Theoretical Derivations of DQPT in Non-Hermitian Quantum Systems

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1 Introduction and Total Phase

In the study of Dynamical Quantum Phase Transitions (DQPT), we monitor the Loschmidt amplitude, which characterizes the overlap between the initial state and the evolved state:

$$g_k(t) = \langle \Psi(0)| e^{-iH_k t} |\Psi(0)\rangle = r_k e^{i\varphi_R} \tag{1}$$

The total phase φ_R is defined through the relation:

$$\varphi_R = -i \ln \left(\frac{g_k(t)}{|g_k(t)|} \right) \tag{2}$$

For a two-level system $H_k = \omega_k \hat{n}_k \cdot \vec{\sigma}$, the initial density matrix is prepared as a thermal-like state:

$$\rho_k(0) = \frac{e^{-\beta H_k}}{\mathrm{tr}(e^{-\beta H_k})} = \frac{1}{2} \left(I - \frac{m}{\omega} H_k \right) \tag{3}$$

where $m = \tanh(\beta\omega_k)$ is the effective magnetization.

2 Detailed Derivation of the Loschmidt Amplitude

The Loschmidt amplitude $g_k(t)$ is defined as the overlap between the initial state and the time-evolved state. In the density matrix formalism, this is expressed as the trace of the product of the initial density matrix and the evolution operator:

$$g_k(t) = \mathrm{tr}[\rho_k(0) U_k(t)]$$

We distinguish between the initial state axis $\vec{n}_k$ and the final (post-quench) Hamiltonian axis $\vec{n}_{k,f}$. Given $\rho_k(0) = \frac{1}{2}(\sigma_0 - m(\vec{n}_k \cdot \vec{\sigma}))$ and $U_k(t) = \cos(\omega_k t)\sigma_0 - i(\vec{n}_{k,f} \cdot \vec{\sigma}) \sin(\omega_k t)$, the expansion is:

$$g_k(t) = \frac{1}{2} \mathrm{tr}\{[\sigma_0 - m(\vec{n}_k \cdot \vec{\sigma})][\cos(\omega_k t)\sigma_0 - i(\vec{n}_{k,f} \cdot \vec{\sigma}) \sin(\omega_k t)]\}$$

We evaluate the trace by expanding the product into four terms:

$$\begin{aligned}
(a) &= \frac{1}{2}\,\mathrm{tr}[\cos(\omega_k t)\sigma_0 \cdot \sigma_0] = \frac{1}{2}\cos(\omega_k t)\,\mathrm{tr}(\sigma_0) = \cos(\omega_k t) \\
(b) &= -\frac{i}{2}\,\mathrm{tr}[\sigma_0(\vec{n}_{k,f}\cdot\vec{\sigma})\sin(\omega_k t)] = -\frac{i}{2}\sin(\omega_k t)\,\mathrm{tr}(\vec{n}_{k,f}\cdot\vec{\sigma}) = 0 \\
(c) &= -\frac{1}{2}\,\mathrm{tr}[m(\vec{n}_k\cdot\vec{\sigma})\cos(\omega_k t)\sigma_0] = -\frac{m}{2}\cos(\omega_k t)\,\mathrm{tr}(\vec{n}_k\cdot\vec{\sigma}) = 0 \\
(d) &= \frac{im}{2}\sin(\omega_k t)\,\mathrm{tr}[(\vec{n}_k\cdot\vec{\sigma})(\vec{n}_{k,f}\cdot\vec{\sigma})]
\end{aligned}$$

Using the identity $(\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B}) = (\vec{A}\cdot\vec{B})I + i\vec{\sigma}\cdot(\vec{A}\times\vec{B})$, we find:

$$\mathrm{tr}[(\vec{n}_k\cdot\vec{\sigma})(\vec{n}_{k,f}\cdot\vec{\sigma})] = \mathrm{tr}[(\vec{n}_k\cdot\vec{n}_{k,f})\sigma_0 + i\vec{\sigma}\cdot(\vec{n}_k\times\vec{n}_{k,f})] = 2(\vec{n}_k\cdot\vec{n}_{k,f})$$

Substituting this back into term (d):

$$(d) = \frac{im}{2}\sin(\omega_k t)\cdot 2(\vec{n}_k\cdot\vec{n}_{k,f}) = im(\vec{n}_k\cdot\vec{n}_{k,f})\sin(\omega_k t)$$

