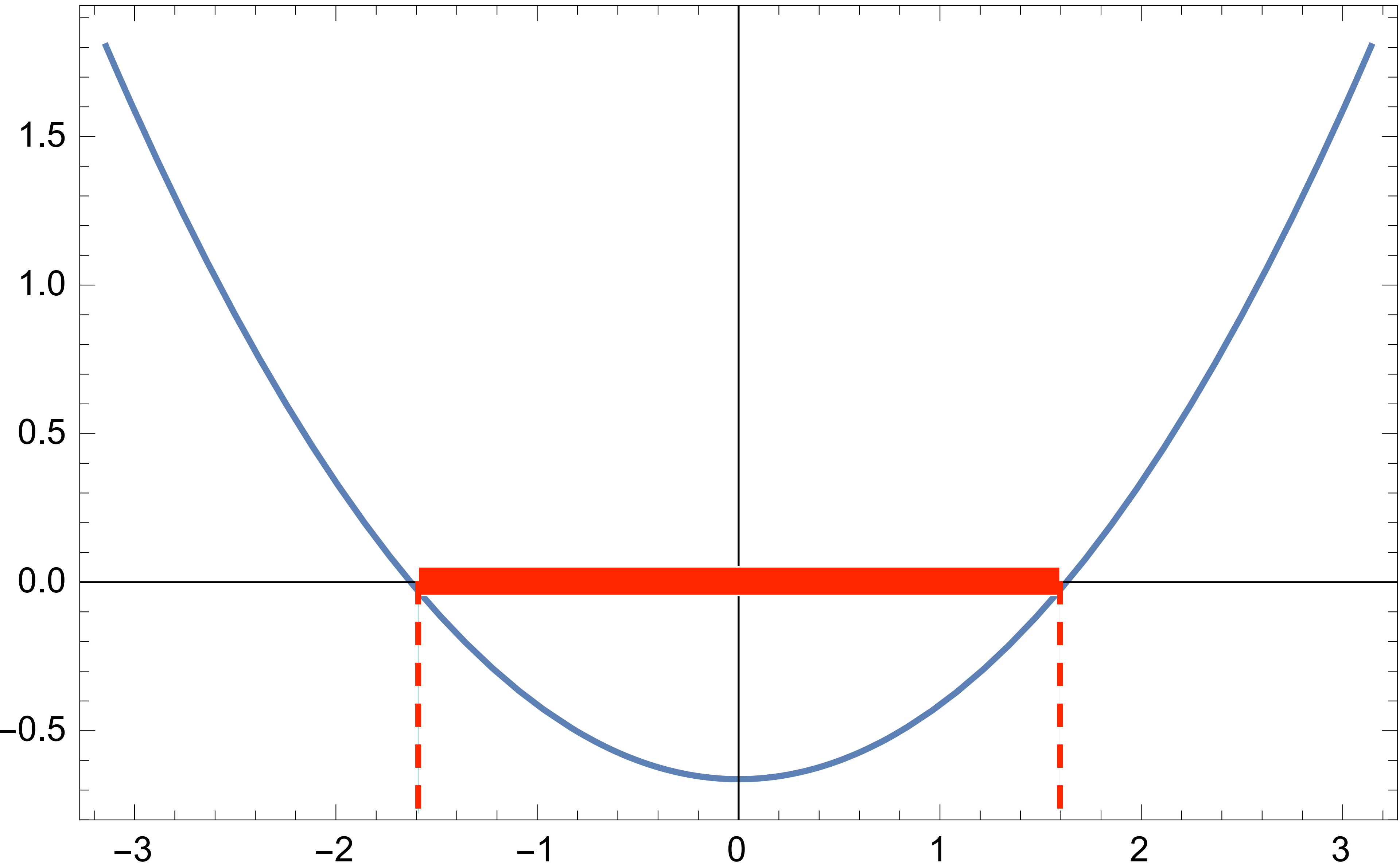
$$\eta(\theta) = \frac{1}{2\pi} - \frac{1}{\pi} \sum_{n=1}^{\infty} n\, b_n \cos(n\theta)$$

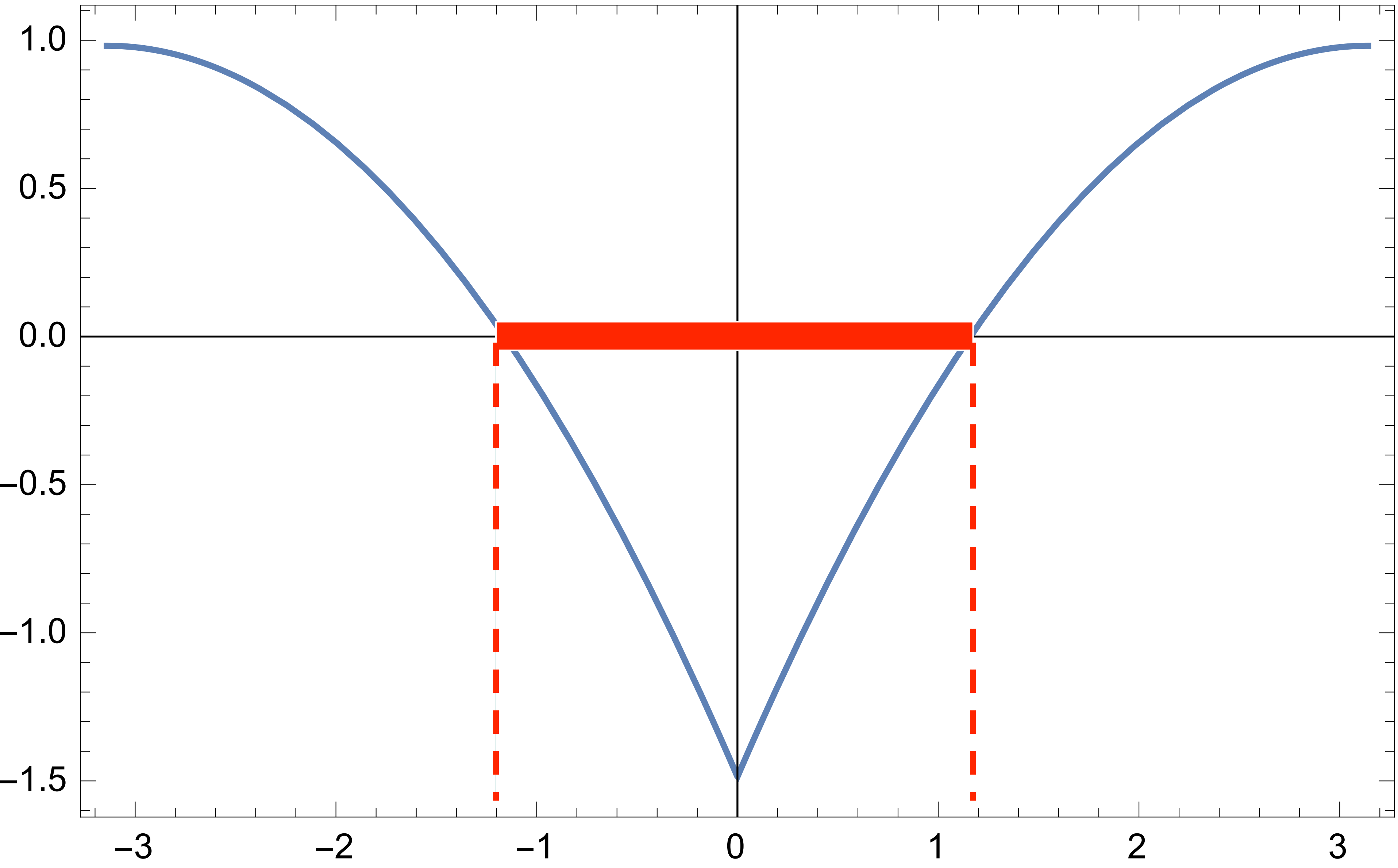
We can resum the series!

$$\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^2} \cos n\theta = \frac{1}{4}\left(\frac{\pi^2}{3} - \theta^2\right)$$

