Supplementary Material: Experimental investigation of Lee-Yang criticality using non-Hermitian quantum system

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S1. EXPERIMENTAL SETUP

The experiments were performed on an optically detected magnetic resonance setup. The 532 nm green laser pulses were modulated by an acousto-optic modulator (ISOMET). The laser beam traveled twice through the acousto-optic modulator before going through an oil objective (Olympus, PLAPON 60*O, NA 1.42). The phonon sideband fluorescence (wavelength, 650-800nm) went through the same oil objective and was collected by an avalanche photodiode (Perkin Elmer, SPCM-AQRH-14) with a counter card. The magnetic field of 503 G was provided by a permanent magnet along the NV symmetry axis so the state of the two-qubit system can be effectively polarized to $|0\rangle_e|1\rangle_n$ by laser pumping. An arbitrary waveform generator (CIQTEK AWG4100) generated MW and radio-frequency (RF) pulses to manipulate the states of the two-qubit system. The MW pulses were modulated by an IQ mixer (Marki Microwave IQ-1545LMP). The RF pulses were amplified by power amplifier (Mini Circuits LZY-22+). Both the MW and RF pulses are fed by a broadband coplanar waveguide with 15 GHz bandwidth. In the state preparation and read out part, single qubit operations of the nuclear spin qubit were realized by applying two channel RF pulses simultaneously. The frequencies of the RF pulses were 2.93 MHz and 5.09 MHz, corresponding to the nuclear spin transition frequencies.

S2. QUANTUM-CLASSICAL CORRESPONDENCE

This note mainly discuss the quantum-classical correspondence between the classical one-dimensional N sites ferromagnetic Ising model $H_{\mathrm{Ising}} = -J\sum_{j=1}^{N}\sigma_j\sigma_{j+1} - ih_{cl}\sum_{j=1}^{N}\sigma_j(h_{cl} \in \mathbb{R})$ and a parity-time (PT) symmetric non-Hermitian Hamiltonian $H_Q = h_x\sigma^x + ih_z\sigma^z$ with real parameters h_x and h_z. Under the periodic boundary condition, the correspondence is based on the equivalence of the partition functions. The partition function for H_{PT} is given by

$$Z_{PT} = \mathrm{Tr}[e^{-\beta H_Q}] = \mathrm{Tr}[e^{\beta H_Q}] = \sum_{\sigma_0=\pm1}\langle\sigma_0|e^{\beta H_Q}|\sigma_0\rangle, \tag{S1}$$

where $|\sigma_0\rangle$ is the eigenstate of σ^z with the eigenvalue $\sigma_0 \in \{+1,-1\}$ and β is the inverse temperature. The quantum-classical correspondence is derived as

$$\begin{aligned}
Z_{PT} &= \lim_{N\to\infty} \sum_{\sigma_0=\pm 1} \langle\sigma_0|[\exp(\frac{\beta h_x}{N}\sigma^x)\exp(i\frac{\beta h_z}{N}\sigma^z)]^N|\sigma_0\rangle \\
&= \lim_{N\to\infty} \sum_{\sigma_0}\cdots\sum_{\sigma_{N-1}}\prod_{k=0}^{N-1}\langle\sigma_{k+1}|\exp(\frac{\beta h_x}{N}\sigma^x)\exp(i\frac{\beta h_z}{N}\sigma^z)|\sigma_k\rangle \\
&= \lim_{N\to\infty} \sum_{\sigma_0}\cdots\sum_{\sigma_{N-1}}\prod_{k=0}^{N-1}\langle\sigma_{k+1}|[\cosh(\frac{\beta h_x}{N})+\sinh(\frac{\beta h_x}{N})\sigma^x]|\sigma_k\rangle\exp(i\frac{\beta h_z}{N}\sigma_k) \\
&= \lim_{N\to\infty} \sum_{\sigma_0}\cdots\sum_{\sigma_{N-1}}\prod_{k=0}^{N-1}[\cosh(\frac{\beta h_x}{N})\delta_{\sigma_{k+1},\sigma_k}+\sinh(\frac{\beta h_x}{N})(1-\delta_{\sigma_{k+1},\sigma_k})]\exp(i\frac{\beta h_z}{N}\sigma_k) \\
&= \lim_{N\to\infty} \sum_{\sigma_0}\cdots\sum_{\sigma_{N-1}}\prod_{k=0}^{N-1}A\exp(\beta_{cl}J\sigma_{k+1}\sigma_k)\exp(i\beta_{cl}h_{cl}\sigma_k) \\
&= \lim_{N\to\infty} \sum_{\sigma_0}\cdots\sum_{\sigma_{N-1}}A^N\exp[\sum_{k=0}^{N-1}(\beta_{cl}J\sigma_{k+1}\sigma_k+i\beta_{cl}h_{cl}\sigma_k)],
\end{aligned} \tag{S2}$$

