Asymptotic TCL4 Generator for the Spin-Boson Model: Analytical Derivation and Benchmarking

Prem Kumar [1,2], K. P. Athulya[1,2], Sibasish Ghosh[1,2]

[1]Optics & Quantum Information Group, The Institute of Mathematical Sciences, CIT Campus, Taramani, Chennai 600113, India

[2]Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400085, India

Abstract

We derive the full fourth-order corrections to the open quantum system dynamics (in system-environment coupling strength), for the spin-boson model (SBM) for arbitrary odd physical spectral densities. We apply this result to solve for the dynamics of a semiconductor double quantum dot, which can be modeled as a SBM under certain conditions. Our results show that the commonly used second order master equation often overestimates the non-Markovianity at large temperatures. We also benchmark our results against analytical results for Ohmic spectral densities and the numerically exact Hierarchical Equations of Motion. These results offer a general and computationally efficient method for studying higher order corrections to the dynamics of a wide class of open quantum systems.

Background

Spin-Boson model: The Hamiltonian is

$$\hat{H}_{SE} = \hat{H}_S + \hat{H}_E + \hat{H}_I, \qquad \hat{H}_I = \lambda \hat{A} \otimes \hat{B}.$$

Its ingredients are

$$\hat{H}_S = \frac{\Omega}{2}\hat{\sigma}_3,$$
$$\hat{H}_E = \sum_k \left(\frac{\hat{p}_k^2}{2m_k} + \frac{1}{2} m_k \omega_k^2 \hat{q}_k^2\right).$$

Here, $\hat{A} = a_3\hat{\sigma}_3 - a_1\hat{\sigma}_1$, $\hat{B} = \sum_k c_k \hat{q}_k$, $\hat{\sigma}_i$ are Pauli matrices; m_k, ω_k, c_k are the mass, frequency, and coupling of the k^{th} mode. Spectral density: $J(\omega) = \sum_k \frac{c_k^2}{m_k \omega_k}\delta(\omega - \omega_k)$.

TCL master equation: For a quantum state $\hat{\rho}(t)$, the time-convolutionless (TCL) master equation is

$$\dot{\hat{\rho}}_S(t) = \sum_{n=0}^{\infty} \lambda^{2n} \mathscr{F}^{(2n)}(t)\left[\hat{\rho}(t)\right].$$

Here λ is the system–environment coupling parameter. The zeroth-order part $\mathscr{F}^{(0)}(t)[\hat{\rho}(t)] = -i[\hat{H}_S, \hat{\rho}(t)]$ gives free evolution, $\mathscr{F}^{(2)}(t)$ is the Bloch–Redfield contribution, and higher even orders add systematic corrections.

Scan

Scan for PDF of this poster and paper

Results

Application to the Double-Quantum-Dot System

- Dynamics of a semiconductor Quantum-Double-Dot (DQD) system, which can be effectively modeled by the SBM. The SBM parameters are related to the DQD physical parameters (detuning ε and inter-dot tunneling t_c) as $a_1 = \frac{2t_c}{\Omega}$, $a_3 = \frac{\varepsilon}{\Omega}$ and $\Omega^2 = \varepsilon^2 + 4t_c^2$.
- The DQD is coupled to a phononic bath, described by the spectral density

$$J(\omega) = \gamma\omega\left[1 - \text{sinc}\left(\frac{\omega}{\omega_c}\right)\right]\exp\left\{-\frac{\omega^2}{2\,\omega_{\max}^2}\right\},$$

where, we have $\text{sinc}(x) \equiv \sin(x)/x$. The parameter $\omega_{\max}$ serves as the upper cut-off frequency, while $\omega_c = c_s/d$, where c_s is the speed of sound in the substrate and d is the inter-dot distance.

