We study parity-time-symmetric non-Hermitian quantum systems at finite temperature, where the Boltzmann distribution law fails to hold. To characterize their abnormal physical properties, a new quantum statistics theory (the so-called quantum Liouvillian statistics theory) was developed, in which the Boltzmann distribution law was replaced by the Liouvillian-Boltzmann distribution law. Using it, we derived analytical results of thermodynamic properties for thermal $\mathcal{PT}$ systems and found that a “continuous” thermodynamic phase transition occurs at the exceptional point, where a zero-temperature anomaly exists.

In statistical mechanics, the Boltzmann distribution (BZ) law plays a central role and governs the equilibrium distribution of different equilibrium states at a particular temperature. According to it, a system will be in a certain state as a function of its energy $E_n$ and of its temperature $T$. As a result, the weights of different (quantum) states obey the BZ law, i.e. $\rho_n \sim e^{-E_n/k_B T}$. This universal distribution law was derived by Boltzmann through an axiomatic way, which involves finding the most likely macrostates for a given the total energy under the assumption that all possible microstates were equally likely to occur. With the help of the BZ law, one can recognize properties of macroscopic quantities of different physical systems at finite temperature (finite-T).

The non-Hermitian (NH) problem in controlled open quantum systems has recently begun to be considered one of the frontiers of physics. A parity-time ($\mathcal{PT}$)-symmetric NH quantum model was proposed by Bender and Boettcher [1–3] in 1998, where $\mathcal{PT}$-symmetry spontaneous breaking ($\mathcal{PT}$-SSB) occurs at a critical point (the so-called “exceptional point” (EP)). $\mathcal{PT}$-symmetry systems have attracted a lot of researches in different fields [4–8] and various approaches were proposed for realizing $\mathcal{PT}$-symmetric NH models[9–38]. However, people are still in the dark about the properties of a $\mathcal{PT}$-symmetric NH quantum model at finite-T (the so-called thermal $\mathcal{PT}$ systems) and nothing is known about their thermodynamic behavior. Hence, immediate questions appear, such as: Do the thermal $\mathcal{PT}$ systems still obey the BZ law? If not, what distribution do they obey? Are there new physical phenomena compared with their Hermitian counterparts for thermal $\mathcal{PT}$ systems?

In this letter, by taking a designed thermal $\mathcal{PT}$ system as an example, we studied this issue and derived reliable results by solving the quantum master equation. According to them, a surprising discovery is that the BZ law is no longer applicable in such systems. As a result, a new theory beyond the usual quantum statistical one is developed in order to completely understand these abnormal physical properties of thermal $\mathcal{PT}$ systems.

To design a thermal $\mathcal{PT}$ system we couple a thermal bath to a $\mathcal{PT}$ system. To reach this goal, we consider a controlled open quantum system $S$ coupling to two separated environments $B$ and $E$. $S$ denotes a tight-binding model of two lattice sites, 1 and 2, with single fermionic particle; $B$ denotes a thermal environment with temperature $T = \frac{1}{k_B \beta_T}$; and $E$ denotes an environment under postselection with fixed particle number of $S$ to be 1.

![FIG. 1: Illustration of a thermal $\mathcal{PT}$ system that comes from the controlled open quantum system $S$ coupling to two separated environments $B$ and $E$. $S$ denotes a tight-binding model of two lattice sites, 1 and 2, with single fermionic particle; $B$ denotes a thermal environment with temperature $T = \frac{1}{k_B \beta_T}$; and $E$ denotes an environment under postselection with fixed particle number of $S$ to be 1.](image-url)
the system B. Here, we assume that $\gamma_1, \gamma_2 \ll \gamma, h$. In particular, there is no direct coupling between the two environments B and E. In the following parts, $h$ is set be the unit.

For the open quantum system S under the Markovian approximation, its non-unitary dynamics is in general expressed by the quantum master equation in the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) form [40–42],

$$\frac{d\rho^S(t)}{dt} = \mathcal{L}\rho^S(t),$$

where $\mathcal{L}$ is a Liouville super-operator acting on the (reduced) density matrix $\rho^S$ of the subsystem S.

In Hermitian systems at finite-T, the quantum statistical mechanics is based on the thermal equilibrium state. To reach it, one can prepare a unique final state under postselection measurements, the quantum jumping term from $\hat{H}^S$ will be projected out [43]. Under these conditions, the temperature of a possible NHTS is also assumed to be the same as that of the thermal environment B.

Next, we trace out B from the combined subsystem S+B and consider it on the NH subsystem S. This issue of NH open quantum systems has never been studied before. We assume that the NH subsystem S has little influence on the environment B and the relaxation time of the environment B is much smaller than S. Besides these conditions, the temperature of a possible NHTS must be a steady state with the eigenvalue 0 corresponding to the Liouville super-operator $\mathcal{L}$. After solving the GKSL equation, $\rho^S_{\text{NHTS}}$ is obtained as

$$\frac{h-\gamma}{\sqrt{h^2-\gamma^2-h^2}} \begin{pmatrix} h+\gamma & 1-e^{-\beta \gamma} \sqrt{h^2-\gamma^2-h^2} \\ 1 & 1 \end{pmatrix}.$$ 

More detailed calculations are provided in the Supplementary Materials.

On the other hand, we study the possible NHTS $\rho^S_{\text{NHTS}}$ in the phase with $\mathcal{PT}$-symmetry ($h > \gamma$). Now, the two energy levels of NH Hamiltonian are purely real, $\pm \sqrt{\gamma^2-h^2}$. As a result, the NHTS must be a steady state with the eigenvalue 0 corresponding to the Liouville super-operator $\mathcal{L}$. After solving the GKSL equation, $\rho^S_{\text{NHTS}}$ is obtained as

$$\begin{pmatrix} \frac{h+\gamma}{h-\gamma} & 1 + e^{-\beta \gamma} \sqrt{h^2-\gamma^2-h^2} \\ 1 & 1 \end{pmatrix}.$$ 

This can be understood as the fact that the state $|\Psi_R\rangle$ decays much more faster than the state $|\Psi_L\rangle$. Eventually, there is only one eigenstate $|\Psi_R\rangle$ with the largest imaginary part of the eigenvalue $+i\sqrt{\gamma^2-h^2}$ left in the system.

Finally, according to the above results from the GKSL equation, we investigate the properties of NHTSs in the thermal $\mathcal{PT}$ system. These results of the expected values of $\sigma_i$ (i = x, y, z), i.e. $n_i = \langle \sigma_i \rangle$, are represented by points on the Bloch sphere in Fig.2(a) and Fig.2(b). Fig.2(a) indicates the existence of a unique NHTS $\rho^S_{\text{NHTS}}$ for $\hat{H}_{\text{NH}}$ with fixed $\gamma$ ($\gamma = 0.2h$), taking the limit $t \to \infty$, different initial states will eventually evolve into the same final state $\rho^S(t \to \infty)$. That means $\rho^S(t \to \infty)$ is just the NHTS $\rho^S_{\text{NHTS}}$; Fig.2(b) indicates the abnormality of the NHTS $\rho^S_{\text{NHTS}}$ for $\hat{H}_{\text{NH}}$ with different values for $\gamma$ ($\gamma = 0.3h, \gamma = 0.9h, \gamma = 1.5h$), from the same initial state, for example, a fully thermalized state described by $\rho^S(t = 0) = \frac{1}{4}I_{2 \times 2}$, the system will eventually evolve into different NHTSs $\rho^S_{\text{NHTS}}(\gamma)$.
Let us check the validity of the BZ law in this thermal $\mathcal{PT}$ system.

For the Hermitian case ($\gamma = 0$), different thermal equilibrium states obey the BZ law, i.e., $P_+^T = e^{-\beta_T E^+}$ and $P_-^T = e^{-\beta_T E^{-}}$, where $E_{\pm} = \pm h$ are energy levels. In Fig.2(c), the blue line and blue triangles represent these expected values of $\sigma_z (n_z)$ from the BZ law and those derived by directly solving the GKSL equation, respectively. The consistency between the results from the BZ law and those derived from the GKSL equation verifies the correctness of both approaches.

Then we study the NH case. For NHTSs with $\gamma = 0.9h$, we can also derive $n_x$ by using the BZ law, i.e., $n_x = \frac{1}{e^{-\beta_T E_x} - e^{-\beta_T H_{R\text{BZ}}}} \text{Tr}(\sigma_x \cdot e^{-\beta_T H_{\text{BZ}}})$. In Fig.2(c), the red line and red triangles represent $n_x$ from the BZ law and those obtained by directly solving the GKSL equation, respectively. One can see that the results derived by means of the two mentioned approaches are noticeably contradictory in this case, which means that the BZ law does not hold in this situation. Consequently, one can safely conclude that the usual BZ law for thermal equilibrium states in Hermitian systems does not work anymore in NH systems! The immediate questions would be how to understand this violation of the BZ law in NHTSs, and whether there exists a new law that explains these abnormal results for a thermal $\mathcal{PT}$ system.

