Lee-Yang Zeros and Critical Times in Decoherence of a Probe Spin Coupled to a Bath

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Phase transitions are not usually seen in the time domain. Here, we report on the finding of critical times at which a physical observable, in the thermodynamic limit, becomes nonanalytic as a function of time. We find that the coherence of a probe spin coupled to a many-body system vanishes at times in one-to-one correspondence to the Lee-Yang zeros of the partition function of the many-body system. In the thermodynamic limit, the Lee-Yang zeros form a continuum cut in the complex plane of fugacity and the probe spin coherence presents sudden death and birth at the critical times corresponding to the Yang-Lee singularities. These results provide new experimental possibilities in many-body physics.

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In 1952, Lee and Yang laid a cornerstone of statistical mechanics by showing that the partition functions of thermal systems vanish at certain points, termed Lee-Yang zeros, on the complex plane of fugacity or a magnetic field [1,2]. They proved the famous unit-circle theorem [2], which states that all the Lee-Yang zeros of a general Ising ferromagnet are located on the unit circle in the complex fugacity plane. In the thermodynamic limit, the Lee-Yang zeros form a continuum cut in the complex plane [1]. Above the critical temperature, the continuum cut has a gap within which the partition function is free of zeros [1]. Kortman and Griffiths [3] pointed out that the two edge points of the continuum cut are singularity points, called Yang-Lee singularities [4]. The Yang-Lee singularities approach the real axis at the critical temperature [1]. The Lee-Yang theorem applies to general ferromagnetic Ising models and has later been generalized to ferromagnetic Ising models of arbitrarily high spin [5–7] as well as other interesting types of interactions [8–10].

The imaginary Lee-Yang zeros have not been regarded as observable since they occur only at an imaginary magnetic field or an imaginary temperature [11], neither of which are physical. High field magnetization data have previously been used to extract densities of Lee-Yang zeros and Yang-Lee singularities in the thermodynamic limit [12,13]. Direct observation of the Lee-Yang zeros and singularities, however, has been elusive. In theoretical physics, a mathematical technique called Wick rotation has been employed to relate the imaginary inverse temperature to time. Therefore, it is conceivable that the imaginary Lee-Yang zeros may be observed in the time domain.

In this Letter, we show that the Lee-Yang zeros can be mapped to zeros in the coherence [14,15] of a probe spin coupled to the many-body system. Moreover, in the thermodynamic limit, the coherence presents sudden death and birth at critical times corresponding to the Yang-Lee singularities if the temperature is above the critical point. While it has been known that nonequilibrium systems can present abrupt changes in their evolutions, the time-domain phase transitions reported in this Letter are essentially an equilibrium-state phenomenon since the probe-bath coupling in principle can be made arbitrarily small.

Let us consider a general Ising model with ferromagnetic interactions under a magnetic field h. The Hamiltonian is

$$H(h) = -\sum_{i,j} J_{ij} s_i s_j - h \sum_j s_j, \tag{1}$$

where the spins s_j take values ± 1 and $J_{ij} \geq 0$. The partition function of N spins at temperature T can be written as an Nth order polynomial of $z \equiv \exp(-2\beta h)$ as

$$Z(\beta, h) = \mathrm{Tr}[e^{-\beta H}] = e^{\beta N h} \sum_{n=0}^{N} p_n z^n, \tag{2}$$

where $\beta = 1/T$ is the inverse temperature (Boltzmann and Planck constants taken as unity) and p_n is the partition function with zero magnetic field under the constraint that n spins are in the state -1. The variable z can be regarded as the scaled field and has the physical meaning of fugacity for a lattice gas described by the Ising model [2]. The N zeros of the partition function, lying on the unit circle in the complex plane of z (corresponding to a complex external field) [2], can be written as $z_n \equiv e^{i\theta_n}$ with $n = 1, 2, \ldots, N$. If the Lee-Yang zeros are determined, the partition function can be readily reconstructed as

