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## Probing Yang–Lee edge singularity by central spin decoherence

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## PAPER

## Probing Yang–Lee edge singularity by central spin decoherence

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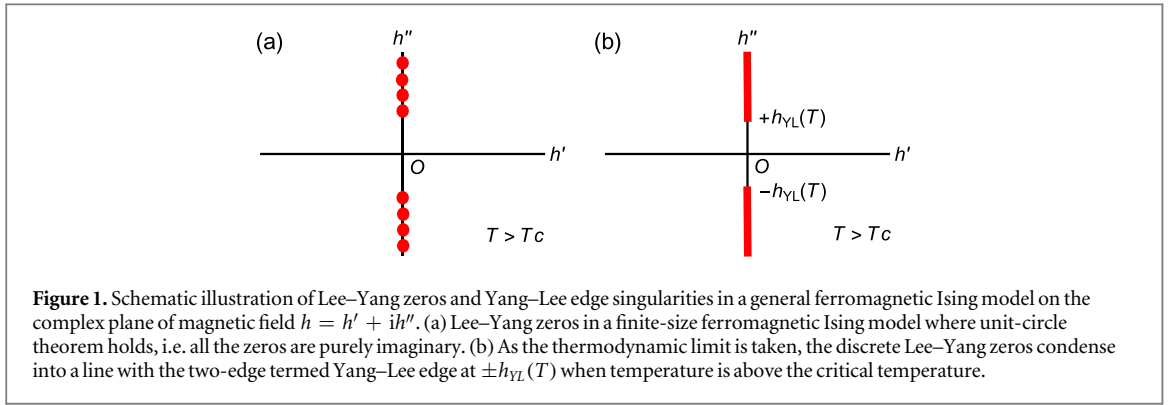
## Abstract

Yang–Lee edge singularities are the branch point of free energy on the complex plane of physical parameters and have been shown to be the simplest universality class of phase transitions. However, Yang–Lee edge singularities have not been regarded as experimentally observable since they occur at complex physical parameters which are unphysical. A recent discovery regarding the relation between partition functions and probe spin coherence makes it experimentally feasible to access the complex plane of physical parameters. However, how to extract the critical point and the critical exponent of Yang–Lee edge singularities in many-body systems, which occurs only at the thermodynamic limit, has still been elusive. Here we show that the quantum coherence of a probe spin coupled to finite-size Ising-type spin systems presents universal scaling behavior near the Yang–Lee edge singularity. The finite-size scaling behavior of the quantum coherence of the probe spin predicts that one can extract the critical point and the critical exponent of the Yang–Lee edge singularity of an Ising-type spin system in the thermodynamic limit from the spin coherence measurement of the probe spin coupled to finite-size Ising-type spin systems. This finding provides a practical approach to studying the nature of Yang–Lee edge singularities of many-body systems.

In 1952, Yang and Lee [1, 2] initiated the examination of phase transitions by studying the partition function zeros, termed Lee–Yang zeros, on the complex plane of a magnetic field  $h$  (or fugacity  $z$  for fluids). They found that for a system above its critical temperature  $T_c$ , the partition function must be nonzero throughout some neighborhood of the real axis of the magnetic field within a gap determined by two edges at  $\pm h_{YL}(T)$ . Therefore the free energy is an analytic function of the real magnetic field. On the other hand, below the critical temperature  $T_c$ , the Lee–Yang zeros will come arbitrarily to the real axis as the thermodynamic limit is taken, destroying the analyticity of the free energy in  $h$  for those real fields at which the Lee–Yang zeros accumulate.

