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

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

. 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.

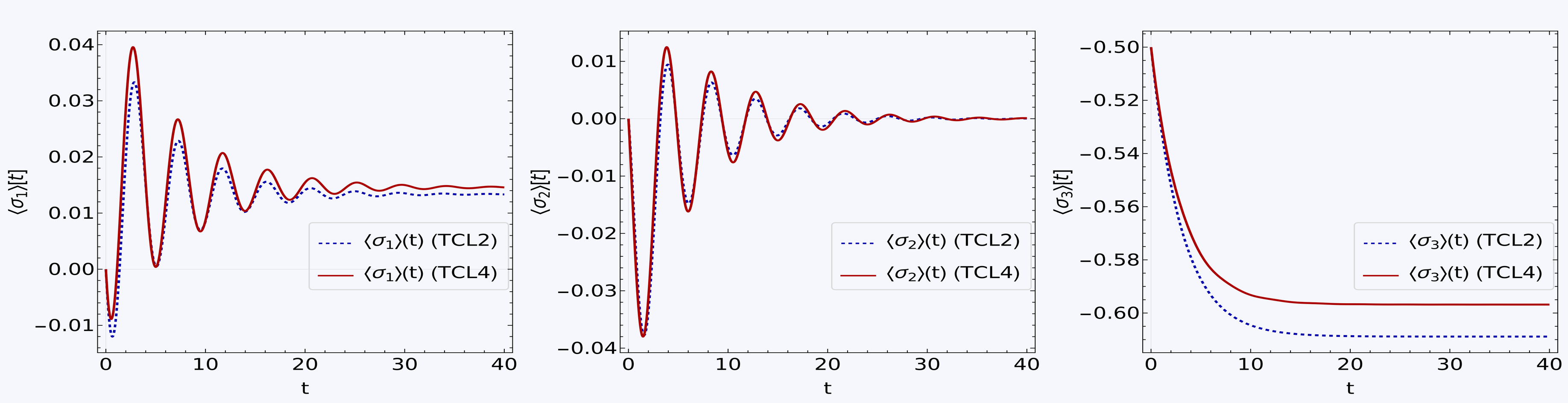

Figure 1: Evolution of Pauli matrix expectation values (a) $\langle\hat{\sigma}_1(t)\rangle$, (b) $\langle\hat{\sigma}_2(t)\rangle$, and (c) $\langle\hat{\sigma}_3(t)\rangle$ for a DQD system using TCL2 (blue lines) and TCL4 (red lines) master equations. The model parameters are $\varepsilon = 1$, $t_c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