$$Z(\beta, h) = p_0 e^{\beta N h} \prod_{n=1}^{N} (z - z_n). \tag{3}$$

We use a probe spin-1/2 coupled to the Ising system (bath), with the probe-bath interaction

$$H_I = -\lambda\sigma_z \otimes \sum_j s_j \equiv \lambda\sigma_z \otimes H_1 \equiv (1/2)\sigma_z B, \quad (4)$$

where λ is a coupling constant, $\sigma_z \equiv |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|$ is the Pauli matrix of the probe spin, and $B \equiv 2\lambda H_1$ acts as the random field for the probe spin. The probe spin is equally coupled to all the N spins in the bath. We note that the quantum coherence of a spin has previously been used to probe quantum criticality [16–18]. We assume that the probe spin is initially prepared in a superposition state as $|\uparrow\rangle + |\downarrow\rangle$ and the bath is at temperature T. The thermal fluctuation of the field B induces a random phase Bt in the probe spin and, in turn, induces probe spin decoherence. The probe spin coherence, given by the ensemble average of the random phase factor, is

$$L(t) = \langle\exp(iBt)\rangle = \mathrm{Tr}[e^{-\beta H(h)} e^{i2\lambda H_1 t}]/Z(\beta, h), \quad (5)$$

which can be written in an intriguing form as

$$\begin{aligned} L(t) &= \frac{Z(\beta, h - 2it\lambda/\beta)}{Z(\beta, h)} \\ &= \frac{e^{-2iN\lambda t}\prod_{n=1}^{N}(e^{-2\beta h + 4i\lambda t} - z_n)}{\prod_{n=1}^{N}(e^{-2\beta h} - z_n)}. \end{aligned} \quad (6)$$

The denominator in the above equation is nonzero for a real magnetic field and temperature. The numerator resembles the form of a partition function but with a complex magnetic field $h - 2it\lambda/\beta$. The probe spin coherence in a finite system vanishes whenever $z' \equiv \exp(4i\lambda t - 2\beta h)$ reaches a Lee-Yang zero. Particularly, for Ising ferromagnets, the Lee-Yang zeros all lie on the unit circle and therefore are mapped to the probe spin coherence zeros (t_n) for the vanishing external field ($h = 0$), with the correspondence relation $\exp(4i\lambda t) = z_n$ or $t_n = \theta_n/(4\lambda)$. Therefore, in a ferromagnetic Ising bath under zero field,

$$L(t) = e^{-2iN\lambda t}\prod_{n=1}^{N}(e^{4i\lambda t} - e^{i\theta_n})/(1 - e^{i\theta_n}). \quad (7)$$

For a bath of a finite number (N) of spins, the probe spin coherence will vanish for N times before the coherence revival at $t = 2\pi/(4\lambda)$. In the thermodynamic limit ($N \to \infty$), the Lee-Yang zeros form a continuum cut in the complex plane; the probe spin coherence would be constant at zero between the edge singularities $\pm\theta_c$ and present a sudden death feature at the critical time $t_c = \theta_c/(4\lambda)$ and a sudden birth feature at the critical time $t_c' = (2\pi - \theta_c)/(4\lambda)$.

To illustrate the above idea, we use the one-dimensional (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 [19,20]. There is no finite-temperature phase transition in the 1D Ising model. The Lee-Yang zeros of the 1D Ising model with N spins have been exactly calculated [2].

Figure 1 shows the Lee-Yang zeros and the probe spin coherence for the 1D Ising model with $N = 10$ spins at various temperatures. At infinite temperature ($\beta = 0$), all the Lee-Yang zeros are degenerate at $z_n = -1$ [Fig. 1(a)]. Correspondingly, the probe spin coherence has one zero at $t = \theta_1/(4\lambda)$ [Fig. 1(b)]. As a finite-size effect, the probe spin coherence presents periodic revivals at integer multiples of $2\pi/(4\lambda)$, as can be seen from Eq. (7). With decreasing temperature, the Lee-Yang zeros disperse on the unit circle [Fig. 1(c)]. As shown in Fig. 1(d), the probe spin coherence has 10 zeros corresponding to the Lee-Yang zeros. As the temperature approaches zero, the Lee-Yang zeros tend to be uniformly distributed on the unit circle [Fig. 1(e)]. From Eq. (7), we see that, if the Lee-Yang zeros are uniformly distributed [$\theta_n \to (2n-1)\pi/N$], the probe spin coherence is fully recovered whenever the time is such that $4\lambda t = n2\pi/N$, and therefore the probe spin coherence oscillates periodically [Fig. 1(f)].