where $\sigma_N = \sigma_0$, and the parameters of the classical and quantum systems are related to each other by

$$\begin{aligned}
\beta_{cl}J &= -\frac{1}{2}\ln[\tanh(\frac{\beta h_x}{N})], \\
\beta_{cl}h_{cl} &= \frac{\beta h_z}{N}, \\
A &= \sqrt{\cosh(\frac{\beta h_x}{N})\sinh(\frac{\beta h_z}{N})}.
\end{aligned} \tag{S3}$$

The right-hand side of Eq. S2 is the partition function for the classical one-dimensional Ising model.

In our case, the quantum system described by a parity-time ($\mathcal{PT}$) symmetric non-Hermitian Hamiltonian

$$H_{PT} = \lambda \begin{pmatrix} ia & 1 \\ 1 & -ia \end{pmatrix}, \tag{S4}$$

where λ is an overall coefficient, is utilized to investigate the Lee-Yang zeros of the 1D Ising model. The corresponding parameters are $h_x = 1$ and $h_z = a$. Eigenvalues of this Hamiltonian are $E_\pm = \pm\lambda\sqrt{1-a^2}$. The partition function of H_{PT} is

$$Z_{PT} \equiv \mathrm{Tr}[e^{-\beta H_{PT}}] = \sum_{p\in\{+,-\}} e^{-\beta E_p}. \tag{S5}$$

The zeros of partition function can be achieved in the $\mathcal{PT}$-symmetry broken regime, where the imaginary part of eigenvalues appear. The condition for the Lee-Yang zeros is given by $\beta\lambda\sqrt{a^2-1} = (n+1/2)\pi$ for non-negative integer n. These zeros appear at $a = \sqrt{(n+1/2)^2\pi^2/\beta^2\lambda^2+1}$. As β increases, the Lee-Yang zeros are more densely distributed as shown in Fig. S1.

S3. HERMITIAN DILATION OF NON-HERMITIAN HAMILTONIANS

Our target is to realize the dynamics of a quantum system governed by Hamiltonian H_{PT}. The state evolution of system s is described by $|\psi(t)\rangle$, so the corresponding Schrödinger equation can be written as

