PHYSICS

Observation of parity-time symmetry breaking in a single-spin system

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Steering the evolution of single spin systems is crucial for quantum computing and quantum sensing. The dynamics of quantum systems has been theoretically investigated with parity-time–symmetric Hamiltonians exhibiting exotic properties. Although parity-time symmetry has been explored in classical systems, its observation in a single quantum system remains elusive. We developed a method to dilate a general parity-time–symmetric Hamiltonian into a Hermitian one. The quantum state evolutions ranging from regions of unbroken to broken $\mathcal{PT}$ symmetry have been observed with a single nitrogen-vacancy center in diamond. Owing to the universality of the dilation method, our result provides a route for further exploiting and understanding the exotic properties of parity-time symmetric Hamiltonian in quantum systems.

In quantum mechanics, the real energies of a system are guaranteed by a fundamental axiom associated with the Hermiticity of physical observables. However, a class of non-Hermitian Hamiltonians satisfying parity-time ($\mathcal{PT}$) symmetry can still exhibit real eigenenergies (*1*). An alternative formulation of quantum mechanics can be established when the axiom of Hermiticity is replaced by the condition of $\mathcal{PT}$ symmetry (*2*, *3*). The physics associated with $\mathcal{PT}$-symmetric Hamiltonian has aroused considerable experimental interest (*4*, *5*). The optical analog of $\mathcal{PT}$-symmetric quantum mechanics was first proposed (*6*) and then extended to other systems, such as electronics (*7*–*9*), microwaves (*10*), mechanics (*11*), acoustics (*12*–*14*), and optical systems with atomic media (*15*–*17*). Experimental study on $\mathcal{PT}$-symmetric classical optical systems has stimulated many applications such as unidirectional light transport (*18*, *19*) and single-mode lasers (*20*, *21*).

Experimentally investigating $\mathcal{PT}$-symmetric physics in quantum systems is challenging, because quantum systems are governed by Hermitian Hamiltonians. A possible approach is to realize a $\mathcal{PT}$-symmetric Hamiltonian in an open quantum system. However, it is difficult in general to realize a controllable $\mathcal{PT}$-symmetric Hamiltonian by controlling the environment (*22*). Some progress has been made with this approach in the system of light-matter quasiparticles (*23*, *24*). A lossy Hamiltonian has been constructed to simulate the quantum dynamics under $\mathcal{PT}$-symmetric Hamiltonians (*25*). However, the additional dissipation introduced in this protocol is usually detrimental to quantum features such as coherence and entanglement. Instead of engineering $\mathcal{PT}$-symmetric Hamiltonians, nonunitary evolution operators have been mimicked in optics (*26*, *27*). Alternatively, two theoretical approaches have been developed to dilate a $\mathcal{PT}$-symmetric Hamiltonian into a Hermitian Hamiltonian with a higher-dimensional Hilbert space (*28*, *29*). However, these dilation methods are limited to the cases of unbroken $\mathcal{PT}$-symmetric Hamiltonians. Thus, observing the transition from the unbroken to the broken $\mathcal{PT}$ symmetry through the exceptional point in a single quantum system, such as a single spin, remains elusive.

For the $\mathcal{PT}$-symmetric Hamiltonian H_s and the quantum state $|\psi(t)\rangle$ satisfying the Schrödinger type equation, $i\frac{d}{dt}|\psi(t)\rangle = H_s|\psi(t)\rangle$, we introduce a dilated state $|\Psi(t)\rangle = |\psi(t)\rangle|-\rangle + \eta(t)|\psi(t)\rangle|+\rangle$, governed by a dilated Hermitian Hamiltonian $H_{s,a}(t)$, wherein $|-\rangle = (|0\rangle - i|1\rangle)/\sqrt{2}$ and $|+\rangle = -i(|0\rangle + i|1\rangle)/\sqrt{2}$ are the eigenstates of σ_y of the introduced ancilla and $\eta(t)$ is an appropriate linear operator. By measuring state $|\Psi(t)\rangle$, the evolution of $|\psi(t)\rangle$ can be obtained in the subspace where the ancilla is $|-\rangle$.

