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

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Abstract

We derive the full fourth-order TCL (TCL4) generator for the spin-boson model (SBM) for arbitrary odd spectral densities and show that the steady state matches the quantum mean-force Gibbs state up to $O(\lambda^2)$. Our results show that the commonly used TCL2 master equation often overestimates non-Markovianity. Benchmarking against analytical results for Ohmic spectral densities and the numerically exact Hierarchical Equations of Motion confirms the accuracy of TCL4. These results offer a general and computationally efficient method for studying steady-state and dynamical properties of a wide class of quantum systems, including semiconductor double quantum dots.

Background

TCL master equation.

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

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

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.

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

$$\hat{H}_S = \tfrac{\Omega}{2}\hat{\sigma}_3,$$
$$\hat{H}_E = \sum_k \left(\frac{\hat{p}_k^2}{2m_k} + \tfrac{1}{2} m_k \omega_k^2 \hat{q}_k^2\right),$$
$$\hat{A} = a_3\hat{\sigma}_3 - a_1\hat{\sigma}_1,$$
$$\hat{B} = \sum_k c_k \hat{q}_k.$$

Spectral density: $J(\omega) = \sum_k \frac{c_k^2}{m_k\omega_k}\delta(\omega - \omega_k)$.

Bloch-vector TCL form.

In Bloch-vector notation,

$$\dot{\mathbf{v}}(t) = \sum_{n=0}^{\infty} \lambda^{2n} F^{(2n)}(t)\,\mathbf{v}(t),$$

with matrix elements

$$F_{mn}^{(2n)}(t) \equiv \mathrm{Tr}\{\hat{\sigma}_m F^{(2n)}(t)[\hat{\sigma}_n]\}$$

. Here λ sets the system–environment coupling; $\hat{\sigma}_i$ are Pauli matrices; m_k, ω_k, c_k are the mass, frequency, and coupling of the k^{th} mode; and a_1, a_3 encode detuning and tunneling.

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

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

where, we have $\mathrm{sinc}(x) \equiv \sin(x)/x$. 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.

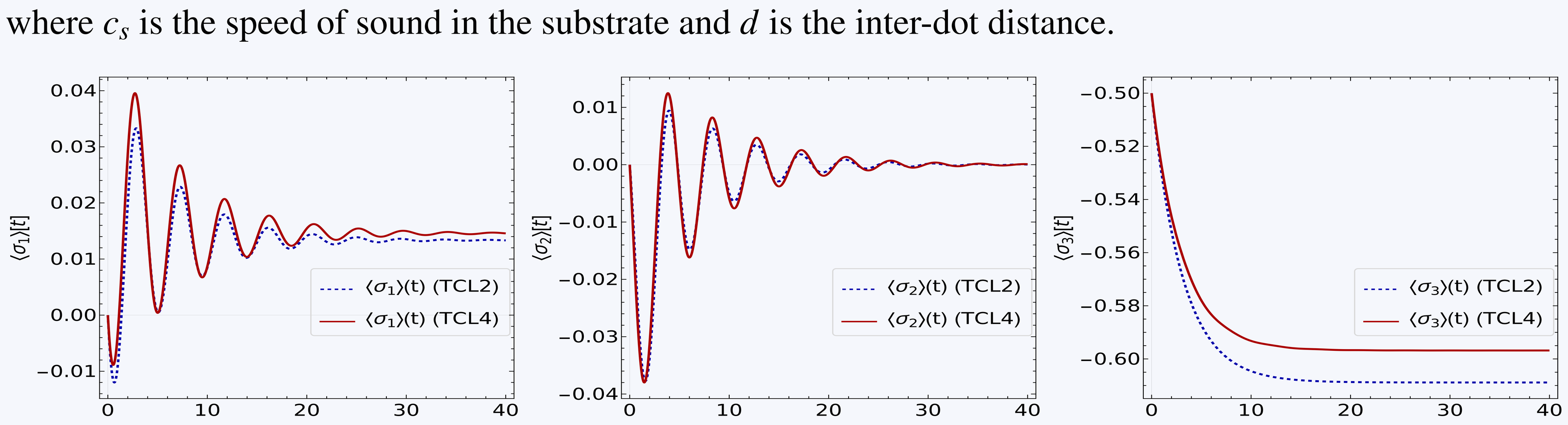

Figure 1: Evolution of Pauli matrix expectation values (a) $\langle\hat{\sigma}_1(t)\rangle$, (b) $\langle\hat{\sigma}_2(t)\rangle$, and (c) $\langle\hat{\sigma}_3(t)\rangle$ for a DQD system using TCL2 (blue lines) and TCL4 (red lines) master equations. The model parameters are $\varepsilon = 1$, $t_c = 0.5$, $\gamma\lambda^2 = 0.4$, $\beta = 1$, $\omega_{\max} = 1$, 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, quantified by the fidelity between $\hat{\rho}_{\mathrm{TCL}}$ and $\hat{\rho}_{\mathrm{H}}$

