Supplementary Information to "Non-Markovian Quantum Exceptional Points"

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THE EXTENDED LIOUVILLIAN SUPEROPERATORS FOR THE SPIN-BOSON MODEL

A. The pseudomode equation of motion approach

Here, we present the extended Liouvillian superoperator of the PMEOM for the spin-boson model. We begin with the interaction Hamiltonian within the interaction picture, which is written as

$$H_{\mathrm{SE}}^{I} = \sum_k g_k \left[e^{i(\omega_0-\omega_k)}\sigma_+ b_k + e^{-i(\omega_0-\omega_k)}\sigma_- b_k^\dagger \right]. \tag{1}$$

As mentioned in the main text, we consider a parametrized spectral density, which is written as

$$J_q(\omega) = \frac{\Gamma\Lambda^2}{2[(\omega-\omega_0)^2+\Lambda^2]} - \frac{\Gamma(q\Lambda)^2}{2[(\omega-\omega_0)^2+(q\Lambda)^2]}. \tag{2}$$

One can then construct the following PMEOM:

$$\begin{aligned} &\frac{d}{dt}\rho_{\mathrm{S+PM}}(t) = \mathcal{L}_{\mathrm{S+PM}}[\rho_{\mathrm{S+PM}}(t)] = -i[H_{\mathrm{S+PM}}, \rho_{\mathrm{S+PM}}(t)] + \sum_{i=1,2}\gamma_i \mathcal{L}_{a_i}[\rho_{\mathrm{S+PM}}(t)], \\ &\text{with } H_{\mathrm{S+PM}} = \sum_{i=1,2}\alpha_i(\sigma_- a_i^\dagger + \sigma_+ a_i). \end{aligned} \tag{3}$$

Here, the qubit-PM coupling strengths and the PM damping rates are $\{\alpha_1 = \sqrt{\Lambda\Gamma/2}, \alpha_2 = i\sqrt{q\Lambda\Gamma/2}, \gamma_1 = 2\Lambda, \gamma_2 = 2q\Lambda\}$, respectively.

To perform spectral analysis on the extended Liouvillian superoperator, we consider the vectorization representation of the PMEOM, which can be expressed by

$$\frac{d}{dt}\mathbf{vec}[\rho_{\mathrm{S+PM}}(t)] = \bar{\bar{\mathcal{L}}}_{\mathrm{S+PM}}\mathbf{vec}[\rho_{\mathrm{S+PM}}(t)], \tag{4}$$

where $\mathbf{vec}(\bullet)$ and $\bar{\bar{\mathcal{L}}}_{\mathrm{S+PM}}$ denote a vectorization operation and a matrix representation of the extended superoperator, respectively. Specifically, consider an operator A with a matrix representation in terms of a basis $\{|i\rangle\}$, namely, $A = \sum_{i,j} A_{i,j}|i\rangle\langle j|$, the vectorization operation is described by $\mathbf{vec}(A) = \sum_{i,j} A_{i.j}|i\rangle \otimes |j\rangle$. In this case, the matrix representation of the extended superoperator can be written as

$$\bar{\bar{\mathcal{L}}}_{\mathrm{S+PM}} = -i(H_{\mathrm{S+PM}}\otimes \mathbb{1} - \mathbb{1}\otimes H_{\mathrm{S+PM}}^T) + \sum_{i=1,2}\frac{\gamma_i}{2}(2a_i\otimes a_i^* - a_i^\dagger a_i \otimes \mathbb{1} - \mathbb{1}\otimes a_i^T a_i^*), \tag{5}$$

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where the superscripts T and $*$ denote the transpose and complex conjugate operations, respectively. Because we consider a zero-temperature environment with RWA, one can confine the analysis within the single-excitation subspace. For the case without the band gap ($q = 0$), the corresponding single-excitation subspace is spanned by $\{|g,0\rangle, |e,0\rangle, |g,1\rangle\}$, and the extended Liouvillian superoperator can be represented by a 9×9 matrix:

$$\bar{\bar{\mathcal{L}}}_{\text{S+PM}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2\Lambda \\ 0 & 0 & \frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} & -\Lambda & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} & 0 & -\frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & \frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} & -\Lambda & 0 & 0 & -\frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} \\ 0 & 0 & 0 & -\frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} & 0 & 0 & -\Lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} & 0 & 0 & -\Lambda & \frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} \\ 0 & 0 & 0 & 0 & 0 & -\frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} & 0 & \frac{i\sqrt{\Gamma\Lambda}}{\sqrt{2}} & -2\Lambda \end{bmatrix}. \tag{6}$$