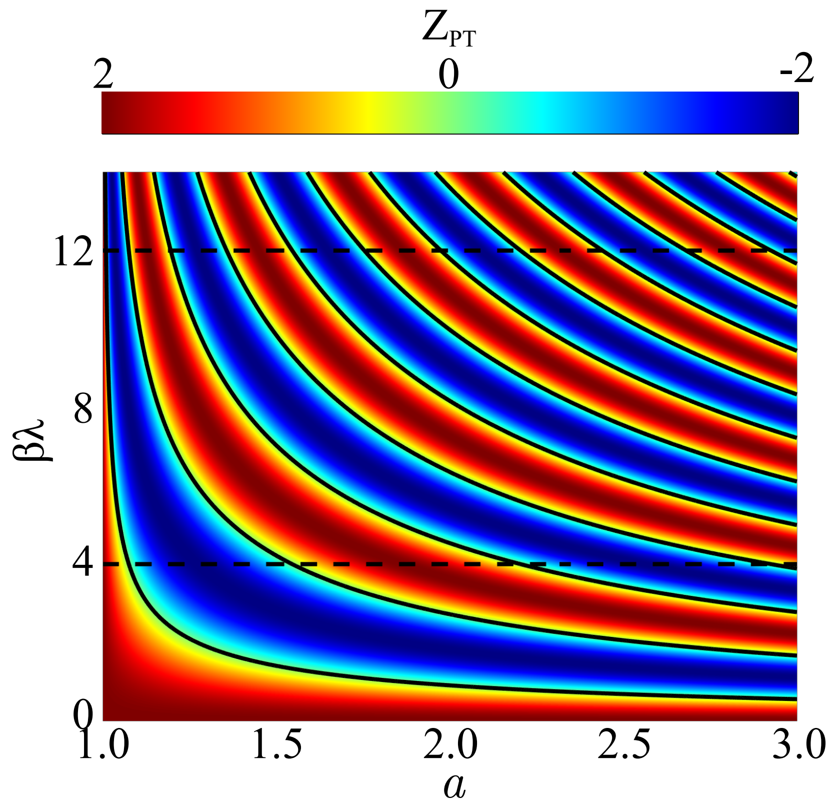

Fig. S1: The partition function with various inverse temperature β and parameter a. The value of the partition function obtained from Eq. S5. The black solid lines characterizes the zeros of partition function. The dashed lines correspond to the cases where the inverse temperature takes $\beta_1 = 4/\lambda$ and $\beta_1 = 12/\lambda$. The overall coefficient λ is 150 kHz.

(natural unit are chosen so that $\hbar = 1$ in this supplementary material)

$$i\frac{d}{dt}|\psi(t)\rangle = H_{PT}|\psi(t)\rangle. \tag{S6}$$

An ancilla qubit is introduced to dilate H_{PT} into a Hermitian Hamiltonian $H_{tot}(t)$ to realize the dynamics in quantum system. The state evolution of the combined system is described by $|\Psi(t)\rangle$, which satisfies the following Schrödinger equation

$$i\frac{d}{dt}|\Psi(t)\rangle = H_{tot}(t)|\Psi(t)\rangle. \tag{S7}$$

$|\Psi(t)\rangle$ is a dilation of $|\psi(t)\rangle$ and can be written as

$$|\Psi(t)\rangle = |\psi(t)\rangle|-\rangle + \eta(t)|\psi(t)\rangle|+\rangle, \tag{S8}$$

where $|-\rangle = \frac{|0\rangle - i|1\rangle}{\sqrt{2}}$ and $|+\rangle = -i\frac{|0\rangle + i|1\rangle}{\sqrt{2}}$ are the eigenstates of Pauli operator σ_y, which forms an orthonormal basis of the ancilla qubit. $\eta(t)$ is a linear operator which can be derived as following,

$$\eta(t) = U(t)[M(t) - I]^{\frac{1}{2}}, \tag{S9}$$

$$M(t) = \mathcal{T}e^{-i\int_0^t H_{PT}^\dagger(t)dt}M(0)\overline{\mathcal{T}}e^{i\int_0^t H_{PT}(t)dt}, \tag{S10}$$

where $\mathcal{T}$ and $\overline{\mathcal{T}}$ are time-ordering and anti-time-ordering operators, respectively. $M(0)$ is an initial operator of operator $M(t)$, which is chosen to ensure that $M(t) - I$ keeps positive for all t. Due to the Hermiticity of

$H_{tot}(t)$, we obtain the form of $H_{tot}(t)$ as

$$H_{tot}(t) = \Lambda(t) \otimes I + \Gamma(t) \otimes \sigma_z, \tag{S11}$$

with

$$\begin{cases} \Lambda(t) = \{H_{PT}(t) + [i\frac{d}{dt}\eta(t) + \eta(t)H_{PT}(t)]\eta(t)\}M^{-1}(t), \\ \Gamma(t) = i[H_{PT}(t)\eta(t) - \eta(t)H_{PT}(t) - i\frac{d}{dt}\eta(t)]M^{-1}(t). \end{cases} \tag{S12}$$

When a measurement is applied on the ancilla qubit and $|-\rangle$ is postselected, the evolution governed by the non-Hermitian Hamiltonian H_{PT} can be produced.