Before developing a systematic theory, we provide a physical explanation. In fact, NHTSs come from NH systems rather than from free ones. To realize a NH system, we controlled the open thermal $\mathcal{PT}$ system by performing a postselection and projecting out the quantum jumping term. The postselection measurement would result in a continuous information backflow from the NH environment $E$ to the subsystem $S$ [39]. These control actions break down the equal probability of different microscopic states and lead to a new distribution law.

In order to better describe this new distribution law, we develop a quantum Liouvillian statistics theory systematically and analytically characterize the thermal $\mathcal{PT}$ systems. In particular, it is a new type of distribution, that we call Liouvillian-Boltzmann distribution (LBZ) that governs the distribution of NHTSs at finite-$T$.

We focus on the case with real energy levels ($h > \gamma$). By doing a similarity transformation (ST) $\hat{S} = e^{\beta T \hat{H}}$, $\hat{H}_{\text{NH}}$ can be transformed into a Hermitian Hamiltonian $\hat{H}_0 = \sqrt{h^2 - \gamma^2} \sigma_x$, i.e., $\hat{H}_{\text{NH}} = \hat{S} \hat{H}_0 \hat{S}^{-1}$. Here, the real number $\beta_{\text{NH}} = \frac{1}{2} \ln \frac{h + \gamma}{h - \gamma}$ characterizes the strength of the NH terms and the Hermitian operator $\hat{H}' = \frac{1}{2} \sigma_z$ determines the form of the NH terms. Under the NH TS $\hat{S}$, the energy levels $E^\pm$ of $\hat{H}_{\text{NH}}$ are same to those of the Hermitian model $\hat{H}_0$. The corresponding eigenstates of $\hat{H}_{\text{NH}}$ become $|\Psi_n^S\rangle = \hat{S} |\Psi_{n,0}\rangle$, where $n = \pm$ and $|\Psi_{n,0}\rangle$ denotes the normalized eigenstates of $\hat{H}_0$. It is obvious that the effect from the NH terms leads to the additional NH TS $\hat{S}$ that breaks down the equal probability of different microscopic states.

Based on these physical quantities, we define the analytical formula of the density matrix $\rho_{\text{NH,NHTS}}^S$.

The density matrix for the thermal state of a NH system at temperature $T = \frac{1}{k_B \beta}$ is given as

$$\rho_{\text{NH,NHTS}}^S = \sum_{n=\pm} |\Psi_{n}^S\rangle e^{-\beta T E_n} \langle \Psi_n^S | = \hat{S} \rho_0 \hat{S}^\dagger,$$

where $\rho_0$ is the density matrix for Hermitian model $\hat{H}_0$. In [47], we provide the reason to write down the above equation (4).

To simplify the Liouvillian physics for NHTSs, we introduce an effective Hamiltonian $\hat{H}_L$ as $e^{-\beta_T \hat{H}_L} = \hat{S} (e^{-\beta_T \hat{H}_0}) \hat{S}^\dagger$ or

$$\hat{H}_L = -\frac{1}{\beta_T} \ln [\hat{S} (e^{-\beta_T \hat{H}_0}) \hat{S}^\dagger].$$

In this paper, we call the temperature-dependent Hamiltonian $\hat{H}_L$ to be Liouvillian Hamiltonian (LH). Its corresponding eigenvalues $E_L^\dagger$ and eigenstates are called Liouvillian energy levels and Liouvillian states, respectively. According to $\hat{H}_L = \hat{H}_L^\dagger$, $E_L^\dagger$ must be real.
For NHTSs in this NH system, although the energy levels do not change under STs, the weights of NHTSs are deformed. Consequently, the usual BZ law \( P_T = \frac{1}{Z_0} e^{-\beta_T E_n} \) is replaced by the Liouvillian-Boltzmann distribution (LBZ) law [48, 49], i.e.,

\[
P_T = \frac{1}{Z_{NHTS}^S} e^{-\beta_T E_n^L},
\]

where \( E_n^L \) is a Liouvillian energy level rather than the energy level \( E_n \) and \( Z_{NHTS}^S = \text{Tr}(e^{\beta_T H_L}) \) are the partition functions for the NHTSs. To distinguish the phenomenon of weights in the thermal PT system from those in Hermitian thermal systems, we call the corresponding weight \( P_T \) the Liouvillian weight.

In particular, when the temperature is high, \( \beta_T \to 0 \), the density matrix \( \rho_{NHTS}^S = e^{-\beta_T H_L} \) for a NH system with real spectra is reduced to \( \rho_{NHTS}^S \sim \hat{S} \hat{S}^\dagger = e^{2\beta_N H'} \), and the Liouvillian weight turns into \( P_T = \frac{1}{Z_{NHTS}^S} e^{-\beta_N (-2E'_n)} \), where \( E'_n \) is the “energy levels” of \( H' \).

By employing the quantum Liouvillian statistical theory, we study thermodynamic properties for the NHTSs \( \rho_{NHTS}^S \) of the thermal PT system.

These physical properties of the original NH system \( \hat{H}_{NH} \) at finite-T correspond to those of a Hermitian system of LH, \( \hat{H}_L \). According to \( e^{-\beta_T \hat{H}_L} = \hat{S}(e^{-\beta_T \hat{H}_0})\hat{S}^\dagger \), we obtain the analytical result as \( e^{-\beta_T \hat{H}_L} = \sigma_x A + \sigma_z B + 1C \), where \( I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \), \( A = -\sinh(\beta_T \sqrt{h^2 - \gamma^2}) \), \( B = \sinh(\beta_N) \cdot \cosh(\beta_T \sqrt{h^2 - \gamma^2}) \) and \( C = \cosh(\beta_N) \cdot \cosh(\beta_T \sqrt{h^2 - \gamma^2}) \). As a result, the LH is derived as

\[
\hat{H}_L = -\frac{1}{\beta_T} \frac{\cosh^{-1} C}{|\vec{r}_{eH}|} \hat{r} \cdot \hat{r}_{eH},
\]

where \( \hat{r} = (\sigma_x, \sigma_y, \sigma_z) \), \( \hat{r}_{eH} = (A, 0, B) \) and \( |\vec{r}_{eH}| = \sqrt{A^2 + B^2} \). Hence, the Liouvillian energy levels (the eigenvalues of \( \hat{H}_L \)) are

\[
E_{\pm} = \pm \frac{1}{\beta_T} \cosh^{-1} \left( \cosh(\beta_N) \cdot \cosh(\beta_T/2) \right),
\]

that are quite different from the energy levels (the eigenvalues for \( \hat{H}_{NH} \)) \( E_{\pm} = \pm \sqrt{h^2 - \gamma^2} \). According to LBZ law, we have

\[
P_T = \frac{1}{Z_{NHTS}^S} \frac{\exp[\cosh^{-1} C \cdot |\vec{r}_{eH}| \cdot (\hat{r} \cdot \hat{r}_{eH})]}{|\vec{r}_{eH}|^N}.
\]

The expected values of \( \sigma_i \) \((i = x, y, z)\) are defined as \( n_i = \langle \sigma_i \rangle = \frac{1}{Z_{NHTS}^S} \text{Tr} \left[ \sigma_i \cdot e^{-\beta_T \hat{H}_L} \right] \).

After straightforward calculations, we have \( \vec{n} = (n_x, n_y, n_z) = (\frac{\alpha}{\sqrt{\beta_N}}, \frac{\beta}{\sqrt{\beta_N}}, \frac{\gamma}{\sqrt{\beta_N}}) \) in the region of \( h > \gamma \). We then check the validity of the LBZ law by comparing its results \((n_x = \frac{\alpha}{\sqrt{\beta_N}}, \frac{\beta}{\sqrt{\beta_N}}, \frac{\gamma}{\sqrt{\beta_N}})\) with those from solving the GKSL equation. As shown in Fig. 2(d), they have the exact consistency of those derived by directly solving the GKSL equation (small triangles). Fig. 3(a) shows the results of \( \vec{n} \). From it, one can see that when \( \beta_N \) increases from zero to infinite, the spin direction changes from the x-direction to the z-direction. In particular, when the temperature is high, \( \beta_T \to 0 \), the expected values of \( \sigma_i \) waver from the z-direction to the y-direction with increasing \( \gamma \).

Finally, we discuss the possible thermodynamic phase transition at the EP \( h = \gamma \).

From the above discussions we concluded that the average spin operator \( n_i \) is always continuous when crossing over the EP. Furthermore, we calculate the derivatives of spin average values \( \frac{\partial \vec{n}}{\partial \beta_T} \). Because \( h = \gamma \) is a transition from real spectra to complex, the NHTSs of both sides \((h > \gamma \) and \( h < \gamma \)) are described by different functions. Thus, \( \frac{\partial \vec{n}}{\partial \beta_T} \) becomes discontinuous at \( h = \gamma \).