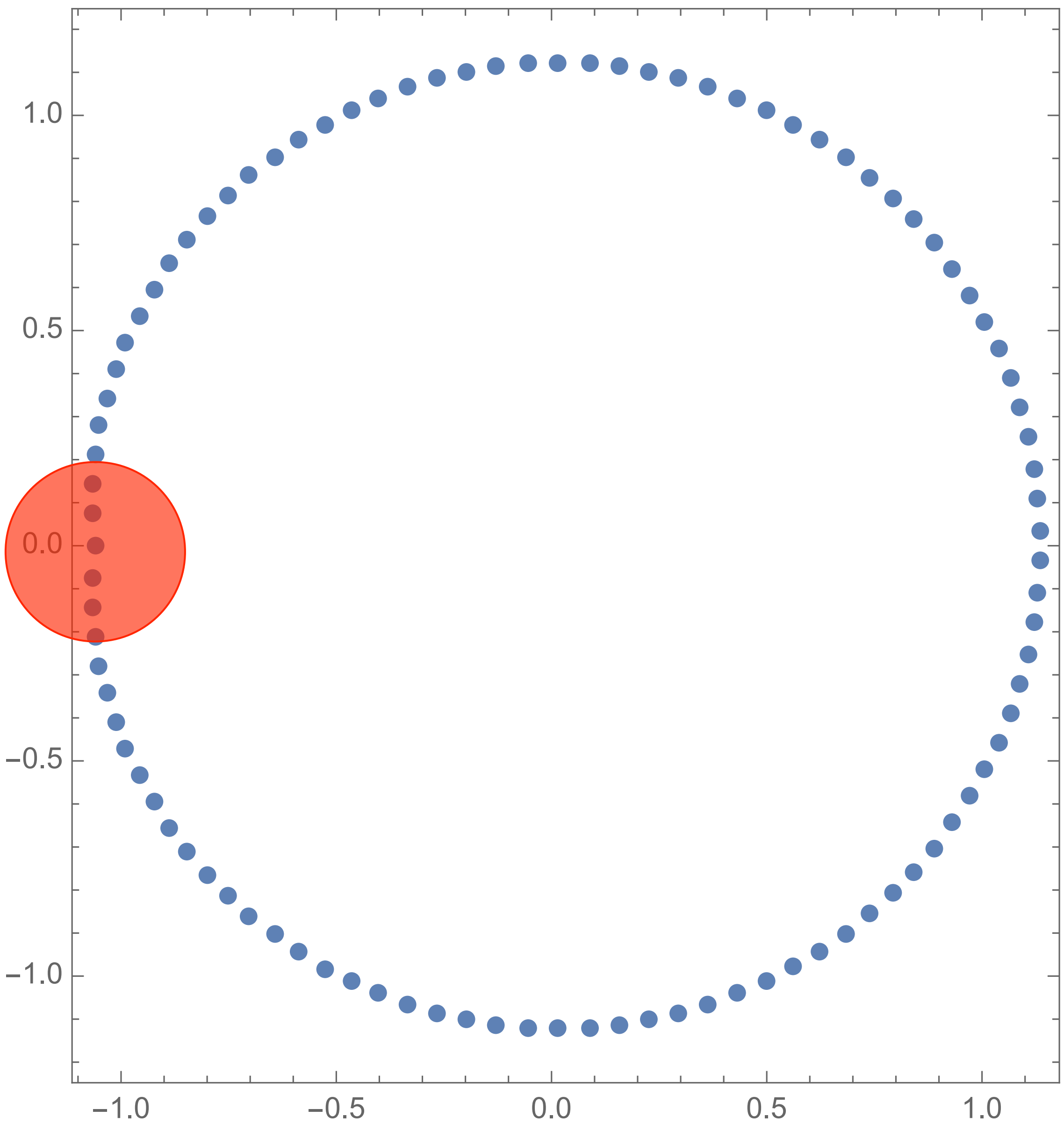
$$\sum_{n=1}^{\infty} \frac{1}{n^2} \cos n\theta = \frac{1}{4}(\pi - |\,\theta\,|)^2 - \frac{\pi^2}{12}$$

$$\cdots\cdots$$


1.5
1.0
0.5
0.0
−0.5
−3
−2
−1
0
1
2
3



1.0
0.5
0.0
−0.5
−1.0
−1.5
−3
−2
−1
0
1
2
3

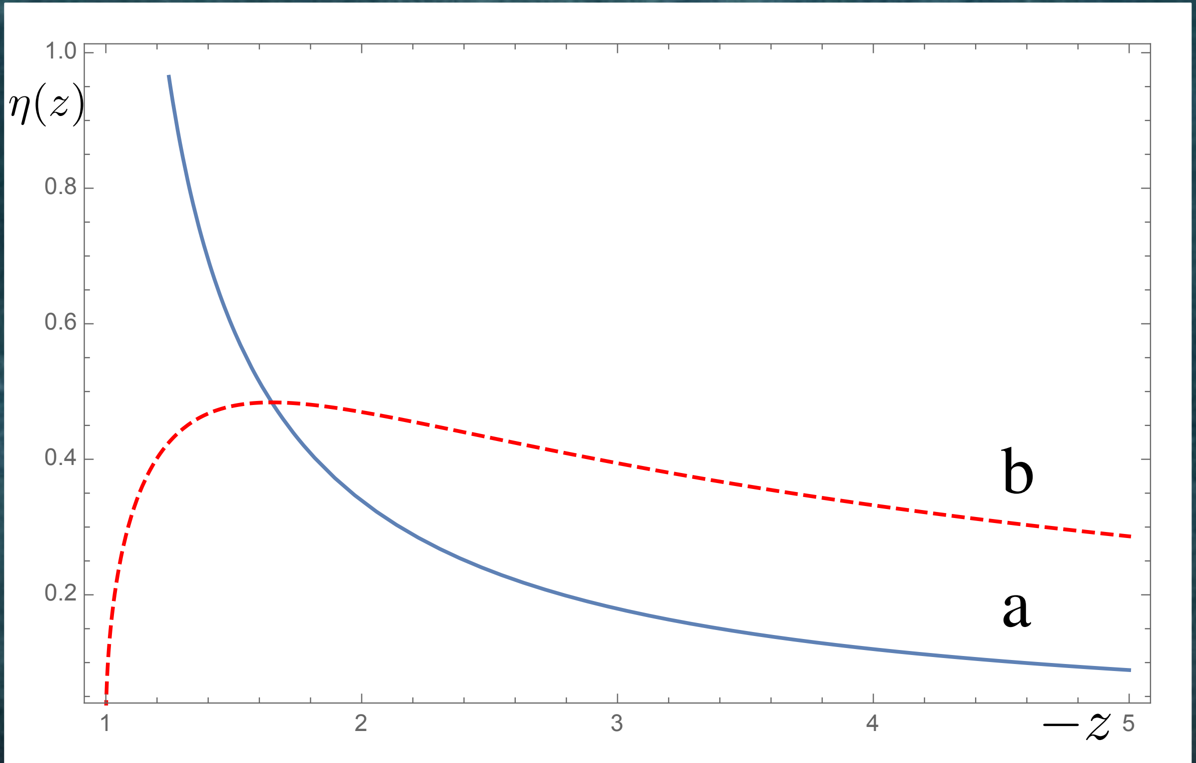


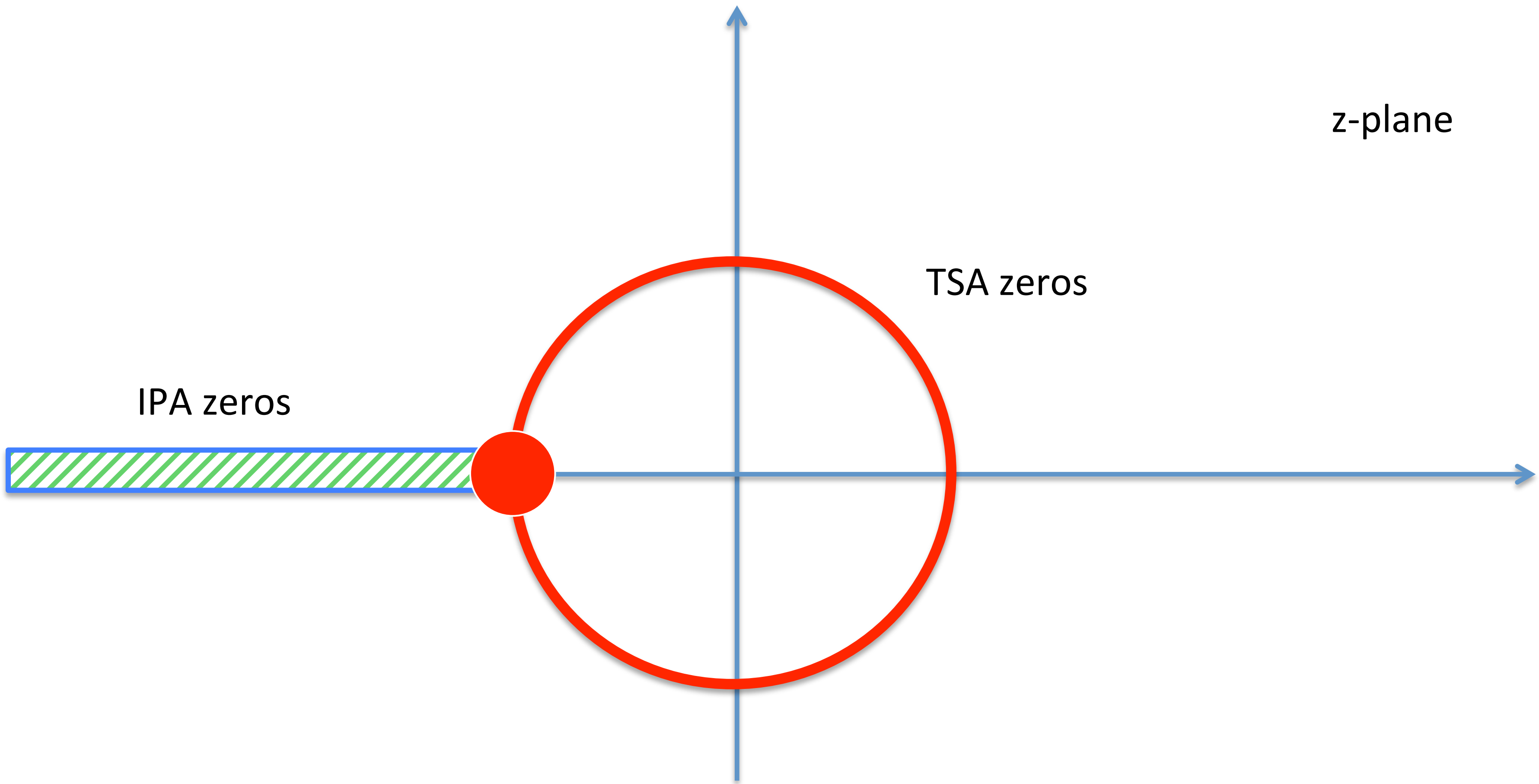
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

Another set of zeros??

$$\Omega(z) = \prod_p \left(1 + z\, e^{-\beta \epsilon_p}\right)$$

$$z_p = -e^{\beta \epsilon_p} \qquad\qquad \eta(z) = g(\epsilon) \left| \frac{d\epsilon}{dz} \right|$$




z-plane
TSA zeros
IPA zeros

Where are the Yang-Lee zeros of the Yang-Lee model?