The Hamiltonian, $H_{s,a}(t)$, can be designed flexibly according to realistic physical systems, as $H_{s,a}(t)$ is not uniquely determined [see supplementary text SM1 (*30*)]. For example, $H_{s,a}(t)$ can be chosen as

$$H_{s,a}(t) = \Lambda(t) \otimes I + \Gamma(t) \otimes \sigma_z \quad (1)$$

where $\Lambda(t) = \{H_s(t) + [i\frac{d}{dt}\eta(t) + \eta(t)H_s(t)]\eta(t)\} M^{-1}(t)$, and $\Gamma(t) = i[H_s(t)\eta(t) - \eta(t)H_s(t) - i\frac{d}{dt}\eta(t)]M^{-1}(t)$. The time-dependent operator $M(t) = \eta^\dagger(t)\eta(t) + I$, where σ_x, σ_y, and σ_z are Pauli operators and I is the identity matrix. We note that this derivation of $H_{s,a}(t)$ holds for an arbitrary Hamiltonian H_s, i.e., our method can be applied to dilate a general $\mathcal{PT}$-symmetric Hamiltonian (SM1).

We investigate the $\mathcal{PT}$-symmetric Hamiltonian of the form

$$H_s = \begin{bmatrix} ir & 1 \\ 1 & -ir \end{bmatrix} \quad (2)$$

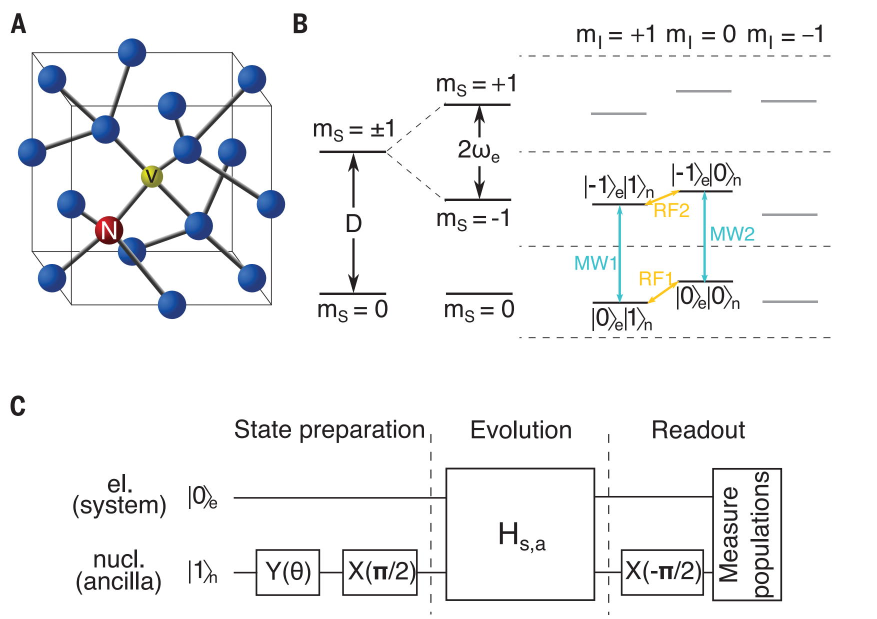

Fig. 1. Constructing a $\mathcal{PT}$-symmetric Hamiltonian in a NV center. (**A**) Schematic atomic structure of the NV center. (**B**) Energy-level structure of the NV center in the ground multiplet states. Two microwave pulses (blue arrows) and two radiofrequency pulses (orange arrows) are applied. (**C**) Quantum circuit of the experiment. The electron (nuclear) spin is taken as the system (ancilla) qubit. X (Y) denotes the nuclear spin rotation around the *x* (*y*) axis. The initial state is prepared by rotations Y(θ) and X(π/2). The two-qubit system evolves under the dilation Hamiltonian $H_{s,a}$. The populations of the four energy levels are measured after the rotation X(−π/2).