The discontinuity of \( \frac{\partial \vec{n}}{\partial \beta_T} \) indicates a “continuous” thermodynamic phase transition. In particular, there exists a \( \nu = \frac{1}{2} \) critical rule for \( \frac{\partial \vec{n}}{\partial \beta_T} \). At finite-T \( T \neq 0 \), \( \frac{\partial \vec{n}}{\partial \beta_T} = (2\beta_T, 0, h^{-1}) \) for \( h \to +0 \) and \( \frac{\partial \vec{n}}{\partial \beta_T} = (0, -(2h)^{-\nu}(\gamma - h)^{-\nu}, -\gamma^{-1}) \) for \( h \to +0 \); at zero temperature \( T = 0 \), \( \frac{\partial \vec{n}}{\partial \beta_T} = ((2h)^{-\nu}(h - \gamma)^{-\nu}, 0, h^{-1}) \) for \( h \to +0 \) and \( \frac{\partial \vec{n}}{\partial \beta_T} = (0, -(2h)^{-\nu}(\gamma - h)^{-\nu}, -\gamma^{-1}) \) for \( h \to +0 \). To emphasize the strangeness of the
ν = 1 critical rule, we call it zero temperature anomaly for the thermodynamic phase transition at EP. See the detailed calculations in the Supplementary Materials.

In this paper we studied the physics of thermal PT systems. Our results show that due to the postselection measurements, for the thermal PT system both the usual BZ law and Equal Probability Principle do not hold anymore. To characterize this abnormal behavior in NH systems at finite-T, a quantum Liouvillian statistics theory was developed, where the usual BZ law \( P_n^T \sim e^{-E_n/k_BT} \) is replaced by the LBZ law \( P_n^T \sim e^{-E_n^L/k_BT} \), where \( E_n^L \) is a Liouvillian energy level rather than an energy level \( E_n \). Based on the new theory, analytical results of thermodynamic properties for the thermal PT system were derived. We found that a “continuous” thermodynamic phase transition occurs at the EP, where there exists a zero-temperature anomaly. In the future, we plan to study the thermal states of more complex NH models and to explore the possible exotic phenomena in NH systems at finite-T.

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Let briefly explain why the density matrix is defined as \[ \hat{\rho}^S_{\text{NHTS}} = \sum_{n=\pm} |\Psi_{n}^R\rangle e^{-\beta T E_n} \langle \Psi_{n}^R| = \hat{S}_0 \hat{S}^\dagger. \]

To develop a theory to describe quantum statistical physics of non-Hermitian systems, there are two choices: one choice is to define density matrix \[ \tilde{\rho}^S_{\text{NHTS}} = \sum_{n=\pm} \hat{\Psi}_{n}^L \rangle e^{-\beta T E_n} \langle \hat{\Psi}_{n}^R| = \hat{S} \rho_0 \hat{S}^{-1}, \]
the other is \[ \rho^S_{\text{NHTS}} = \sum_{n=\pm} |\Psi_{n}^R\rangle e^{-\beta T E_n} \langle \Psi_{n}^R| = \hat{S} \rho_0 \hat{S}^\dagger. \]

From the results by solving GKSL equation, we found \[ \rho^S_{\text{NHTS}} \text{ is real}. \]
However, the density matrix \[ \tilde{\rho}^S_{\text{NHTS}} \text{ is always complex}, \]
i.e., \[ (\hat{S} \rho_0 \hat{S}^{-1})^\dagger \neq \hat{S}^{-1} \rho_0 \hat{S}; \]
the density matrix \[ \rho^S_{\text{NHTS}} = \sum_{n=\pm} |\Psi_{n}^R\rangle e^{-\beta T E_n} \langle \Psi_{n}^R| \]
is real, i.e., \[ (\hat{S} \rho_0 \hat{S}^\dagger)^\dagger = \hat{S}^\dagger \rho_0 \hat{S}. \]

Therefore, we may guess the density matrix from \[ \rho^S_{\text{NHTS}} \text{ is correct}. \]
Furthermore, to confirm the conclusion, we do both calculations from directly solving GKSL equation and those from \[ \rho^S_{\text{NHTS}} = \sum_{n=\pm} |\Psi_{n}^R\rangle e^{-\beta T E_n} \langle \Psi_{n}^R|. \]
The consistence between the results from them verifies the correctness of the definition of \[ \rho^S_{\text{NHTS}} = \sum_{n=\pm} |\Psi_{n}^R\rangle e^{-\beta T E_n} \langle \Psi_{n}^R|. \]

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Supplemental Material for “Physics of PT-Symmetric Quantum Systems at Finite Temperature”

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I. THE DETAILED CALCULATIONS OF THE DENSITY MATRIX FOR THE NON-HERMITIAN THERMAL STATE IN THE PHASE WITH \( \mathcal{PT} \)-SYMMETRY

\((h > \gamma)\)

In this section, we directly solve Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) equation and obtain the density matrix \( \rho_{\text{NHTS}}^S \) for a non-Hermitian thermal state (NHTS) in the phase with \( \mathcal{PT} \)-symmetry \((h > \gamma)\). The followings are detailed calculations.

Firstly, we derive an effective non-Hermitian (NH) Hamiltonian after the postselection measurements based on the GKSL equation.

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For the total system S+B+E, we trace out E from it and get the GKSL equation of the reduced density matrix $\rho^{S+B}$

$$\frac{d\rho^{S+B}}{dt} = -i[H_{S+B}, \rho^{S+B}] - \frac{1}{2}\{L^\dagger_{ES}L_{ES}, \rho^{S+B}\} + L_{ES}\rho^{S+B}L^\dagger_{ES},$$

(1)

where the Lindblad operator is $L_{ES} = \sqrt{2\gamma}(c_1 + ic_2) \otimes \hat{I}_B$. We make the postselection measurement for the number of particles of the subsystem S $$(c_1^\dagger c_1 + c_2^\dagger c_2) \otimes \hat{I}_B$$ so that it is always 1. After the postselection measurements, the quantum jumping term $L_{ES}\rho^{S+B}L^\dagger_{ES}$ will be projected out. Then $\rho^{S+B}$ becomes

$$\frac{d\rho^{S+B}}{dt} = -i(H_{S+B,eff}\rho^{S+B} - \rho^{S+B}H^\dagger_{S+B,eff}),$$

(2)

where

$$H_{S+B,eff} = H_{NH} \otimes \hat{I}_B + \hat{H}_S \otimes \hat{H}_B + \hat{H}_{BS}$$

with

$$H_{NH} = (h + \gamma)c_1^\dagger c_2 + (h - \gamma)c_2^\dagger c_1 - i\gamma(c_1^\dagger c_1 + c_2^\dagger c_2)$$

and

$$H_{BS} = \gamma_1c_1^\dagger c_1 \otimes \hat{B}_1 + \gamma_2c_2^\dagger c_2 \otimes \hat{B}_2.$$  

Because we have fixed the number of particles in subsystem S to 1 by postselection, the third term of $H_{NH}$ become a constant $-i\gamma$. During the postselection measurements, $\rho^{S+B}$ at each moment needs to be normalized and thus we can ignore the term $-i\gamma$.

When considering the postselection process, the subsystem S can be effectively described by an effective NH Hamiltonian

$$H_{NH} = (h + \gamma)c_1^\dagger c_2 + (h - \gamma)c_2^\dagger c_1.$$

(3)

In the case of $h > \gamma$, its eigenvalues are $E_- = -\sqrt{h^2 - \gamma^2}$ with the right eigenstate $|\rangle_R = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ y \end{pmatrix}^T$ and the left eigenstate $|\rangle_L = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ x \end{pmatrix}^T$, $E_+ = \sqrt{h^2 - \gamma^2}$ with the right eigenstate $|\rangle_R = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -y \end{pmatrix}^T$ and the left eigenstate $|\rangle_L = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -x \end{pmatrix}^T$, respectively. Here, we have $x = \sqrt{\frac{h + \gamma}{h - \gamma}}, y = 1/x$.

Secondly, we calculate the Liouville super-operator $\mathcal{L}$ under the Born-Markov approximation in the interaction picture for the NH open quantum system, which has never been studied before.
In general, the derivation of a quantum Markovian master equation is performed in the interaction picture. Thus, we write Eq. \ref{eq:interaction} as in the interaction picture

\[
\frac{d}{dt}\rho_{I}^{S+B}(t) = -i(\hat{V}_{I}(t)\rho_{I}^{S+B}(t) - \rho_{I}^{S+B}(t)\hat{V}_{I}^{\dagger}(t)), \tag{4}
\]

where \(\rho_{I}^{S+B}(t) = e^{iH_{\text{int},\alpha}t}\rho^{S+B}(t)e^{-iH_{\text{int},\alpha}t}\), \(\hat{V}_{I}(t) = e^{iH_{\text{int},\alpha}t}\hat{H}_{\text{BSE}}e^{-iH_{\text{int},\alpha}t}\) and \(\hat{H}_{\text{eff},0} = \hat{H}_{\text{NH}} \otimes \hat{I}_{B} + \hat{I}_{S} \otimes \hat{H}_{B}\). Its equivalent integral form is

\[
\rho_{I}^{S+B}(t) = \rho_{I}^{S+B}(0) - i\int_{0}^{t} ds \left[ \hat{V}_{I}(s) \rho_{I}^{S+B}(s) - \rho_{I}^{S+B}(s) \hat{V}_{I}^{\dagger}(s) \right]. \tag{5}
\]