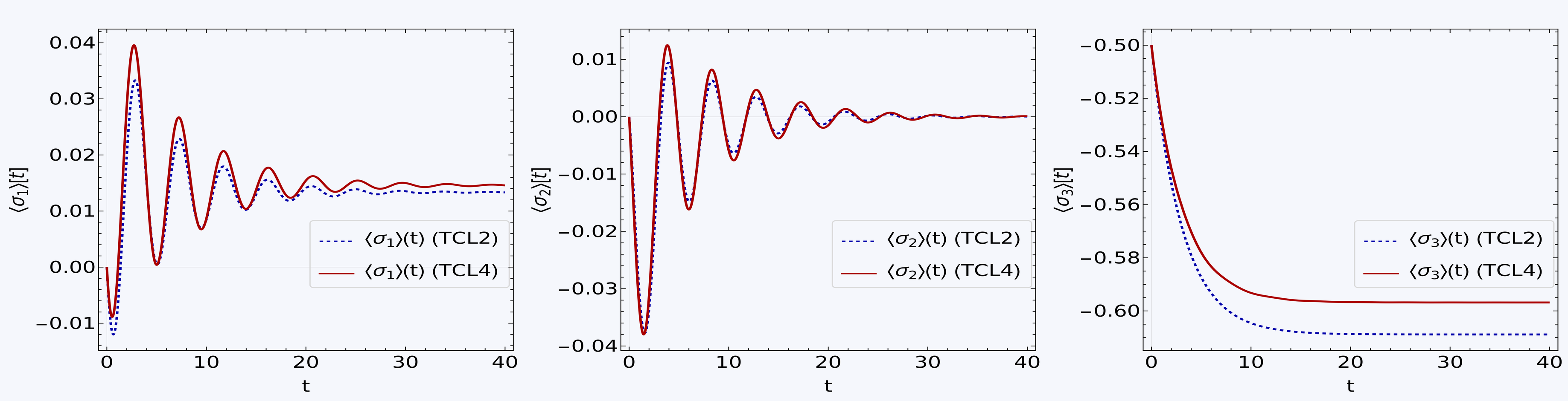


Figure 1: Evolution of Pauli matrix expectation values (a) $\langle\hat{\sigma}_1(t)\rangle$, (b) $\langle\hat{\sigma}_2(t)\rangle$, and (c) $\langle\hat{\sigma}_3(t)\rangle$ for a DQD system using TCL2 (blue dotted lines) and TCL4 (red lines) master equations. The model parameters are $\varepsilon = 1$, $t_c = 0.5$, $\gamma\lambda^2 = 0.4$, $\beta = 1$, $\omega_{\max} = 1$, and $\omega_c = 1$. The initial expectation values are $\langle\hat{\sigma}_1\rangle = 0$, $\langle\hat{\sigma}_2\rangle = 0$, and $\langle\hat{\sigma}_3\rangle = -0.5$.

Numerical verification and benchmarking

- We compare TCL2 and TCL4 dynamics with HEOM for the Ohmic spectral density with Drude cutoff case $\left(J_D(\omega) = \frac{\gamma\Lambda^2\omega}{\Lambda^2+\omega^2}\right)$, quantified by the fidelity between $\hat{\rho}_{\text{TCL}}$ and $\hat{\rho}_{\text{H}}$

$$F(\hat{\rho}_{\text{TCL}}(t), \hat{\rho}_{\text{H}}(t)) = \text{Tr}\sqrt{\sqrt{\hat{\rho}_{\text{H}}(t)}\hat{\rho}_{\text{TCL}}(t)\sqrt{\hat{\rho}_{\text{H}}(t)}}. \tag{1}$$

