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Original citation & hyperlink:
Krasnytska, K. , Berche, B. , Holovatch, Y. and Kenna, R. (2015) Violation of Lee-Yang circle theorem for Ising phase transitions on complex networks. EPL, volume 111 (6)
http://dx.doi.org/10.1209/0295-5075/111/60009

DOI 10.1209/0295-5075/111/60009
ISSN 0295-5075

Publisher: IOP

Violation of Lee-Yang circle theorem for Ising phase transitions on complex networks

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PACS 05.50.+q – Lattice theory and statistics (Ising, Potts, etc.)
PACS 64.60.aq – Networks
PACS 64.60F- – Equilibrium properties near critical points, critical exponents

Abstract –The Ising model on annealed complex networks with degree distribution decaying algebraically as $p(K) \sim K^{-\lambda}$ has a second-order phase transition at finite temperature if $\lambda > 3$. In the absence of space dimensionality, λ controls the transition strength; mean-field theory applies for $\lambda > 5$ but critical exponents are λ-dependent if $\lambda < 5$. Here we show that, as for regular lattices, the celebrated Lee-Yang circle theorem is obeyed for the former case. However, unlike on regular lattices where it is independent of dimensionality, the circle theorem fails on complex networks when $\lambda < 5$. We discuss the importance of this result for both theory and experiments on phase transitions and critical phenomena. We also investigate the finite-size scaling of Lee-Yang zeros in both regimes as well as the multiplicative logarithmic corrections which occur at $\lambda = 5$.

Due to an abundance of natural and man-made network-like structures [1], phase transitions on complex networks are found in systems ranging from the physical to the sociological and form a fast developing theme of research [2, 3]. Investigations have centered on moments of the partition function and how they scale close to critical points. Inspired by the fundamental theorem of algebra, the Lee-Yang approach, on the other hand, is based upon the zeros of the partition function, which it interrogates directly instead of through its moments [4]. We investigate the Ising model on complex networks through Lee-Yang zeros, to reveal an unexpected feature of importance for theoretical and experimental studies.

For scale-free networks, the probability that a node has degree K decreases for large K as

$$p(K) \sim K^{-\lambda}. \tag{1}$$

Models on such networks have qualitatively similar critical behavior to those on lattice systems. In particular, in the absence of a space dimension d, the exponent λ determines collective behaviour. There are lower and upper critical values of λ for networks, analogous to critical dimensions for lattices. At the upper critical values scaling behaviour is modified by logarithmic corrections, while above them, critical exponents assume mean-field values [5]. (This analogy has limitations; e.g., in complex networks the mean number of second neighbors decreases with increasing λ, while for lattices it increases with dimensionality.) Between the critical values, critical exponents, amplitude ratios and other universal quantities are λ- or d-dependent. For the Ising model, as most models with discrete symmetry group, the lower critical values are $\lambda_{\rm lc} = 3$, $d_{\rm lc} = 1$, while the upper ones are $\lambda_{\rm uc} = 5$ and $d_{\rm uc} = 4$.

From its inception, the Lee-Yang approach profoundly influenced modern-day statistical mechanics [6]. The idea is to generalize the magnetic field to the complex plane and consider the partition function as a polynomial in a related parameter [4]. Fisher extended this idea to the complex temperature plane [7]. The free energy is analytic in regions free from zeros. This is important because phase transitions are manifestations of nonanalyticities. These appear only when the density of zeros accumulate in the thermodynamic limit. Moments such as the susceptibility are directly expressible in terms of partition function zeros which contain all of the thermodynamic information accessible through standard approaches [8]. In particular, critical exponents are determinable through scaling of zeros near the critical point and amplitude ratios from the angle at which they impact onto the real parameter axis.

The full locus of partition function zeros contains additional information. The Lee-Yang theorem states that, under very general conditions, all zeros are purely imaginary in the complex field plane or on the unit circle after a change of variable. This circle theorem was proven for the Ising model on lattices independent of dimensionality d, size, and boundary conditions of the lattice and range of the interactions. It has since been extended to a wider class of regular-lattice models. (For a review see [8].) Recently, the Lee-Yang zeros of an Ising system were experimentally accessed for the first time using an approach which relied crucially on the validity of the circle theorem [9].

