Dynamical quantum phase transition in a non-Hermitian Hubbard model

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We reveal the dynamical quantum phase transition unique to non-Hermitian systems. A system initially in a symmetry-unbroken state suddenly falls into a symmetry-broken state as time goes by. This is in stark contrast to that in Hermitian systems since an order parameter of spontaneous symmetry breaking shows non-analyticity at a critical time, that is, spontaneous symmetry breaking occurs as a function of time. By the quantum Monte Carlo, we simulate the time evolution of a non-Hermitian Hubbard model and show the non-analyticity of a magnetic correlation function in the infinite volume limit.

Introduction Understanding the dynamics of dissipative quantum many-body systems has been one of the key topics in recent years. Among them, two nonunitary dynamics are found to serve a new platform of physics: One is the conditional dynamics, which is obtained by post-selecting quantum trajectories from the unconditional Lindbladian dynamics of open quantum systems. The other is the monitored dynamics, which is a hybrid quantum system composed of the unitary evolution and repeated projective measurements. Intriguing phenomena such as the entanglement phase transition have been found so far [1–4], but many-body phenomena unique to them are yet to be elucidated.

As aforementioned, theoretically, and also experimentally, the stochastically unraveling dynamics is investigated instead of directly handling the quantum master equation. In this procedure, one solves the time evolution of a wave function under some stochasticity instead of that of a density matrix. If we employ the quantum trajectory method [5, 6], the dynamics is decomposed into two parts: One is the nonunitary evolution described by the Schrödinger equation with an effective non-Hermitian Hamiltonian. The other is the quantum jump process, which is a stochastic loss event. Although we can reconstruct the density matrix under the Lindbladian dynamics by averaging the loss event, or equivalently, the many trial wave functions, we restrict ourselves to follow the single trial wave function that experiences no loss event. The dynamics of the constrained wave function leads us to study the non-Hermitian quantum mechanics (see, e.g., Ref. [7] for a review). However, genuine many-body physics is yet to be elucidated [8–16], and in particular, it still lacks the reliable methods for accurate large-scale numerical simulations.

In this Letter, we reveal an exotic dynamical quantum phase transition, which has no counterpart in Hermitian quantum systems. To this end, we study the time evolution of a non-Hermitian Hubbard model in which the coupling strength of the Hubbard interaction is pure-imaginary. In fact, such a non-Hermitian Hubbard model with complex coupling strength can be realized, e.g., in dissipative ultracold atoms, and its dynamical properties are intensively investigated [17–22]. We compute the time evolution of magnetic correlation functions after a quantum quench, and show that the system initially set in a symmetry-unbroken state suddenly turns into a symmetry-broken state during the time evolution. In contrast to the dynamical quantum phase transition in Hermitian systems [23], an order parameter of spontaneous symmetry breaking exhibits non-analyticity at a critical time in the infinite volume limit, that is, spontaneous symmetry breaking as a function of time. It paves the way towards understanding unique properties of non-Hermitian many-body systems.

As a computational tool, we adopt a large-scale simulation of the fermionic quantum Monte Carlo. The simulation is ab initio and unbiased. We show that it does not suffer from the notorious sign problem, although one may suspect that the complex weights associated with the real-time evolution hinder the importance sampling. This enables us to study many-body phenomena with a large number of degrees of freedom, e.g., the critical properties of the phase transition on the basis of the finite-size scaling analysis.

Model and formulation We consider two-component fermions on a three-dimensional cubic lattice \( r = (x, y, z) \). The unitary evolution is described by the free Hamiltonian,

\[
H = -w \sum_{r,j,\sigma} \left( c_{r+\sigma,j}^\dagger c_{r,\sigma} + c_{r,\bar{\sigma}}^\dagger c_{r+\bar{\sigma},j} \right),
\]

where \( c_{r,\uparrow,\downarrow}^\dagger \) and \( c_{r,\uparrow,\downarrow} \) are the creation and annihilation operators of the \( \uparrow \)- and \( \downarrow \)-component of fermions at a site \( r \), respectively. \( w \) is a hopping parameter between the nearest neighbor sites, and \( j = \hat{x}, \hat{y}, \hat{z} \) is the unit lattice vector along the \( j \) direction. We consider the dissipative dynamics in the presence of the particle loss due to inelastic collisions. When the \( \uparrow \)- and \( \downarrow \)-fermions occupy a site simultaneously, they acquire the kinetic energy from inelastic collisions and quickly escape from the system. Such a loss process is described by the quantum master equation in the Lindblad form [6],