Kortman and Griffiths [3] pointed out that the edges of Lee–Yang zeros of a many-body system in the thermodynamic limit are singularity points, termed Yang–Lee edge singularities [4]. Fisher [4] proposed that the Yang–Lee edge singularity could be considered as a new second order phase transition point with associated critical exponents. Renormalization group analyses [4] show that the Yang–Lee edge singularity is associated with an  $i\varphi^3$  theory and the crossover dimensionality of the Yang–Lee edge singularity is  $d_c = 6$ . Later, the investigation of the Yang–Lee edge singularity has been extended to many other models, such as the classical  $n$ -vector model [5], the quantum Heisenberg model [5], the spherical model [6], the quantum one-dimensional (1D) transverse Ising model [7], the hierarchical model [8], branched polymers [9], the directed-site animals-enumeration problem [10], Ising models on fractal lattices [11], Ising systems with correlated disorder [12], fluid models with repulsive-core interactions [13], the antiferromagnetic Ising model [14] etc. A comprehensive review of the study of Yang–Lee edge singularities can be found in [15, 16]. Recently, Kibble–Zurek scaling was shown to appear at the Yang–Lee edge singularity [17], which supports that the Yang–Lee edge singularity is similar to conventional second order phase transitions.

Yang–Lee edge singularity occurs in the ferromagnetic Ising models above its critical temperatures in a purely imaginary magnetic field  $ih''$  (figure 1). For  $h'' > h_{YL}(T)$ , the partition function acquires zeros, which becomes dense on the line with  $\Im h > h_{YL}(T)$ . The density of Lee–Yang zeros  $g(T, h'')$  in the thermodynamic limit behaves as  $g(T, h'') \sim |h'' - h_{YL}(T)|^\sigma$  when  $h'' \rightarrow h_{YL}(T)$  from above, with  $\sigma$  being the universal critical



exponent of the Yang-Lee edge singularity. Fisher showed that [18] for 1D systems with classical finite range interactions, the critical exponent of Yang-Lee edge singularity takes a universal value  $\sigma = -1/2$ , independent of the temperature and the details of the Hamiltonian. Cardy showed that [19]  $\sigma = -1/6$  for a Yang-Lee edge singularity in two-dimensional (2D) systems. The exponent  $\sigma = 1/2$  for dimensionality  $d \geq d_c$  [4]. From the density of Lee-Yang zeros, we know that the free energy density near the Yang-Lee edge [15, 16] behaves as  $f(T, h'') \sim A_{\pm} |h'' - h_{YL}(T)|^{\sigma+1}$  where the amplitudes  $A_{\pm}$  may depend on the sign of  $h'' - h_{YL}(T)$ . It follows that the susceptibility,  $\chi \sim \partial^2 f / \partial h^2$  diverges with an exponent  $\gamma = 1 - \sigma$ . The correlation function of two spins with distance  $R$  apart near the Yang-Lee edge singularity for an Ising-type system behaves as  $G(R, T, h'') \sim D(R\tilde{h}'') / R^{d-2+\eta}$  when  $\tilde{h}'' \equiv h'' - h_{YL}(T) \rightarrow 0$  and  $R \rightarrow \infty$ . Similarly, hyperscaling relations,  $\sigma = (d - 2 + \eta) / (d + 2 - \eta)$  and  $\gamma = 2(2 - \eta) / (d + 2 - \eta)$  are verified up to upper critical dimension  $d_c = 6$  [4–6].

Although Yang-Lee edge singularities appear ubiquitous in many-body systems, experimental observation of Yang-Lee edge singularities has, however, not been achieved before. Previous experiments could only indirectly derive the densities of Lee-Yang zeros from susceptibility measurements plus analytic continuation [20, 21]. The difficulty is intrinsic: Yang-Lee edge singularities would occur only at complex values of external fields, which are unphysical. A recent theoretical discovery [22] about the relation between partition functions and probe spin coherence makes it experimentally feasible to access the complex plane of physical parameters and more generally the thermodynamic on the complex plane [23, 24]. Wei and Liu [22] found that the quantum coherence of a central spin embedded in an Ising-type spin bath is equivalent to the partition function of the Ising spin bath under a complex magnetic field. Then the Lee-Yang zeros of the partition function are one-to-one mapped to the zeros of the central spin coherence, which are directly measurable. This leads to the first experimental observation of Lee-Yang zeros [25, 26]. However, how to locate the critical points and the critical exponents of the Yang-Lee edge singularity, which occurs in the thermodynamic limit of a many-body system, has remained elusive.