The validity or otherwise of the circle theorem for lattice systems is dimensional independent. Given the parallel roles played by λ and d outlined above, one may expect an analogous statement to hold for annealed complex networks. However, here we show that, while the theorem holds for the Ising model on a complex network provided $\lambda \geq \lambda_{\rm uc}$, it fails when $\lambda < \lambda_{\rm uc}$. This represents a striking difference between the $\lambda \geq \lambda_{\rm uc}$ and $\lambda < \lambda_{\rm uc}$ fat-tailed cases and an unexpected difference between models on networks and lattices. The finding has consequences for experimental realizations of Lee-Yang zeros, and therefore for further investigations of phase transitions, on networks. We discuss these consequences after presenting our analysis.

The Hamiltonian of the Ising model on a complex network is

$$-\mathcal{H} = \frac{1}{2}\sum_{l\neq m} J_{lm} S_l S_m + H\sum_l S_l\,. \qquad (2)$$

Here, $S_l = \pm 1$ is a spin variable, H an external magnetic field, the sum $\sum_{l\neq m}$ spans all pairs of N nodes, and the adjacency matrix J_{lm} contains information about the network structure in that $J_{lm}=1$ if the nodes are linked and $J_{lm}=0$ otherwise. In general, the degree $K_l=\sum_m J_{lm}$ varies for different l and may be characterized by a distribution $p(K)$. For annealed networks, the links fluctuate on the same time scale as the spin variables. Therefore the partition function is averaged with respect to the link distribution as well as the Boltzmann distribution [10]. To implement this, each node l is assigned a hidden variable k_l, the distribution of which is given by (1). The probability of a link between nodes l and m is then given by $p_{lm} = k_l k_m/(N\langle k\rangle)$. It is easy to check that the expected node degree value is then $\mathrm{E}[K_l] = \sum_m p_{lm} = k_l$. The above choice for p_{lm} leads to the Hamiltonian (2) with separable interaction.

Applying the Hubbard-Stratonovich transformation, averaging over the spins can be performed exactly, leading to the representation for the partition function,

$$Z_N(T,H) = \int_{-\infty}^{+\infty} \exp\Big\{\frac{-N\langle k\rangle x^2}{2T} + \sum_l \ln\cosh[(xk_l+H)/T]\Big\}dx\,, \qquad (3)$$

having dropped, for clarity, pre-factors insignificant for the purpose of this study.

The sum over nodes l may be rewritten in terms of a suitable integral over k with distribution function $p(k) = c_\lambda k^{-\lambda}$, in which c_λ is a normalizing constant. One obtains [11]

$$Z_N(T,H) = \int_0^{+\infty} e^{-\frac{\langle k\rangle x^2 T}{2}}\left(e^{I^+_\lambda(x)} + e^{I^-_\lambda(x)}\right)dx, \qquad (4)$$

where

$$I^{\pm}_\lambda(x) = c_\lambda \frac{x^{\lambda-1}}{N^{\frac{\lambda-3}{2}}}\int_{\frac{2x}{\sqrt{N}}}^{\infty}\frac{dy}{y^\lambda}\ln\cosh\Big(\pm y + \frac{H}{T}\Big)\,. \qquad (5)$$

This partition function sets the phase diagram of the Ising model on an annealed scale-free network [1,2]. There is no phase transition for $\lambda\leq 3$. For $\lambda>3$ a second-order transition occurs at finite temperature $T_c = \langle k^2\rangle/\langle k\rangle$. In the region $3<\lambda<5$ it is governed by λ-dependent exponents which, in standard notation for the thermal behaviour of the specific heat, magnetization, susceptibility and the field-dependency of the magnetization, are [12]

$$\alpha = \frac{\lambda-5}{\lambda-3},\;\; \beta=\frac{1}{\lambda-3},\;\; \gamma=1,\;\; \delta=\lambda-2\,. \qquad (6)$$

For $\lambda>5$ the exponents attain their usual Ising mean-field values $\alpha=0$, $\beta=1/2$, $\gamma=1$, and $\delta=1/3$ enhanced by the logarithmic corrections at $\lambda=5$. Thus the global variable λ determines the critical behaviour in a manner similar to the space dimensionality for lattice models.

We are interested in the zeros of the partition function (4) at the critical temperature. Substitute $T=T_c$ in (4) and make an asymptotic expansion keeping the leading terms in $1/N$ and H, to find

$$Z(h) = \begin{cases} \int_0^{+\infty} e^{-x^{\lambda-1}}\cosh(hx)dx\,, & 3<\lambda<5,\\ \int_0^{+\infty} e^{-x^4}\cosh(hx)dx\,, & \lambda\geq 5\,. \end{cases} \qquad (7)$$