We substitute Eq. \ref{eq:interaction} into Eq. \ref{eq:interaction} and obtain

\[
\frac{d}{dt}\rho_{I}^{S+B}(t) = -i\left[ \hat{V}_{I}(t)\rho_{I}^{S+B}(0) - \rho_{I}^{S+B}(0)\hat{V}_{I}^{\dagger}(t) \right]
- \left\{ \hat{V}_{I}(t) \int_{0}^{t} ds \left[ \hat{V}_{I}(s) \rho_{I}^{S+B}(s) - \rho_{I}^{S+B}(s) \hat{V}_{I}^{\dagger}(s) \right] \right\}
- \int_{0}^{t} ds \left[ \hat{V}_{I}(s) \rho_{I}^{S+B}(s) - \rho_{I}^{S+B}(s) \hat{V}_{I}^{\dagger}(s) \right] \hat{V}_{I}^{\dagger}(t) \right\}. \tag{6}
\]

Taking the partial trace over the degrees of freedom of the environment B for the above equation, we give the reduced density matrix \(\rho_{I}^{S}(t)\) in the subsystem S

\[
\frac{d}{dt}\rho_{I}^{S}(t) = -itr_{B}\left[ \hat{V}_{I}(t)\rho_{I}^{S+B}(0) - \rho_{I}^{S+B}(0)\hat{V}_{I}^{\dagger}(t) \right]
- tr_{B}\left\{ \hat{V}_{I}(t) \int_{0}^{t} ds \left[ \hat{V}_{I}(s) \rho_{I}^{S+B}(s) - \rho_{I}^{S+B}(s) \hat{V}_{I}^{\dagger}(s) \right] \right\}
- \int_{0}^{t} ds \left[ \hat{V}_{I}(s) \rho_{I}^{S+B}(s) - \rho_{I}^{S+B}(s) \hat{V}_{I}^{\dagger}(s) \right] \hat{V}_{I}^{\dagger}(t) \right\}. \tag{7}
\]

Here, we assume \[1\]

\[
tr_{B}\left[ \hat{V}_{I}(t)\rho_{I}^{S+B}(0) - \rho_{I}^{S+B}(0)\hat{V}_{I}^{\dagger}(t) \right] = 0. \tag{8}
\]

Additionally, we use the Born approximation that the subsystem S has little influence on the environment B, so \(\rho_{I}^{S+B}(s) \sim \rho_{I}^{S}(s) \otimes \rho_{I}^{B}\). By the Markov approximation \(\rho_{I}^{S}(s) \sim \rho_{I}^{S}(t)\), we have

\[
\frac{d}{dt}\rho_{I}^{S}(t) = -tr_{B}\left\{ \hat{V}_{I}(t) \int_{0}^{t} ds \left[ \hat{V}_{I}(s) \left( \rho_{I}^{S}(t) \otimes \rho_{I}^{B} \right) - \left( \rho_{I}^{S}(t) \otimes \rho_{I}^{B} \right) \hat{V}_{I}^{\dagger}(s) \right] \right\}
- \int_{0}^{t} ds \left[ \hat{V}_{I}(s) \left( \rho_{I}^{S}(t) \otimes \rho_{I}^{B} \right) - \left( \rho_{I}^{S}(t) \otimes \rho_{I}^{B} \right) \hat{V}_{I}^{\dagger}(s) \right] \hat{V}_{I}^{\dagger}(t) \right\}. \tag{9}
\]

We substitute \(s\) by \(t - s\), the above equation can be expressed as

\[
\frac{d}{dt}\rho_{I}^{S}(t) = tr_{B}\int_{0}^{t} ds [\hat{V}_{I}(t - s) \rho_{I}^{S}(t) \otimes \rho_{I}^{B} \hat{V}_{I}^{\dagger}(t) - \hat{V}_{I}(t) \hat{V}_{I}(t - s) \rho_{I}^{S}(t) \otimes \rho_{I}^{B}] + h.c.. \tag{10}
\]
Using eigenstates of the $\hat{H}_{NH}$ in $h > \gamma$, we insert the identity operator $\hat{I} = \sum_{m=+,-} |m\rangle_R \langle m|_L \otimes \hat{I}_B$ in $\hat{V}_I(t) = e^{i\hat{H}_{at}} \hat{H}_{BS} e^{-i\hat{H}_{at}}$ and get

$$\hat{V}_I(t) = e^{iD_{at}t} \left[ \sum_a \sum_{m=+,-} |m\rangle_R \langle m|_L \gamma_a c_d^t c_a \sum_{n=+,-} |n\rangle_R \langle n|_L \otimes \hat{B}_a \right] e^{-iD_{at}t}$$

$$= \sum_a \sum_{m=+,-} \sum_n e^{iE_n t} |m\rangle_R \langle m|_L \gamma_a c_d^t c_a |n\rangle_R \langle n|_L e^{-iE_n t} \otimes \hat{B}_a (t)$$

$$= \sum_a \sum_{m=+,-} \sum_{\omega} e^{-i\omega t} |m\rangle_R \langle m|_L \gamma_a c_d^t c_a |m+\omega\rangle_R \langle m+\omega|_L \otimes \hat{B}_a (t), \tag{11}$$

where $\omega = E_m - E_m$ is real and $|m+\omega\rangle$ means the state with energy $E_m = E_m + \omega$. Here we define an operator $\hat{A}_a(\omega)$,

$$\hat{A}_a(\omega) = \sum_{m=+} |m\rangle_R \langle m|_L \gamma_a c_d^t c_a |m+\omega\rangle_R \langle m+\omega|_L \tag{12}$$

with $a = 1, 2$.

Now, $\hat{V}_I(t)$ is written as

$$\hat{V}_I(t) = \sum_a \sum_{\omega} e^{-i\omega t} \hat{A}_a(\omega) \otimes \hat{B}_a (t). \tag{13}$$

Substituting this form of $\hat{V}_I(t)$ to Eq. (10), we get

$$\frac{d}{dt} \rho_S^b(t) = \sum_a \sum_{\omega} \sum_{\omega_1} e^{i(\omega - \omega_1)t} \hat{A}_a(\omega) \rho_S^b(t) \hat{A}_a^\dagger(\omega_1) \int_0^t ds e^{i\omega s} \text{tr}_B \left( \hat{B}_b(t-s) \rho_I^B \hat{B}_a^\dagger(t) \right)$$

$$- \sum_a \sum_{\omega_1} \sum_{b} \sum_{\omega} e^{i(\omega - \omega_1)t} \hat{A}_a(-\omega_1) \hat{A}_b(\omega) \rho_I^B(t) \int_0^t ds e^{i\omega s} \text{tr}_B \left( \hat{B}_a^\dagger(t) \hat{B}_b(t-s) \rho_I^B \right)$$

$$+ \sum_a \sum_{\omega_1} \sum_{b} \sum_{\omega} e^{-i(\omega - \omega_1)t} \hat{A}_a(\omega_1) \rho_S^b(t) \hat{A}_b^\dagger(\omega) \int_0^t ds e^{-i\omega s} \text{tr}_B \left( \rho_I^B \hat{B}_b(t-s) \hat{B}_a(t) \right)$$

$$- \sum_b \sum_{\omega_1} \sum_{a} \sum_{\omega} e^{-i(\omega - \omega_1)t} \rho_I^B(t) \hat{A}_b^\dagger(\omega) \hat{A}_a(-\omega_1) \int_0^t ds e^{-i\omega s} \text{tr}_B \left( \rho_I^B \hat{B}_b(t-s) \hat{B}_a(t) \right). \tag{14}$$

We employ the reservoir correlation functions of the environment B

$$\Gamma_{ab}(\omega) = \int_0^t ds e^{i\omega s} \text{tr}_B \left( \hat{B}_a^\dagger(t) \hat{B}_b(t-s) \rho_I^B \right),$$

$$\Gamma_{ba}(\omega) = \int_0^t ds e^{-i\omega s} \text{tr}_B \left( \rho_I^B \hat{B}_b^\dagger(t-s) \hat{B}_a(t) \right).$$
to simply the Eq. (14) equation. Eventually, \( \frac{d}{dt} \rho^S_I(t) \) of the subsystem S in the interaction picture is

\[
\frac{d}{dt} \rho^S_I(t) = \sum_{a,b} \sum_{\omega} \sum_{\omega_1} e^{i(\omega_1 - \omega)t} \Gamma_{ab}(\omega) \left( \hat{A}_b(\omega) \rho^S_I(t) \hat{A}_a^\dagger(\omega_1) - \hat{A}_a(-\omega_1) \hat{A}_b(\omega) \rho^S_I(t) \right) \\
+ \sum_{a,b} \sum_{\omega} \sum_{\omega_1} e^{-i(\omega_1 - \omega)t} \Gamma_{ba}^*(\omega) \left( \hat{A}_a(\omega_1) \rho^S_I(t) \hat{A}_b^\dagger(\omega) - \rho^S_I(t) \hat{A}_b(\omega) \hat{A}_a^\dagger(-\omega_1) \right). \tag{15}
\]