In this paper we show that the quantum coherence of the probe spin coupled to a finite-size many-body system presents universal scaling behavior around the Yang-Lee edge singularity. The universal finite-size scaling of the quantum coherence of the probe spin predicts the critical point and the critical exponent of the Yang-Lee edge singularity accurately and systematically. By measuring the quantum coherence of the probe spin which is coupled to finite-size systems, one can extract the critical point and the critical exponent of the Yang-Lee edge singularity of an infinite system and verify the universality of the Yang-Lee edge singularity.

Let us consider a general Ising model with ferromagnetic interactions  $J_{ij} \geq 0$  under a magnetic field  $h$ . The Hamiltonian is

$$H(h) = -\sum_{i,j} J_{ij} s_i s_j - h \sum_j s_j \equiv H_0 + hH_1, \quad (1)$$

where the spins  $s_j$  take values  $\pm 1$ . We use a probe spin-1/2 coupled to the Ising system (bath), with probe-bath interaction  $H_I = -\lambda S_z \otimes \sum_j s_j \equiv \lambda S_z \otimes H_1$  and  $\lambda$  being a coupling constant and  $S_z \equiv (|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|) / 2$  being the Pauli matrix of the probe spin. If we initiate the probe spin in a superposition state as  $(|\uparrow\rangle + |\downarrow\rangle) / \sqrt{2}$  and the bath at inverse temperature  $\beta = 1/T$  described by  $\rho_0 = e^{-\beta H} / Z(\beta, h)$  with  $Z(\beta, h) = \text{Tr}[e^{-\beta H}]$  being the partition function. Then the quantum coherence of the probe spin, defined as  $L(t) = \langle S_x \rangle + i \langle S_y \rangle$ , has the intriguing form of [22, 23]

$$L(t) = \frac{Z(\beta, h - it\lambda/\beta)}{Z(\beta, h)}. \quad (2)$$

The denominator in the above equation is nonzero for real magnetic field and temperature. The numerator resembles the form of a partition function but with a complex magnetic field  $h - it\lambda/\beta$ . The probe spin coherence in a finite system vanishes whenever  $h - it\lambda/\beta$  reaches a Lee-Yang zero. Particularly for Ising ferromagnets, the Lee-Yang zeros all lie on the unit circle, the  $n$ th Lee-Yang zeros  $h_n = ih_n''$ ,  $n = 1, 2, \dots, N$ ,

and therefore are mapped to the probe spin coherence zeros ( $t_n$ ) for vanishing external field ( $h = 0$ ), with the correspondence relation  $t_n = h_n''/\lambda$ . This leads to the first experimental observation of Lee–Yang zeros [25, 26].

To probe Yang–Lee edge singularities, which occurs only at the thermodynamic limit, is non-trivial because any realistic experiment is always performed on finite-sized samples. To extract the properties of an infinite system from the experimental data for finite-sized systems, one needs to employ the finite-size scaling technique invented by Fisher and Barber [27]. The central idea of finite-size scaling is that the physical observable of a finite-sized system with spatial extent characterized by a length  $N$  only depends on the universal ratio  $N/\xi$  with  $\xi$  being the correlation length of the infinite system. Finite-size scaling has been an important tool for the understanding and development of statistical mechanics of systems which are close to a critical point [28] and was later shown to be a natural consequence of renormalization group theory [29].

