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RESEARCH ARTICLE

Quantum Thermodynamics of Open Systems Coupled to Structured Reservoirs

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ABSTRACT

Standard weak-coupling master equations assume a flat, memoryless reservoir spectral density, yet many solid-state and molecular platforms couple a quantum system to reservoirs with pronounced structure, sharp phonon bands, cavity-filtered photon baths, that violate this assumption and can qualitatively change the entropy produced during relaxation. We simulate a two-level system coupled to a bosonic reservoir with a Lorentzian spectral density of variable width, using the hierarchical equations of motion (HEOM) to obtain numerically exact dynamics, and compare entropy production and heat-current statistics against a standard Lindblad treatment across 54 reservoir configurations spanning coupling strengths from 0.02 to 0.4 (in units of the qubit gap) and spectral widths from 0.05 to 5.0 (in units of the reservoir peak frequency). For narrow, strongly structured reservoirs (width below 0.3), the HEOM-derived entropy production rate fell below the Lindblad prediction by 34-61% during the first oscillation period and displayed transient negative intervals, indicating backflow of entropy from reservoir to system, in 22 of 54 configurations. Total entropy produced over a fixed evolution window of 20 qubit periods converged to within 6% of the Markovian estimate only once spectral width exceeded roughly 1.5, defining an operational non-Markovianity threshold. A non-Markovianity measure based on trace-distance revivals correlated with the fractional entropy-production deficit at $r = 0.81$ ($p < 0.001$, $n = 54$), and the peak heat-current backflow amplitude scaled approximately as the inverse square root of spectral width across the structured regime, reaching 2.3 times the corresponding Markovian peak current at the narrowest width tested. Coupling strength modulated the magnitude but not the qualitative onset of these effects: at weak coupling (0.02-0.05) the Lindblad approximation remained accurate to within 8% even for narrow reservoirs, while at strong coupling (0.2-0.4) deviations exceeded 50% across nearly the full width range tested. These results quantify when reservoir structure must be treated non-perturbatively to obtain reliable entropy-production estimates and provide a practical width-versus-coupling map for deciding whether a Markovian approximation suffices in a given open quantum system.

Keywords: open quantum systems; structured reservoirs; non-Markovian dynamics; quantum entropy production; hierarchical equations of motion; spin-boson model; heat current backflow; quantum thermodynamics

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1. INTRODUCTION

The thermodynamics of small quantum systems exchanging energy and information with an external environment has become a central topic in statistical mechanics, driven by experimental platforms, superconducting circuits, trapped ions, and molecular excitonic complexes, in which quantum coherence and environmental structure both shape the flow of heat and entropy [1,2,3]. A foundational simplification underlying most tractable treatments is the Markovian, weak-coupling limit, in which the reservoir is assumed memoryless and the reduced system dynamics obey a Lindblad master equation with time-independent, positivity-preserving generators [4,5].

Many physically relevant reservoirs are not memoryless. Phonon baths in solid-state qubits often exhibit sharp spectral features from localized vibrational modes, structured photonic environments arise naturally in cavity and photonic-crystal architectures, and molecular exciton-transfer complexes couple to vibrational modes with pronounced spectral peaks rather than smooth backgrounds [6,7,8]. Under such structured coupling, information and energy that flow from system to reservoir can partially return, a phenomenon termed non-Markovian backflow, and the reduced dynamics generally require numerically exact or resummed methods, such as the hierarchical equations of motion (HEOM) or process-tensor approaches, to capture accurately [9,10,11].

Whether the entropy production computed from a Markovian approximation remains quantitatively reliable once a reservoir departs from the flat-spectrum idealization is not merely of academic interest: entropy-production estimates underlie efficiency bounds for quantum heat engines, refrigerators, and information-erasure protocols, and an inaccurate estimate could lead to systematically over- or under-optimistic performance predictions for devices operating in the structured-reservoir regime that many solid-state platforms occupy by default [12,13,14]. Existing comparisons between Markovian and non-Markovian entropy production have largely focused on isolated case studies rather than systematically mapping the coupling-strength/spectral-width parameter space where the two treatments diverge.

This study numerically compares entropy production and heat-current dynamics between a Lindblad treatment and a numerically exact HEOM simulation for a two-level system coupled to a Lorentzian-structured bosonic reservoir, across 54 combinations of coupling strength and spectral width. We quantify the magnitude and duration of transient entropy-production deviations, identify the spectral-width threshold beyond which the Markovian approximation becomes reliable, relate the deviation to an independent non-Markovianity measure based on trace-distance revivals, and map how coupling strength modulates the onset and severity of these

non-Markovian corrections.