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

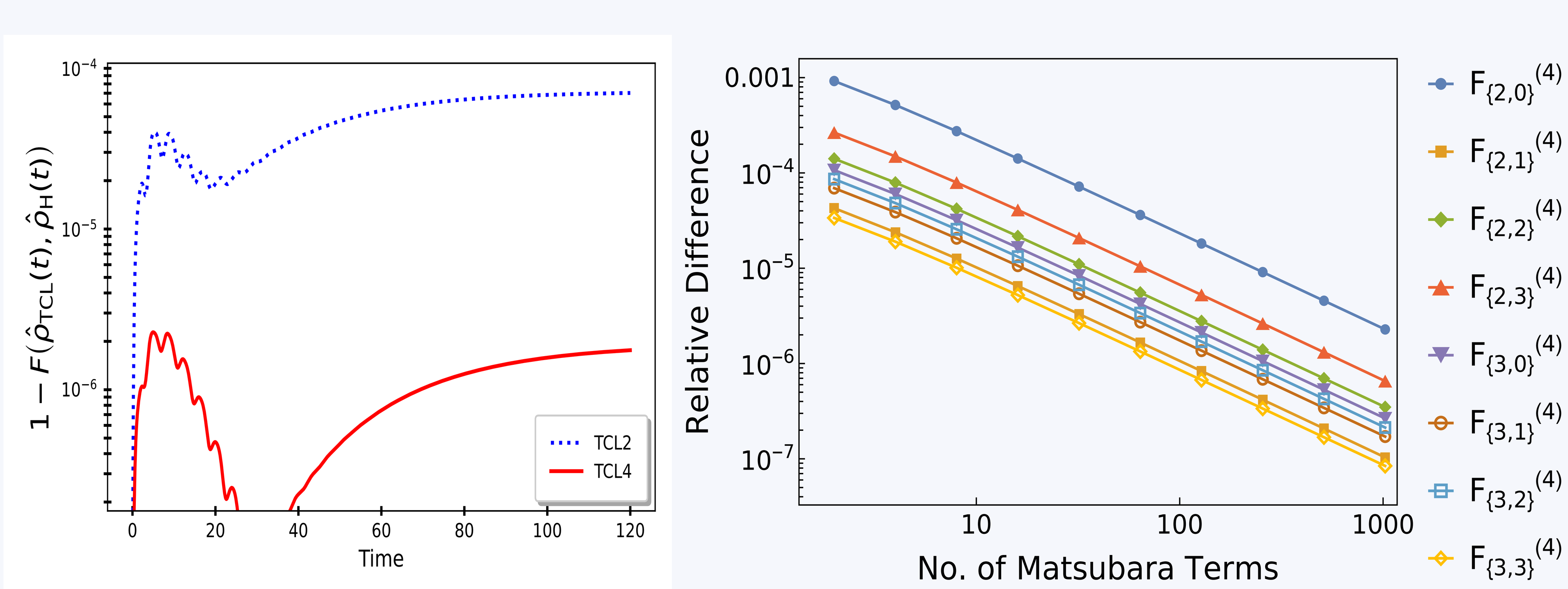

Figure 2: These figures plot a) One minus the Fidelity of the system state evolved by HEOM and TCL-ME (blue line is TCL2 and red line is TCL4), b)Relative difference between asymptotic TCL4 generator elements for the Ohmic–Drude case, obtained from our general odd-spectral-density result and from specialized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

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 $J_D(\omega) = \frac{\gamma\Lambda^2\omega}{\Lambda^2+\omega^2}$.
- The degree of non-Markovianity of dynamics is defined by

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

where $\sigma(t, \hat{\rho}_{1,2}(0)) = \frac{d}{dt} D[\Phi_t(\hat{\rho}_1(0)), \Phi_t(\hat{\rho}_2(0))]$.