Figure 2 shows the Lee-Yang zeros and the probe spin coherence with the bath size increasing toward the

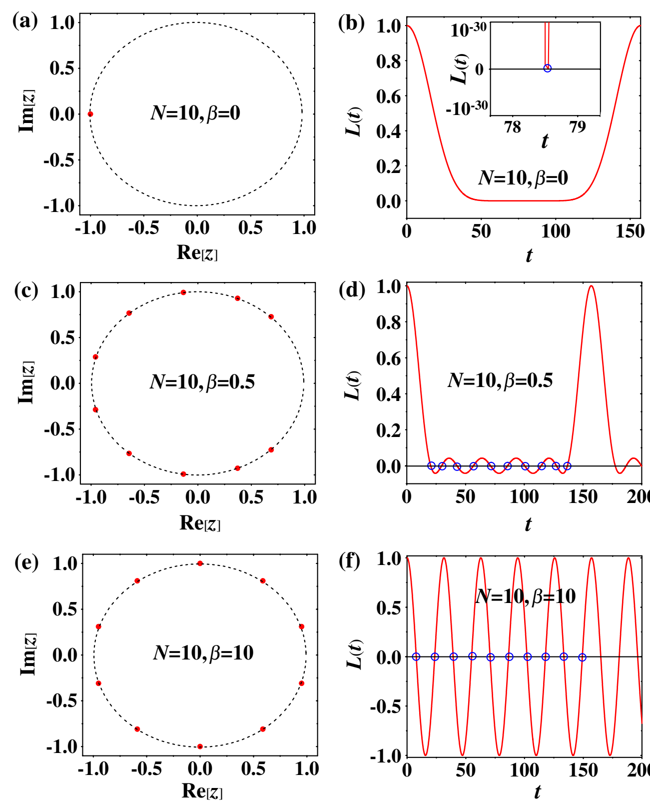

FIG. 1 (color online). Correspondence between the Lee-Yang zeros and the coherence zeros of a probe spin. (a),(c),(e) The Lee-Yang zeros (red circles) for a 1D Ising model of 10 spins at inverse temperatures $\beta = 0$, 0.5, and 10, correspondingly. The black dashed lines are the unit circles. (b),(d),(f) Probe spin coherence as a function of time corresponding to (a), (c), and (e). The inset in (b) zooms into the coherence zero. The small blue circles in (b), (d), and (f) mark the coherence zeros. The probe-bath coupling is $\lambda = 0.01$.