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where r is a real number. The eigenvalues of H_s are $E = \pm\sqrt{1-r^2}$. In the region $|r| < 1$, the eigenvalues E are real, and the system is in an unbroken-symmetry region. Especially, the Hamiltonian H_s is Hermitian with $r = 0$. When $|r| > 1$, the imaginary part of E appears, and the system is in a broken-symmetry region. The point $|r| = 1$ is known as the exceptional point. By taking $\eta(0) = \eta_0 I$, with η_0 being a real number, the corresponding $H_{s,a}$ can be written in terms of Pauli operators as follows

$$H_{s,a}(t) = A_1(t)\sigma_x \otimes I + A_2(t) I \otimes \sigma_z + A_3(t)\sigma_y \otimes \sigma_z + A_4(t)\sigma_z \otimes \sigma_z \quad (3)$$

where $A_1(t)$, $A_2(t)$, $A_3(t)$, and $A_4(t)$ are real-valued functions determined by H_s (SM1 and fig. S3).

A single nitrogen-vacancy (NV) center in diamond (Fig. 1A) is used to demonstrate our proposal. The Hamiltonian of the NV center is $H_{NV} = 2\pi(DS_z^2 + \omega_e S_z + QI_z^2 + \omega_n I_z + AS_z I_z)$, where S_z (I_z) is the spin operator of the electron (nuclear) spin, $D = 2.87$ GHz is the electronic zero-field splitting, $Q = -4.95$ MHz is the nuclear quadrupolar interaction, and $A = -2.16$ MHz is the hyperfine interaction. A magnetic field is applied along the NV symmetry axis ([1 1 1] crystal axis), yielding the electron (nuclear) Zeeman frequencies ω_e (ω_n). A subspace of the total system is utilized to form a two-qubit system, which is spanned by the four energy levels $|m_S, m_I\rangle = |0,1\rangle, |0,0\rangle, |-1,0\rangle$, and $|-1,1\rangle$ relabeled with $|0\rangle_e|1\rangle_n, |0\rangle_e|0\rangle_n, |-1\rangle_e|0\rangle_n$, and $|-1\rangle_e|1\rangle_n$ (Fig. 1B).

To realize the $H_{s,a}(t)$ in Eq. 3, we apply on the electron spin of the two-spin system two selective microwave pulses with time-dependent amplitudes, frequencies, and phases. The pulses can be described by the following Hamiltonian

$$H_c = 2\pi\sqrt{2}\Omega_1(t)\cos\left[\int_0^t \omega_1(\tau)d\tau + \phi_1(t)\right] S_x \otimes |1\rangle_{nn}\langle 1| + 2\pi\sqrt{2}\Omega_2(t)\cos\left[\int_0^t \omega_2(\tau)d\tau + \phi_2(t)\right] S_x \otimes |0\rangle_{nn}\langle 0| \quad (4)$$

where $\Omega_{1,2}(t)$, $\omega_{1,2}(t)$ and $\phi_{1,2}(t)$ correspond to the amplitudes, angular frequencies, and phases of the two pulses. The evolution of the two-qubit system follows $H_{s,a}$ in Eq. 3 (in the interaction picture) when the frequencies of the two microwave pulses $\omega_1(t) = \omega_{MW1} + 2A_4(t)$ and $\omega_2(t) = \omega_{MW2} - 2A_4(t)$, the amplitudes $\Omega_1(t) = \Omega_2(t) = \sqrt{A_1^2(t) + A_3^2(t)}/\pi$ and the phases $\phi_1(t) = -\phi_2(t) = -\text{arctan2}(A_3(t), A_1(t))$ (see SM2 and fig. S4 for the derivation and numerical results).

The experiment was performed on an optically detected magnetic resonance setup. The static magnetic field was set to 506 G, and the NV center was polarized into the state $|0\rangle_e|1\rangle_n$ via laser pulses (*31*). Then the initial state was prepared to $|\Psi\rangle = |0\rangle_e|-\rangle_n + \eta_0|0\rangle_e|+\rangle_n$ by the rotations $Y(\theta)$ followed by $X(\pi/2)$ applied on the nuclear spin (Fig. 1C), where $\theta = 2\arctan\eta_0$. Two selective MW pulses applied to the electron spin were generated by an arbitrary waveform generator. Finally, the nuclear spin rotation $X(-\pi/2)$ transformed the state $|\Psi(t)\rangle = |\psi(t)\rangle_e|-\rangle_n + \eta(t)|\psi(t)\rangle_e|+\rangle_n$ into $|\Phi(t)\rangle = |\psi(t)\rangle_e|1\rangle_n + \eta(t)|\psi(t)\rangle_e|0\rangle_n$ for measurement. Populations of the electron spin states (denoted as P_0 and P_1) when nuclear spin is $|1\rangle_n$ were obtained by a proper renormalization of the experimentally measured data (SM3).