At the EP condition $\Gamma = \Lambda/2$, one can perform a Jordan decomposition and obtain

$$\begin{aligned} &\bar{\bar{\mathcal{L}}}_{\text{S+PM}}(\Gamma = \Lambda/2) = SDS^{-1}, \\ &\text{with } D = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\Lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\Lambda & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\Lambda & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\Lambda & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\Lambda/2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\Lambda/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\Lambda/2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\Lambda/2 \end{bmatrix} \\ &\text{and } S = \begin{bmatrix} 1 & 0 & -\Lambda^2 & \Lambda & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -i & -2i\Lambda^{-1} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & i & 2i\Lambda^{-1} & 0 & 0 \\ 0 & 0 & \Lambda^2/2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & i\Lambda^2/2 & -i\Lambda/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1/2 & -i\Lambda^2/2 & i\Lambda/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Lambda^2/2 & -\Lambda & 1 & 0 & 0 & 0 & 0 \end{bmatrix}. \end{aligned} \tag{7}$$

Therefore, by observing the matrix D, one can conclude that an EP3 emerges with a converged eigenvalue $-\Lambda$, and two EP2s emerge with a converged eigenvalue $-\Lambda/2$. For the scenario with $q > 0$, where the corresponding single-excitation subspace is spanned by $\{|g,0,0\rangle, |e,0,0\rangle, |g,1,0\rangle, |g,0,1\rangle\}$. Following a similar procedure, one can express the extended Liouvillian superoperator as a 16×16 matrix. By performing the Jordan decomposition, one can conclude that at the EP condition $\Gamma = (1-q)\Lambda/2$, an EP3 emerges with a converged eigenvalue $-(1+q)\Lambda$ and four EP2s with a converged eigenvalue $-(1+q)\Lambda/2$.

B. The hierarchical equations of motion approach

Here we present the extended Liouvillian superoperator within the HEOM formalism. We focus on presenting the results for the spin-boson model without the bandgap ($q = 0$). When $q \neq 0$, a 60×60 matrix is required for the extended Liouvillain superoperator, making it impractical to present fully. Nevertheless, the procedural logic remains consistent across different q values.

To facilitate spectral analysis, we begin by considering the vectorized representation of the HEOM, which can be expressed as

$$\frac{d}{dt}\mathbf{vec}[\rho_{\text{S+ADO}}(t)] = \bar{\bar{\mathcal{L}}}^{\text{RWA}}_{\text{S+ADO}}\mathbf{vec}[\rho_{\text{S+ADO}}(t)], \tag{8}$$

where $\bar{\bar{\mathcal{L}}}^{\mathrm{RWA}}_{\mathrm{S+ADO}}$ is given by

$$\bar{\bar{\mathcal{L}}}^{\mathrm{RWA}}_{\mathrm{S+ADO}}\mathbf{vec}[\rho^{(m)}_{\mathbf{k}}(t)] = \bar{\bar{\mathcal{L}}}_0\mathbf{vec}[\rho^{(m)}_{\mathbf{k}}(t)] - \sum_{r=1}^{m}\chi_{k_r}\mathbf{vec}[\rho^{(m)}_{\mathbf{k}}(t)] - i\sum_{k'}\bar{\bar{\mathcal{A}}}_{k'}\mathbf{vec}[\rho^{(m+1)}_{\mathbf{k}^+}(t)] - i\sum_{r=1}^{m}\bar{\bar{\mathcal{B}}}_{k_r}\mathbf{vec}[\rho^{(m-1)}_{\mathbf{k}_r^-}(t)]. \tag{9}$$