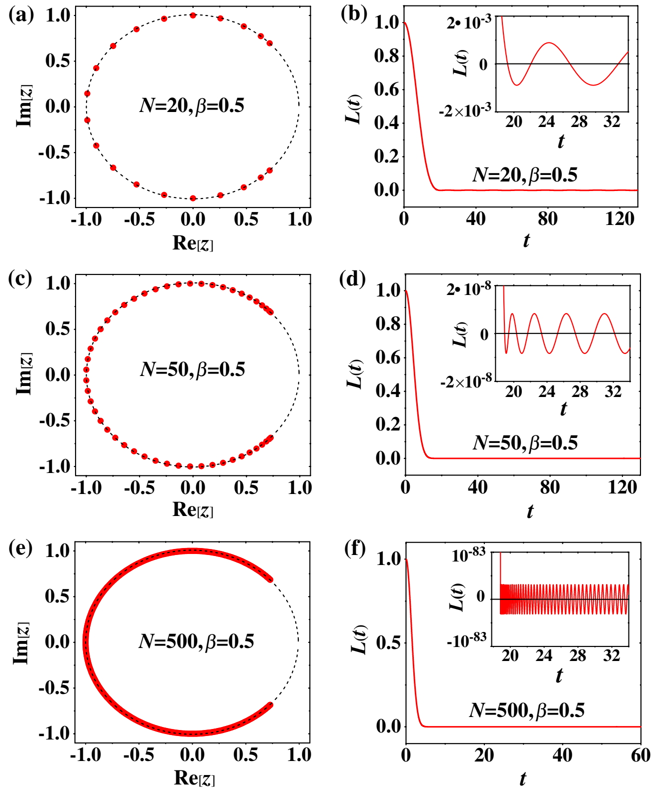

FIG. 2 (color online). Yang-Lee singularities and critical times in probe spin decoherence. (a),(c),(e) The Lee-Yang zeros for a 1D Ising model with the numbers of spins $N = 20$, 50, and 500, correspondingly. As the thermodynamic limit is approached, the zeros form a continuum cut in the complex plane ended by two singularity points. (b),(d),(f) Probe spin coherence as a function of time corresponding to (a), (c), and (e). The insets zoom into the sudden death point. The parameters are such that $\beta = 0.5$ and $\lambda = 0.01$.

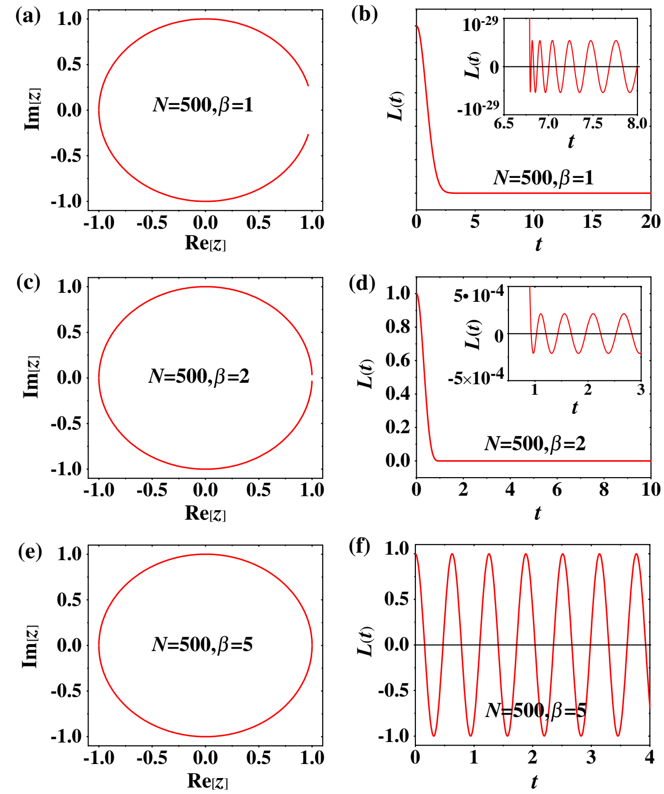

FIG. 3 (color online). Temperature dependence of Yang-Lee singularities and probe spin coherence sudden death. (a),(c),(e) Lee-Yang zeros for a 1D Ising model of 500 spins at inverse temperatures $\beta = 1$, 2, and 5, correspondingly. (b),(d),(f) Probe spin coherence as a function of time corresponding to (a), (c), and (e). The insets of (b) and (d) zoom into the sudden death point. The probe-bath coupling is $\lambda = 0.01$.

thermodynamic limit ($N \to \infty$). With increasing N, the Lee-Yang zeros become denser and denser between the two edge singularities. The probe spin coherence becomes almost constant at zero after the critical time corresponding to the first edge singularity [$t_c = \theta_c/(4\lambda)$], until a sudden birth at $t_c' = (2\pi - \theta_c)/(4\lambda)$ corresponding to the second edge singularity. For a large bath size ($N = 500$) that approximates the thermodynamic limit, the coherence presents nearly sudden death and birth at the critical times. The probe spin coherence does not appear smooth at these singularity points, although it is an analytic function, by definition, for any finite-size system. Note that such coherence sudden death, being a phase transition in the time domain, is fundamentally different from the previously discovered entanglement sudden death [21,22], which is instead caused by the nonanalyticity in the definition of entanglement.