Defining $B_k = -m(\vec{n}_k\cdot\vec{n}_{k,f})$, the Loschmidt amplitude becomes:

$$g_k(t) = \cos(\omega_k t) - iB_k\sin(\omega_k t)$$

3 Analytical Calculation of Critical Times

Dynamical Quantum Phase Transitions (DQPT) occur when $g_k(t) = 0$. Using the derived form:

$$\cos(\omega_k t) - iB_k\sin(\omega_k t) = 0 \implies \cot(\omega_k t) = iB_k$$

Applying the identity $\cot(x) = i\coth(ix)$, we obtain:

$$\coth(i\omega_k t) = B_k$$

Solving for the complex time $i\omega_k t$:

$$\begin{aligned}
i\omega_k t = \coth^{-1}(B_k) &= \frac{1}{2}\ln\left(\frac{B_k+1}{B_k-1}\right) \\
&= \frac{1}{2}\ln\left[(-1)\frac{1+B_k}{1-B_k}\right] = \frac{1}{2}\ln(-1) + \tanh^{-1}(B_k)
\end{aligned}$$

With $\ln(-1) = i(2n+1)\pi$, the discrete set of critical times $t_{n,k}$ is:

$$t_{n,k} = \left(n+\frac{1}{2}\right)\frac{\pi}{\omega_k} - \frac{i}{\omega_k}\tanh^{-1}(B_k)$$

When the temperature is zero ($\beta\to\infty$) and the states are perfectly orthogonal ($\vec{n}_k\cdot\vec{n}_{k,f} = 0$), B_k vanishes, and the critical times are purely real:

$$t_{n,k} = \left(n+\frac{1}{2}\right)\frac{\pi}{\omega_k}$$

4 Non-Hermitian Biorthogonal Evolution

For non-Hermitian Hamiltonians where $[H, H^\dagger] \neq 0$, the standard Hermitian orthogonality fails. We invoke the biorthogonal basis $\{|s^r\rangle, |s^l\rangle\}$ satisfying:

$$H|s^r\rangle = s\omega|s^r\rangle, \quad H^\dagger|s^l\rangle = s\omega^*|s^l\rangle, \quad \langle s^l|s'^r\rangle = \delta_{s,s'} \quad (s = \pm 1) \tag{4}$$

The evolution operators for the right and left states are:

$$U^r(t) = e^{-i\omega t}|+^r\rangle\langle +^l| + e^{i\omega t}|-^r\rangle\langle -^l| \tag{5}$$

$$U^{l\dagger}(t) = e^{i\omega^* t}|+^r\rangle\langle +^l| + e^{-i\omega^* t}|-^r\rangle\langle -^l| \tag{6}$$

The product operator resulting from the biorthogonal evolution is:

$$U^{l\dagger}U^r = e^{2\,\mathrm{Im}(\omega)t}|+^r\rangle\langle +^l| + e^{-2\,\mathrm{Im}(\omega)t}|-^r\rangle\langle -^l| \tag{7}$$

Remark on sign convention. Here $\omega = \omega_R + i\omega_I$ with $\omega_I = \mathrm{Im}(\omega)$. A positive ω_I corresponds to an amplifying (gain) mode, while a negative ω_I corresponds to a decaying (loss) mode. The exponential factors in Eq. (7) follow directly from:

$$e^{-i\omega t} \cdot e^{i\omega^* t} = e^{-i(\omega-\omega^*)t} = e^{2\,\mathrm{Im}(\omega)t} \tag{8}$$

which makes the gain/loss asymmetry between the $|+^r\rangle$ and $|-^r\rangle$ sectors explicit.

5 Exhaustive Term-by-Term Trace Calculations

The trace in the biorthogonal framework is defined as the sum over the diagonal elements: $\mathrm{tr}(A) = \left\langle +^l \right| A \left|+^r\right\rangle + \left\langle -^l \right| A \left|-^r\right\rangle$. We now expand every term for the operators required in the dynamical phase integral.

5.1 Expansion of $\mathrm{tr}\big(U^{l\dagger}U^r\big)$

Substituting the expansion of $U^{l\dagger}U^r$:

