Lee–Yang zeros in the age of Rydberg atoms

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Lee–Yang (LY) zeros play a fundamental role in the formulation of statistical physics in terms of (grand) partition functions, and assume theoretical significance for the phenomenon of phase transitions. In this paper, motivated by recent progress in cold Rydberg atom experiments, we explore the LY zeros in classical Rydberg blockade models. We prove that all the LY zeros are real for such models with arbitrary blockade radii, and show how the zeros redistribute as one interpolates between nearest- and next-nearest-neighbor blockade. We also discuss possible experimental measurements of these zeros.

I. INTRODUCTION

Much of modern statistical physics builds on the concept of (grand) partition functions. For finite systems in general, they are positive, analytic functions in terms of physical quantities, and, in particular, are smooth functions with regard to temperature $T$ when the latter is finite. Historically, this fact caused some confusion as to how discontinuity, as occurs in phase transitions, can emerge from such a smooth function, before it became clear that phase transitions can only happen in the thermodynamic limit. However, it wasn’t until the work of Lee and Yang [1, 2] when a more detailed description of the relation between the analyticity of partition functions and phase transitions was put forward.

Exactly 70 years ago in 1952, in two seminal papers [1, 2], Lee and Yang proposed to study the complex zeros of the (grand) partition function as a polynomial of some sorts of fugacity, and showed how the distribution of such zeros in the thermodynamic limit relates to the existence and properties of phase transitions. They proved that if there exists a region containing part of the positive real axis with no zeros inside, in the corresponding regime of physical parameters no phase transition can happen. Conversely, if the zeros accumulate to a point on the positive real axis in the thermodynamic limit, phase transitions will generally ensue. As a concrete example, they considered the Ising model with arbitrary ferromagnetic couplings, and proved that all the zeros are located on the unit circle with the fugacity defined as $\exp(-\beta h)$, where $h$ is the magnetic field. A direct corollary is that phase transitions are not possible unless $h = 0$ in the Ising model.

The original construction of Lee and Yang focused on spin-$1/2$ Ising ferromagnets, or equivalently attractive lattice gases. Generalizations of this program to higher spins and Heisenberg models soon followed [3–10]. In the next decades, results on other geometries and interactions, in particular antiferromagnetic Ising models, became available [11–18]. The endeavor of characterizing complex zeros of real polynomials with positive coefficients has attracted interest from the mathematics community alike [19–22].

While originally a purely theoretical discussion with no direct experimental relevance envisioned, Lee–Yang (LY) zeros turn out experimentally measurable using nuclear magnetic resonance (NMR) techniques [23, 24]. The idea is to carefully couple a collection of spins to a probe spin, and extract the zeros from its quantum evolution. Recently, cold Rydberg atoms have attracted extensive research efforts for their versatile control and measurements together with strong dipole interactions. Two major frontiers are unfolding — First, various novel phases and phase transitions emerge from geometries enabled by the single-atom manipulations, including one dimensional (1d) chains [25, 26] and two dimensional (2d) square [27–30] and kagome lattices [31–35]. Even in the seemingly innocuous 1d case, there are some debates on the nature of the phase transitions [36–41], a caricature of the rich and subtle physics in such systems. Second, the constrained Hilbert space drastically changes the dynamical behavior, leading to violations of the eigenstate thermalization hypothesis (ETH) [25], which is in turn closely related to the quantum many body scar states [42, 43].

Motivated by these exciting progresses, we study how the LY zeros distribute in classical Rydberg atom systems. Here by “classical” we mean that all the terms in the Hamiltonian commute with each other, yet the Hilbert space is still constrained by the Rydberg blockade. It turns out that in 1d for any blockade radius the zeros are real (and therefore negative). A proof using elementary techniques is given and some other numerical and analytical results are stated. We then show how the zeros redistribute as the Rydberg blockade interpolates from nearest- to next-nearest-neighbor. Finally, we discuss how such zeros can be experimentally measured in the cold atom settings.
II. RYDBERG BLOCKADE HAMILTONIAN, PARTITION FUNCTION, AND ZEROS