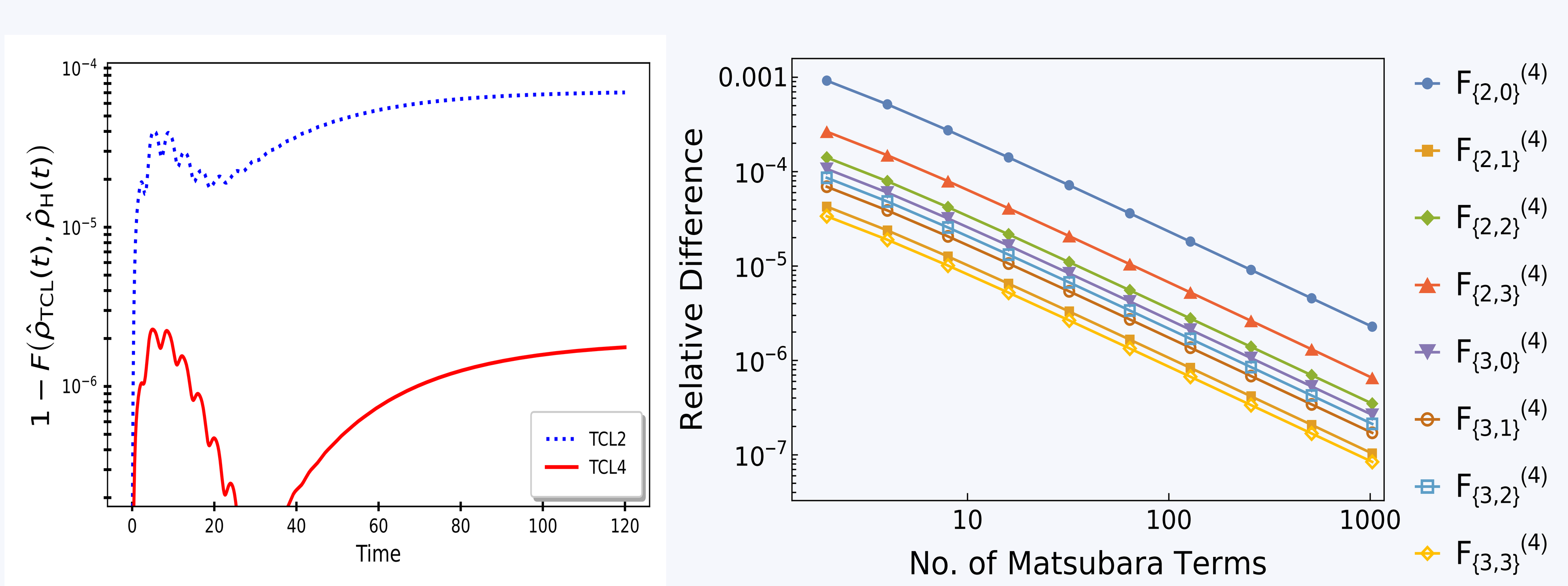


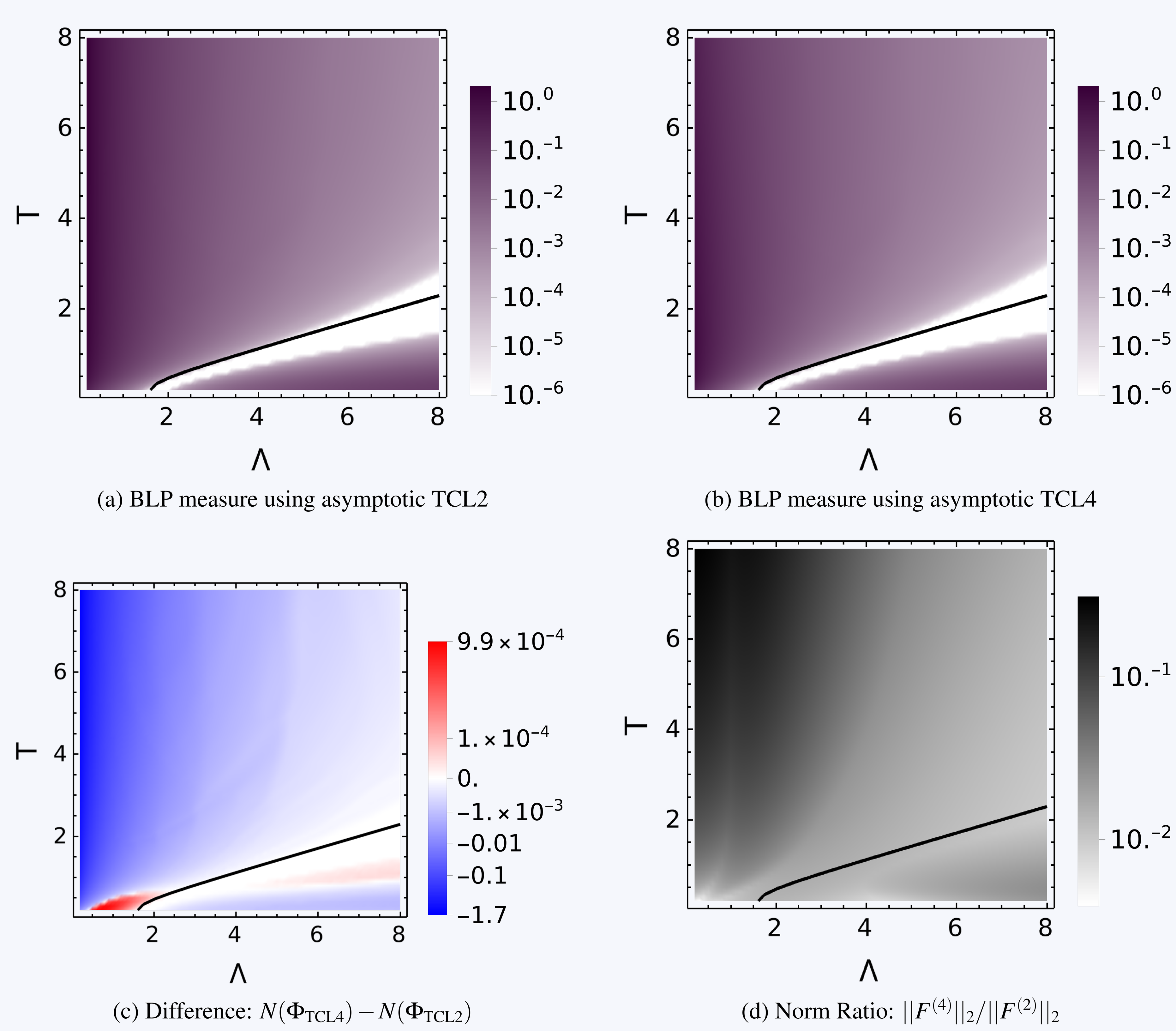
Figure 2: These figures plot a) One minus the Fidelity of the system state evolved by HEOM and TCL-ME (blue dotted line is TCL2 and red line is TCL4), b) Relative difference between asymptotic TCL4 generator elements for the Ohmic–Drude case, obtained from our general odd-spectral-density result and from specialized calculations, plotted against the number of Matsubara terms used in the latter calculation.