\[
\frac{d\rho}{dt} = -i(H \rho - \rho H) + \sum_r \gamma_r \left( \Gamma_r \rho \Gamma_r^\dagger - \frac{1}{2} \Gamma_r^\dagger \Gamma_r \rho - \frac{1}{2} \rho \Gamma_r \Gamma_r^\dagger \right).
\]
where $\rho$ is the density matrix of the system. The first and second lines determine the unitary and dissipative dynamics, respectively, where $\Gamma_r$ is the quantum jump operator and $\gamma_r$ is the strength of dissipation. In our case, $\Gamma_r$ removes the pair of fermions occupying the site $r$ at rate $\gamma_r$, so that the quantum jump operator is given as $\Gamma_r = c_r \dagger c_r$. Since the loss rate is independent of the site, we take $\gamma_r = 2\gamma$, where the factor of 2 is introduced for notational convenience.

We employ the quantum trajectory method [5]. Then, the dynamics is decomposed into the unitary evolution and quantum jump process. By post-selecting the quantum trajectories, we follow the time evolution of the wave function that experiences no particle loss, which can be recovered from the non-Hermitian quantum mechanics described by

$$i \frac{d}{dt} |\Psi(t)\rangle = H_{\text{eff}} |\Psi(t)\rangle,$$

and the non-Hermitian Hamiltonian,

$$H_{\text{eff}} = -w \sum_{r,j,\sigma} \left[ c_{r,\sigma}^\dagger c_{r+j,\sigma} + c_{r+j,\sigma}^\dagger c_{r,\sigma} \right] - i\gamma \sum_r c_{r,\uparrow}^\dagger c_{r,\downarrow}^\dagger c_{r,\downarrow} c_{r,\uparrow}.$$

These define our model investigated in this Letter. As an initial condition, we consider the Néel state, that is, the half-filled state with even (odd) sites being occupied by the $\uparrow$- ($\downarrow$-) components. Since $|\Psi(t)\rangle|\Psi(t)\rangle$ gives the persistent probability that no quantum jump occurs, by taking the conditional probability into account, the expectation values of physical observable $\hat{O}$ under the conditional dynamics is given as

$$\langle \hat{O} \rangle = \frac{\langle \Psi(t) | \hat{O} | \Psi(t) \rangle}{\langle \Psi(t) | \Psi(t) \rangle}.$$

Using the total number of the fermions $N = \sum_r c_{r,\sigma}^\dagger c_{r,\sigma}$, we rescale the wave function as $|\Psi(t)\rangle = e^{-\frac{i}{2} N t} |\tilde{\Psi}(t)\rangle$. Since $N$ is conserved during time evolution, that is, it is a classical number fixed by the initial condition, Eq. (5) is invariant under $|\tilde{\Psi}(t)\rangle = e^{-\frac{i}{2} N t} |\Psi(t)\rangle$. The time evolution of $|\tilde{\Psi}(t)\rangle$ obeys

$$i \frac{d}{dt} |\tilde{\Psi}(t)\rangle = \left( H_{\text{eff}} + \frac{i\gamma}{2} \sum_{r,\sigma} c_{r,\sigma}^\dagger c_{r,\sigma} \right) |\tilde{\Psi}(t)\rangle \equiv \tilde{H}_{\text{eff}} |\tilde{\Psi}(t)\rangle.$$

The transformation is essential for the sign-free auxiliary-field quantum Monte Carlo. Below we always use the latter representation, and omit the tilde index for notational simplicity.

Using the second-order Suzuki-Trotter decomposition, we write the persistent probability as

$$\langle \Psi(t) | \tilde{\Psi}(t) \rangle = \langle \Psi(0) | e^{iH_{\text{eff}}t} e^{-iH_{\text{eff}}t} |\Psi(0)\rangle = \langle \Psi(0) \prod_m U_m \prod_n \langle U_n | \Psi(0) \rangle,$$

where

$$U_n = e^{-i \Delta t K/2} e^{-i \Delta t/2} e^{-i \Delta t K/2},$$

$$K = -w \sum_{r,j,\sigma} \left[ c_{r,\sigma}^\dagger c_{r+j,\sigma} + c_{r+j,\sigma}^\dagger c_{r,\sigma} \right],$$