Here, the H- and N-dependencies are adsorbed in a single variable h, the explicit form for which differs in different regions of λ:

$$h = \begin{cases} H\frac{\langle k\rangle^2}{\langle k^2\rangle}a(\lambda)^{1/(1-\lambda)}N^{\frac{\lambda-2}{\lambda-1}}\,, & 3<\lambda<5,\\ H\frac{\langle k\rangle^2}{\langle k^2\rangle}\Big(\frac{24}{\ln N}\Big)^{1/4}N^{3/4}\,, & \lambda=5,\\ H\frac{\langle k\rangle^2}{\langle k^2\rangle}\Big(\frac{12}{\langle k^4\rangle}\Big)^{1/4}N^{3/4}\,, & \lambda>5\,. \end{cases} \qquad (8)$$

Note that $Z(h)$ is independent of λ when $\lambda\geq 5$. In particular, the logarithmic corrections at $\lambda=5$ reside in the form of h in the middle expression of (8). Therefore, working in terms of the reduced variable h, the loci of partition function zeros for $\lambda=5$ and $\lambda>5$ are the same. For $\lambda<5$ the values of the coefficients

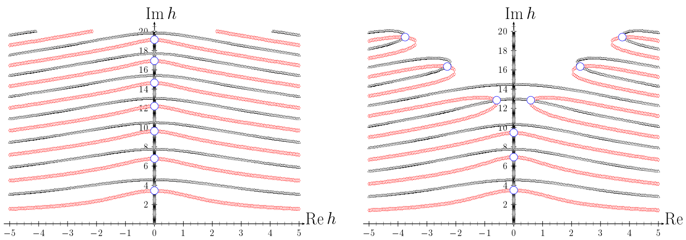

Fig. 1: Solutions of the system of equations Re $Z(h)=0$ (diamonds, red online) and Im $Z(h)=0$ (triangles, including along the imaginary axis) for the partition function (7) when $\lambda \geq 5$ (left) and $\lambda = 4.5$ (right). The Lee-Yang zeros are given by the intersections of contours of different types and are denoted by circles (blue online). All zeros are imaginary only when $\lambda \geq 5$.

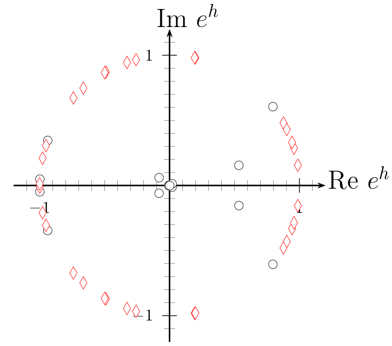

Fig. 2: Lee-Yang zeros in the complex e^h-plane. The diamonds (red online) correspond to $\lambda \geq 5$ and the circles to $\lambda = 4.5$. The plot depicts only those zeros that fit into the region shown.

$a(\lambda) = -c_\lambda \int_0^\infty dy\, y^{-\lambda}(\ln\cosh y - y^2/2) > 0$ can be found numerically and are listed in [13].

Let us now consider the partition function (7) in complex magnetic field $h = \text{Re } h + i \text{ Im } h$. We are interested in its zeros h_j at the critical point. The index j identifies the sequence of zeros relative to the origin in the upper half-plane with $j = 1$ identifying zero closest to $h = 0$. Increasing N, the zeros approach the origin and their scaling at criticality is governed by the exponent σ [14]:

$$H_j(N) \sim \left(\frac{j}{N}\right)^\sigma . \tag{9}$$

Comparing (8) and (9) one finds

$$\sigma = \begin{cases} \frac{\lambda-2}{\lambda-1}, & 3 < \lambda \leq 5, \\ 3/4, & \lambda \geq 5. \end{cases} \tag{10}$$

Therefore, σ becomes λ-dependent in the region $3 < \lambda < 5$, similar to the other critical exponents (6). Moreover, the validity of the scaling relation $\sigma = \beta\delta/(2-\alpha)$ is verified [14]. Also, from (8), a logarithmic correction appears in the marginal case $\lambda = 5$: $H_j \sim N^{-3/4}(\ln N)^{1/4}$. Again, the power of the logarithm complies with the corresponding scaling relation [15].