We begin with the classical Rydberg blockade Hamiltonian,

\[ H = -\Delta \sum_i n_i, \]  

where \( n_i = 0, 1 \) is the number of Rydberg excitation on each site \( i \) and \( \Delta \) is the detuning. Generally there is a Rabi oscillation term that couples the ground state and the Rydberg state, which we assume to be small and ignore here. The effect of the Rydberg blockade is taken into account by requiring that no two atoms can be excited within a radius of \( r \), or that there can be at most one Rydberg atom in each consecutive \((r+1)\) sites. For a chain with \( n \) sites and open boundary conditions, the number of different configurations with \( m \) Rydberg atoms, \( F_n^m \), is

\[ F_n^m = \binom{n-r(m-1)}{m} \]

from elementary combinatorics. These coefficients satisfy a recursion relation

\[ F_{n+1}^m = F_n^m + F_{n-r}^{m-1}. \]

To see this, notice that either the \((n+1)\)-th site is unoccupied, in which case one is free to put \( m \) Rydberg atoms in the first \( n \) sites, giving the first term, or the \((n+1)\)-th site is occupied, blocking sites \( n-r+1 \) to \( n \), giving the second term. To proceed we introduce the fugacity \( y = \exp(\beta \Delta) \), and the partition function is

\[ Z_n(y) = \sum_{m=0}^{\left\lfloor (N-1)/(r+1) \right\rfloor} F_n^m y^m, \]

where \( \lfloor \cdot \rfloor \) denotes the floor function. The partition function in turn satisfies

\[ Z_{n+1}(y) = Z_n(y) + y Z_{n-r}(y), \]

with initial conditions

\[ Z_n(y) = 1 + ny, \quad 1 \leq n \leq r+1. \]

From now on we deem \( y \) as a complex variable and explore the complex roots (zeros) of the partition function as a polynomial in \( y \). The first main result we obtain is

**Proposition 1.** For any \( r, n \), all the zeros of the partition function as a polynomial of \( y \) are real and negative.

The proof is elementary yet slightly involved and is presented in the next section. Some other results are summarized in Sec. IV.

III. PROOF OF PROPOSITION 1

The main idea of the proof is as follows, which is similar to the one given in [12]: for any fixed \( r \), we already know that the partition function is a polynomial of degree \( \lfloor (n-1)/(r+1) \rfloor + 1 \). That is, as \( n \) increases, the first \((r+1)\) polynomials have degree one, the next \((r+1)\) ones degree two, and so on. The claim is proved by finding \( \lfloor (n-1)/(r+1) \rfloor + 1 \) real roots of the polynomials in each group. This follows from the following lemma.

**Lemma 1.** For each \( i \geq 0 \) and \( j = 1, \ldots, r+1 \), the \( i+1 \) roots of \( Z_n=(r+1)_{i+j}(y) \) are real and different. Furthermore, when they are ordered by \( 0 > y_{1,n} > y_{2,n} > \cdots > y_{i+1,n} \), they satisfy

\[ y_{1,(r+1)i+r+1} > y_{1,(r+1)i+r} > \cdots > y_{1,(r+1)i+1} \]
\[ > y_{2,(r+1)i+r+1} > y_{2,(r+1)i+r} > \cdots > y_{2,(r+1)i+1} \]
\[ > \cdots \]
\[ > y_{i+1,(r+1)i+r+1} > y_{i+1,(r+1)i+r} > \cdots > y_{i+1,(r+1)i+1}. \]

**Proof.** We prove the case \( r = 2 \) for simplicity, see Fig. 1, but the same proof works for any \( r \). The first \( 3 \) polynomials \((i = 0)\) obviously satisfy the lemma. If the lemma is satisfied for \( Z_{3i+1}, Z_{3i+2}, Z_{3i+3} \), from continuity we know the sign of the polynomial in each segment partitioned by the zeros. For example, \( Z_{3i+k}(y) > 0 \) when \( y_{1,3i+k} < y < 0, k = 1, 2, 3 \). We obtain from the recursion relation

\[ Z_{3(i+1)+1}(0) > 0 \]
and
\[
Z_{3(i+1)+1}(y_{1,3i+3}) = Z_{3i+3}(y_{1,3i+3}) + y_{1,3i+3}Z_{3i+1}(y_{1,3i+3}) = y_{1,3i+3}Z_{3i+1}(y_{1,3i+3}) < 0.
\]

Therefore, there exists a zero of \(Z_{3(i+1)+1}\), namely \(y_{1,3(i+1)+1}\), in the open interval \((y_{1,3i+3}, 0)\) by the intermediate value theorem. Similar calculations give the other \(i + 1\) zeros, \(y_{m,3(i+1)+1}\), in the intervals \((y_{m,3i+3}, y_{m-1,3i+3})\), where \(y_{i+2,3i+3} = -\infty\). Next, the zeros of \(Z_{3(i+1)+2}, Z_{3(i+1)+3}\) can be found in the same way, giving inequalities including \(y_{m,3(i+1)+1} < y_{m,3(i+1)+2} < y_{m-1,3i+3}\) and \(y_{m,3(i+1)+1} < y_{m,3(i+1)+2} < y_{m-1,3i+3}\). Combining the results above, we find
\[
y_{m,3(i+1)+1} < y_{m,3(i+1)+2} < y_{m,3(i+1)+3} < y_{m-1,3i+3+1},
\]
which concludes the proof.