$$U = i\gamma \sum_r \left[ -c_{r,\uparrow}^\dagger c_{r,\downarrow}^\dagger c_{r,\downarrow} + \frac{1}{2} (c_{r,\uparrow}^\dagger c_{r,\uparrow} + c_{r,\downarrow}^\dagger c_{r,\downarrow}) \right],$$

and $\Delta t = t/N_t$ with $N_t$ being the number of the Suzuki-Trotter step. Each component of $U$ can be rewritten by introducing the auxiliary binary field $s$ as

$$e^{-\gamma \Delta t (c_{r,\uparrow}^\dagger c_{r,\downarrow} - \frac{1}{2}) (c_{r,\downarrow}^\dagger c_{r,\uparrow} - \frac{1}{2}) + \frac{\gamma}{2} \Delta t} = \frac{\gamma}{2} \sum_{s=\pm 1} e^{igs(c_{r,\uparrow}^\dagger c_{r,\downarrow} + c_{r,\downarrow}^\dagger c_{r,\uparrow} - 1)},$$

where $\cos(g) = e^{-\gamma \Delta t/2}$. Therefore, the nonunitary evolution $e^{-iH_{\text{eff}}t}$ is reformulated as the unitary evolution under the space-time binary disorder. Now we have [24]

$$\langle \Psi(t) | \tilde{\Psi}(t) \rangle = \mathcal{N} \sum_{s(n,r)} e^{-i g s(n,r)} \prod_{\sigma} \prod_{\{s(n,r)\}} \det \left[ P_{\sigma}^j B_{2N_t} \cdots B_1 P_{\sigma} \right],$$

where $\mathcal{N} = \langle \Psi(0) \rangle \langle \Psi(0) \rangle = \langle \Psi(0) \rangle \langle \Psi(0) \rangle$. (II) Each spin state is expressed by a Slater determinant with the $V \times V^2$ rectangular matrix $P_{\sigma}$:

$$\langle \Psi_{\sigma}(0) \rangle = \prod_{r'} \prod_\sigma c_{r',\sigma}^\dagger c_{r',\sigma} = \left[ P_{\sigma}^j r_{j} \right] / \langle \Psi_{\sigma}(0) \rangle,$$

where $\langle 0 \rangle$ is the Fock vacuum, and $r'$ runs for even (odd) sites for the $\uparrow$- ($\downarrow$-) component.

We consider the particle-hole transformation only for the $\downarrow$-component: $c_{r,\downarrow} \rightarrow c_{r,\downarrow}^\dagger$. Then, occupied and unoccupied states are swapped for the $\downarrow$-component, so that $|\Psi_{\sigma}(0)\rangle = |\Psi_{\downarrow}(0)\rangle$, and $P_{\downarrow} = P_{\uparrow}$ (up to an irrelevant phase). Also, the transfer matrix is transformed as $e^{-i \sigma \sum_{n,r} B_n} \rightarrow B_n^*$, and thus the integrand of $\langle \Psi(t) | \tilde{\Psi}(t) \rangle$ is actually positive definite:

$$\langle \Psi(t) | \tilde{\Psi}(t) \rangle = \mathcal{N} \sum_{s(n,r)} \left| \det \left[ P_{\sigma}^j B_{2N_t} \cdots B_1 P_{\sigma} \right] \right|^2.$$

The summation of the auxiliary fields can be evaluated on the basis of the importance sampling, and the physical observable can by ensemble average (with the help of the Wick theo-
The initial state is the Néel state.

rem) as is commonly done in the projector quantum Monte Carlo (see, e.g., Ref. [24]). There is also another way to prove the positivity. We consider a unitary transformation $c_{r\uparrow} \rightarrow i^{x+y+z} c_{r\uparrow}$, and $c_{r\downarrow} \rightarrow (-i)^{x+y+z} c_{r\downarrow}$. Then the non-Hermitian Hamiltonian (4) reads

$$H_{\text{eff}} = -iw \sum_{\mathbf{r},\mathbf{j}} \left[ c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}+\mathbf{j}\downarrow} - c_{\mathbf{r}+\mathbf{j}\uparrow}^\dagger c_{\mathbf{r}\downarrow} \right] + iw \sum_{\mathbf{r},\mathbf{j}} \left[ c_{\mathbf{r}\downarrow}^\dagger c_{\mathbf{r}+\mathbf{j}\downarrow} - c_{\mathbf{r}+\mathbf{j}\uparrow}^\dagger c_{\mathbf{r}\downarrow} \right] - i\gamma \sum_{\mathbf{x}} c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}\uparrow} c_{\mathbf{r}\downarrow}^\dagger c_{\mathbf{r}\downarrow}$$

$$\equiv -iH_{\text{new}}. \quad (16)$$

The real-time evolution in the original basis $e^{-iH_{\text{eff}}t}$ is mapped to the imaginary-time one $e^{-H_{\text{new}}t}$ with the spin-dependent Hatano-Nelson type hopping, which does not suffer from the sign problem at half filling [16]. This mapping is very suggestive. By changing the expectation value of a pure initial state to the trace average of all initial states, we can study the finite-temperature phase of $H_{\text{new}}$ via the time evolution of $H_{\text{eff}}$.