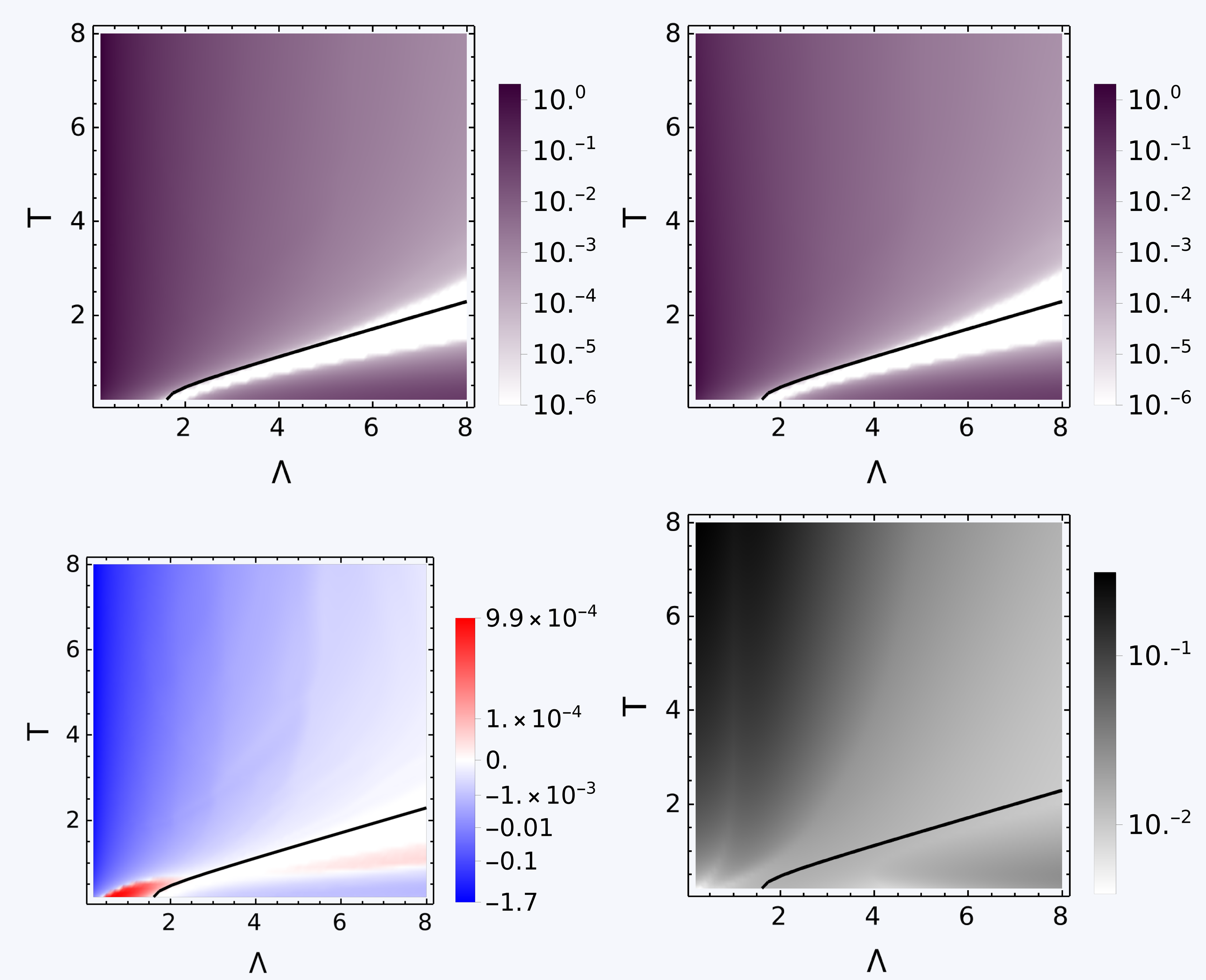

Figure 3: These figures plot the BLP measure ($N(\Phi)$) as logarithmic color plot calculated using (a) TCL2 and (b) TCL4 as a function of Λ and T. Part (c) plots the difference between these two quantities ($N(\Phi_{\mathrm{TCL4}}) - N(\Phi_{\mathrm{TCL2}})$), while (d) shows the L_2 norm ratio $||F^{(4)}||_2/||F^{(2)}||_2$, highlighting the regime where TCL4 remains valid. 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

- For Ohmic-Drude spectral density, TCL2 overestimates non-Markovianity across a wide range of T and Λ.
- TCL4 is benchmarked against analytical Drude results and exact HEOM, showing closer agreement across tested regimes.