Series Solution of the TBA eqs.

Threefold way

$$\epsilon(\beta, z) \;\rightarrow\; F(\beta, z) \;\rightarrow\; \Omega(\beta, z)$$

Series Solution of the TBA eqs.

$$\epsilon(\theta, z) = m\beta \cosh\theta - \int_{-\infty}^{\infty} \frac{d\theta'}{2\pi} \varphi(\theta - \theta') \log\left(1 + z\, e^{-\epsilon(\theta', z)}\right)$$

$$\epsilon(\theta, z) = \sum_{n=0}^{\infty} \epsilon_n(\theta)\, z^n$$

$$\epsilon_0(\theta) = \beta \cosh(\theta)$$

$$\epsilon_1(\theta) = -\int_{-\infty}^{\infty} d\theta' \varphi(\theta - \theta') e^{-\epsilon_0(\theta')}$$

$$\epsilon_2(\theta) = \frac{1}{2!} \int_{-\infty}^{\infty} d\theta' \varphi(\theta - \theta') [2\epsilon_1 e^{-\epsilon_0(\theta')} + e^{-2\epsilon_0(\theta')}]$$

Series Solution of the TBA eqs.

$$F(z) \;=\; mL \int_{-\infty}^{+\infty} \cosh\theta \log\left(1 + z\, e^{-\epsilon(\theta,z)}\right) \frac{d\theta}{2\pi}$$

$$F(z) \;=\; \sum_{n=0}^{\infty} f_n\, z^n$$

$$f_0(\beta) \;=\; 0$$

$$f_1(\beta) = \frac{L}{\beta} \int_{-\infty}^{\infty} \frac{d\theta}{2\pi} \cosh(\theta) e^{-\epsilon_0(\theta)}$$

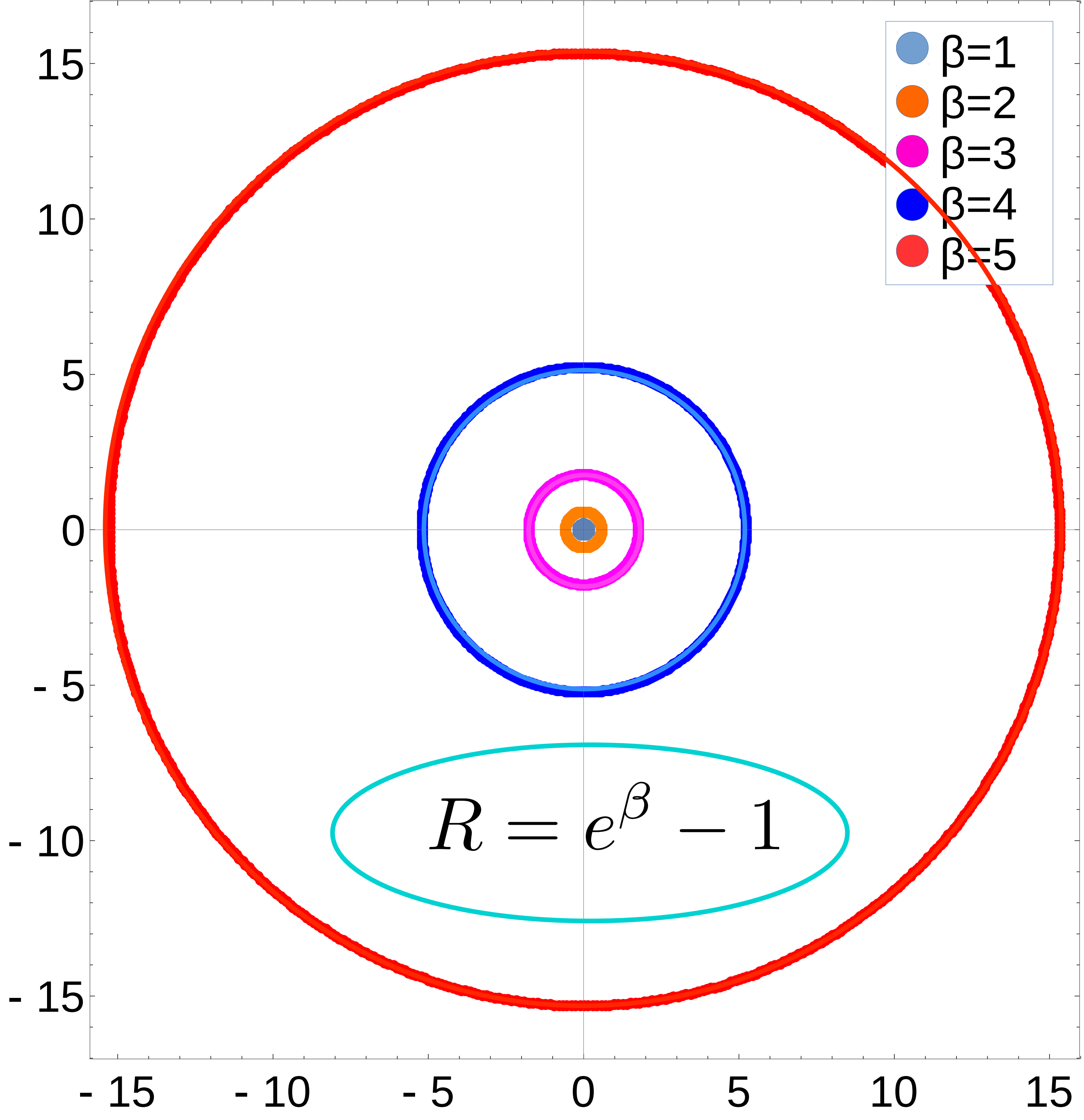
$$f_2(\beta) = -\frac{L}{2!\beta} \int_{-\infty}^{\infty} \frac{d\theta}{2\pi} \cosh(\theta)[2\epsilon_1 e^{-\epsilon_0(\theta')} + e^{-2\epsilon_0(\theta')}]$$

Series Solution of the TBA eqs.

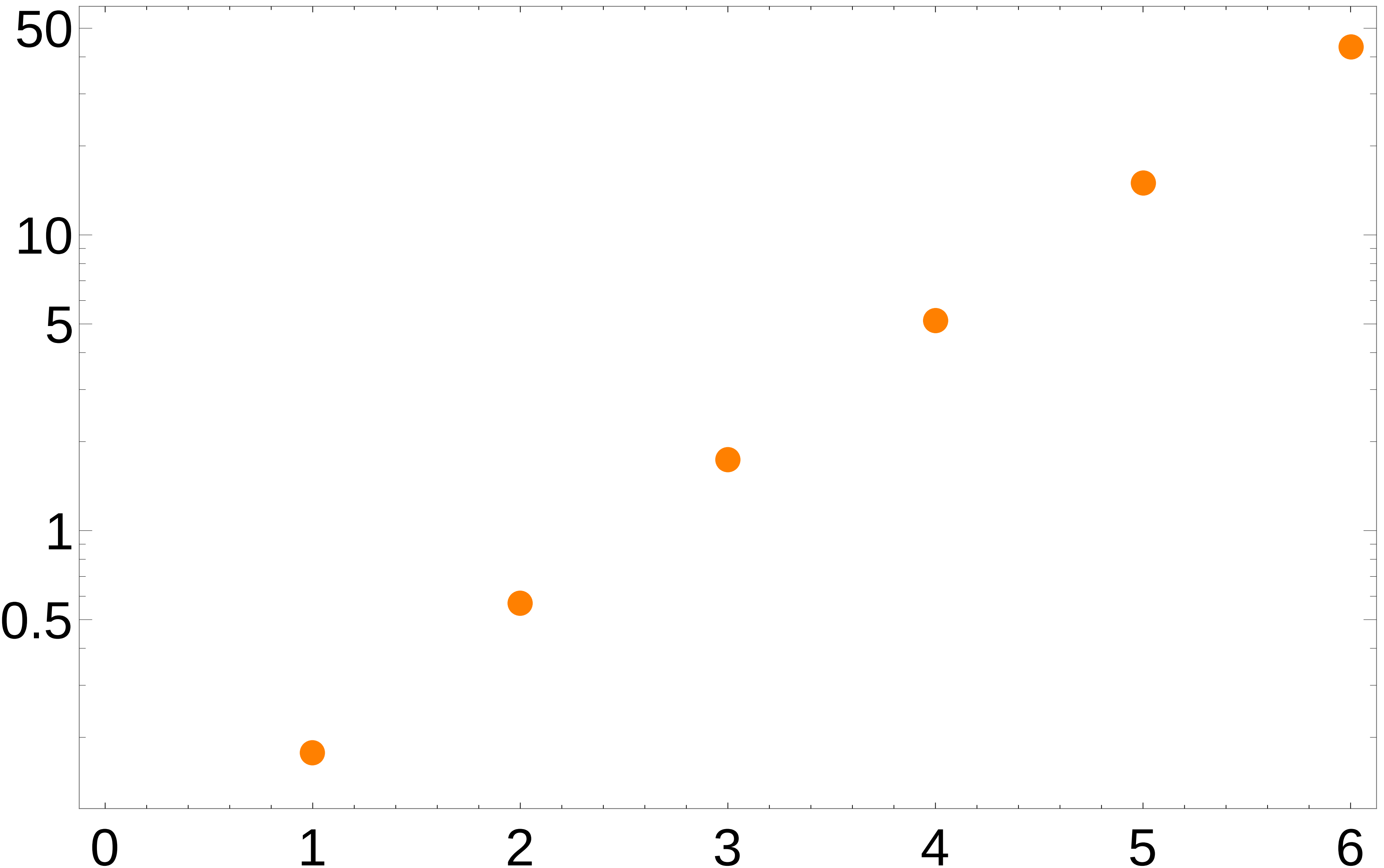
$$\Omega(\beta, z) \;=\; e^{F(\beta, z)}$$