**IV. OTHER RESULTS**

It is possible to formally solve the recursion relation in Eq. (5). We first simplify the initial condition by extending \(n\) to negative. One easily sees that
\[
Z_n(y) = 1, \quad -r \leq n \leq 0,
\]
\[
Z_n(y) = 0, \quad -2r \leq n \leq -r - 1.
\]
We then have
\[
Z_n = (1, 0, \cdots, 0) \begin{pmatrix} Z_n & Z_{n-1} \vdots & Z_{n-r-1} \end{pmatrix} \begin{pmatrix} y \end{pmatrix}^{n+r} = (1, 0, \cdots, 0) \begin{pmatrix} 1 & 1 & \cdots & 1 \end{pmatrix} \begin{pmatrix} Z_{-r} & Z_{-r+1} \vdots & Z_{-2r} \end{pmatrix} \begin{pmatrix} y \end{pmatrix}^{n+r} = (1, 0, \cdots, 0) \begin{pmatrix} 1 & 1 & \cdots & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \vdots & 0 \end{pmatrix}.
\]
To proceed we need to diagonalize
\[
A = \begin{pmatrix} 1 & y \\ 1 & 1 \\ \vdots & \vdots \\ 1 & 1 \end{pmatrix},
\]

The characteristic polynomial reads
\[
\lambda^{r+1} - \lambda^r - y = 0.
\]
Assuming all the eigenvalues \(\lambda_i\) to be different, we see that \(A\) is diagonalized by
\[
U = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ \lambda_1^{-1} & \lambda_2^{-1} & \cdots & \lambda_{r+1}^{-1} \\ \lambda_1^{-2} & \lambda_2^{-2} & \cdots & \lambda_{r+1}^{-2} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_1^{-r} & \lambda_2^{-r} & \cdots & \lambda_{r+1}^{-r} \end{pmatrix},
\]
which is a Vandermonde matrix of \(\lambda_i^{-1}\). We arrive at
\[
Z_n = (U \operatorname{diag} \{\lambda_1^{n+r}, \ldots, \lambda_{r+1}^{n+r}\} U^{-1})_{1,1} = \frac{1}{\prod \lambda_i} \sum_i \prod \left(\lambda_i - \lambda_j^{-1}\right).
\]
For \(r = 1\), or nearest-neighbor blockade, \(\lambda_{1,2} = (1 \pm \sqrt{1+4y})/2\),
\[
Z_n = \frac{\lambda_1^{n+2} - \lambda_2^{n+2}}{\lambda_1 \lambda_2 (\lambda_1^{-1} - \lambda_2^{-1})} = \frac{\lambda_1^{n+2} - \lambda_2^{n+2}}{\lambda_1 - \lambda_2} = \frac{1}{\sqrt{4y + 1}} \times \left(\frac{1 + \sqrt{4y + 1}}{2}\right)^{n+2} - \left(\frac{1 - \sqrt{4y + 1}}{2}\right)^{n+2}.
\]
To find the zeros we set \(Z_n(y) = 0\) and get
\[
\left(\frac{1 + \sqrt{4y + 1}}{1 - \sqrt{4y + 1}}\right)^{n+2} = 1.
\]
It’s straightforward to find
\[
y = -\frac{1 + \tan^2(\phi/2)}{4},
\]
where
\[
\phi = 2\pi m/(n + 2), m = 1, \cdots, [(n + 1)/2],
\]
which is real, negative and always smaller than \(-1/4\).

Looking back at the characteristic polynomial Eq. (14), we note that as \(y\) goes from 0 to \(-\infty\), there is a value of \(y\) at which the number of real roots of Eq. (14) changes. To find this point we set \((d/d\lambda)(\lambda^{r+1} - \lambda^r) = 0\), or \(\lambda = r/(r+1)\), and correspondingly \(y_0 = -r^r/(r + 1)^{r+1}\). Indeed, we have the following result.