Applying the finite-size scaling hypothesis [27] to Yang–Lee edge singularities, the singular part of the free energy density of a finite system  $f_N$  with spatial extension  $N$  presents finite-size scaling behavior,

$$\frac{f_N(\tilde{h})}{f_\infty(\tilde{h})} = \Phi(N/\xi) \quad (3)$$

where  $\tilde{h} = h' + ih'' - h_c(T)$ ,  $h_c(T)$  is the position of the Yang–Lee edge singularity,  $\xi \sim \tilde{h}^{-\nu}$  is the correlation length near the Yang–Lee edge singularity for an infinite system, and  $\Phi(x)$  is a universal scaling function. Because the singular part of the free energy density near the Yang–Lee edge singularity for an infinite system behaves as  $f_\infty(\tilde{h}) \sim \tilde{h}^{\sigma+1}$  [15, 16] and the hyperscaling relation  $\nu = (\sigma + 1)/d$ , the singular part of the free energy density  $f_N$  of a finite system presents finite-size scaling behavior [15, 30],

$$f_N(\tilde{h}) = N^{-d}\tilde{\Phi}(\tilde{h}N^{d/(\sigma+1)}), \quad (4)$$

where  $d$  is the dimensionality of the system,  $\sigma$  is the universal critical exponent associated with the Yang–Lee edge singularity, and  $\tilde{\Phi}(x)$  is a new universal scaling function. The free energy of the system can be written as sum of two parts,  $f = f_s + f_{ns}$  with  $f_s$  being the singular part and  $f_{ns}$  being the non-singular part [31]. This means that the partition function takes a product form of two factors  $Z = Z_s Z_{ns}$  with  $f_{s/ns} \equiv -k_B T \ln Z_{s/ns}$ . Thus the singular part of the partition function is  $Z_s = Z/Z_{ns}$ , which presents universal scaling behavior because it is related to the singular part of the free energy. Note that the non-singular part of the free energy  $f_{ns}$  does not depend on the size for systems with periodic boundary conditions [31–33]. Near the critical point, one can assume that the non-singular part of the free energy  $f_{ns}$  is a constant  $f_0(\beta)$  and then the non-singular part of the partition function is  $Z_{ns} = \exp(-\beta N^d f_0(\beta))$ . The relation between the probe spin coherence and partition function with a complex parameter in equation (2) implies that the rescaled probe spin coherence coupled to an Ising-type spin bath presents finite-size scaling behavior,

$$\tilde{L}(t) = Z_s(\beta, h + i\lambda t/\beta), \quad (5)$$

$$= \frac{Z(\beta, h + i\lambda t/\beta)}{Z_{ns}(\beta, h + i\lambda t/\beta)}, \quad (6)$$