We use the rotating wave approximation to average out the high frequency part of quantum transition processes and ignore the case of \( \omega \neq \omega_1 \), then get

\[
\frac{d}{dt} \rho^S_I(t) = \sum_{a,b} \sum_{\omega} \left[ \Gamma_{ab}(\omega) \left( \hat{A}_b(\omega) \rho^S_I(t) \hat{A}_a^\dagger(\omega) - \hat{A}_a(-\omega) \hat{A}_b(\omega) \rho^S_I(t) \right) + h.c. \right]. \tag{16}
\]

Because the imaginary part of \( \Gamma_{ab} \) only provides a shift of energy levels and does not affect the NHTS that we will focus on, we ignore them in the calculation below and get

\[
\Gamma_{ab} = \frac{1}{2} \gamma_{ab}, \tag{17}
\]

where \( \gamma_{ab} = \int_{-\infty}^{\infty} dt e^{i\omega t} \left\langle \hat{B}_a^\dagger(t) \hat{B}_b(0) \right\rangle = \int_{-\infty}^{\infty} dt e^{i\omega t} \text{tr}_B \left( \hat{B}_a^\dagger(t) \hat{B}_b(t - s) \rho_I^B \right) \) is the real part of \( \Gamma_{ab} \). Using the Kubo-Martin-Schwinger (KMS) condition \left\langle \hat{B}_a^\dagger(t) \hat{B}_b(0) \right\rangle = \left\langle \hat{B}_b(0) \hat{B}_a^\dagger(t + i\frac{1}{T}) \right\rangle, \) we derive the temperature dependent behavior of \( \gamma_{ab} \), i.e.,

\[
\gamma_{ab}(-\omega) = e^{-\omega/k_B T} \gamma_{ba}(\omega). \tag{18}
\]

For the effective NH Hamiltonian \( \hat{H}_{NH} \), we have \( \omega = \pm \omega_0, \) 0 with \( \omega_0 = |E_+ - E_-| = \)
Thus, the GKSL equation becomes

\[
\frac{d}{dt} \rho_I^S(t) = \sum \omega \left[ \hat{A}_1(\omega) \rho_I^S(t) \hat{A}_1^\dagger(\omega) - \hat{A}_1^\dagger(-\omega) \hat{A}_1(\omega) \rho_I^S(t) \right] \\
+ \sum \omega \left[ \hat{A}_2(\omega) \rho_I^S(t) \hat{A}_2^\dagger(\omega) - \hat{A}_2^\dagger(-\omega) \hat{A}_2(\omega) \rho_I^S(t) \right] \\
+ \sum \omega \left[ \hat{A}_3(\omega) \rho_I^S(t) \hat{A}_3^\dagger(\omega) - \hat{A}_3^\dagger(-\omega) \hat{A}_3(\omega) \rho_I^S(t) \right] \\
+ \sum \omega \left[ \hat{A}_4(\omega) \rho_I^S(t) \hat{A}_4^\dagger(\omega) - \hat{A}_4^\dagger(-\omega) \hat{A}_4(\omega) \rho_I^S(t) \right] \\
+ \sum \omega \left[ \hat{A}_5(\omega) \rho_I^S(t) \hat{A}_5^\dagger(\omega) - \hat{A}_5^\dagger(-\omega) \hat{A}_5(\omega) \rho_I^S(t) \right] \\
+ \sum \omega \left[ \hat{A}_6(\omega) \rho_I^S(t) \hat{A}_6^\dagger(\omega) - \hat{A}_6^\dagger(-\omega) \hat{A}_6(\omega) \rho_I^S(t) \right].
\]

(19)

We use \(\begin{pmatrix} A & B \\ C & D \end{pmatrix}\) to denote \(\rho_I^S(t)\). In combination with \(\Gamma_{ab} = \frac{1}{2} \gamma_{ab}\) and \(\hat{A}_{a,b}(\omega)\), we have the first term

\[
\sum \omega \left[ \hat{A}_1(\omega) \rho_I^S(t) \hat{A}_1^\dagger(\omega) - \hat{A}_1^\dagger(-\omega) \hat{A}_1(\omega) \rho_I^S(t) \right] \\
= \Gamma_{11}(\omega_0) \left[ \hat{A}_1(\omega_0) \rho_I^S(t_0) \hat{A}_1^\dagger(\omega_0) - \hat{A}_1^\dagger(-\omega_0) \hat{A}_1(\omega_0) \rho_I^S(t_0) \right] \\
+ \Gamma_{11}(-\omega_0) \left[ \hat{A}_1(-\omega_0) \rho_I^S(t_0) \hat{A}_1^\dagger(-\omega_0) - \hat{A}_1^\dagger(\omega_0) \hat{A}_1(-\omega_0) \rho_I^S(t_0) \right] \\
+ \Gamma_{11}(0) \left[ \hat{A}_1(0) \rho_I^S(t_0) \hat{A}_1^\dagger(0) - \hat{A}_1^\dagger(0) \hat{A}_1(0) \rho_I^S(t_0) \right] \\
= \frac{1}{32} e^{\omega_0/k_BT} \gamma_{11}(-\omega_0) \gamma_1^2 \begin{pmatrix} -A + xB - xC + x^2D & -Ay - 3B - C - 3xD \\ -3yA - B - 3C & -xD \end{pmatrix} \\
+ \frac{1}{32} \gamma_{11}(-\omega_0) \gamma_1^2 \begin{pmatrix} -A - xB + xC + x^2D & Ay - 3B - C + 3xD \\ 3Ay - B - 3C & y^2A + yB - yC - D \end{pmatrix}. \quad (20)
\]
The second term is

\[
\sum_{\omega} \Gamma_{11}(\omega) [\hat{A}_1(\omega) \rho_1^S(t) \hat{A}_1^\dagger(\omega) - \rho_1^S(t) \hat{A}_1^\dagger(\omega) \hat{A}_1(\omega)]
\]

\[
= \frac{1}{32} e^{\omega_0/k_B T} \gamma_{11}(\omega) \left( -A - xB + xC + x^2 D + 3Ay - 3B - C - xD \\
- yA - B - 3C - 3yD - y^2 A + yB - yC - D \right)
\]

\[+ \frac{1}{32} \gamma_{11}(\omega) \left( -A + xB - xC + x^2 D + 3Ab - 3B - C + xD \\
yA - B - 3C + 3xD + y^2 A - yB + yC - D \right). \tag{21}\]

The third term is

\[
\sum_{\omega} \Gamma_{22}(\omega) [\hat{A}_2(\omega) \rho_2^S(t) \hat{A}_2^\dagger(\omega) - \hat{A}_2(\omega) \rho_2^S(t)]
\]

\[
= \frac{1}{32} e^{\omega_0/k_B T} \gamma_{22}(\omega) \left( -A + xB - xC + x^2 D - Ay - 3B - C - 3xD \\
- 3yA - B - 3C - xD - y^2 A - yB + yC - D \right)
\]

\[+ \frac{1}{32} \gamma_{22}(\omega) \left( -A - xB + xC + x^2 D + 3Ab - 3B - C + 3xD \\
3Ay - B - 3C + xD + y^2 A + yB - yC - D \right). \tag{22}\]

The fourth term is

\[
\sum_{\omega} \Gamma_{22}^s(\omega) [\hat{A}_2^s(\omega) \rho_2^S(t) \hat{A}_2^\dagger(\omega) - \rho_2^S(t) \hat{A}_2^\dagger(\omega) \hat{A}_2(\omega)]
\]

\[
= \frac{1}{32} e^{\omega_0/k_B T} \gamma_{22}^s(\omega) \left( -A - xB + xC + x^2 D - 3yA - 3B - C - xD \\
- Ay - B - 3C - 3xD - y^2 A + yB - yC - D \right)
\]

\[+ \frac{1}{32} \gamma_{22}^s(\omega) \left( -A + xB - xC + x^2 D + 3Ay - 3B - C + xD \\
Ay - B - 3C + 3xD + y^2 A - yB + yC - D \right). \tag{23}\]