$$\Omega_N(\beta, z) \;=\; 1 + \sum_{k=1}^{N} \gamma_k \, z^k$$

$$= \; 1 + \gamma_1 \, z^1 + \gamma_2 \, z^2 + \cdots \gamma_N \, z^N$$



β=1
β=2
β=3
β=4
β=5
$R = e^{\beta} - 1$
15
10
5
0
- 5
- 10
- 15



50
10
5
1
0.5
0
1
2
3
4
5
6

- **Large β**

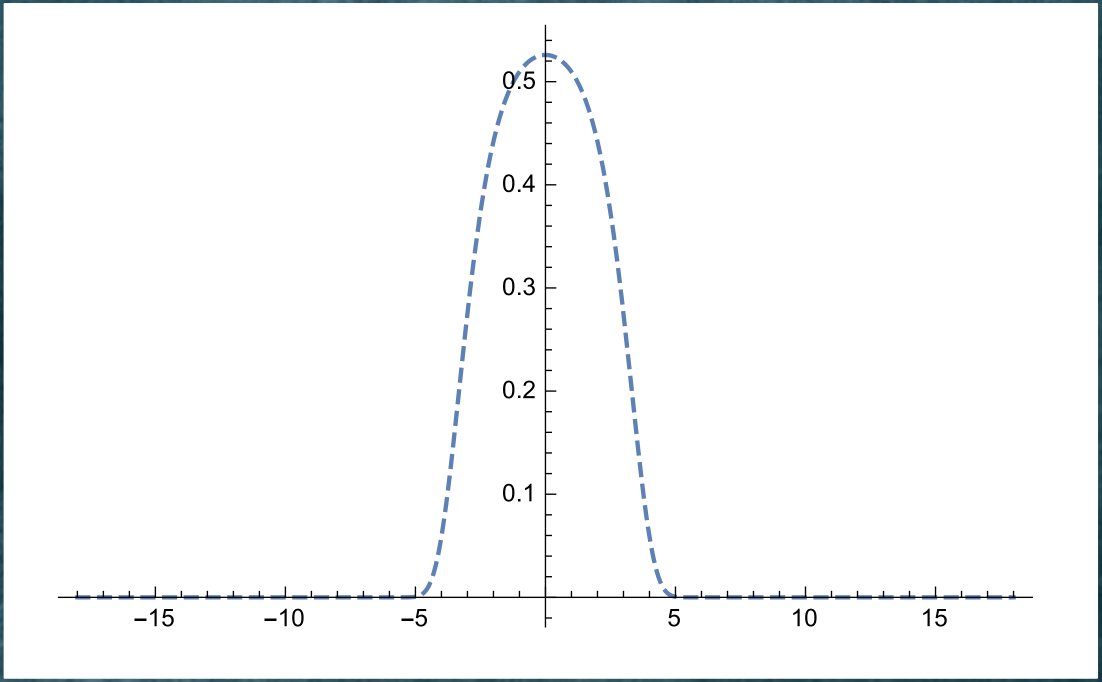
$$\Omega(z) = \exp\left[\sum_{n=1}^{\infty} \frac{1}{n} K_1(n\beta m) z^n\right]$$