The contours in Fig. 1 depict curves in the complex plane along which the real and imaginary parts of the partition functions (7) vanish at $T = T_c$ for $\lambda \geq 5$ and $3 < \lambda < 5$, exemplified by $\lambda = 4.5$. Note that Im$Z(h)$ vanishes when h itself is imaginary because the partition function is an even function of h. The intersections of the different contours give the locations of the Lee-Yang zeros. When $\lambda \geq 5$ all zeros plotted are on the imaginary axis. But for $\lambda = 4.5$ only the first three zeros are imaginary and zeros of higher order (h_j for $j > 3$) have non-vanishing real parts. This type of behaviour is found for all other values of λ in the region $3 < \lambda < 5$; there is a finite number, $\mathcal{N}$, such that h_j is imaginary for $j \leq \mathcal{N}$ and has non-vanishing real part for $j > \mathcal{N}$. Moreover, $\mathcal{N}$ decreases with decreasing λ. The numerically determined values of Lee-Yang zeros are listed in Table 1 for various values of $\lambda < \lambda_{\text{uc}} = 5$, and for $\lambda \geq 5$. When $\lambda = 4$, $\mathcal{N} = 2$ while for $\lambda = 3.5$, $\mathcal{N} = 1$.

The picture is reaffirmed in Fig. 2 which demonstrates that the circle theorem holds in the complex e^h-plane for the Ising model on the annealed scale-free network for $\lambda \geq 5$. However it does not hold for $\lambda < 5$, where only a few low index zeros lie on the unit circle, the rest being scattered on the complex plane.

Thus, while our numerical examples hint that the Lee-Yang theorem holds for $\lambda \geq 5$, we have established the surprising result that it does not hold when $\lambda < 5$. To gain analytical insight, we can determine an asymptotic form for the partition function (7) when Re $h = 0$ in the limit of large Im h. We employ the Erdelyi lemma; if

$$F(y) = \int_0^a x^{\beta-1} f(x) e^{iyx^\alpha} dx, \tag{11}$$

where $\alpha \geq 1$, $\beta > 0$ and the function $f(x)$ together with all derivatives vanishes at the upper integration limit, the large-y asymptotic behaviour is [16]

$$F(y) \sim \sum_{k=0}^\infty a_k y^{-\frac{k+\beta}{\alpha}}, \tag{12}$$

where $a_k = \frac{f^k(0)}{k!\alpha}\Gamma\left(\frac{k+\beta}{\alpha}\right)\exp\left[\frac{i\pi(k+\beta)}{2\alpha}\right]$. Putting $h = ir$ one can represent the partition function for $3 < \lambda < 5$ in the form (11):

$$Z(ir) = \frac{5}{\lambda-1}\text{Re } \int_0^\infty x^{\frac{5}{\lambda-1}-1} e^{-x^5} e^{irx^{5/(\lambda-1)}} dx . \tag{13}$$

From (12), the asymptotic expansion is

$$Z(ir) \sim (\lambda-1)\sum_{k=0}^\infty b_k r^{-\frac{k(\lambda-1)}{5}-1}, \qquad r \to \infty, \tag{14}$$

with coefficients

$$b_k = \frac{f^k(0)}{5k!}\Gamma\left[\frac{k(\lambda-1)}{5}+1\right]\cos\left[\frac{\pi(k(\lambda-1)+5)}{10}\right]. \tag{15}$$

Table 1: The first five zeros h_j for different values of λ.

	$\lambda \geq 5$	$\lambda = 4.5$	$\lambda = 4$	$\lambda = 3.5$
$j = 1$	$i3.495$	$i3.495$	$i3.569$	$i3.762$
$j = 2$	$i6.784$	$i6.933$	$i7.823$	$1.875 + i7.212$
$j = 3$	$i9.636$	$i9.474$	$2.418 + i11.466$	$3.659 + i9.496$
$j = 4$	$i12.229$	$0.589 + i12.848$	$4.014 + i14.174$	$5.138 + i11.351$
$j = 5$	$i14.650$	$2.297 + i16.346$	$5.446 + i16.574$	$6.435 + i12.983$

The asymptotics for the $\lambda \geq 5$ partition function (7) can be evaluated by steepest descent, leading to

$$Z(ir) \sim \exp\left[-\frac{3}{2}\left(\frac{r}{4}\right)^{\frac{4}{3}}\right]\cos\left[\frac{3\sqrt{3}}{2}\left(\frac{r}{4}\right)^{\frac{4}{3}}\right], \quad r \to \infty, \ \lambda \geq 5. \qquad (16)$$

The trigonometric function in (16) ensures the partition function alters in sign as a function of r. This signals that it vanishes on the imaginary axis for large (infinite) values of r, suggesting that $\mathcal{N}$ is infinite. If the pattern of zeros observed in Fig.1 is generic in that h_j has a non-vanishing real part only when $j > \mathcal{N}$, this indicates that all zeros are on the imaginary-h axis, suggesting that the Lee-Yang circle theorem is obeyed in the complex fugacity plane.