**Proposition 2.** All the zeros of the partition function as in Proposition 1 are smaller than \(y_0\).

**Proof.** We only need to prove that when \(y_0 \leq y < 0\), \(Z_n(y)\) is always greater than zero. We prove it by showing a stronger condition,
\[
\frac{Z_{n+1}}{Z_n} > \frac{r}{r+1}.
\]
This obviously holds for \( Z_n, n = -r, \cdots, -1 \). Assume this to be true for \( Z_n, n = i, \cdots, i + r - 1 \), then
\[
\frac{Z_{i+r}}{Z_i} > \left(\frac{r}{r + 1}\right)^r.
\] (22)

The recursion relation gives
\[
\frac{Z_{i+r+1}}{Z_{i+r}} = 1 + y \frac{Z_i}{Z_{i+r}} > 1 + y \left(\frac{r + 1}{r}\right)^r.\] (23)

Then we have
\[
\frac{Z_{i+r+1}}{Z_{i+r}} > \frac{r}{r + 1} \Leftrightarrow 1 + y \left(\frac{r + 1}{r}\right)^r \geq \frac{r}{r + 1} \Leftrightarrow y \geq y_0.
\] (24)

We also have the following corollary:

**Corollary 1.** For \( y_0 \leq y < 0 \), we have \( Z_n(y) \to 0 \) as \( n \to \infty \).

**Proof.** Using the recursion relation and Proposition 2, we have
\[
\frac{Z_{n+1}(y)}{Z_n(y)} = 1 + y \frac{Z_{n-r}(y)}{Z_n(y)} < 1.
\] (25)

Thus, \( Z_n \) decreases monotonically with index \( n \). By realizing
\[
\frac{Z_{n-r}(y)}{Z_n(y)} > 1,
\] (26)

Eq. (25) can be made stronger
\[
\frac{Z_{n+1}(y)}{Z_n(y)} = 1 + y \frac{Z_{n-r}(y)}{Z_n(y)} < 1 + y.\] (27)

At last, the squeeze theorem gives
\[
\lim_{n \to \infty} Z_n(y) = 0, \forall y \in [y_0, 0].
\] (28)

**V. FROM NEAREST- TO NEXT-NEAREST-NEIGHBOR BLOCKADE**

We wish to understand how the zeros redistribute as the blockade radius increases, and to begin with we focus on the case \( r = 1 \) to \( r = 2 \), or nearest- to next-nearest-neighbor blockade. For this purpose we add a next-nearest-neighbor interacting term to the \( r = 1 \) Hamiltonian and the new Hamiltonian reads
\[
H = -\Delta \sum_i n_i + V \sum_i n_in_{i+2}.
\] (29)

The partition function is then
\[
Z = \sum_n y^n \sum_{\{n_i\}} \exp(-\beta V \sum_i n_in_{i+2}).
\] (30)

We numerically calculate the zeros for \( N = 24, 36 \). While for negative \( V \) the zeros are in general complex, we find that when \( V \) is positive the zeros are real. There is a sharp difference between the distributions of the largest \( N/3 \) zeros and the others: the former approach that of the \( r = 2 \) result, while the latter decrease to \( -\infty \) exponentially. The results for \( N = 36 \) are shown in Fig. 2.

**VI. EXPERIMENTAL MEASUREMENT OF THE LY ZEROS**

Amenability to individual manipulations and measurements empowers cold Rydberg atoms as an ideal platform to measure LY zeros experimentally. Here we propose a setup similar to those in [23, 24] where the zeros can be measured dynamically.

We first assemble atoms (system, denoted by s) uniformly on a circle, either to a C-shaped arc for open boundary condition or an O-shaped circle for periodic boundary condition, with detuning \( \Delta \) and inverse temperature \( \beta \), see Fig. 3(a, b). Then we put a probe (denoted by p) atom on the axis of the circle, not necessarily in the same plane as the circle to allow for more general couplings while maintaining a homogeneous one-to-all in-
Motivated by the recent advances in cold Rydberg atom experiments, we study LY zeros in one-dimensional classical Rydberg blockade systems. We prove that for general blockade radii the LY zeros are real and numerically find that they keep being so when one turns on a next-nearest-neighbor repulsive interaction to interpolate between the nearest- and next-nearest-neighbor blockades. These results can be experimentally verified by coupling the system to a probe atom and performing dynamical measurements thereon.

VII. CONCLUSIONS

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