$$\simeq \exp\left[\sum_{n=1}^{\infty} \frac{1}{n} e^{-n\beta m} z^n\right]$$

$$\mu\, e^{\beta} \leq |z_i| \leq \nu\, e^{\beta}$$

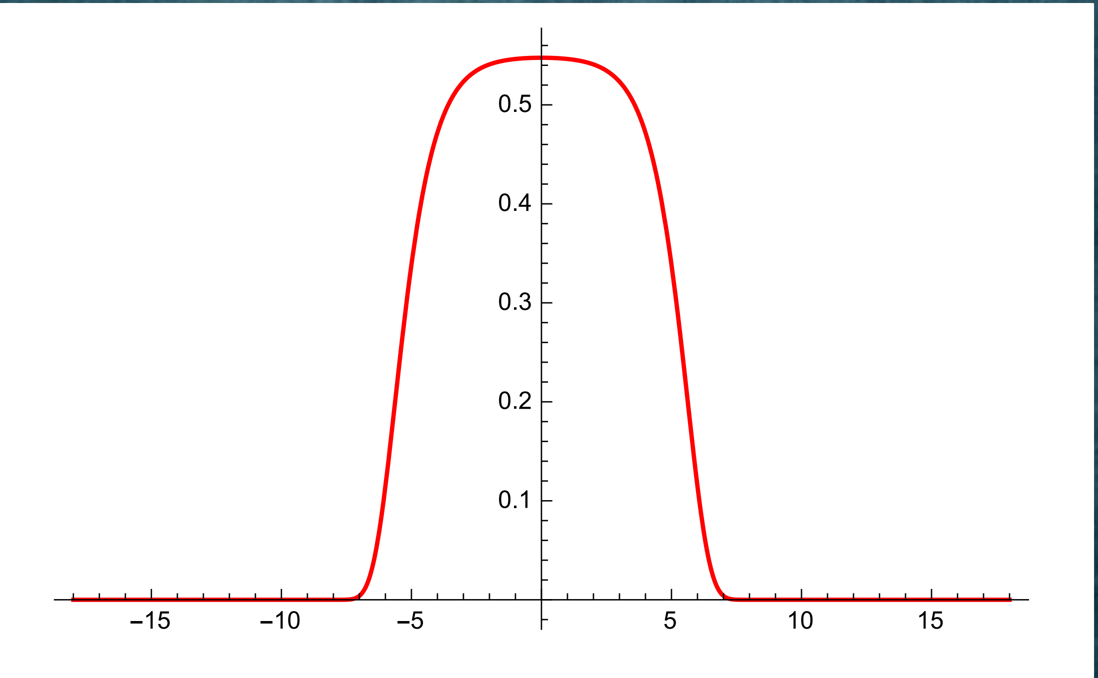
- **Small β**

$$\Omega(z) \simeq \exp\left[\frac{1}{\beta} f(z)\right]$$



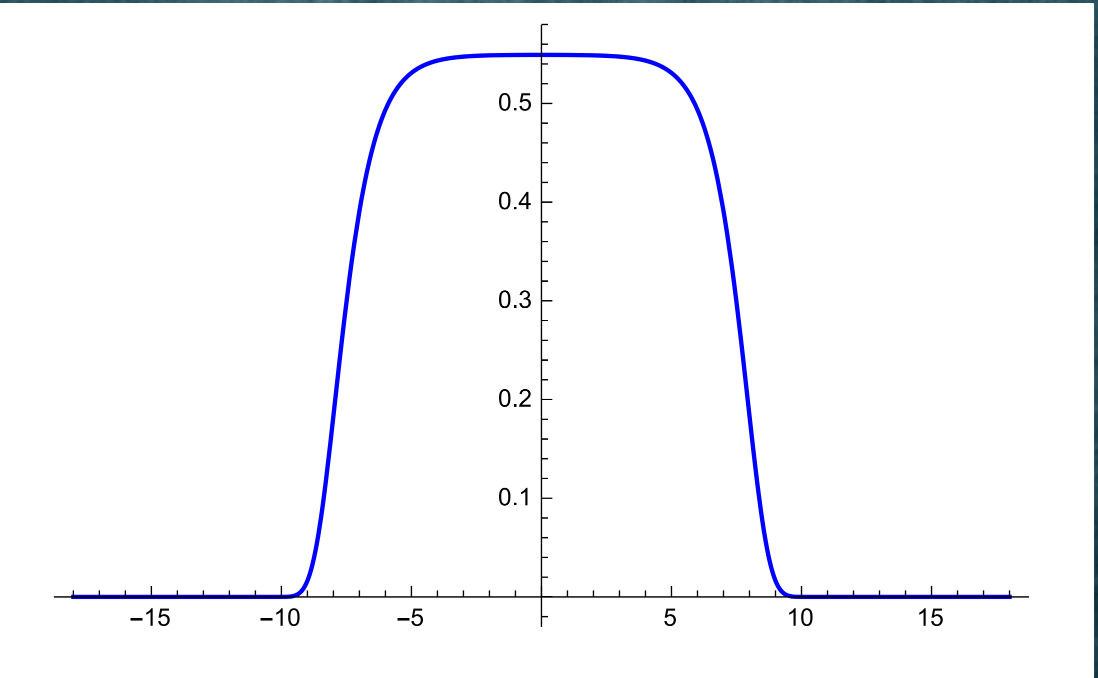
- **Small β**

$$\Omega(z) \simeq \exp\left[\frac{1}{\beta} f(z)\right]$$



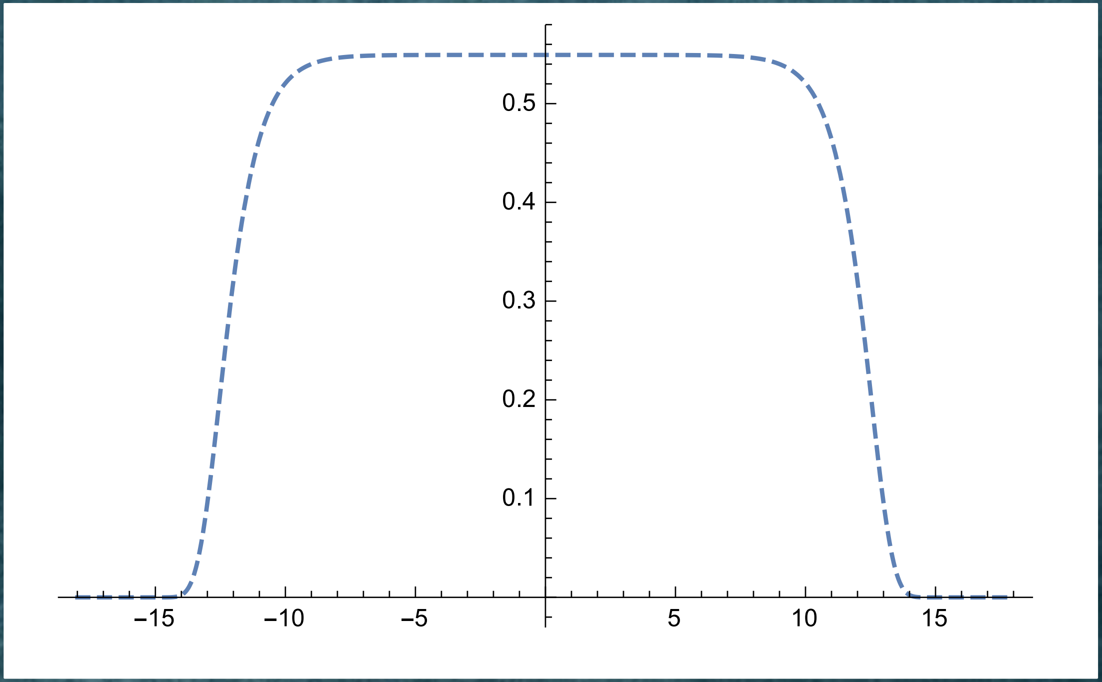
- **Small β**

$$\Omega(z) \simeq \exp\left[\frac{1}{\beta} f(z)\right]$$



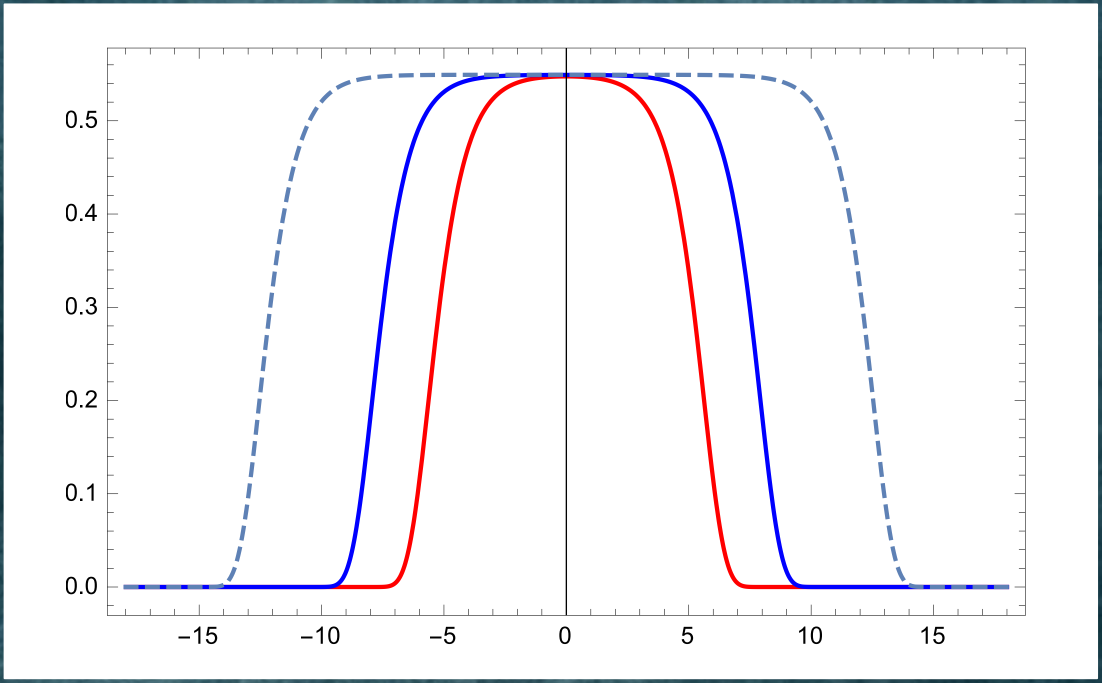
- **Small β**

$$\Omega(z) \simeq \exp\left[\frac{1}{\beta} f(z)\right]$$



- **Small β**

$$\Omega(z) \simeq \exp\left[\frac{1}{\beta} f(z)\right]$$

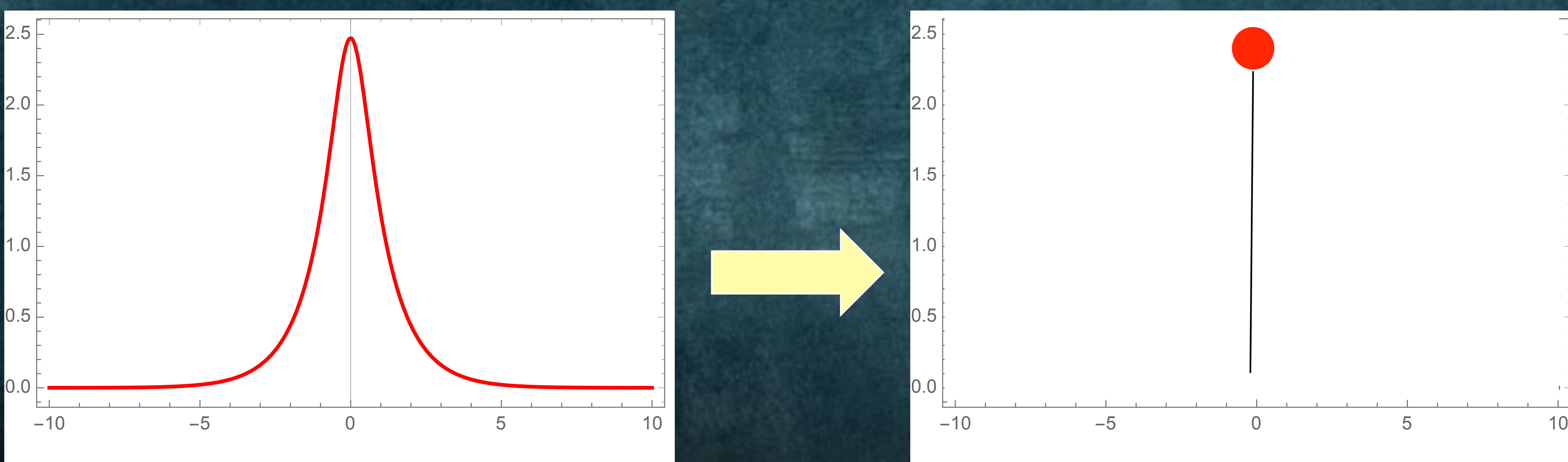


$$\rho\,\beta \leq |z_i| \leq \gamma\,\beta$$

Alternative method

$$\Omega(z) \;=\; \exp\left[mL\int_{-\infty}^{+\infty}\cosh\theta\,\log\left(1+z\,e^{-\epsilon(\theta,z)}\right)\frac{d\theta}{2\pi}\right]$$