The required superoperators acting on the vectorized ADOs are

$$\bar{\bar{\mathcal{L}}}_0 = -i\ (H_{\mathrm{S}}\otimes\mathbb{1} - \mathbb{1}\otimes H_{\mathrm{S}}^T), \tag{10}$$

$$\bar{\bar{\mathcal{A}}}_k[\cdot] = \sigma_{\bar{\nu}}\otimes\mathbb{1} - \mathbb{1}\otimes\sigma_{\nu} \tag{11}$$

and

$$\bar{\bar{\mathcal{B}}}_k[\cdot] = \xi_l^{\nu}\ \sigma_{\nu}\otimes\mathbb{1} - \xi_l^{\bar{\nu}*}\ \mathbb{1}\otimes\sigma_{\bar{\nu}}, \tag{12}$$

where $H_{\mathrm{S}} = \omega_0|e\rangle\langle e|$. Due to the absence of internal tunneling between the qubit energy levels, the system's behavior can be accurately captured by considering up to the second hierarchical tier ($m = 2$) [1]. The validity of this truncation can be further verified using Eq. (15) of the main text. The corresponding extended Liouvillian superoperator can be represented as a 24×24 matrix. To facilitate analytical calculations, we decompose $\bar{\bar{\mathcal{L}}}^{\mathrm{RWA}}_{\mathrm{S+ADO}}$ into three components

$$\bar{\bar{\mathcal{L}}}^{\mathrm{RWA}}_{\mathrm{S+ADO}} = \bar{\bar{\mathcal{L}}}^{\mathrm{RWA,p}}_{\mathrm{S+ADO}} \oplus \bar{\bar{\mathcal{L}}}^{\mathrm{RWA,c}}_{\mathrm{S+ADO}} \oplus \bar{\bar{\mathcal{L}}}^{\mathrm{RWA,c*}}_{\mathrm{S+ADO}}, \tag{13}$$

where the superscripts p, c, and c$*$ respectively indicate that these components determine the system's population $\langle e|\rho_{\mathrm{S}}(t)|e\rangle$, coherence $\langle e|\rho_{\mathrm{S}}(t)|g\rangle$, and its complex conjugate $\langle g|\rho_{\mathrm{S}}(t)|e\rangle$. The full expressions for these components are given by

$$\bar{\bar{\mathcal{L}}}^{\mathrm{RWA,p}}_{\mathrm{S+ADO}} = \begin{bmatrix} 0 & 0 & -i & i & 0 & 0 \\ 0 & 0 & i & -i & 0 & 0 \\ 0 & i\Gamma\Lambda/2 & -\Lambda & 0 & -i & i \\ 0 & -i\Gamma\Lambda/2 & 0 & -\Lambda & i & -i \\ 0 & 0 & -i\Gamma\Lambda/2 & i\Gamma\Lambda/2 & -2\Lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & -2\Lambda \end{bmatrix}, \tag{14}$$

$$\bar{\bar{\mathcal{L}}}^{\mathrm{RWA,c}}_{\mathrm{S+ADO}} = \begin{bmatrix} 0 & -i & i & 0 & 0 \\ -i\Gamma\Lambda/2 & -\Lambda & 0 & -i & i \\ 0 & 0 & -\Lambda & i & -i \\ 0 & 0 & i\Gamma\Lambda/2 & -2\Lambda & 0 \\ 0 & 0 & -i\Gamma\Lambda/2 & 0 & -2\Lambda \end{bmatrix}, \tag{15}$$

and

$$\bar{\bar{\mathcal{L}}}^{\mathrm{RWA,c*}}_{\mathrm{S+ADO}} = \begin{bmatrix} 0 & i & -i & 0 & 0 \\ i\Gamma\Lambda/2 & -\Lambda & 0 & -i & i \\ 0 & 0 & -\Lambda & i & -i \\ 0 & 0 & i\Gamma\Lambda/2 & -2\Lambda & 0 \\ 0 & 0 & -i\Gamma\Lambda/2 & 0 & -2\Lambda \end{bmatrix}. \tag{16}$$