In Fig. 3 we compare numerically calculated absolute values of the integral $|Z(ir)|$ (7) with its asymptotic expansions (14) and (16) for different λ. The behaviour for $\lambda \geq 5$ is qualitatively different from that at $\lambda < 5$: whereas in the former case the function oscillates even in the asymptotic regime (meaning that the number of zeros is unbounded), this is not the case for $\lambda < 5$. There, after a finite number of oscillations the function approaches its asymptotic, bounding the regime of zeros. Moreover, the number of oscillation decreases with decreasing λ.

In summary, besides delivering finite-size scaling, we found an unexpected result for the locus of Lee-Yang zeros for the Ising model on annealed scale-free networks, namely, while the circle theorem is obeyed for $\lambda \geq \lambda_{\rm uc} = 5$, it fails for $\lambda < \lambda_{\rm uc} = 5$. This is surprising because it means that the similarity between roles played by λ (for complex networks) and d (for regular lattices), which control universal aspects of phase transitions, do not extend to the fundamental Lee-Yang level.

Recently Peng et al. related imaginary magnetic fields associated with a bath of Ising spins to the quantum coherence of a probe [9]. This allowed them to identify the experimentally obtained times at which the quantum coherence disappears as imaginary Lee-Yang zeros. This demonstration of a physical manifestation of Lee-Yang zeros is important at a fundamental level and points to new, experimental ways of studying zeros in many-bodied materials. However, an identification of the type made in [9] relies crucially on the Lee-Yang theorem in that it can only be made for imaginary zeros [17]. The results herein show that while these are accessible for lattices and complex networks for sufficiently large λ, not all network zeros are accessible in this manner for $\lambda < 5$. A challenge for experiment is to find another way to access them.

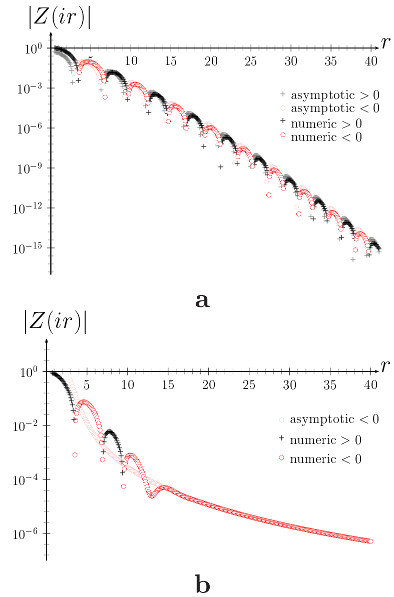

Fig. 3: Numerically calculated absolute values of the partition function along the imaginary axis: $|Z(ir)|$ with $r = \mathrm{Im}\, h$. The asymptotic expansions using Eq. (14) and (16) in the limit $r \to \infty$ are also plotted. The symbols "+" indicate $Z(ir) > 0$ (black and gray online correspondingly) and circles indicate $Z(ir) < 0$ (red and pink red online). Panel (a) is for $\lambda \geq 5$ and Panel (b) for $\lambda = 4.5$. The number of zeros is finite for $\lambda < 5$.

Finally we address the question of why the theorem is obeyed for some but not all values of λ. It was proven [18] that the theorem holds for any Ising-like model with ferromagnetic interactions. One may therefore anticipate that the Hamiltonian (2) for a single network realization should have the Lee-Yang property, since the adjacency matrix elements J_{ij} are non-negative. However, averaging over an ensemble of networks amounts to taking a sum (or integral) of functions and there is no guarantee for $\lambda < 5$ that the zeros of the sum preserves the property. Indeed, one can consider heuristically the Landau free energy for scale-free networks, $F(M) \sim M^2 + M^{\lambda-1} + M^4 + \ldots$ [19]. When $\lambda < 5$ the second term on the right is dominant for small order parameter M, delivering λ-dependent critical exponents. The partition function is also λ-dependent and its zeros are complex. When $\lambda > 5$, however, the first term on the right dominates. This leads to mean-field critical behaviour which is independent of λ. Since mean-field theory obeys the Lee-Yang theorem, so too must averaged annealed complex networks with $\lambda > 5$.

Acknowledgements. – This work was supported in part by FP7 EU IRSES projects No.269139 (DCP-PhysBio), No. 295302 (Spider), IIF Project No.300206 (RAVEN), and by the Collège Doctoral "Statistical Physics of Complex Systems" Coventry-Leipzig-Lviv-Nancy. We thank Yuri Kozitsky, Taras Krokhmalskii, Jean-Yves Fortin and Nikolay Izmailian for comments and discussions.

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