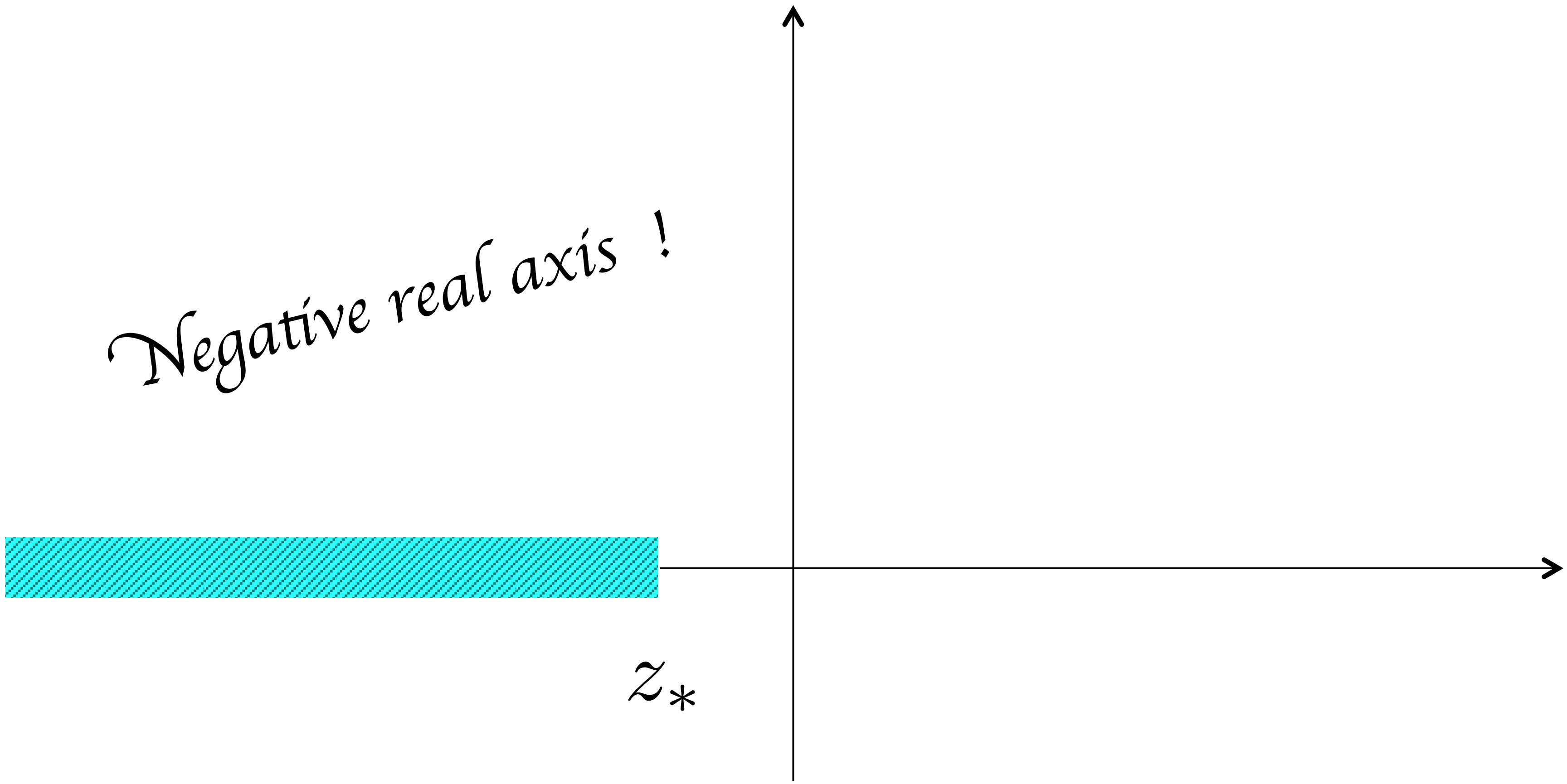
$$\epsilon(\theta,z) \;=\; m\beta\,\cosh\theta - \int_{-\infty}^{\infty}\frac{d\theta'}{2\pi}\,\varphi(\theta-\theta')\,\log\left(1+z\,e^{-\epsilon(\theta',z)}\right)$$



Alternative method

$$\epsilon(\theta, z) \;=\; -\log\left[\frac{-1+\sqrt{1+4ze^{-m\beta\cosh\theta}}}{2z}\right]$$

$$F(z) \;=\; \int_{-\infty}^{\infty} \cosh\theta\; \log\left[1+\sqrt{1+4z\,e^{-m\beta\cosh\theta}}\right]\; d\theta$$



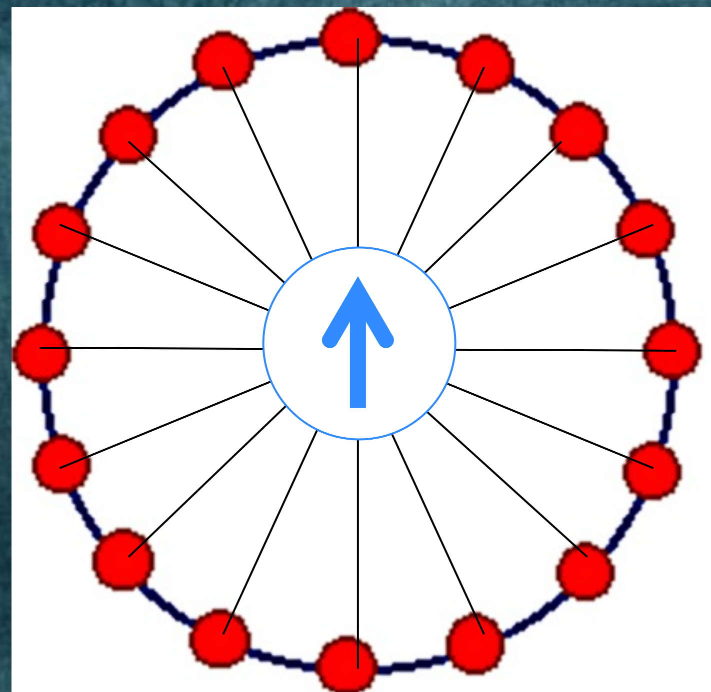
$$z \leq z_* = -\frac{1}{4} e^{-m\beta \cosh \theta}$$

Experimental Observation of Yang-Lee zeros

This can be done measuring decoherence of a probe spin coupled to a spin bath

Wei-Liu Phys. Rev. Lett. 109, 185701 (2012)
Peng et al. Phys. Rev. Lett. 114, 010601 (2015)