S4. CONSTRUCT THE DILATED HAMILTONIAN IN NV CENTER

Considering the form of the H_{PT}, $H_{tot}(t)$ in equation S11 reduces to

$$H_{tot}(t) = A_1(t)\sigma_x \otimes I + A_2(t)I \otimes \sigma_z + A_3(t)\sigma_y \otimes \sigma_z + A_4(t)\sigma_z \otimes \sigma_z, \tag{S13}$$

where $A_i(t)$, $i \in [1, 4]$, are the corresponding decomposition coefficients (real parameters). Next, we construct the Hamiltonian $H_{tot}(t)$ shown in equation S13 in the NV center. By applying an external magnetic field B_0 along the NV axis, the Hamiltonian of NV center can be written as

$$H_{\mathrm{NV}} = 2\pi(DS_z^2 + \omega_e S_z + QI_z^2 + \omega_n I_z + AS_z I_z), \tag{S14}$$

where $\omega_e = -\gamma_e B_0/2\pi$ ($\omega_n = -\gamma_n B_0/2\pi$) is the Zeeman splitting of the electron (^{14}N nuclear) spin, with γ_e (γ_n) being the electron (^{14}N nuclear) gyromagnetic ratio. S_z and I_z are the spin operators of the electron spin (spin-1) and the ^{14}N nuclear spin (spin-1), respectively. $D = 2.87$ GHz is the axial zero-field splitting parameter for the electron spin. $Q = -4.95$ MHz is the quadrupole splitting parameter of the ^{14}N nuclear spin. $A = -2.16$ MHz is the hyperfine coupling parameter.

The experiment is performed in the two qubit subspace spanned by $|m_s = 0, m_I = 1\rangle$, $|m_s = 0, m_I = 0\rangle$, $|m_s = -1, m_I = 1\rangle$, and $|m_s = -1, m_I = 0\rangle$, labeled by $|0\rangle_e|1\rangle_n, |0\rangle_e|0\rangle_n, |-1\rangle_e|1\rangle_n$ and $|-1\rangle_e|0\rangle_n$, in which the Hamiltonian can be simplified as

$$H_0 = \pi[-(D - \omega_e - \frac{A}{2})\sigma_z \otimes I + (Q + \omega_n - \frac{A}{2})I \otimes \sigma_z + \frac{A}{2}\sigma_z \otimes \sigma_z]. \tag{S15}$$

To construct $H_{tot}(t)$ in NV center, we can apply two slightly detuned microwave (MW) pulses to selectively drive the two electron spin transitions, as depicted in Fig. 1a in the main text. The total Hamiltonian in the two qubit subspace when applying MW pulses can be written as

$$\begin{aligned} H_{\mathrm{all}} = \pi[&-(D - \omega_e - \frac{A}{2})\sigma_z \otimes I + (Q + \omega_n - \frac{A}{2})I \otimes \sigma_z + \frac{A}{2}\sigma_z \otimes \sigma_z] \\ &+ 2\pi\Omega_1(t)\cos[\int_0^t \omega_1(\tau)d\tau + \phi_1(t)]\sigma_x \otimes |1\rangle_{n\,n}\langle 1| \\ &+ 2\pi\Omega_2(t)\cos[\int_0^t \omega_2(\tau)d\tau + \phi_2(t)]\sigma_x \otimes |0\rangle_{n\,n}\langle 0|, \end{aligned} \tag{S16}$$

where $\Omega_1(t)$, $\omega_1(t)$ and $\phi_1(t)$ ($\Omega_2(t)$, $\omega_2(t)$ and $\phi_2(t)$) are the Rabi frequency, angular frequency and phase of the MW pulses which drive the electron spin transition if the nuclear spin is $|1\rangle_n$ ($|0\rangle_n$). By choosing interaction picture

$$U_{rot} = e^{i\int_0^t [H_0 - A_2(\tau)I\otimes\sigma_z - A_4(\tau)\sigma_z\otimes\sigma_z]d\tau}, \tag{S17}$$

the total Hamiltonian transforms to

$$H_{rot} = A_2(t) I \otimes \sigma_z + A_4(t)\sigma_z \otimes \sigma_z + \pi\Omega(t)\cos[\phi(t)]\sigma_x \otimes I + \pi\Omega(t)\sin[\phi(t)]\sigma_y \otimes I. \tag{S18}$$

Comparing equation S18 with equation S15, we can choose

$$\begin{cases} \omega_1(t) = \omega_{MW1} + 2A_4(t) \\ \omega_2(t) = \omega_{MW2} - 2A_4(t) \\ \Omega_1(t) = \Omega_2(t) = \dfrac{\sqrt{A_1^2(t) + A_3^2(t)}}{2\pi} \\ -\phi_1(t) = \phi_2(t) = \arctan \dfrac{A_3(t)}{A_1(t)} \end{cases} \tag{S19}$$

to realize Hamiltonian $H_{tot}(t)$ with $\omega_{MW1}(\omega_{MW2})$ being the transition frequency between $|0\rangle_e|1\rangle_n$ and $|-1\rangle_e|1\rangle_n$ ($|0\rangle_e|0\rangle_n$ and $|-1\rangle_e|0\rangle_n$).