$$= \frac{L(t)Z(\beta, h)}{\exp(-\beta N^d f_0(\beta))}, \quad (7)$$

$$= \tilde{\Psi}((h - i\lambda t/\beta - h_c)N^{d/(\sigma+1)}). \quad (8)$$

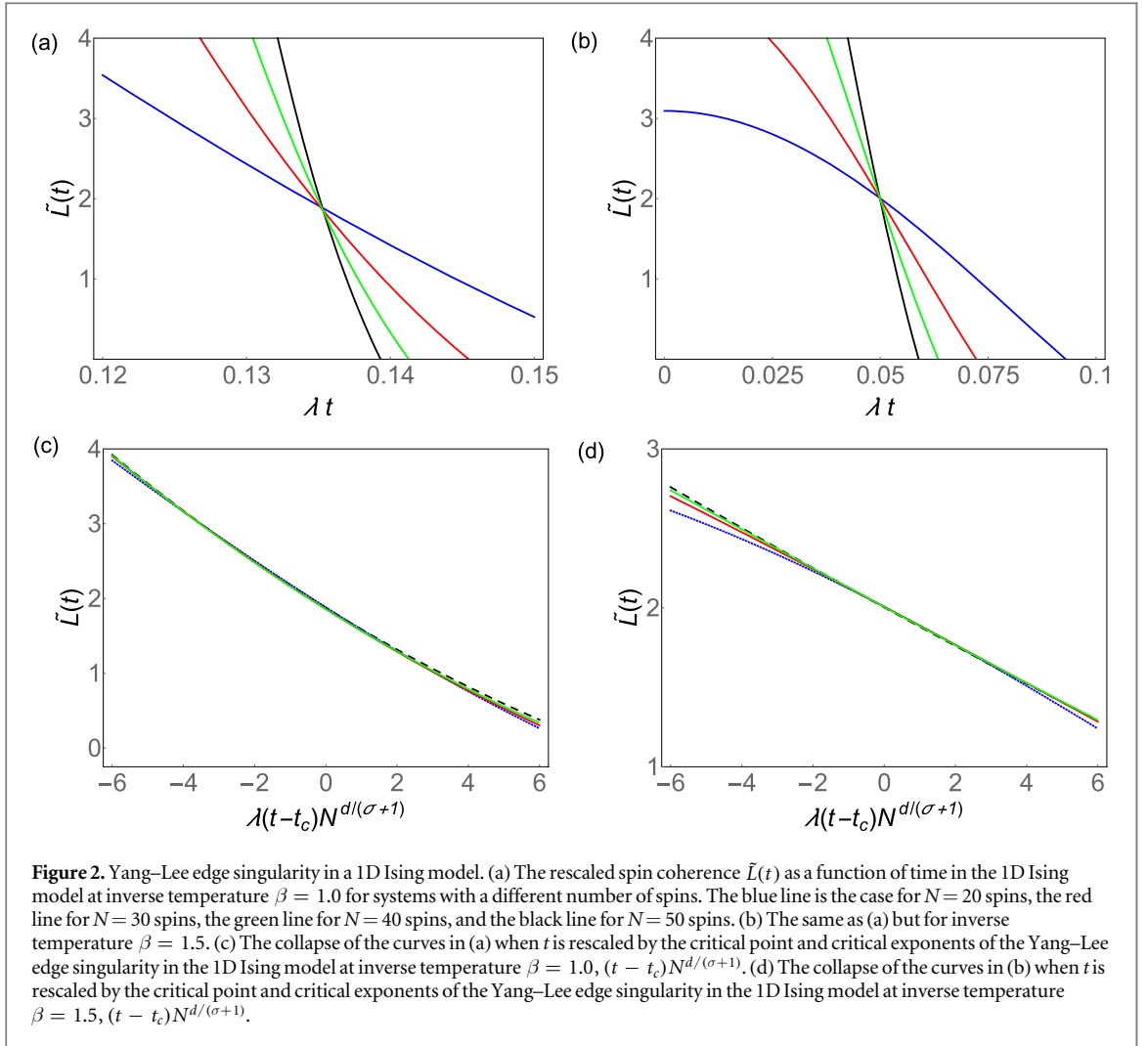
Here  $\tilde{\Psi}(x)$  is a universal scaling function. In particular, for Ising ferromagnets the Yang–Lee edge singularity is purely imaginary  $h_c = ih_{YL}(T)$  and therefore we study the probe spin coherence for the vanishing external field  $h = 0$ . For more general spin models, the Yang–Lee edge singularity may not lie on the imaginary axis [15]. In such a case, one needs to study the probe spin coherence which is coupled to a spin model at a finite magnetic field with the field strength being the real part of the Yang–Lee edge singularity.

According to the finite-size scaling hypothesis, the rescaled probe spin coherence which is coupled to a ferromagnetic Ising-type spin bath at zero magnetic field presents a universal finite-scaling behavior,

$$\tilde{L}(t) = \frac{L(t)Z(\beta, 0)}{\exp(-\beta N^d f_0(\beta))} = \Psi(\lambda(t - t_c)N^{d/(\sigma+1)}). \quad (9)$$

Here  $\Psi(x)$  is a universal scaling function and analytic for finite-sized systems and  $t_c = \beta h_{YL}/\lambda$ . This universal finite-size scaling behavior of quantum coherence is powerful for studying the nature of Yang–Lee edge singularities:

- (1) *Identifying the critical point of the Yang–Lee edge singularity.* If we plot  $\tilde{L}(t)$  as a function of time for systems with different sizes at a fixed temperature  $T$ , all curves cross at  $t = t_c = \beta h_{YL}(T)/\lambda$  if the non-singular part of the free energy  $f_0(\beta)$  is properly chosen and all the curves cross at  $\tilde{L}(t_c) = \Psi(0)$ . From the crossing point of  $\tilde{L}(t)$  for different system sizes with a fixed temperature, we therefore can locate the Yang–Lee edge singularity for an infinite system.