Yang-Lee zeros of Ising Model

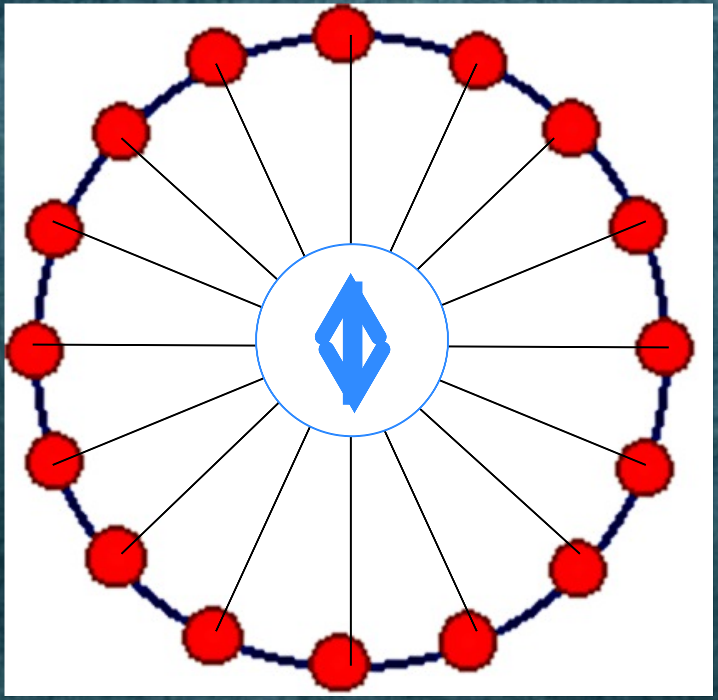


$$H_0 = -J\sum_{i=1}^{N}\sigma_i\sigma_{i+1}$$

$$H = H_0 - \lambda S_1$$

$$-h\sum_{i=1}^{N}\sigma_i \qquad \sum_{i=1}^{N}\sigma_i$$

Yang-Lee zeros of Ising Model



$$H = H_0 - \lambda \mathbf{S} \sum_{i=1}^{N} \sigma_i$$

Yang-Lee zeros of Ising Model

$$|\Psi(0)> = \frac{1}{\sqrt{2}}(|+> + |->) \otimes |E>$$

$$|\Psi(t)> = \frac{1}{\sqrt{2}}|+> \otimes e^{-iH_+ t}|E> +$$

$$+ \frac{1}{\sqrt{2}}|-> \otimes e^{-iH_- t}|E>$$

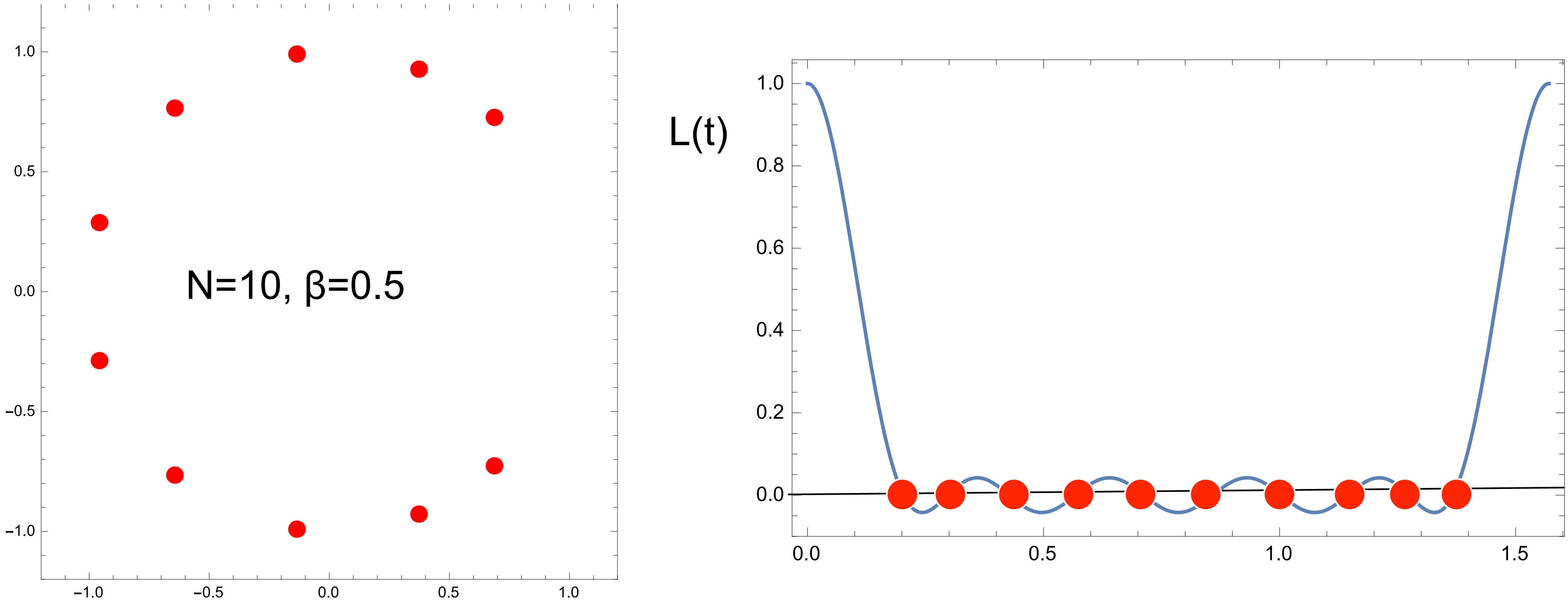
Yang-Lee zeros of Ising Model

Decoherence of the probe spin coupled to the spin bath

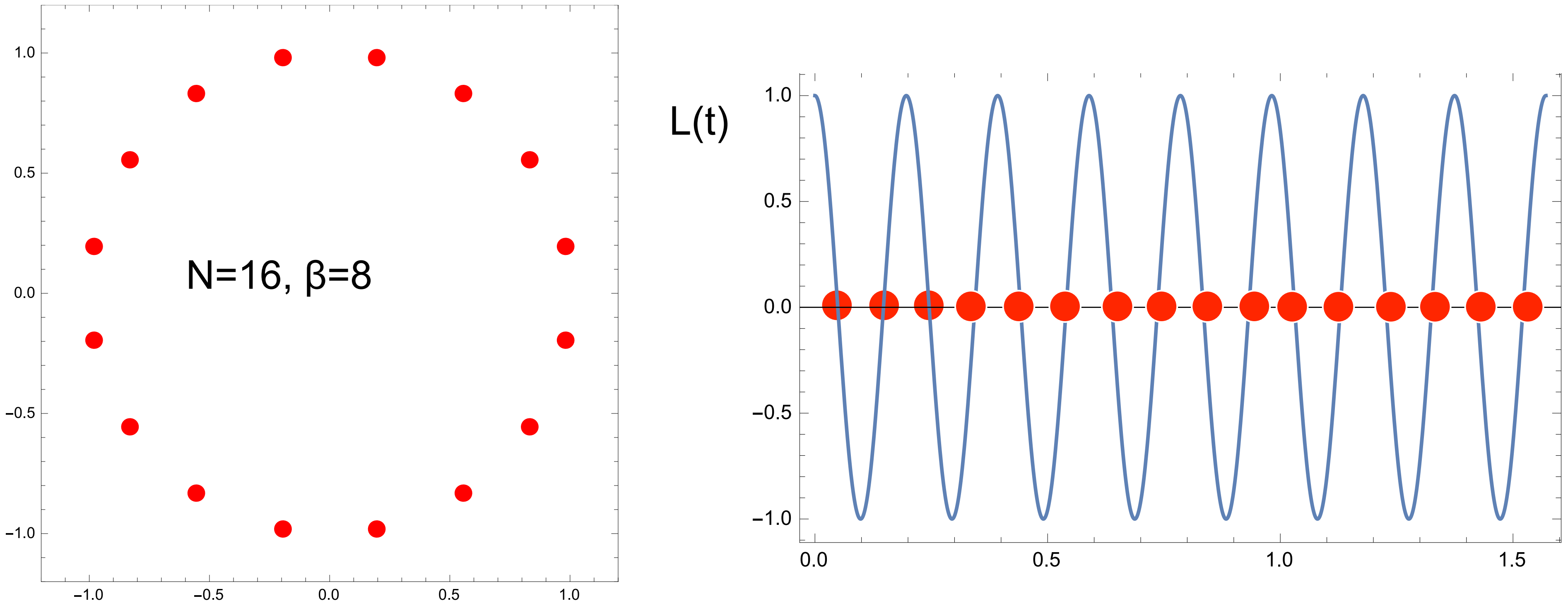
$$< \Psi(t) \,|\, S_x \,|\Psi(t) > = < E \,|e^{-i(H_+ - H_-)t} \,|\, E >$$

$$= \mathrm{Tr}\left[e^{-\beta H_0} \, e^{2i\lambda \sum_k \sigma_k \, t} \right] / \Omega(\beta, h)$$

$$= \frac{\Omega(\beta, h - 2i\lambda t)}{\Omega(\beta, h)} \quad = \frac{\prod_{n=1}^{N} \left(e^{-2\beta h + 4i\lambda t} - z_n \right)}{\left(e^{-2\beta t} - z_n \right)}$$



N=10, β=0.5
L(t)


N=16, β=8
L(t)

Selected for a Viewpoint in *Physics*
PRL **114**, 010601 (2015) PHYSICAL REVIEW LETTERS week ending 9 JANUARY 2015

Experimental Observation of Lee-Yang Zeros

Xinhua Peng,[1,*] Hui Zhou,[1] Bo-Bo Wei,[2] Jiangyu Cui,[1] Jiangfeng Du,[1,†] and Ren-Bao Liu[2,‡]
[1]*Hefei National Laboratory for Physical Sciences at Microscale, Department of Modern Physics, and Synergetic Innovation Center of Quantum Information & Quantum Physics, University of Science and Technology of China, Hefei 230026, China*
[2]*Department of Physics, Centre for Quantum Coherence, and Institute of Theoretical Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, China*
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Lee-Yang zeros are points on the complex plane of physical parameters where the partition function of a system vanishes and hence the free energy diverges. Lee-Yang zeros are ubiquitous in many-body systems and fully characterize their thermodynamics. Notwithstanding their fundamental importance, Lee-Yang zeros have never been observed in experiments, due to the intrinsic difficulty that they would occur only at complex values of physical parameters, which are generally regarded as unphysical. Here we report the first observation of Lee-Yang zeros, by measuring quantum coherence of a probe spin coupled to an Ising-type spin bath. The quantum evolution of the probe spin introduces a complex phase factor and therefore effectively realizes an imaginary magnetic field. From the measured Lee-Yang zeros, we reconstructed the free energy of the spin bath and determined its phase transition temperature. This experiment opens up new opportunities of studying thermodynamics in the complex plane.