The fifth term is

\[
\sum_{\omega} \Gamma_{12}(\omega) [\hat{A}_2(\omega) \rho_1^S(t) \hat{A}_1^\dagger(\omega) - \hat{A}_1(\omega) \rho_1^S(t)]
\]

\[
= -\frac{1}{32} e^{\omega_0/k_B T} \gamma_{21}(\omega) \left( -A + xB - xC + x^2 D - Ay - 3B - C - 3xD \\
- 3yA - B - 3C - xD - y^2 A - yB + yC - D \right)
\]

\[+ \frac{1}{32} \gamma_{21}(\omega) \left( -A - xB + xC + x^2 D + Ay - 3B - C + 3xD \\
3Ay - B - 3C + xD + y^2 A + yB - yC - D \right). \tag{24}\]
The sixth term is

\[
\sum_{\omega} \Gamma_{21}^{s}(\omega) \left[ \hat{A}_{1}(\omega) \rho_{f}^{S}(t) \hat{A}_{1}^\dagger(\omega) - \rho_{f}^{S}(t) \hat{A}_{2}^{\dagger}(\omega) \hat{A}_{1}^{\dagger}(-\omega) \right]
\]

\[= -\frac{1}{32} e^{\omega_{0}/k_{B}T} \gamma_{21} (-\omega_{0}) \gamma_{1} \gamma_{2} \left( \begin{array}{c} -A - xB + xC + x^{2}D - 3yA - 3B - C - xD \\ -Ay - B - 3C - 3xD - y^{2}A + yB - yC - D \end{array} \right) \]

\[ - \frac{1}{32} \gamma_{1} \gamma_{2} \left( \begin{array}{c} -A + xB - xC + x^{2}D \ 3Ay - 3B - C + xD \\ Ay - B - 3C + 3xD \ y^{2}A - yB + yC - D \end{array} \right). \tag{25} \]

The seventh term is

\[
\sum_{\omega} \Gamma_{21}^{s}(\omega) \left[ \hat{A}_{1}(\omega) \rho_{f}^{S}(t) \hat{A}_{2}^{\dagger}(\omega) - \hat{A}_{2}(\omega) \hat{A}_{1}^{\dagger}(\omega) \rho_{f}^{S}(t) \right]
\]

\[= -\frac{1}{32} e^{\omega_{0}/k_{B}T} \gamma_{12} (-\omega_{0}) \gamma_{1} \gamma_{2} \left( \begin{array}{c} -A + xB - xC + x^{2}D - Ay - 3B - C - 3xD \\ -3yA - B - 3C - 3xD - y^{2}A - yB + yC - D \end{array} \right) \]

\[ - \frac{1}{32} \gamma_{21} (-\omega_{0}) \gamma_{1} \gamma_{2} \left( \begin{array}{c} -A - xB + xC + x^{2}D \ Ay - 3B - C + 3xD \\ 3Ay - B - 3C + 3xD \ y^{2}A + yB - yC - D \end{array} \right). \tag{26} \]

The eighth term is

\[
\sum_{\omega} \Gamma_{12}^{s}(\omega) \left[ \hat{A}_{2}(\omega) \rho_{f}^{S}(t) \hat{A}_{1}^{\dagger}(\omega) - \rho_{f}^{S}(t) \hat{A}_{1}^{\dagger}(\omega) \hat{A}_{2}^{\dagger}(-\omega) \right]
\]

\[= -\frac{1}{32} e^{\omega_{0}/k_{B}T} \gamma_{12} (-\omega_{0}) \gamma_{1} \gamma_{2} \left( \begin{array}{c} -A - xB + xC + x^{2}D - 3yA - 3B - C - xD \\ -Ay - B - 3C - 3xD - y^{2}A + yB - yC - D \end{array} \right) \]

\[ - \frac{1}{32} \gamma_{21} (-\omega_{0}) \gamma_{1} \gamma_{2} \left( \begin{array}{c} -A + xB - xC + x^{2}D \ 3Ay - 3B - C + xD \\ Ay - B - 3C + 3xD \ y^{2}A - yB + yC - D \end{array} \right). \tag{27} \]

Combining them together, we get

\[
\frac{d}{dt} \rho_{f}^{S}(t) = \gamma_{0} e^{\omega_{0}/k_{B}T} \left( \begin{array}{c} -A + x^{2}D \ -2Ay - 3B - C - 2xD \\ -2yA - B - 3C - 2xD \ y^{2}A - D \end{array} \right) + \gamma_{0} \left( \begin{array}{c} -A + x^{2}D \ 2yA - 3B - C + 2xD \\ 2yA - B - 3C + 2xD \ y^{2}A - D \end{array} \right), \tag{28} \]

where

\[
\gamma_{0} = \frac{1}{16} [\gamma_{11} (-\omega_{0}) \gamma_{1}^{2} + \gamma_{22} (-\omega_{0}) \gamma_{2}^{2} - (\gamma_{12} (-\omega_{0}) + \gamma_{21} (-\omega_{0})) \gamma_{1} \gamma_{2}]. \tag{29} \]

According to the quantum master equation in the GKSL form \(\frac{d \rho_{f}^{S}(t)}{dt} \equiv \mathcal{L} \rho_{f}^{S}(t)\), we derive
\[
\frac{dA}{dt} = -\gamma_0 \left(e^{\omega_0/k_B T} + 1\right) A + \gamma_0 \left(e^{\omega_0/k_B T} + 1\right) D,
\]
\[
\frac{dB}{dt} = -2\gamma_0 y \left(e^{\omega_0/k_B T} - 1\right) A - 3\gamma_0 \left(e^{\omega_0/k_B T} + 1\right) B - \gamma_0 \left(e^{\omega_0/k_B T} + 1\right) C - 2\gamma_0 x \left(e^{\omega_0/k_B T} - 1\right) D,
\]
\[
\frac{dC}{dt} = -2\gamma_0 y \left(e^{\omega_0/k_B T} - 1\right) A - \gamma_0 \left(e^{\omega_0/k_B T} + 1\right) B - 3\gamma_0 \left(e^{\omega_0/k_B T} + 1\right) C - 2\gamma_0 x \left(e^{\omega_0/k_B T} - 1\right) D,
\]
\[
\frac{dD}{dt} = \gamma_0 \left(e^{\omega_0/k_B T} + 1\right) b^2 A - \gamma_0 \left(e^{\omega_0/k_B T} + 1\right) D.
\]

Eventually, we have
\[
\mathcal{L} = \begin{pmatrix}
-\gamma_0 (1 + e^{\omega_0/k_B T}) & 0 & 0 & \gamma_0 (1 + e^{\omega_0/k_B T}) \\
-2\gamma_0 (e^{\omega_0/k_B T} - 1) \sqrt{\frac{h+\gamma}{h-\gamma}} & -3\gamma_0 (1 + e^{\omega_0/k_B T}) & -\gamma_0 (1 + e^{\omega_0/k_B T}) & -2\gamma_0 (e^{\omega_0/k_B T} - 1) \sqrt{\frac{h+\gamma}{h-\gamma}} \\
-2\gamma_0 (e^{\omega_0/k_B T} - 1) \sqrt{\frac{h+\gamma}{h-\gamma}} & -\gamma_0 (1 + e^{\omega_0/k_B T}) & -3\gamma_0 (1 + e^{\omega_0/k_B T}) & -2\gamma_0 (e^{\omega_0/k_B T} - 1) \sqrt{\frac{h+\gamma}{h-\gamma}} \\
\gamma_0 (1 + e^{\omega_0/k_B T}) \frac{h-\gamma}{h+\gamma} & 0 & 0 & -\gamma_0 (1 + e^{\omega_0/k_B T})
\end{pmatrix}.
\]

Thirdly, we derive the reduced density matrix \(\rho_{\text{NHTS}}^S\) for the NHTS according to the Liouville super-operator \(\mathcal{L}\).

The eigenvalues of \(\mathcal{L}\) are \(-4\gamma_0 (1 + e^{\omega_0/T})\), \(-2\gamma_0 (1 + e^{\omega_0/T})\) (double degeneracy), and 0 in the interaction picture. We have \(\gamma_0 > 0\) because \(\gamma_0\) and \(\gamma\) are independent. For the Hermitian system \(\gamma = 0\), which the postselection measurement does not affect system evolution, the maximum eigenvalue of \(\mathcal{L}\) must be 0. The first three will dissipate, the rest 0 will form a NHTS that is also a steady state. Thus, the density matrix \(\rho_{\text{NHTS}}^S\) for a NHTS corresponding to the eigenvalue of the Liouville super-operator \(\mathcal{L}\) with maximum real part is obtained as
\[
\rho_{\text{NHTS}}^S = \frac{h - \gamma}{2h} \left(\begin{array}{cc}
\frac{h+\gamma}{h-\gamma} & \sqrt{\frac{h+\gamma}{h-\gamma}} \left(1 - e^{-\omega_0 T}\right) \\
\sqrt{\frac{h+\gamma}{h-\gamma}} & \frac{1}{1 + e^{-\omega_0 T}}
\end{array}\right).
\]