- (2) *Data collapse.* If we draw  $\tilde{L}(t)$  as a function of  $\lambda(t - t_c)N^{d/(\sigma+1)}$ , then the curves for different system sizes collapse around the Yang–Lee edge singularity because  $\Psi(x)$  is a universal scaling function.
- (3) *Extracting the universal critical exponent of the Yang–Lee edge singularity.* Since the universal scaling function  $\Psi(x)$  is an analytic function for finite-sized systems, Taylor expansion of  $\Psi(x)$  around  $x = 0$  in equation (9) leads to

$$\tilde{L}(t) = \Psi(0) + \Psi'(0)\lambda(t - t_c)N^{d/(\sigma+1)} + o(t - t_c)^2. \quad (10)$$

Differentiating both sides of equation (10) with respect to  $\lambda t$  and taking  $t = t_c$ , we obtain

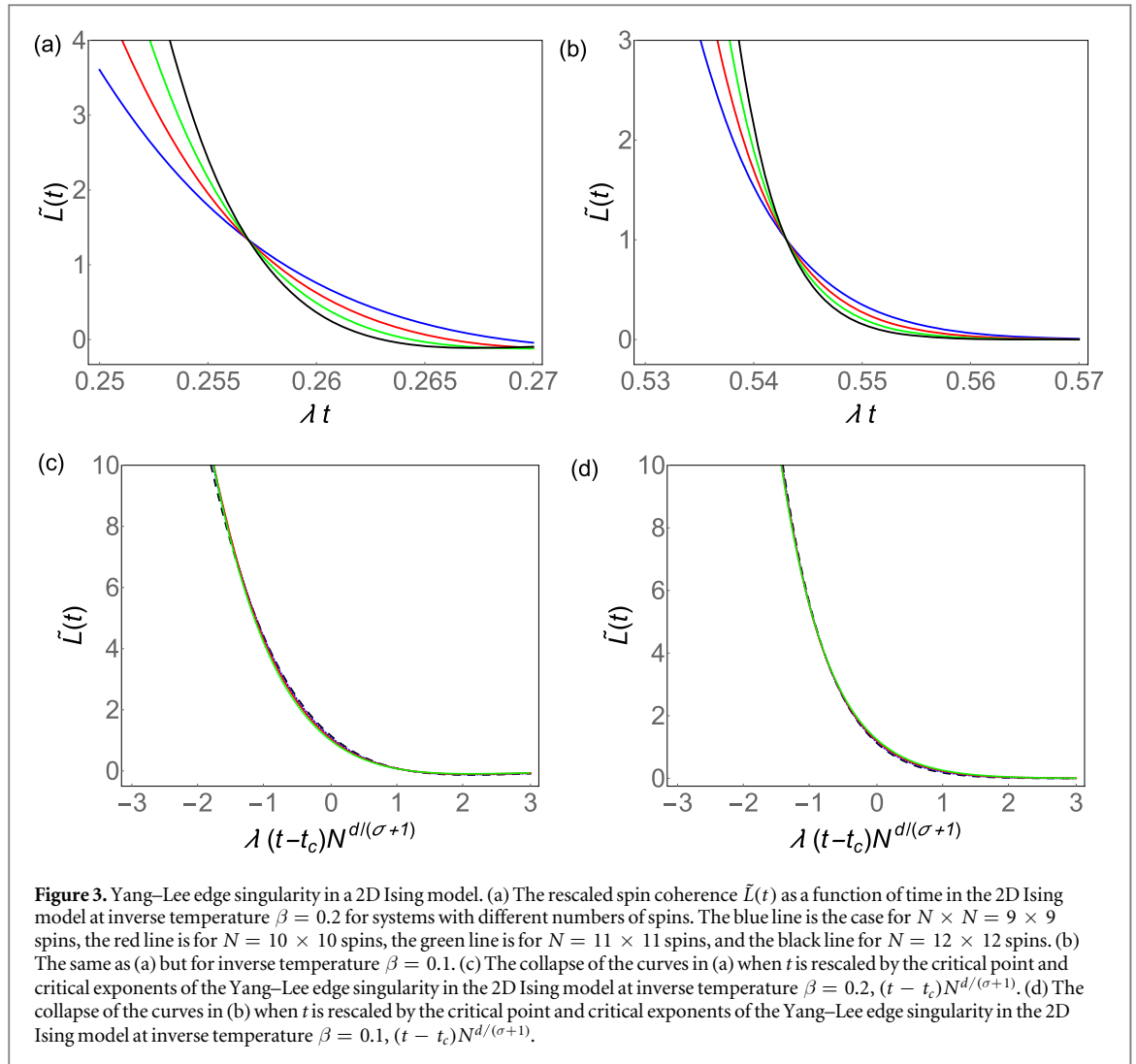
$$\tilde{L}(t_c)' = \Psi'(0)N^{d/(\sigma+1)}. \quad (11)$$