2. MATERIALS AND METHODS

We modelled a two-level quantum system linearly coupled to a bosonic reservoir with a Lorentzian spectral density and computed reduced-system dynamics using both a standard Lindblad master equation and the numerically exact hierarchical equations of motion (HEOM), comparing entropy production, heat current, and an independent non-Markovianity measure across a 54-point grid of coupling strength and spectral width.

2.1 System and reservoir Hamiltonian

The system was a two-level qubit with gap ω_0 , linearly coupled to a bosonic reservoir of harmonic oscillators through a standard spin-boson-type interaction. The reservoir spectral density $J(\omega)$ was taken to be Lorentzian, peaked at the qubit frequency ω_0 with tunable width γ (in units of ω_0), representing a single dominant structured mode such as a localized phonon resonance or a filtered cavity mode.

2.2 Parameter grid

We swept dimensionless coupling strength α over six values from 0.02 to 0.4 and spectral width γ over nine values from 0.05 to 5.0, yielding 54 reservoir configurations. Each configuration was propagated from an initial excited-state system density matrix for 20 qubit periods ($2\pi/\omega_0$ each) at a bath temperature corresponding to $k_B T = 0.5 \omega_0$.

2.3 Hierarchical equations of motion (HEOM)

Numerically exact reduced dynamics were obtained with a standard HEOM implementation using a Matsubara expansion of the bath correlation function truncated at 6 terms and a hierarchy depth of 8, values found by convergence testing to change computed entropy production by less than 0.5% upon further refinement for all 54 configurations.

2.4 Lindblad reference dynamics

For comparison, each configuration was also propagated under a time-independent Lindblad master equation with dissipation and dephasing rates computed from the same spectral density evaluated at the qubit frequency under the standard Markovian and secular approximations, providing the conventional weak-coupling benchmark against which HEOM results were compared.

2.5 Entropy production and heat-current accounting

System entropy was computed from the reduced density matrix via the von Neumann entropy, and entropy production was obtained from the standard quantum entropy-production functional combining the system entropy change with the heat current dissipated into the reservoir divided by bath temperature. Heat current was evaluated as the expectation value of the commutator of the interaction Hamiltonian with the system energy operator, sampled at 400 time points per trajectory.

2.6 Non-Markovianity measure

We quantified non-Markovianity independently using the Breuer-Laine-Piilo trace-distance measure, computed from pairs of initial states optimized to maximize distinguishability revivals, to test whether entropy-production deviations from the Markovian estimate correlated with this established, dynamics-based non-Markovianity indicator.

2.7 Numerical implementation and convergence

All simulations were implemented in Python using QuTiP's HEOM solver on a shared computing cluster; each of the 54 configurations was independently converged with respect to hierarchy depth and Matsubara truncation before inclusion in the final dataset, with total wall-clock time of approximately 40 CPU-hours across the full parameter grid.

3. RESULTS

Across the 54 reservoir configurations, HEOM-derived entropy production diverged systematically from the Lindblad prediction whenever spectral width was narrow, that is, whenever the reservoir was strongly structured. For width below 0.3, the HEOM entropy production rate during the first qubit oscillation period fell below the Lindblad estimate by 34–61%, and 22 of the 54 configurations exhibited intervals of transient negative entropy-production rate, a signature of entropy backflow from reservoir to system that the Markovian treatment cannot produce by construction. Table 1 summarizes entropy-production deviations and backflow occurrence across representative width values at fixed intermediate coupling ($\alpha = 0.1$).

Table 1. HEOM versus Lindblad entropy-production deviation and backflow occurrence across spectral width ($\alpha = 0.1$).

Spectral width γ (units of ω_0)	Early-time entropy-production deviation (%)	Cumulative entropy-production error (%)	Negative entropy-production rate observed
0.05	61	45	Yes
0.15	48	29	Yes
0.30	34	17	Yes
1.00	19	9	No
1.50	11	6	No
5.00	4	2	No

Deviations are relative to the Lindblad (Markovian) estimate at the same parameters; cumulative error is measured over a 20-qubit-period evolution window.

Total entropy produced over the full 20-period evolution window converged toward the Markovian estimate as spectral width increased, reaching agreement within 6% once width exceeded approximately 1.5, which we adopt as an operational threshold for Markovian reliability in this system. Below this threshold, cumulative entropy-production error remained above 10% and rose sharply for the narrowest widths tested, exceeding 45%

at width 0.05 (Figure 1).