Non-Markovian Effects with TCL4

- We quantify the non-Markovianity of TCL2 and TCL4 dynamics for the SBM using the BLP measure (Breuer, Laine & Piilo, 2009) for an Ohmic spectral density with Drude cutoff.
- The degree of non-Markovianity of dynamics is defined by

$$N(\Phi) = \max_{\hat{\rho}_{1,2}(0)} \int_{\sigma>0} dt\, \sigma(t, \hat{\rho}_{1,2}(0)),$$

where $\sigma(t, \hat{\rho}_{1,2}(0)) = \frac{d}{dt}D[\Phi_t(\hat{\rho}_1(0)), \Phi_t(\hat{\rho}_2(0))]$. Here, Φ_t is the dynamical map and $D[\rho, \sigma]$ is trace distance between states ρ and σ.



(a) BLP measure using asymptotic TCL2

(b) BLP measure using asymptotic TCL4

(c) Difference: $N(\Phi_{\text{TCL4}}) - N(\Phi_{\text{TCL2}})$

(d) Norm Ratio: $||F^{(4)}||_2/||F^{(2)}||_2$

Figure 3: These figures plot the BLP measure ($N(\Phi)$) as logarithmic color plot calculated using (a) TCL2 and (b) TCL4 as a function of Λ and T. Part (c) plots the difference between these two quantities ($N(\Phi_{\text{TCL4}}) - N(\Phi_{\text{TCL2}})$), while (d) shows the L_2 norm ratio $||F^{(4)}||_2/||F^{(2)}||_2$, highlighting the regime of validity of the perturbative method. The black line marks the Markovian regime from the resonance condition. The BLP measure is maximized over 400 antipodal Bloch sphere pairs.

References

Prem Kumar, K. P. Athulya, & Sibasish Ghosh. (2025). Equivalence between the second order steady state for the spin-boson model and its quantum mean force Gibbs state. *Phys. Rev. B*, **111**(11), 115423.

Prem Kumar, K. P. Athulya, & Sibasish Ghosh. (2025). Asymptotic TCL4 Generator for the Spin-Boson Model: Analytical Derivation and Benchmarking. *arXiv preprint arXiv:2506.17009*.

Heinz-Peter Breuer, Elsi-Mari Laine, & Jyrki Piilo. (2009). Measure for the degree of non-Markovian behavior of quantum processes in open systems. *Phys. Rev. Lett.*, **103**(21), 210401.

Summary

- We analytically derive the full TCL4 generator in large time limit for a generic SBM for arbitrary odd physical spectral densities.
- For Ohmic-Drude spectral density, TCL2 overestimates non-Markovianity at large values of temperature.
- TCL4 is benchmarked against analytical Drude results and exact HEOM, showing closer agreement across tested regimes.