We now study how the coherence sudden death changes with decreasing temperature, in particular, toward the critical temperature (which is zero in the 1D Ising model). As shown in Fig. 3 for an Ising model of 500 spins at various temperatures, the gap between the Yang-Lee singularities tends to close as temperature decreases toward zero. At high temperatures, the probe spin coherence displays a sudden death, as expected. The sudden death occurs at earlier times as the temperature decreases, which is consistent with the narrowing gap between the Yang-Lee singularities. When the temperature is close to the critical point [Figs. 3(e) and 3(f)], the Lee-Yang zeros become almost uniformly distributed [as is more clearly seen in Fig. 1(e) for a smaller Ising bath] and the probe spin coherence displays pronounced oscillations. For larger baths, the oscillation features would appear for a temperature closer to the critical point (figure not shown). In the thermodynamic limit, only at the critical temperature would the sudden death change to the oscillation feature.

We further study how the Lee-Yang zeros appear in the probe spin coherence below the critical temperature by considering the two-dimensional (2D) Ising model, which has a finite-temperature phase transition. We consider a 2D Ising model on a square lattice with nearest-neighbor coupling $J = 1$ and periodic boundary conditions. This model under zero field is exactly solvable [23] and has a finite-temperature phase transition at $\beta \simeq 0.44$. For a finite field and finite-time evolution, we use the transfer matrix approach to map the 2D model to a 1D Ising model with both longitudinal and transverse fields [20] and then employ exact numerical diagonalization. Figure 4 plots the Lee-Yang zeros and the probe spin coherence in a 2D Ising model of 8×50 spins for various temperatures. Above the critical temperature ($\beta = 0.2$ and 0.4), the Lee-Yang zeros have a gap across the positive real axis. The corresponding probe spin coherence shows a well-developed sudden death feature (though not strictly nonanalytic due to the finite size of the bath). The sudden death appears at earlier times for lower temperatures since the gap between the Yang-Lee edge singularities is smaller. Below the critical temperature ($\beta = 0.5$ and 0.8), the Lee-Yang zeros are almost uniformly distributed along the unit circle and the probe spin coherence oscillates coherently with a period $2\pi/(2N\lambda)$, as a signature of the ferromagnetic phase.