The state evolution under H_s is explored by monitoring P_0 in the time range of 0 to 8 μs, with the Hermitian case $r = 0$ (Fig. 2A), $\mathcal{PT}$ unbroken case $r = 0.6$ (Fig. 2B), exceptional point $r = 1.0$ (Fig. 2C) and $\mathcal{PT}$ broken case $r = 1.4$ (Fig. 2D). The measured dependence of the state evolution under H_s with r (Fig. 2F), shows good agreement with the theoretical predictions (Fig. 2E). The transition from the unbroken to the broken $\mathcal{PT}$ symmetry through the exceptional point has been clearly demonstrated in Fig. 2. When $|r| < 1$, H_s has real-valued eigenvalues and determines an oscillatory dynamics (Fig. 2B). When $|r| > 1$, the eigenvalues become imaginary, leading to the breakdown of the oscillation (Fig. 2D). Physically, the dynamics of P_0 in the region of unbroken $\mathcal{PT}$ symmetry is due to the nonvanished oscillatory amplitudes of microwave pulses. While in the region of broken $\mathcal{PT}$ symmetry, the amplitudes of microwave

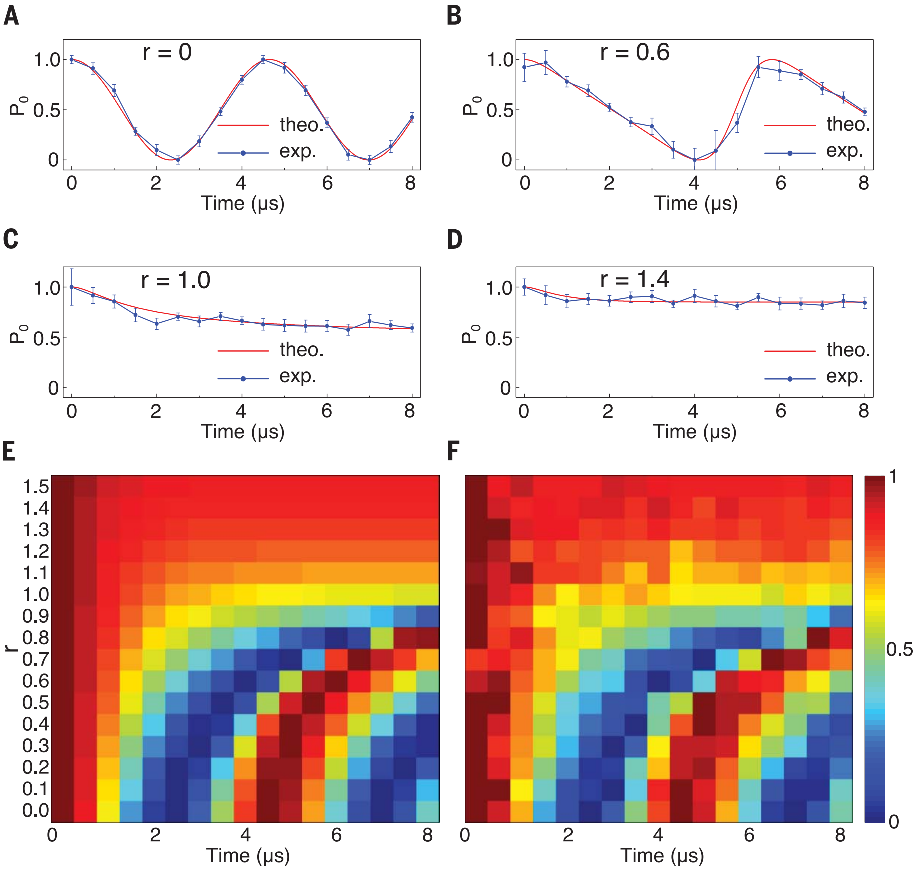

Fig. 2. State evolution under H_s. (**A** to **D**) Experimental dynamics of renormalized population P_0 when $r = 0$ (A), $r = 0.6$ (B), $r = 1.0$ (C), and $r = 1.4$ (D). All data were collected with 0.5 million averages. Blue dots with error bars are experimental results, and red lines are the theoretical predictions. (**E** and **F**) Plot of theoretical results (E) and experimental results (F) for various r values. The color bar stands for P_0.