**II. THE GENERALIZED BAKER–CAMPBELL–HAUSDORFF FORMULATION**

*Generalized Baker–Campbell–Hausdorff formulation:* For the case of \(\sigma_1^2 = 1\) and \(\sigma_2^2 = 1\), we have the following equation,
\[
\rho = e^{\vec{r}_1 \cdot \vec{\sigma}} \cdot e^{\vec{r}_2 \cdot \vec{\sigma}} \cdot e^{\vec{r}_1 \cdot \vec{\sigma}} = \alpha + |\vec{r}_{\text{eff}}| \cdot \sigma_{\text{eff}} = e^{\vec{r}_{\text{eff}} \cdot \vec{\sigma}},
\]
where
\[ c = \frac{1}{2} \ln(\alpha^2 - |\vec{r}_{\text{eff}}|^2) \] (37)

and
\[ |\vec{r}| = \tanh^{-1}\left(\frac{|\vec{r}_{\text{eff}}|}{\alpha}\right) \] (38)

with
\[ \alpha = \cosh(2r_1) \cdot \cosh r_2 + (\vec{n}_1 \cdot \vec{n}_2) \sinh(2r_1) \cdot \sinh r_2, \]
\[ |\vec{r}_{\text{eff}}| = \sqrt{[\sinh(2r_1) \cdot \cosh r_2 + 2 (\vec{n}_1 \cdot \vec{n}_2) \sinh^2 r_1 \cdot \sinh r_2]^2 + (\sinh r_2)^2}, \]
\[ \sigma_{\text{eff}} = |\vec{r}_{\text{eff}}|^{-1} \cdot (\sigma_1 \sinh(2r_1) \cdot \cosh r_2 + 2 (\vec{n}_1 \cdot \vec{n}_2) \sinh^2 r_1 \cdot \sinh r_2 + \sigma_2 \sinh r_2), \]
\[ r_1 = |\vec{r}_1| \text{ and } r_2 = |\vec{r}_2|. \]

We then prove the above generalized Baker–Campbell–Hausdorff (BCH) formulation. Firstly, for \( \sigma_{\text{eff}}^2 = 1 \), we have
\[ e^{\vec{r} \cdot \vec{\sigma}} = \cosh r + \sigma_n \sinh r, \] (39)

where \( |\vec{r}| = r \) with \( \cosh^2 r - \sinh^2 r = 1 \) and \( \sigma_n = \frac{\vec{r} \cdot \vec{\sigma}}{r} \). On the other hand, for the case of \( X = \vec{d} + \vec{e} \cdot \vec{\sigma} \) with \( e = |\vec{e}| \), we have \( X = e^{\vec{c} + \vec{r} \cdot \vec{\sigma}} \) where
\[ e \cosh r = d, \quad e \sinh r = e. \] (40)

Then, we have \( r = \tanh^{-1}\left(\frac{c}{d}\right) \) and \( c = \frac{1}{2} \ln(d^2 - e^2) \).

Next, we calculate \( \rho = e^{\vec{r}_1 \cdot \vec{\sigma}} \cdot e^{\vec{r}_2 \cdot \vec{\sigma}} \cdot e^{\vec{r}_1 \cdot \vec{\sigma}} \) and get
\[ \rho = e^{\vec{r}_1 \cdot \vec{\sigma}} \cdot e^{\vec{r}_2 \cdot \vec{\sigma}} \cdot e^{\vec{r}_1 \cdot \vec{\sigma}} \\
= (\cosh r_1 + \sigma_1 \sinh r_1) \\
\cdot (\cosh r_2 + \sigma_2 \sinh r_2) \\
\cdot (\cosh r_1 + \sigma_1 \sinh r_1), \] (41)

where \( r_1 = |\vec{r}_1| \) and \( r_2 = |\vec{r}_2| \). The result is obtained as
\[ \rho = (\cosh r_1 \cdot \cosh r_2 + \sigma_1 \sinh r_1 \cdot \cosh r_2 \\
+ \sigma_2 \cosh r_1 \cdot \sinh r_2 + \sigma_1 \sigma_2 \sinh r_1 \cdot \sinh r_2) \\
\cdot (\cosh r_1 + \sigma_1 \sinh r_1) \\
= \cosh(2r_1) \cdot \cosh r_2 + (\vec{n}_1 \cdot \vec{n}_2) \sinh(2r_1) \cdot \sinh r_2 \\
+ \sigma_1 \sinh(2r_1) \cdot \cosh r_2 + 2 (\vec{n}_1 \cdot \vec{n}_2) \sinh^2 r_1 \cdot \sinh r_2 \\
+ \sigma_2 \sinh r_2, \] (42)
where \( \vec{n}_1 = \frac{\vec{r}_1}{|\vec{r}_1|} \) and \( \vec{n}_2 = \frac{\vec{r}_2}{|\vec{r}_2|} \). Here, we have used \( \{\sigma_1, \sigma_2\} = 2(\vec{n}_1 \cdot \vec{n}_2) \).

Thirdly, we show the final result:

\[
\rho = \alpha + |\vec{r}_{\text{eff}}| \cdot \sigma_{\text{eff}}
\]

\[
= e^{c + \vec{r} \cdot \vec{\sigma}},
\]

where

\[
c = \frac{1}{2} \ln(\alpha^2 - |\vec{r}_{\text{eff}}|^2),
\]

\[
r = \tanh^{-1}\left(\frac{|\vec{r}_{\text{eff}}|}{\alpha}\right)
\]

with \( \alpha = \cosh 2r_1 \cdot \cosh r_2 + (\vec{n}_1 \cdot \vec{n}_2) \sinh 2r_1 \cdot \sinh r_2 \),

\[
|\vec{r}_{\text{eff}}| = \sqrt{[\sinh (2r_1) \cdot \cosh r_2 + 2(\vec{n}_1 \cdot \vec{n}_2) \sinh^2 r_1 \cdot \sinh r_2]^2 + (\sinh r_2)^2}
\]

and

\[
\sigma_{\text{eff}} = |\vec{r}_{\text{eff}}|^{-1} \cdot \{\sigma_1[\sinh (2r_1) \cdot \cosh r_2 + 2(\vec{n}_1 \cdot \vec{n}_2) \sinh^2 r_1 \cdot \sinh r_2] + \sigma_2 \sinh r_2\}.
\]

In general, according to \( \alpha^2 - |\vec{r}_{\text{eff}}|^2 = 1 \), we have

\[
c = \frac{1}{2} \ln(\alpha^2 - |\vec{r}_{\text{eff}}|^2) \equiv 0.
\]

So

\[
\rho = e^{\frac{\cosh^{-1} \alpha}{|\vec{r}_{\text{eff}}|^2} (\vec{\sigma} \cdot \vec{r}_{\text{eff}})} = e^{\cosh^{-1} \alpha \sigma_{\text{eff}}}. \tag{45}
\]

### III. THE DETAILED CALCULATIONS OF THE EXPECTED VALUES OF PHYSICAL OPERATORS \( \sigma_i \)

In the case of real energy levels \( (h > \gamma) \), we have a steady state (or the NHTS for this case) for the original NH system \( \hat{H}_{\text{NH}} \) at finite temperature. By doing similarity transformation (ST) \( \hat{S} = e^{\beta_{\text{NH}} \hat{H}'} \), \( \hat{H}_{\text{NH}} \) can be transformed into a Hermitian Hamiltonian

\[
\hat{H}_0 = \sqrt{h^2 - \gamma^2} \sigma_x, \tag{46}
\]

i.e.,

\[
\hat{H}_{\text{NH}} = \hat{S} \hat{H}_0 \hat{S}^{-1}. \tag{47}
\]
Here, the real number $\beta_{NH} = \frac{1}{2} \ln \frac{h^2 + \gamma^2}{h^2}$ characterizes the strength of NH terms, and the Hermitian operator $\hat{H}' = \frac{1}{2} \sigma_z$ determines the form of the NH terms.

According to the definition of $e^{-\beta_T \hat{H}_L} = \hat{S}(e^{-\beta_T \hat{H}_0})\hat{S}^\dagger$, we have

$$e^{-\beta_T \hat{H}_L} = \sigma_x A + \sigma_z B + IC \quad (48)$$

where $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$,

$$A = -\sinh(\beta_T \sqrt{h^2 - \gamma^2}),$$

$$B = \sinh(\beta_{NH}) \cdot \cosh(\beta_T \sqrt{h^2 - \gamma^2}),$$

$$C = \cosh(\beta_{NH}) \cdot \cosh(\beta_T \sqrt{h^2 - \gamma^2}). \quad (49)$$

From the generalized BCH formulation, the Liouvillian Hamiltonian is obtained as

$$\hat{H}_L = -\frac{1}{\beta_T} \cosh^{-1} C \left( \sigma \cdot \vec{r}_{\text{eff}} \right), \quad (50)$$

where $\vec{r}_{\text{eff}} = (A, 0, B)$, $|\vec{r}_{\text{eff}}| = \sqrt{A^2 + B^2}$, and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. Specifically,

$$\hat{H}_L = -\frac{1}{\beta_T} \cosh^{-1} \left[ \cosh \beta_{NH} \cosh \left( \beta_T \sqrt{h^2 - \gamma^2} \right) \right] \cdot \left[ \sinh \left( \beta_T \sqrt{h^2 - \gamma^2} \right) \cdot \sigma_x - \sinh \beta_{NH} \cosh \left( \beta_T \sqrt{h^2 - \gamma^2} \right) \cdot \sigma_z \right] \cdot \cosh \left( \beta_T \sqrt{h^2 - \gamma^2} \right). \quad (51)$$

After diagonalizing $\hat{H}_L$, the Liouvillian energy levels $E_{\pm}^L$ are

$$E_{\pm}^L = \pm \frac{1}{\beta_T} \cosh^{-1} \left[ \cosh \beta_{NH} \cdot \cosh(\beta_T \sqrt{h^2 - \gamma^2}) \right] \quad (52)$$

that are quite different from the energy levels (the eigenvalues for $\hat{H}_{NH}$) $E_{\pm} = \pm \sqrt{h^2 - \gamma^2}$, as shown in Fig.1. As a result, the Liouvillian energy gap is

$$\Delta = 2 |\epsilon| = \frac{2}{\beta_T} \cosh^{-1} \left[ \cosh \beta_{NH} \cdot \cosh(\beta_T \sqrt{h^2 - \gamma^2}) \right]. \quad (53)$$

At the EP, $\Delta$ diverges, i.e., when $\beta_{NH} \to \infty$, $\Delta \to \infty$. Remember the energy gap for $\hat{H}_{NH}$ at EP turns to zero, i.e., when $\beta_{NH} \to \infty$, $\omega_0 = 2 \sqrt{h^2 - \gamma^2} \to 0$.