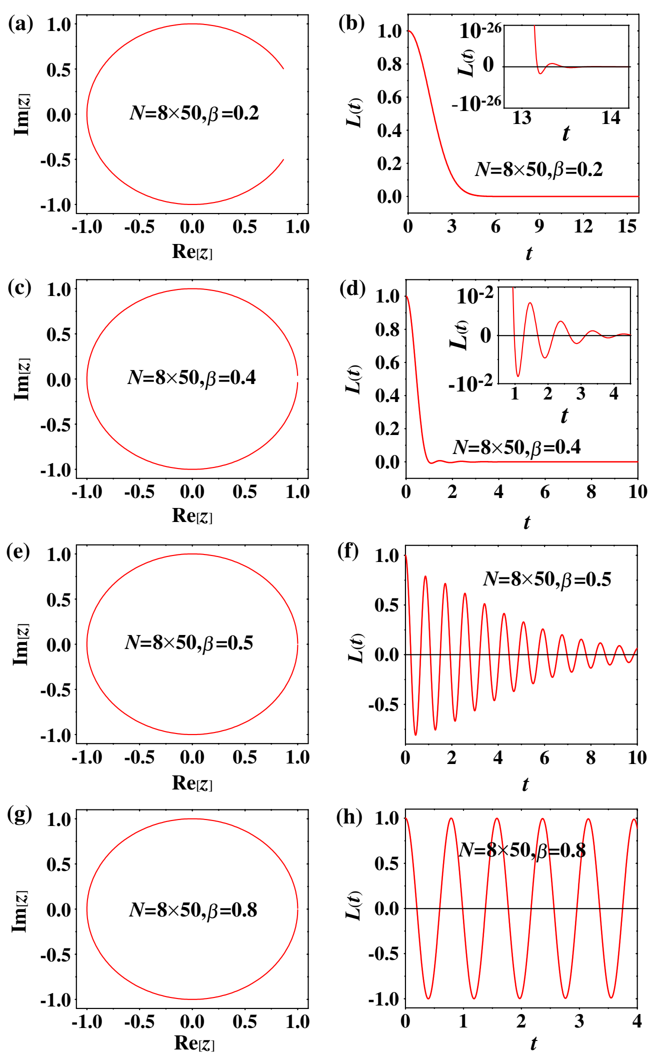

FIG. 4 (color online). Lee-Yang zeros and probe spin coherence in a 2D Ising model at various temperatures. (a),(c),(e),(g) Lee-Yang zeros for a 2D Ising model in an 8×50 lattice at inverse temperatures $\beta = 0.2$, 0.4, 0.5, and 0.8, correspondingly. (b),(d),(f),(h) Probe spin coherence as a function of time t corresponding to (a), (c), (e), and (g). The insets of (b) and (d) zoom into the sudden death region. The probe-bath coupling is $\lambda = 0.01$.

To observe the effects, one can employ magnetic resonance spectroscopy. The nuclear magnetic resonance technique demonstrated in [17] can be adapted to study the Lee-Yang zeros of small-size Ising models. The detection of dynamics in spin baths by central spin decoherence has been experimentally demonstrated [24–30]. With certain modifications, similar techniques may be used to study the Lee-Yang zeros. It follows from Ref. [9] that the probe-bath coupling need not be uniform and that the unit-circle theorem applies to ferromagnetic Heisenberg-Ising models (a large class of spin models). This offers some feasibility and flexibility for experiments. To study the time-domain phase transitions, a sufficiently large spin bath is needed to approximate the thermodynamic limit and the bath spins should be placed on a regular lattice. Furthermore, the bath and the probe should be well isolated from the larger environment. Such challenges are nontrivial. With recent advances in the precise positioning and coupling of single spins in solids [31–33], observation of the critical phenomena in probe spin decoherence is not inconceivable. There also exist alternative methods to the spin resonance technique. For example, a linearly polarized light can act as a probe. If the photons have long wavelength compared with the size of the sample (bath), the probe-bath coupling can be taken as uniform. Magneto-optical Faraday rotation has been used to detect magnetization fluctuations in equilibrium spin systems [30,34,35]. The coherence function in Eq. (5) is related to the Faraday rotation measurement by

$$L(t) = \langle e^{2i\lambda H_1 t} \rangle = \langle e^{2i\lambda M t} \rangle = \langle e^{i\phi_F t} \rangle, \tag{8}$$

where M is the random magnetization of the bath, ϕ_F is the Faraday rotation, and t is the interaction time between the photons and bath spins.

In summary, the coherence of a probe spin coupled to a many-body system presents zeros at times in one-to-one correspondence to the Lee-Yang zeros of the many-body system. In the thermodynamic limit, the probe spin coherence presents sudden death and birth at critical times corresponding to the Yang-Lee edge singularities. The Lee-Yang theorem, and hence the discoveries presented here, apply to a large class of spin systems, including the ferromagnetic Ising and Heisenberg-Ising models, regardless of the interaction range, geometry configurations, disorders, and dimensionality [9]. For other systems (e.g., antiferromagnetic Ising models), the Lee-Yang zeros may not lie on a unit circle. However, one can apply an external field h and get all the zeros of modulus $\exp(-2\beta h)$, according to Eq. (6). The time-domain phase transitions associated with the Yang-Lee edge singularities in such systems, however, are not as straightforward as for the ferromagnetic Ising models and need further investigation.

With the Lee-Yang zeros determined, the partition function of an interacting many-body system can, in principle, be reconstructed, from which all physical properties can be calculated. Thus, measuring the quantum coherence of a single probe spin provides a new approach to studying the interacting many-body systems.

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