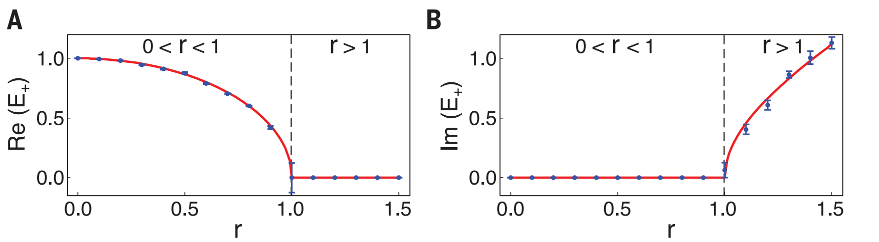

Fig. 3. Experimental observation of the breaking of the $\mathcal{PT}$ symmetry. (**A** and **B**) Real and imaginary part of the eigenvalue, E_+, of H_s as the function of parameter r. The blue dots with error bars are experimental results, and red lines are theoretical predictions. The interval of $0 < r < 1$ indicates the $\mathcal{PT}$ unbroken region and the interval of $r > 1$ indicates the $\mathcal{PT}$ broken region. The exceptional point occurs at $r = 1$.

pulses decay with time, and the system approaches to a steady state (fig. S4).

The $\mathcal{PT}$ phase transition is also characterized by eigenvalues of the $\mathcal{PT}$-symmetric Hamiltonians derived from experimental data (Fig. 3). The eigenvalues of the H_s are expressed as $E_\pm = \pm\sqrt{1 - r_{\mathrm{exp}}^2}$, where the parameter r_{exp} is obtained by curve fitting the experimental time evolution of the population P_0 to theoretical predictions under $\mathcal{PT}$-symmetric Hamiltonian H_s (SM4). When $r < 1$, the eigenvalues $E_\pm$ remain real as r approaches 1 from 0. At the exceptional point $r = 1$, the eigenvalues $E_\pm$ coalesce to 0. When $r > 1$, the system is in the $\mathcal{PT}$-symmetry broken region, and the real parts of the two eigenvalues are zero and the imaginary parts appear. The experimental results show excellent agreement with the corresponding theoretical predictions.

Our work makes NV center a desirable platform for investigating important non-Hermitian physics, such as new topological invariants (*32*–*35*), quantum thermodynamics (*36*), and information criticality (*29*) in this scenario. This platform can be used to investigate various models of decoherence and dissipation in open quantum systems (SM5 and fig. S6). Furthermore, the feature of the exceptional point can be used to improve the sensitivity of quantum sensing (*37*, *38*). This is expected to enhance the performance of NV-based quantum sensor with a variety of applications.

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SUPPLEMENTARY MATERIALS

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Materials and Methods
Supplementary Text
Figs. S1 to S6
Table S1
References (*39*–*41*)

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Breaking symmetry with single spins

The energetics of quantum systems are typically described by Hermitian Hamiltonians. The exploration of non-Hermitian physics in classical parity-time (PT)–symmetric systems has provided fertile theoretical and experimental ground to develop systems exhibiting exotic behavior. Wu *et al.* now demonstrate that non-Hermitian physics can be found in a solid-state quantum system. They developed a protocol, termed dilation, which transformed a PT-symmetric Hamiltonian into a Hermitian one. This allowed them to investigate PT-symmetric physics with a single nitrogen-vacancy center in diamond. The results provide a starting point for exploiting and understanding the exotic properties of PT-symmetric Hamiltonians in quantum systems.

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