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

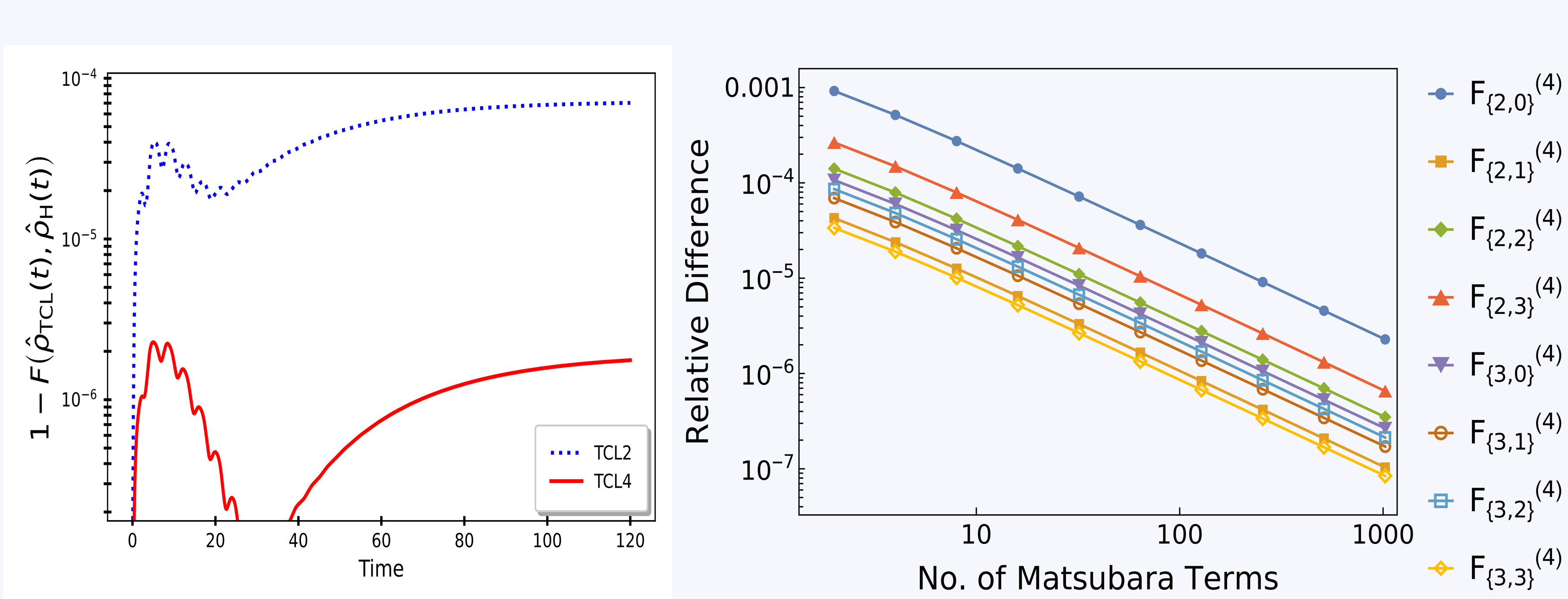

Figure 2: These figures plot a) One minus the Fidelity of the system state evolved by HEOM and TCL-ME (blue line is TCL2 and red line is TCL4), b)Relative difference between asymptotic TCL4 generator elements for the Ohmic–Drude case, obtained from our general odd-spectral-density result and from specialized 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 $\sigma(t, \hat{\rho}_{1,2}(0)) = \frac{d}{dt} D[\Phi_t(\hat{\rho}_1(0)), \Phi_t(\hat{\rho}_2(0))]$.

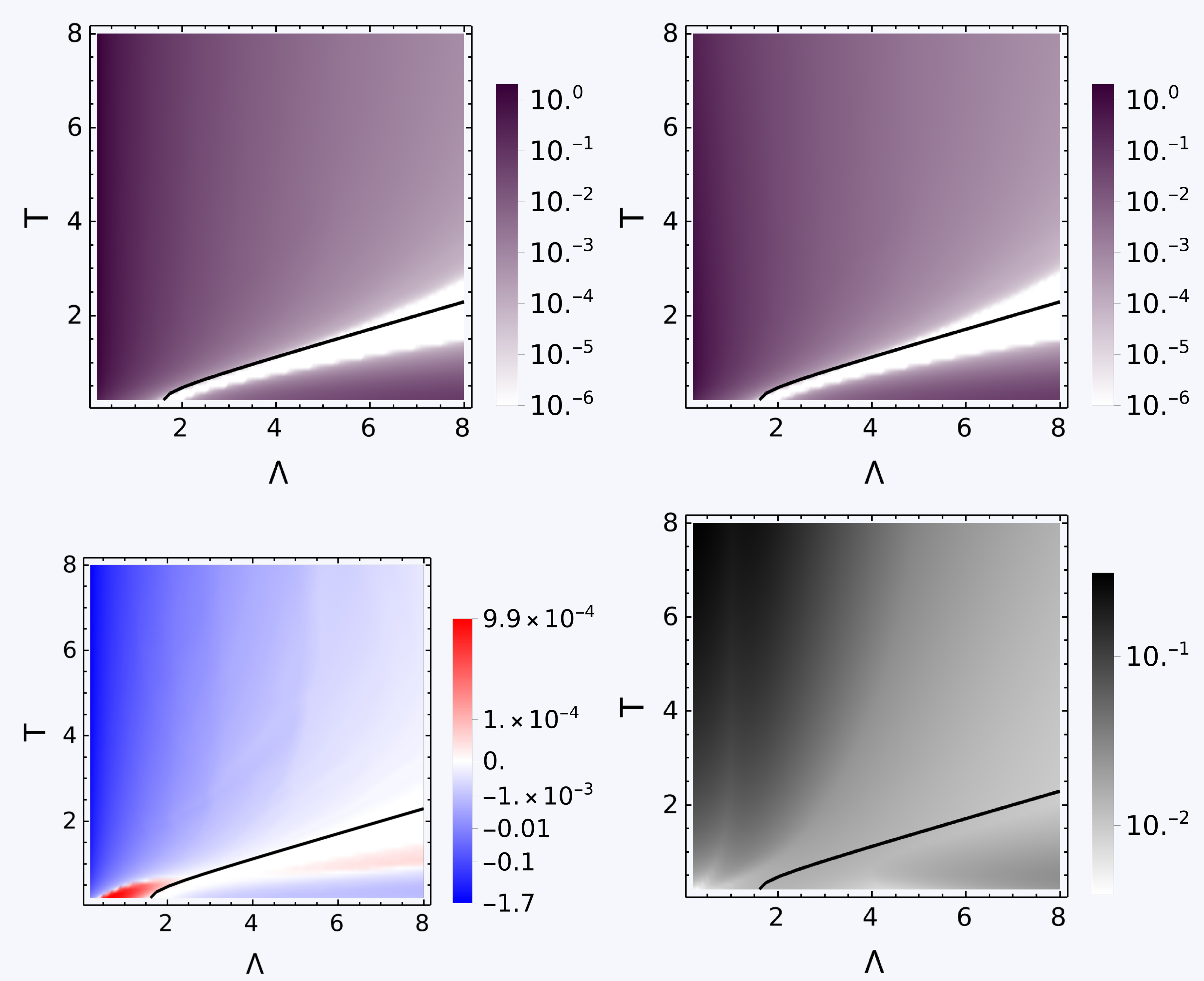

Figure 3: These figures plot the BLP measure ($N(\Phi)$) as logarithmic color plot calculated using (a) TCL2 and (b) TCL4 as a function of Λ and T. Part (c) plots the difference between these two quantities ($N(\Phi_{\mathrm{TCL4}}) - N(\Phi_{\mathrm{TCL2}})$), while (d) shows the L_2 norm ratio $||F^{(4)}||_2/||F^{(2)}||_2$,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

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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.