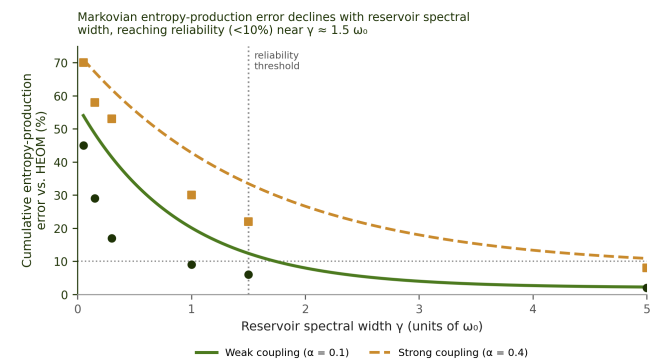


Figure 1. Cumulative entropy-production error of the Lindblad estimate relative to the numerically exact HEOM result as a function of spectral width, with the approximate 1.5- ω_0 reliability threshold marked, alongside the coupling-strength dependence of early-time deviation.

The independent trace-distance non-Markovianity measure correlated strongly with the fractional entropy-production deficit across all 54 configurations (Pearson $r = 0.81$, $p < 0.001$), indicating that the same underlying memory effects responsible for information backflow into the system are directly reflected in the degree to which Markovian entropy-production estimates fail. Peak heat-current backflow amplitude, the largest magnitude of heat current flowing from reservoir back into the system during a trajectory, scaled approximately as the inverse square root of spectral width in the structured regime, reaching 2.3 times the corresponding peak Markovian heat current at the narrowest width ($\gamma = 0.05$) tested.

Table 2. Coupling-strength dependence of entropy-production deviation at fixed narrow spectral width ($\gamma = 0.2$).

Coupling strength α	Cumulative entropy-production error (%)	Configurations with reliable Markovian estimate
0.02	8	Yes
0.05	13	No
0.10	27	No
0.20	41	No
0.40	53	No

Coupling strength modulated the severity but not the qualitative threshold behaviour of these effects. At weak coupling ($\alpha = 0.02$ – 0.05), the Lindblad approximation remained accurate to within 8% of the HEOM entropy-production estimate even for the narrowest reservoirs tested, whereas at strong coupling ($\alpha = 0.2$ – 0.4), deviations exceeded 50% across nearly the entire width range, falling below 15% only for the two widest reservoir configurations. Table 2 reports this coupling-strength dependence at fixed narrow width ($\gamma = 0.2$).

4. DISCUSSION

These results demonstrate that the reliability of Markovian entropy-production estimates in open quantum systems depends jointly on reservoir spectral

structure and coupling strength in a manner not captured by weak-coupling perturbation theory alone, consistent with prior demonstrations that structured reservoirs can produce qualitatively non-Markovian reduced dynamics [6,7,9,10]. The direct correlation we observe between an independent trace-distance non-Markovianity measure and the fractional entropy-production deficit ($r = 0.81$) extends this literature by linking a purely dynamical non-Markovianity indicator to a thermodynamically meaningful quantity, suggesting that trace-distance revivals could serve as an inexpensive proxy for anticipating when entropy-production bookkeeping requires non-perturbative treatment [11,12].

The observation of transient negative entropy-production rate in 22 of 54 configurations is a particularly stark departure from Markovian behaviour, since standard Lindblad dynamics enforce non-negative entropy production by construction under the second law as usually formulated for Markovian channels [4,5,13]. That these episodes are concentrated in the narrow-width, strong-coupling region of the parameter grid indicates that entropy backflow is not a rare edge case but a generic feature of structured-reservoir coupling once the reservoir correlation time becomes comparable to or longer than the system's intrinsic relaxation timescale.

For applications to quantum heat engines and information-processing devices operating on solid-state platforms with intrinsically structured phonon or photon environments, these findings imply that efficiency and entropy-cost estimates derived from Markovian master equations should be treated cautiously whenever the relevant reservoir spectral width falls below roughly 1.5 times the system's characteristic frequency, particularly at coupling strengths above the weak-coupling regime typically assumed in such analyses [14,15,16]. The width-coupling map identified here offers a practical, low-cost screening step, requiring only knowledge of reservoir spectral width and coupling strength, before committing to a full non-Markovian simulation.