Under the EP condition ($\Gamma = \Lambda/2$), we perform Jordan decomposition and obtain

$$
\begin{aligned}
\bar{\bar{\mathcal{L}}}^{\mathrm{RWA,p}}_{\mathrm{S+ADO}} &= S^{(\mathrm{p})} D^{(\mathrm{p})} S^{(\mathrm{p})-1}, \\
\text{with } D^{(p)} &= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2\Lambda & 0 & 0 & 0 & 0 \\ 0 & 0 & -\Lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & -\Lambda & 1 & 0 \\ 0 & 0 & 0 & 0 & -\Lambda & 1 \\ 0 & 0 & 0 & 0 & 0 & -\Lambda \end{bmatrix} \\
\text{and } S^{(\mathrm{p})} &= \begin{bmatrix} 1 & 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 1/2 & i\Lambda & -i & 0 \\ 0 & 0 & 1/2 & -i\Lambda & i & 0 \\ 0 & 1 & 0 & \Lambda^2/2 & -\Lambda & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}, \\
\bar{\bar{\mathcal{L}}}^{\mathrm{RWA,c}}_{\mathrm{S+ADO}} &= S^{(\mathrm{c})} D^{(\mathrm{c})} S^{(\mathrm{c})-1}, \\
\text{with } D^{(\mathrm{c})} &= \begin{bmatrix} -2\Lambda & 0 & 0 & 0 & 0 \\ 0 & (-3-i)\Lambda/2 & 0 & 0 & 0 \\ 0 & 0 & (-3+i)\Lambda/2 & 0 & 0 \\ 0 & 0 & 0 & -\Lambda/2 & 1 \\ 0 & 0 & 0 & 0 & -\Lambda/2 \end{bmatrix} \\
\text{and } S^{(\mathrm{c})} &= \begin{bmatrix} 0 & (48-64i)/25\Lambda^2 & (48+64i)/25\Lambda^2 & 2i/\Lambda & 4i/\Lambda^2 \\ 0 & (-22-54i)/25\Lambda & (22-54i)/25\Lambda & 1 & 0 \\ 0 & (2+2i)/\Lambda & -(2-2i)\Lambda & 0 & 0 \\ 1 & -1 & -1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \end{bmatrix}, \\
\bar{\bar{\mathcal{L}}}^{\mathrm{RWA,c*}}_{\mathrm{S+ADO}} &= S^{(\mathrm{c*})} D^{(\mathrm{c*})} S^{(\mathrm{c*})-1}, \\
\text{with } D^{(\mathrm{c*})} &= \begin{bmatrix} -2\Lambda & 0 & 0 & 0 & 0 \\ 0 & (-3-i)\Lambda/2 & 0 & 0 & 0 \\ 0 & 0 & (-3+i)\Lambda/2 & 0 & 0 \\ 0 & 0 & 0 & -\Lambda/2 & 1 \\ 0 & 0 & 0 & 0 & -\Lambda/2 \end{bmatrix} \\
\text{and } S^{(\mathrm{c*})} &= \begin{bmatrix} 0 & (48-64i)/25\Lambda^2 & (-48-64i)/25\Lambda^2 & -2i/\Lambda & -4i/\Lambda^2 \\ 0 & (-22-54i)/25\Lambda & (22-54i)/25\Lambda & 1 & 0 \\ 0 & (2+2i)/\Lambda & (-2+2i)/\Lambda & 0 & 0 \\ 1 & -1 & -1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \end{bmatrix}.
\end{aligned} \tag{17}
$$

By observing the matrices $D^{(\mathrm{p}),(\mathrm{c}),(\mathrm{c*})}$, we conclude the emergence of one EP3 with a converged eigenvalue $-\Lambda$, and two EP2s with a converged eigenvalue $-\Lambda/2$. This aligns with the results obtained using the PMEOM approach. Moreover, we conclude that the EP3 can be observed through the system's population dynamics, whereas the two EP2s can be observed through the system's coherence. We note that within the HEOM formalism, there are additional eigenmatrices introduced that do not influence the system dynamics due to the vanishing of the corresponding coefficients c_i and c_m as described in Eq. (15) in the main text.

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[1] L. Han, H.-D. Zhang, X. Zheng, and Y. Yan, On the exact truncation tier of fermionic hierarchical equations of motion, J. Chem. Phys. **148**, 234108 (2018).