Here  $\tilde{L}(t_c)' \equiv \frac{1}{\lambda} \frac{d\tilde{L}(t)}{dt} \Big|_{t=t_c}$ . Taking a logarithm on both sides of equation (11), we obtain

$$\ln \tilde{L}(t_c)' = \ln(\Psi'(0)) + \frac{d}{\sigma + 1} \ln N. \quad (12)$$

Equation (12) predicts that  $\ln \tilde{L}(t_c)'$  is a linear function of  $\ln N$  with the slope being  $d/(\sigma + 1)$ . Thus we can also extract the critical exponent for Yang–Lee edge singularities from the probe spin coherence measurement for finite-sized systems.

Note that in equation (9), it is not the central spin coherence  $L(t)$  but the rescaled central spin coherence  $\tilde{L}(t)$ , which is equal to the central spin coherence times partition function at zero magnetic field, that presents finite-size scaling behavior. Since the Yang–Lee edge singularity only occurs for temperatures above the critical temperature, one can obtain the partition function at zero magnetic field from the high temperature expansion method [34, 35]. An alternative method to obtain the partition function of a finite system at high temperature is the cluster correlation expansion method [36, 37]. The non-singular part of the partition function near the



Yang–Lee edge singularity can be treated as a constant, independent of magnetic field,  $Z_{\text{ns}}(\beta, i\lambda t/\beta) = \exp(-\beta N^d f_0(\beta))$ .

To illustrate the above idea, we study the 1D Ising model with nearest-neighbor ferromagnetic coupling  $J = 1$  and the periodic boundary condition. The 1D Ising model can be exactly solved through the transfer matrix method [38] and there is no finite temperature phase transition in the 1D Ising model, i.e.  $T_c = 0$ . Figure 2 shows the extraction of the Yang–Lee edge singularity in a 1D Ising model from probe spin coherence measurements. At inverse temperature  $\beta = 1.0$ , which is above the critical temperature of the 1D Ising model, we choose  $f_0$  so that the rescaled probe spin coherence for systems with different sizes  $N = 20, 30, 40, 50$ , cross at point  $t = t_c$  as predicted from finite-size scaling theory (figure 2(a)) and we found that  $f_0(\beta = 1.0) = 0.005$ . From this procedure we obtain an approximate value for  $t_c$ . We then choose different parameters  $t_c$  and  $\sigma$  so that all curves in figure 2(a) for different system sizes collapse around the Yang–Lee edge singularity (figure 2(c)). We found that  $t_c = 0.1354$ ,  $\sigma = -0.491$ . We can see the finite-size predictions match the exact solution  $t_c = \sin^{-1}(e^{-2}) \approx 0.1357$  and  $\sigma = -1/2$  very well. With temperature decreasing but still above the critical temperature, the Yang–Lee edge singularity point moves towards the real axis. As shown in figure 2(b), the rescaled probe spin coherence for different system sizes  $N = 20, 30, 40, 50$  at inverse temperature  $\beta = 1.5$  cross at one point when we choose  $f_0(\beta = 1.5) = 0.001$ . Then we choose  $t_c$  and  $\sigma$  so that all curves in figure 2(b) collapse (figure 2(d)). We found that  $t_c = 0.0499$  and  $\sigma = -0.492$ , which agree well with the exact solution  $t_c = \sin^{-1}(e^{-3}) \approx 0.0498$  and  $\sigma = -1/2$ . Thus it is feasible to extract the critical point and the universal critical exponent of Yang–Lee edge singularities from central spin coherence measurements.