$$\begin{aligned}
\mathrm{tr}\big(U^{l\dagger}U^r\big) &= \left\langle +^l\right| \left(e^{2\mathrm{Im}(\omega)t}\left|+^r\right\rangle\left\langle +^l\right| + e^{-2\mathrm{Im}(\omega)t}\left|-^r\right\rangle\left\langle -^l\right|\right)\left|+^r\right\rangle \\
&+ \left\langle -^l\right| \left(e^{2\mathrm{Im}(\omega)t}\left|+^r\right\rangle\left\langle +^l\right| + e^{-2\mathrm{Im}(\omega)t}\left|-^r\right\rangle\left\langle -^l\right|\right)\left|-^r\right\rangle \\
&= e^{2\mathrm{Im}(\omega)t}\left\langle +^l\middle|+^r\right\rangle\left\langle +^l\middle|+^r\right\rangle + e^{-2\mathrm{Im}(\omega)t}\left\langle +^l\middle|-^r\right\rangle\left\langle -^l\middle|+^r\right\rangle \\
&+ e^{2\mathrm{Im}(\omega)t}\left\langle -^l\middle|+^r\right\rangle\left\langle +^l\middle|-^r\right\rangle + e^{-2\mathrm{Im}(\omega)t}\left\langle -^l\middle|-^r\right\rangle\left\langle -^l\middle|-^r\right\rangle
\end{aligned} \tag{9}$$

Applying $\left\langle s^l\middle|s'^r\right\rangle = \delta_{s,s'}$:

$$\mathrm{tr}\big(U^{l\dagger}U^r\big) = e^{2\mathrm{Im}(\omega)t}(1)(1) + 0 + 0 + e^{-2\mathrm{Im}(\omega)t}(1)(1) = 2\cosh[2\mathrm{Im}(\omega)t] \tag{10}$$

5.2 Expansion of $\mathrm{tr}\big(U^{l\dagger}HU^r\big)$

Substituting the spectral decomposition of the Hamiltonian $H = \omega\left|+^r\right\rangle\left\langle +^l\right| - \omega\left|-^r\right\rangle\left\langle -^l\right|$:

$$\begin{aligned}
\mathrm{tr}\big(U^{l\dagger}HU^r\big) &= \left\langle +^l\right| (e^{2\mathrm{Im}(\omega)t}\left|+^r\right\rangle\left\langle +^l\right| + e^{-2\mathrm{Im}(\omega)t}\left|-^r\right\rangle\left\langle -^l\right|)H\left|+^r\right\rangle \\
&+ \left\langle -^l\right| (e^{2\mathrm{Im}(\omega)t}\left|+^r\right\rangle\left\langle +^l\right| + e^{-2\mathrm{Im}(\omega)t}\left|-^r\right\rangle\left\langle -^l\right|)H\left|-^r\right\rangle \\
&= e^{2\mathrm{Im}(\omega)t}\left\langle +^l\middle|+^r\right\rangle\left\langle +^l\right|H\left|+^r\right\rangle + e^{-2\mathrm{Im}(\omega)t}\left\langle -^l\middle|-^r\right\rangle\left\langle -^l\right|H\left|-^r\right\rangle \\
&= e^{2\mathrm{Im}(\omega)t}(1)(\omega) + e^{-2\mathrm{Im}(\omega)t}(1)(-\omega) \\
&= \omega(e^{2\mathrm{Im}(\omega)t} - e^{-2\mathrm{Im}(\omega)t}) = 2\omega\sinh[2\mathrm{Im}(\omega)t]
\end{aligned} \tag{11}$$

5.3 Expansion of $\mathrm{tr}\big(U^{l\dagger} H U^r H\big)$

Using $H^2 = \omega^2(\left|+^r\right\rangle\left\langle+^l\right| + \left|-^r\right\rangle\left\langle-^l\right|) = \omega^2 I_{biorth}$:

$$
\begin{aligned}
\mathrm{tr}\big(U^{l\dagger} H U^r H\big) &= \mathrm{tr}\big(U^{l\dagger} U^r H^2\big) \\
&= \left\langle+^l\right| U^{l\dagger} U^r H^2 \left|+^r\right\rangle + \left\langle-^l\right| U^{l\dagger} U^r H^2 \left|-^r\right\rangle \\
&= e^{2\mathrm{Im}(\omega)t} \left\langle+^l\middle|+^r\right\rangle \left\langle+^l\right| H^2 \left|+^r\right\rangle + e^{-2\mathrm{Im}(\omega)t} \left\langle-^l\middle|-^r\right\rangle \left\langle-^l\right| H^2 \left|-^r\right\rangle \\
&= e^{2\mathrm{Im}(\omega)t}(1)(\omega^2) + e^{-2\mathrm{Im}(\omega)t}(1)(\omega^2) \\
&= \omega^2(e^{2\mathrm{Im}(\omega)t} + e^{-2\mathrm{Im}(\omega)t}) = 2\omega^2 \cosh[2\mathrm{Im}(\omega)t]
\end{aligned}
\tag{12}
$$