**Numerical simulation** We compute the time evolution of the antiferromagnetic spin structure factor

$$S_{AF} = \left\langle \frac{1}{V} \sum_{\mathbf{r}} \left( -i^{x+y+z} S_{\mathbf{r}} \right)^2 \right\rangle,$$  \quad (17)

and the ferromagnetic spin structure factor

$$S_{FF} = \left\langle \left( \frac{1}{V} \sum_{\mathbf{r}} S_{\mathbf{r}} \right)^2 \right\rangle,$$  \quad (18)

where $S_{\mathbf{r}}$ is the spin operator, and is given explicitly as

$$S_{\mathbf{r}} = (S_{\mathbf{r}\uparrow}^x, S_{\mathbf{r}\downarrow}^z, S_{\mathbf{r}\downarrow}^z) = (c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}\downarrow} + c_{\mathbf{r}\downarrow}^\dagger c_{\mathbf{r}\uparrow}, -ic_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}\downarrow} + ic_{\mathbf{r}\downarrow}^\dagger c_{\mathbf{r}\uparrow}, c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}\downarrow} - c_{\mathbf{r}\downarrow}^\dagger c_{\mathbf{r}\uparrow})/2,$$

which commutes with the Hamiltonian $H_{\text{eff}}$. We fixed the Trotter step with $\Delta t = 0.05/w$. We have checked the convergence of the numerical results by changing $\Delta t$. We imposed periodic boundary conditions. We show the results at $\gamma/w = 4.0$ with $V = L^4 = 4^3, 6^3, 8^3, 10^3, 12^3$ in Figs. 1 and 2. From Fig. 1, we see that the antiferromagnetic correlation decays exponentially fast. This indicates that the initial-state dependence is quickly lost after a very short time. A more interesting thing happens in the ferromagnetic spin structure factor in Fig. 2. We clearly see that the magnetic correlation suddenly changes from paramagnetic to ferromagnetic at a certain time. The volume dependence suggests that this change can be regarded as a dynamical quantum phase transition in the infinite volume limit; the system initially in a symmetry-unbroken state non-analytically falls into a symmetry-broken state at a critical time. There is a sharp contrast with the conventional dynamical quantum phase transition [23], which is probed by the non-analyticity of the Loshmidt echo, that is, the overlap between time-evolved and reference (usually initial) states. The dynamical quantum phase transition here is accompanied by spontaneous symmetry breaking and probed by the magnetic correlation function. Amazingly, it is just like the equilibrium phase transition. We note that the longitudinal spin correlation $\langle \Psi(t) | S_\mathbf{r}^z S_\mathbf{p}^z | \Psi(t) \rangle / \langle \Psi(t) | \Psi(t) \rangle$ is always exponentially fall off (i.e., gapped) at a large distance since the total $S^z$ is fixed by the initial state, and only the transverse spin correlation $\langle \Psi(t) | S_\mathbf{r}^x S_\mathbf{p}^x + S_\mathbf{r}^y S_\mathbf{p}^y | \Psi(t) \rangle / \langle \Psi(t) | \Psi(t) \rangle$ shows the long-range order. In other words, the initial state explicitly breaks the SU(2) to SO(2)×U(1), and the remaining symmetry is spontaneously broken.

To deepen our understanding of the dynamical phase transition, we performed the finite-size scaling analysis near the critical time as shown in Fig. 3. After the critical time, the spin structure factor clearly shows the linear scaling and becomes nonzero in the infinite volume limit, while it shows the trivial volume-law scaling before the critical time. By fitting the data
as the initial state is a symmetry-unbroken state.