We further study the 2D Ising model with nearest-neighbor ferromagnetic coupling  $J = 1$  and the periodic boundary condition. The 2D Ising model has been exactly solved by Onsager in 1944 [39] and there is a finite temperature phase transition at  $\beta_c = \ln(1 + \sqrt{2})/2$  [39]. For the 2D Ising model under a finite magnetic field, there is no exact solution available but one can map the problem into a 1D quantum Ising model with both a longitudinal and transverse field using the transfer matrix method [40]. Figure 3 shows the extraction of the

Yang–Lee edge singularity in the 2D Ising model from central spin coherence measurements. At inverse temperature  $\beta = 0.2$ , which is above the critical temperature of the 2D Ising model, the rescaled probe spin coherence data for different systems sizes  $N \times N = 9 \times 9, 10 \times 10, 11 \times 11, 12 \times 12$ , respectively, cross at one point (figure 3(a)) when we choose  $f_0(\beta = 0.2) = -3.010$ . We then choose  $t_c$  and  $\sigma$  so that all curves in figure 3(a) collapse perfectly (figure 3(c)). We found that  $t_c = 0.2571$  and  $\sigma = -0.151$ . One can see that the estimated value is close to the exact value  $\sigma = -1/6 \approx -0.167$ . The Yang–Lee edge singularity point moves away from the real axis as temperature increases. We show  $\tilde{L}(t)$  as a function of time for different system sizes,  $N \times N = 9 \times 9, 10 \times 10, 11 \times 11, 12 \times 12$ , respectively, at inverse temperature  $\beta = 0.1$  in figure 3(b). One can see that the rescaled probe spin coherences for different systems sizes cross at one point when we choose  $f_0(\beta = 0.1) = -3.981$ . We then choose  $t_c$  and  $\sigma$  so that all curves in figure 3(b) collapse completely (figure 3(d)) and we find that  $t_c = 0.5420$  and  $\sigma = -0.149$ . The estimated value is close to the exact value  $\sigma = -1/6 \approx 0.167$ . These results prove the feasibility of the central spin decoherence measurement for studying the nature of the Yang–Lee edge singularity.

In summary, we show that the quantum coherence of a probe spin coupled to a finite-size Ising-type spin bath presents universal finite-size scaling behavior near the Yang–Lee edge singularity. The universal finite-size scaling of the quantum coherence of the probe spin predicts the critical point and the critical exponent of the Yang–Lee edge singularity. Thus by measuring quantum coherence of a probe spin which is coupled to finite-size many-body systems, one can extract the critical point and the critical exponent of the Yang–Lee edge singularity of the infinite system. In particular for ferromagnetic Ising models, the unit-circle theorem holds regardless of the interaction range, geometry configurations, disorders, and dimensionality. Such universality offers a great deal of feasibility and flexibility for experimental observation of Yang–Lee edge singularities. For other systems (e.g. antiferromagnetic Ising models), the Yang–Lee edge singularities may not lie on the imaginary axis. However, one can apply an external field  $h$ , and obtain the Yang–Lee edge singularity of the real part  $h$ . Thus measuring the quantum coherence of a single spin provides a universal tool to probe the singularity point of many-body systems on the complex plane of physical parameters, and in more general the thermodynamics on the complex plane. In the complex plane of temperature, there are also singularities [41] termed Fisher edge singularities. Thus one may expect that similar finite-size scaling techniques can be applied to probe the universal nature of Fisher edge singularities.

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