S5. EXPERIMENTAL ACQUISITION OF THE EIGENVALUES OF $\mathcal{PT}$ SYMMETRIC HAMILTONIANS

By fitting the experimental evolution curve to the theoretical evolution curve we can get the parameter a_{exp}, then the eigenvalues of $\mathcal{PT}$ symmetric Hamiltonian H_{PT} can be calculated by $E_\pm^{\text{exp}} = \pm\sqrt{1 - a_{\text{exp}}^2}$. The Hamiltonian we realized in our experimental system is

$$H_{PT} = \begin{pmatrix} ia & 1 \\ 1 & -ia \end{pmatrix}. \tag{S20}$$

The time evolution operator corresponding to H_{PT} takes the form

$$U(t) = \begin{cases} \begin{pmatrix} \frac{e^{t\sqrt{a^2-1}}(a+\sqrt{a^2-1}) - e^{-t\sqrt{a^2-1}}(a-\sqrt{a^2-1})}{2\sqrt{a^2-1}} & \frac{ie^{-t\sqrt{a^2-1}} - ie^{t\sqrt{a^2-1}}}{2\sqrt{a^2-1}} \\ \frac{ie^{-t\sqrt{a^2-1}} - ie^{t\sqrt{a^2-1}}}{2\sqrt{a^2-1}} & \frac{e^{t\sqrt{a^2-1}}(-a+\sqrt{a^2-1}) - e^{-t\sqrt{a^2-1}}(-a-\sqrt{a^2-1})}{2\sqrt{a^2-1}} \end{pmatrix} & a \neq 1 \\ \begin{pmatrix} 1+t & -it \\ -it & 1-t \end{pmatrix} & a = 1 \end{cases} \tag{S21}$$

The initial state we choose is $|\psi(0)\rangle = |0\rangle = (1, 0)^T$. Then the final state at time t, after the evolution governed by Hamiltonian H_{PT}, is

$$|\psi(t)\rangle = \begin{cases} \dfrac{1}{2\sqrt{a^2-1}} \begin{pmatrix} e^{t\sqrt{a^2-1}}(a + \sqrt{a^2-1}) - e^{-t\sqrt{a^2-1}}(a - \sqrt{a^2-1}) \\ ie^{-t\sqrt{a^2-1}} - ie^{t\sqrt{a^2-1}} \end{pmatrix} & a \neq 1 \\ \begin{pmatrix} 1+t \\ -it \end{pmatrix} & a = 1 \end{cases} \tag{S22}$$

So the population of state $|0\rangle$ at moment t is

$$P_0 = \begin{cases} \dfrac{|e^{t\sqrt{a^2-1}}(a + \sqrt{a^2-1}) - e^{-t\sqrt{a^2-1}}(a - \sqrt{a^2-1})|^2}{|e^{t\sqrt{a^2-1}}(a + \sqrt{a^2-1}) - e^{-t\sqrt{a^2-1}}(a - \sqrt{a^2-1})|^2 + |ie^{-t\sqrt{a^2-1}} - ie^{t\sqrt{a^2-1}}|^2} & a \neq 1 \\ \dfrac{(t+1)^2}{(t+1)^2 + t^2} & a = 1 \end{cases} \tag{S23}$$

We use formula S23 to fit our experimental data to get the parameter a_{exp}. The fitting result is shown on Table S1.

Table S1: **Parameter a_{exp} obtained from the time evolution under $\mathcal{PT}$ symmetric Hamiltonian.** a is the parameter at which the experiment implemented. a_{exp} is obtained by fitting the evolution curve. δa_{exp} is the fitting error.

a	1.000	1.040	1.100	1.143	1.200	1.250	1.300	1.317	1.350	1.400
a_{exp}	1.002	1.044	1.108	1.141	1.213	1.243	1.303	1.316	1.373	1.417
δa_{exp}	0.004	0.010	0.014	0.014	0.021	0.029	0.023	0.016	0.025	0.060