We finally comment on the universality class of the phase transition. By considering the strong-coupling expansion of the non-Hermitian Hubbard model [21], its real-time evolution is reduced to the imaginary-time one of the ferromagnetic Heisenberg model. Thus, we expect that the observed phase transition has the same universality class as the finite-temperature one in the Heisenberg model. To check the scenario, we perform the Binder analysis in Fig. 5. Since \( S^z \) is gapped at a large distance, the critical behavior of the Heisenberg model would be the same as that of the classical XY model, and thus, we employ \( \eta = 0.038 \) [25]. The spin structure factor shows scale invariance, which strongly supports the same universality class as the three-dimensional XY model.

Conclusion We have discovered the dynamical quantum phase transition in a non-Hermitian Hubbard model on the basis of the quantum Monte Carlo. The phase transition and its universality class were probed by the long-range order of ferromagnetism, and so described by spontaneous symmetry breaking. It is notable that spontaneous symmetry breaking was analyzed as a function of time. This is strikingly different from the ordinary one induced by varying parameters such as a coupling constant or temperature. Time is the intrinsic parameter inducing this spontaneous symmetry breaking.

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[1] A. Chan, R. M. Nandkishore, M. Pretko, and G. Smith, Phys. Rev. B 99, 224307 (2019).
[2] B. Skinner, J. Ruhman, and A. Nahum, Phys. Rev. X 9, 031009
[3] Y. Li, X. Chen, and M. P. A. Fisher, Phys. Rev. B 100, 134306 (2019).
[4] C.-M. Jian, Y.-Z. You, R. Vasseur, and A. W. W. Ludwig, Phys. Rev. B 101, 104302 (2020).
[5] A. J. Daley, Adv. Phys. 63, 77 (2014).
[6] H.-P. Breuer and F. Petruccione, The Theory of Open Quantum Systems (Oxford University Press, Oxford, 2007).
[7] Y. Ashida, Z. Gong, and M. Ueda, Adv. Phys. 69, 3 (2020).
[8] T. E. Lee and C.-K. Chan, Phys. Rev. X 4, 041001 (2014).
[9] Y. Ashida, S. Furukawa, and M. Ueda, Nature Communications 8, 15791 (2017).
[10] J. A. S. Lourenço, R. L. Eneias, and R. G. Pereira, Phys. Rev. B 98, 085126 (2018).
[11] M. Nakagawa, N. Kawakami, and M. Ueda, Phys. Rev. Lett. 123, 203001 (2019).
[12] R. Hamazaki, K. Kawabata, and M. Ueda, Phys. Rev. Lett. 123, 090603 (2019).
[13] S. Mu, C. H. Lee, L. Li, and J. Gong, Phys. Rev. B 102, 081115 (2020).
[14] T. Liu, J. J. He, T. Yoshida, Z.-L. Xiang, and F. Nori, Phys. Rev. B 102, 235151 (2020).
[15] S. Gopalakrishnan and M. J. Gullans, Phys. Rev. Lett. 126, 170503 (2021).
[16] T. Hayata and A. Yamamoto, Phys. Rev. B 104, 125102 (2021).
[17] K. Sponselee, L. Freystatzky, B. Abeln, M. Diem, B. Hundt, A. Kochanke, T. Ponath, B. Santra, L. Mathey, K. Sengstock, and C. Becker, Quantum Science and Technology 4, 014002 (2019).
[18] T. Tomita, S. Nakajima, I. Danshita, Y. Takashita, and Y. Takahashi, Science Advances 3, e1701513 (2017).
[19] T. Tomita, S. Nakajima, Y. Takashita, and Y. Takahashi, Phys. Rev. A 99, 031601 (2019).
[20] K. Yamamoto, M. Nakagawa, K. Adachi, K. Takasan, M. Ueda, and N. Kawakami, Phys. Rev. Lett. 123, 123601 (2019).
[21] M. Nakagawa, N. Tsuji, N. Kawakami, and M. Ueda, Phys. Rev. Lett. 124, 147203 (2020).
[22] K. Yamamoto, M. Nakagawa, N. Tsuji, M. Ueda, and N. Kawakami, Phys. Rev. Lett. 127, 055301 (2021).
[23] M. Heyl, Rept. Prog. Phys. 81, 054001 (2018).
[24] F. Assaad and H. Evertz, World-line and determinantal quantum monte carlo methods for spins, phonons and electrons, in Computational Many-Particle Physics, edited by H. Fehske, R. Schneider, and A. Weiße (Springer Berlin Heidelberg, Berlin, Heidelberg, 2008) pp. 277–356.
[25] M. Campostrini, M. Hasenbusch, A. Pelissetto, P. Rossi, and E. Vicari, Phys. Rev. B 63, 214503 (2001).