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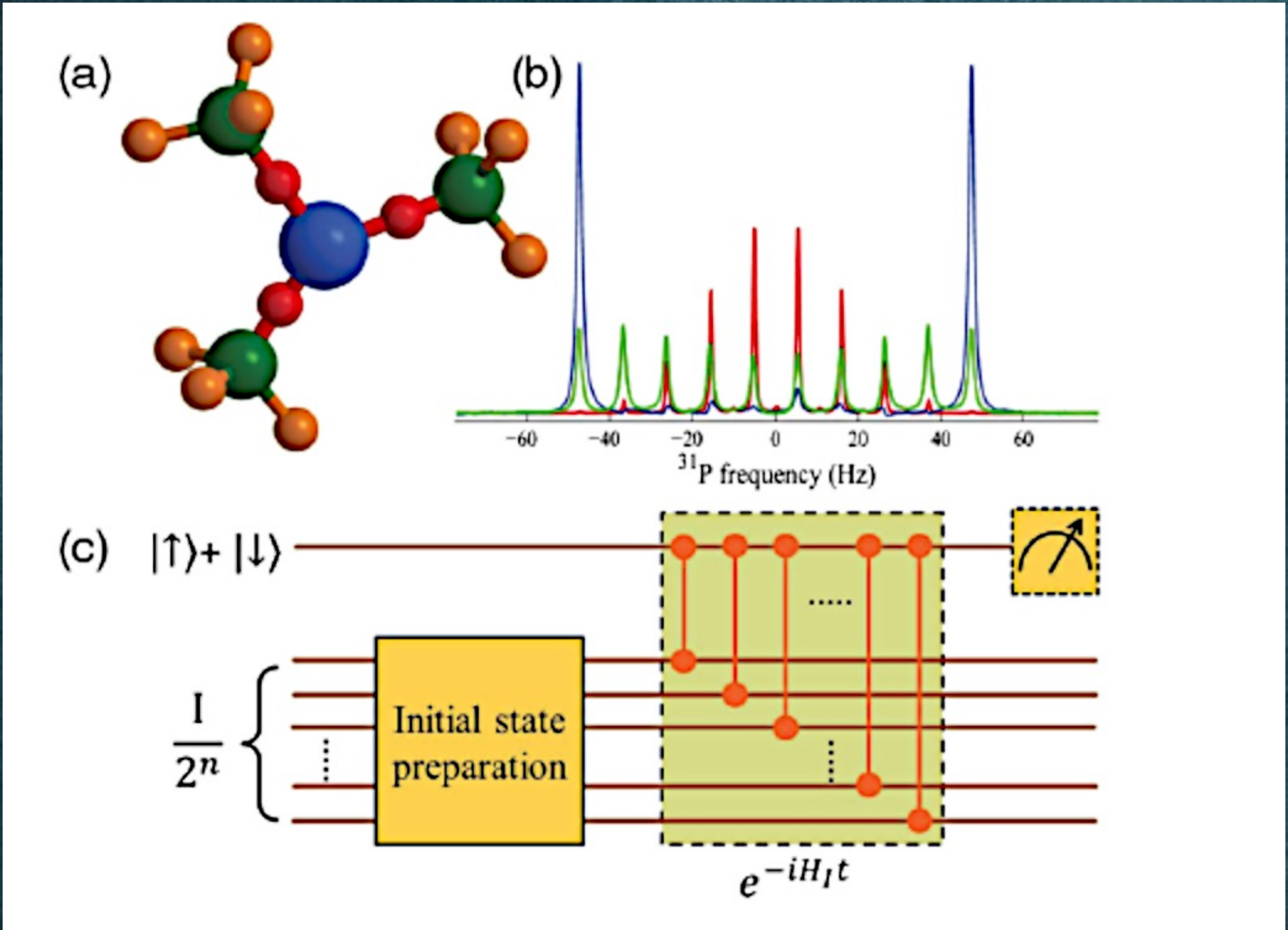
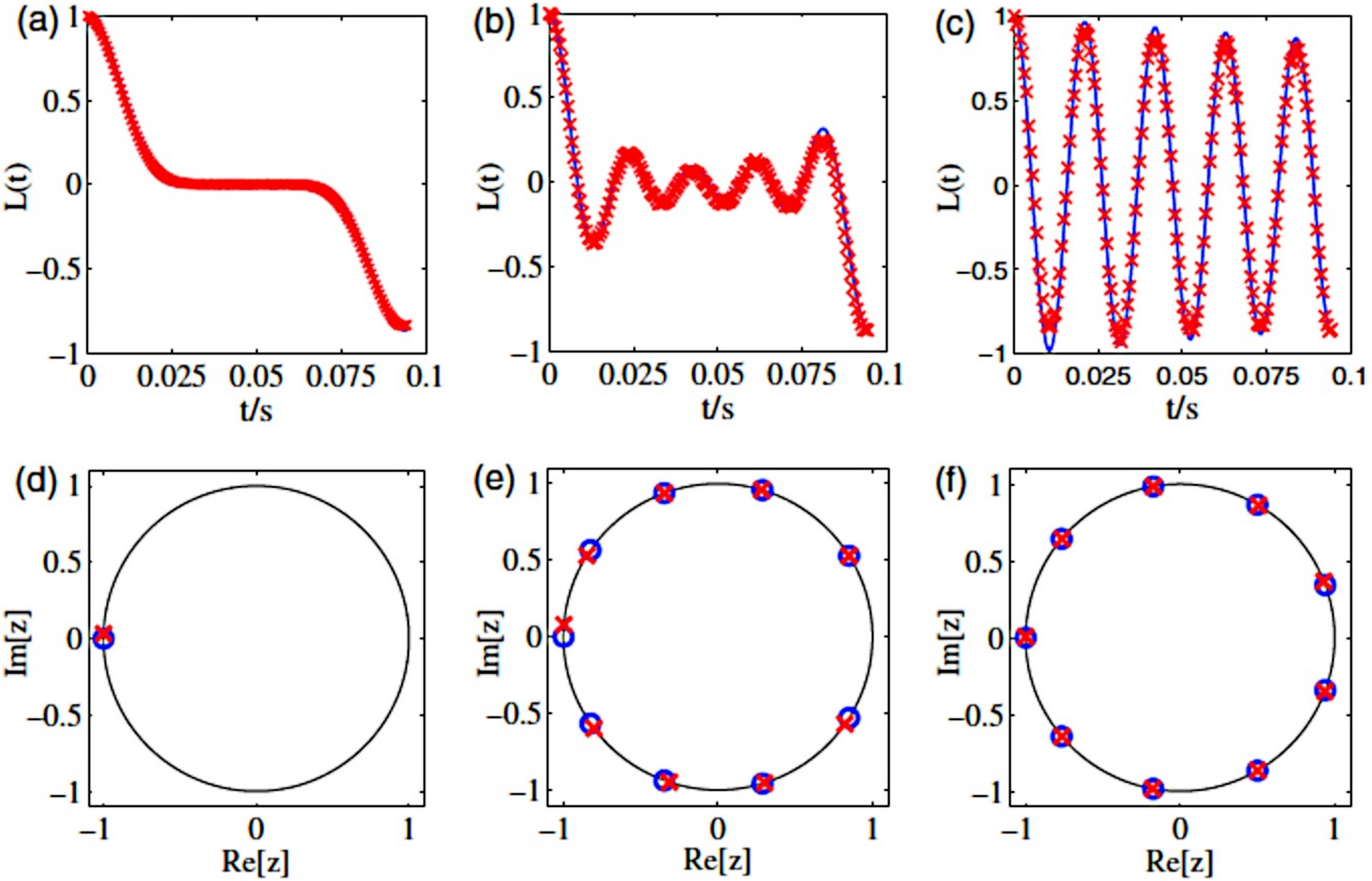
After the pioneering works by van der Waals [1,2], Mayer [3,4], and van Hove [5], it has been known that different phases (e.g., liquid and gas phases) of a thermodynamic system have the same microscopic interactions but the free energy of the system encounters a singularity (nonanalytic) point in the physical parameter space where the phase transition occurs. A rigorous relation between the analytic properties of free energies and thermodynamics (in particular, phase transitions) was established by Yang and Lee in a seminal paper published in 1952 through continuation of the free energy to the complex plane of physical parameters [6]. Lee and Yang considered a general Ising model with the ferromagnetic interaction $J_{ij} > 0$ under a magnetic field h with the Hamiltonian $H(h) = -\sum_{i,j} J_{ij}s_i s_j - h\sum_j s_j$, where the spins s_j take values $\pm 1/2$. The partition function of N spins at temperature T (or inverse temperature $\beta \equiv 1/T$) $\Xi(\beta,h) \equiv \sum_{\text{all states}} \exp(-\beta H)$ can be written into an Nth order polynomial of $z \equiv \exp(-\beta h)$ as $\Xi = \exp(\beta N h/2)\sum_{n=0}^{N} p_n z^n$, where $\exp(-\beta H)$ is the Boltzmann factor (the probability in a state with energy H, up to a normalization factor) and the coefficients p_n can be interpreted as the partition function in a zero magnetic field under the constraint that n spins are at state $-1/2$. The free energy F is related to the partition function by $F = -T\ln(\Xi)$. Obviously, the zeros of the partition function (where $\Xi = 0$) are the singularity points of the free energy and hence fully determine the analytic properties of the free energy. If the Lee-Yang zeros are determined, the partition function can be readily reconstructed as $\Xi = p_0 \exp(\beta N h/2) \prod_{n=1}^{N}(z - z_n)$. Since the Boltzmann factor is always positive for real interaction parameters and real temperature, zeros of the partition function would occur only on the complex plane of the physical parameters. Lee and Yang proved that for the ferromagnetic Ising model the N zeros of the partition function all lie within an arc on the unit circle in the complex plane of z (corresponding to pure imaginary values of the external field) [7]. At sufficiently low temperature ($T \le T_C$), the end points of the arc, i.e., the Yang-Lee singularity edges [8,9] approach the real axis of h at the thermodynamic limit ($N \to \infty$). Thus the free energy encounters a singularity point on the real axis of the magnetic field, which means the onset of a phase transition.

The Lee-Yang zeros exist universally in many-body systems. These include a broad range of physical systems described by the Ising models, such as anisotropic magnets, alloys, and lattice gases. The Lee-Yang theorem, first proved for ferromagnetic Ising models of spin-1/2, was later generalized to general ferromagnetic Ising models of arbitrarily high spin [10–12] and to other interesting types of interactions [13–16]. For general many-body systems, the Lee-Yang zeros may not be distributed along a unit circle but otherwise present similar features as in ferromagnetic Ising models. Lee-Yang zeros have also been generalized to zeros of partition functions in the complex plane of other physical parameters (such as Fisher zeros in the complex plane of temperature [17]). The Lee-Yang zeros (or their generalizations) fully characterize the analytic properties of free energies and hence thermodynamics of the systems. Therefore, determining the Lee-Yang zeros is not only fundamentally important for a complete picture of thermodynamics and statistical physics (by continuation to the



(a)
(b)
-60
-40
-20
0
20
40
60
^{31}P frequency (Hz)
(c)
$|\uparrow\rangle + |\downarrow\rangle$
$\frac{I}{2^n}$
Initial state preparation
$e^{-iH_I t}$



(a)
(b)
(c)
(d)
(e)
(f)
L(t)
t/s
Im[z]
Re[z]
1
0.5
0
−0.5
−1
0.025
0.05
0.075
0.1

Conclusions

- Pattern of Yang-Lee zeros for integrable QFT
- Easy to extend to other integrable models, such as, for instance, the Lieb-Liniger model
- Realistic possibility to measure the YL zeros in cold atom experiments of decoherence
- Interesting avenue to discover new physical statistical systems through appropriate distributions of the zeros in the complex plane