6 Dynamical Phase Integration

The integrated Pancharatnam dynamical phase for $\rho(0) = \frac{1}{2}(I - \frac{m}{\omega}H)$ is:

$$
\begin{aligned}
\varphi_D &= -\frac{1}{\hbar}\int_0^\tau \frac{\frac{1}{2}\left[\mathrm{tr}\big(U^{l\dagger}U^r H\big) - \frac{m}{\omega}\mathrm{tr}\big(U^{l\dagger} H U^r H\big)\right]}{\frac{1}{2}\left[\mathrm{tr}(U^{l\dagger}U^r) - \frac{m}{\omega}\mathrm{tr}(U^{l\dagger} H U^r)\right]} dt \\
&= -\frac{1}{\hbar}\int_0^\tau \omega \frac{\sinh[2\mathrm{Im}(\omega)t] - m\cosh[2\mathrm{Im}(\omega)t]}{\cosh[2\mathrm{Im}(\omega)t] - m\sinh[2\mathrm{Im}(\omega)t]} dt = -\frac{1}{\hbar}\int_0^\tau \omega \frac{\tanh[2\mathrm{Im}(\omega)t] - m}{1 - m\tanh[2\mathrm{Im}(\omega)t]} dt
\end{aligned}
\tag{13}
$$

7 Conclusion and Geometric Phase

7.1 Decomposition of the Total Phase

Recall from Section 1 that the total phase $\phi_R(k,t)$ is extracted from the Loschmidt amplitude via:

$$
\phi_R(k,t) = -i\ln\left(\frac{g_k(t)}{|g_k(t)|}\right) \tag{14}
$$

In the Hermitian case, the standard Pancharatnam decomposition gives:

$$
\phi_R(k,t) = \phi_G(k,t) + \phi_D(k,t) \tag{15}
$$

where ϕ_D is the dynamical phase accumulated by the energy expectation value, and ϕ_G is the purely geometric contribution. Inverting this relation defines the geometric phase:

$$
\phi_G(k,t) = \phi_R(k,t) - \phi_D(k,t) \tag{16}
$$

In a non-Hermitian system the eigenvalues $\omega \in \mathbb{C}$, so the dynamical phase computed in Section 6,

$$
\phi_D(k,t) = -\frac{1}{\hbar}\int_0^t \omega\,\frac{\tanh[2\,\mathrm{Im}(\omega)t'] - m}{1 - m\tanh[2\,\mathrm{Im}(\omega)t']}\,dt' \;\in\; \mathbb{C}, \tag{17}
$$

is generically complex. Decompose it as:

$$
\phi_D(k,t) = \mathrm{Re}\{\phi_D(k,t)\} + i\,\mathrm{Im}\{\phi_D(k,t)\} \tag{18}
$$

Only the real part of ϕ_D contributes to the phase decomposition, and Eq. (16) is replaced by:

$$
\boxed{\phi_G(k,t) = \phi_R(k,t) - \mathrm{Re}\{\phi_D(k,t)\}} \tag{19}
$$

7.2 Hermitian Limit and Recovery of the Topological Invariant

Taking $\mathrm{Im}(\omega) \to 0$, the two cases compare as follows:

$$\phi_D\big|_{\text{non-Herm}} = -\frac{\omega}{\hbar}\int_0^t \frac{\tanh[2\,\mathrm{Im}(\omega)t'] - m}{1 - m\tanh[2\,\mathrm{Im}(\omega)t']}\,dt' \;\in\; \mathbb{C} \tag{20}$$

$$\phi_D\big|_{\text{Herm}} = -\frac{\omega_R}{\hbar}\int_0^t \frac{0 - m}{1 - 0}\,dt' = \frac{m\omega_R}{\hbar}\,t \;\in\; \mathbb{R} \tag{21}$$

Since $\phi_D|_{\text{Herm}} \in \mathbb{R}$, we have $\mathrm{Re}\{\phi_D\} = \phi_D$, and Eq. (19) reduces to Eq. (16):

$$\boxed{\phi_G(k,t)\big|_{\text{Herm}} = \phi_R(k,t) - \frac{m\omega_k}{\hbar}\,t} \tag{22}$$

7.3 Winding Number

The geometric phase $\phi_G(k,t)$ defined in Eq. (19) serves as the foundation for the topological characterization of DQPTs. The winding number is defined by integrating the k-gradient of ϕ_G across the full Brillouin zone:

$$\nu(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \partial_k\,\phi_G(k,t)\,dk \tag{23}$$

$\nu(t)$ takes integer values and changes discontinuously at the critical times $t = t_{n,k}$ derived in Section 3, signalling a DQPT. A non-zero winding number indicates that the geometric phase $\phi_G(k,t)$ winds non-trivially around the Brillouin zone.