The partition function $Z_{NHTS}^S$ is given by

$$Z_{NHTS}^S = \text{Tr}(\rho_{NHTS}^S) = \text{Tr}(e^{-\beta_T \hat{H}_L})$$

$$= \text{Tr}(\sigma_x A + \sigma_z B + IC) = 2C. \quad (54)$$
FIG. 1: (a) The energy level $E_+ = \sqrt{h^2 - \gamma^2}$ versus temperature $T$ and $\gamma$ for non-Hermitian Hamiltonian $\hat{H}_{\text{NH}}$. (b) The Liouvillian energy level $E^L_+ = \frac{1}{\beta T} \cosh^{-1}\left[\cosh \beta_{\text{NH}} \cdot \cosh(\beta T \sqrt{h^2 - \gamma^2})\right]$ versus temperature $T$ and $\gamma$ for the Liouvillian Hamiltonian $\hat{H}_{\text{L}}$.

We then calculate the expected values of $\sigma_i$ ($i = x, y, z$), i.e., $n_i = \langle \sigma_i \rangle$. The expected value of physical operator $\sigma_i$ is defined as

$$\langle \sigma_i \rangle = \frac{1}{Z^S_{\text{NHTS}}} \text{Tr}(\sigma_i \cdot e^{-\beta_T \hat{H}_L})$$

$$= \frac{1}{Z^S_{\text{NHTS}}} \text{Tr}[\sigma_i \cdot (\sigma_x A + \sigma_y B + IC)]. \quad (55)$$

After straightforward calculations, we have

$$\langle \sigma_x \rangle = \frac{A}{C} = \frac{-\tanh(\beta T \sqrt{h^2 - \gamma^2})}{\cosh \beta_{\text{NH}}},$$

$$\langle \sigma_y \rangle = 0,$$

$$\langle \sigma_z \rangle = \frac{B}{C} = \tanh \beta_{\text{NH}}. \quad (56)$$

In the case of imaginary energy levels ($h < \gamma$), the NHTS $\rho^S_{\text{NHTS}}$ is

$$\rho^S_{\text{NHTS}} = |\Psi^R_+\rangle \langle \Psi^R_+|$$

$$= \frac{1}{2} \left( \frac{1}{\sqrt{h-\gamma \over h+\gamma}} \right) \left( 1 - \sqrt{h-\gamma \over h+\gamma}^* \right)$$

$$= \frac{1}{2} \left( \frac{1}{\sqrt{h-\gamma \over h+\gamma}} - \sqrt{h-\gamma \over h+\gamma}^* \right). \quad (57)$$
Then, its partition function \( Z_{\text{NHTS}}^S \) is

\[
Z_{\text{NHTS}}^S = \text{Tr}(\rho_{\text{NHTS}}^S) = \frac{1}{2} + \frac{1}{2} \frac{\gamma - h}{h + \gamma} = \frac{\gamma}{h + \gamma}.
\]

Similarly, we use \( \langle \sigma_i \rangle = \frac{1}{Z_{\text{NHTS}}^S} \text{Tr}(\sigma_i \cdot \rho_{\text{NHTS}}^S) \) and can see that

\[
\langle \sigma_x \rangle = 0,
\langle \sigma_y \rangle = -\sqrt{\frac{\gamma^2 - h^2}{\gamma}},
\langle \sigma_z \rangle = \frac{h}{\gamma}.
\]

\( \langle \sigma_i \rangle \)

**IV. THE DETAILED CALCULATIONS FOR THERMODYNAMIC PHASE TRANSITION AT THE EXCEPTIONAL POINT**

According to the results in main content, the average spin operator \( \vec{n} = (n_x, n_y, n_z) = (\langle \sigma_x \rangle, \langle \sigma_y \rangle, \langle \sigma_z \rangle) \) is obtained as

\[
\vec{n} = \left( \frac{A}{C}, 0, \frac{B}{C} \right) = \left( -\tanh\left( \frac{\beta_T \sqrt{h^2 - \gamma^2}}{\cosh \beta_{\text{NH}}} \right), 0, \tanh \beta_{\text{NH}} \right)
\]

for \( h > \gamma \) and

\[
\vec{n} = (0, -\sqrt{1 - \left( \frac{h}{\gamma} \right)^2}, \frac{h}{\gamma})
\]

for \( h < \gamma \).

We can see that the average spin operator \( \langle \sigma_i \rangle \) is always continuous crossing over the exceptional point (EP). So we calculate the derivatives of spin average values \( \frac{\partial \vec{n}}{\partial \gamma} \),

\[
\frac{\partial n_x}{\partial \gamma} = \left\{ \frac{1}{h} \tanh \left( \beta_T \sqrt{h^2 - \gamma^2} \right) + \frac{1}{h} \sqrt{h^2 - \gamma^2} \left[ 1 - \tanh^2 \left( \beta_T \sqrt{h^2 - \gamma^2} \right) \right] \beta_T \right\} \frac{\gamma}{\sqrt{h^2 - \gamma^2}},
\]

\[
\frac{\partial n_y}{\partial \gamma} = 0,
\]

\[
\frac{\partial n_z}{\partial \gamma} = \frac{1}{h},
\]

\( \frac{\partial \vec{n}}{\partial \gamma} \)
for $h > \gamma$ and

\[
\begin{align*}
\frac{\partial n_x}{\partial \gamma} &= 0, \\
\frac{\partial n_y}{\partial \gamma} &= -\frac{1}{\sqrt{1 - (h/\gamma)^2}} \frac{h^2}{\gamma^3}, \\
\frac{\partial n_z}{\partial \gamma} &= -\frac{h}{\gamma^2},
\end{align*}
\]

(63)

for $h < \gamma$.

Fig. 2 shows the result of $\frac{\partial n}{\partial \gamma}$. We can see that $\frac{\partial n_x}{\partial \gamma}$ depends on $\gamma$ and temperature $T$, and $\frac{\partial n_y}{\partial \gamma}$ and $\frac{\partial n_z}{\partial \gamma}$ depends only on $\gamma$. Moreover, at finite temperature $T \neq 0$, $\frac{\partial n}{\partial \gamma}$ is discontinued at the $\gamma = h$. It means a "second-order" phase transition at the EP: there exists a $\nu = \frac{1}{2}$ critical rule for $\frac{\partial n}{\partial \gamma}$:

\[
\frac{\partial n_x}{\partial \gamma} = 2\beta_T
\]

(64)

for $h \to \gamma + 0^+$ in the phase with $\mathcal{PT}$-symmetry ($h \geq \gamma$) and

\[
\frac{\partial n_y}{\partial \gamma} = -(2h)^{\frac{1}{2}} (\gamma - h)^{-\nu}
\]

(65)

for $\gamma \to h + 0^+$ in the phase with $\mathcal{PT}$-symmetry breaking ($h < \gamma$). While at zero temperature $T = 0$,

\[
\frac{\partial n_x}{\partial \gamma} = (2h)^{-\frac{1}{2}} (h - \gamma)^{-\nu}
\]

(66)

for $h \to \gamma + 0^+$ and

\[
\frac{\partial n_y}{\partial \gamma} = -(2h)^{-\frac{1}{2}} (\gamma - h)^{-\nu}
\]

(67)

for $\gamma \to h + 0^+$. The results illustrate a zero temperature anomaly for the thermodynamic phase transition at EP!

\[1\] H. P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002).
FIG. 2: The derivatives of spin average values $\frac{\partial \langle \sigma_i \rangle}{\partial \gamma} = \frac{\partial \langle \vec{\sigma} \rangle}{\partial \gamma}$ of the thermal $\mathcal{PT}$ system versus $\gamma$ or temperature $T$. (a), (d) and (g) are $\frac{\partial \langle \sigma_i \rangle}{\partial \gamma}$ versus $\gamma$ at the temperature $k_B T = 0.01h$, respectively. (b), (e) and (h) are $\frac{\partial \langle \sigma_i \rangle}{\partial \gamma}$ versus $\gamma$ at the temperature $k_B T = 100h$, respectively. (c), (f) and (i) are $\frac{\partial \langle \sigma_i \rangle}{\partial T}$ versus temperature $T$ at $\gamma = 0.999h$, respectively.