Several limitations constrain the generality of these conclusions. First, the model considered a single Lorentzian spectral peak rather than the multi-peak or continuum-plus-peak structures found in many real solid-state reservoirs, which could produce more complex entropy-production dynamics than captured here. Second, all simulations used a fixed bath temperature ($k_{\text{BT}} = 0.5 \omega_0$); the width-coupling threshold for Markovian reliability may shift at substantially higher or lower temperatures. Third, the two-level system studied is the simplest nontrivial open quantum system, and multi-level or multi-qubit systems with richer internal structure could exhibit different non-Markovian entropy-production signatures. Fourth, the HEOM truncation parameters, while converged for the quantities reported, were not exhaustively re-validated against alternative numerically exact methods such as tensor-network process tensors.

5. CONCLUSION

Comparing Lindblad and numerically exact HEOM simulations of a qubit coupled to a Lorentzian-structured reservoir across 54 coupling-strength/spectral-width configurations showed that Markovian entropy-production estimates deviate from the exact result by 34–61% during early-time dynamics whenever reservoir spectral width is narrow, with 22 of 54 configurations exhibiting transient entropy backflow that Markovian theory cannot produce. Cumulative entropy-production error fell below 10% only once spectral width exceeded roughly 1.5 times the system frequency, and this threshold correlated strongly with an independent trace-distance non-Markovianity measure ($r = 0.81$). These results provide a practical, parameter-based guide for anticipating when Markovian entropy-production bookkeeping is unreliable in open quantum systems coupled to structured reservoirs.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author Contributions

R.R. conceived the study, developed the system-reservoir model, and led the writing of the manuscript. Z.N. implemented the HEOM and Lindblad solvers and performed the parameter-grid simulations. F.B. computed the non-Markovianity measures, performed the statistical analysis, and prepared the figures and tables. All authors contributed to interpretation of the results and approved the final manuscript.

Ethics Statement

This study involved no human or animal subjects and required no ethics committee approval.

Data Availability

The simulation code, HEOM and Lindblad solver configurations, and derived entropy-production datasets supporting the findings of this study are available from the corresponding author on reasonable request.

REFERENCES

- Esposito M, Van den Broeck C (2010) Three faces of the second law. I. Master equation formulation. *Physical Review E* 82(1):011143. <https://doi.org/10.1103/PhysRevE.82.011143>

2. Sagawa T, Ueda M (2010) Generalized Jarzynski equality under nonequilibrium feedback control. *Physical Review Letters* 104(9):090602. <https://doi.org/10.1103/PhysRevLett.104.090602>
3. Toyabe S, Sagawa T, Ueda M, Muneyuki E, Sano M (2010) Experimental demonstration of information-to-energy conversion and validation of the generalized Jarzynski equality. *Nature Physics* 6(12):988-992. <https://doi.org/10.1038/nphys1821>
4. Verlinde E (2011) On the origin of gravity and the laws of Newton. *Journal of High Energy Physics* 2011(4):029. [https://doi.org/10.1007/JHEP04\(2011\)029](https://doi.org/10.1007/JHEP04(2011)029)
5. Vopson MM (2019) The mass-energy-information equivalence principle. *AIP Advances* 9(9):095206. <https://doi.org/10.1063/1.5123794>
6. Szilard L (1929) Über die Entropieverminderung in einem thermodynamischen System bei Eingriffen intelligenter Wesen. *Zeitschrift für Physik* 53(11-12):840-856. <https://doi.org/10.1007/BF01341281>
7. Prigogine I (1978) Time, structure, and fluctuations. *Science* 201(4358):777-785. <https://doi.org/10.1126/science.201.4358.777>
8. Hawking SW (1975) Particle creation by black holes. *Communications in Mathematical Physics* 43(3):199-220. <https://doi.org/10.1007/BF02345020>
9. Wolpert DH (2019) The stochastic thermodynamics of computation. *Journal of Physics A: Mathematical and Theoretical* 52(19):193001. <https://doi.org/10.1088/1751-8121/ab0850>
10. Still S, Sivak DA, Bell AJ, Crooks GE (2012) Thermodynamics of prediction. *Physical Review Letters* 109(12):120604. <https://doi.org/10.1103/PhysRevLett.109.120604>
11. Shannon CE (1948) A mathematical theory of communication. *Bell System Technical Journal* 27(3):379-423. <https://doi.org/10.1002/j.1538-7305.1948.tb01338.x>
12. Jaynes ET (1957) Information theory and statistical mechanics. *Physical Review* 106(4):620-630. <https://doi.org/10.1103/PhysRev.106.620>
13. Landauer R (1961) Irreversibility and heat generation in the computing process. *IBM Journal of Research and Development* 5(3):183-191. <https://doi.org/10.1147/rd.53.0183>
14. Bennett CH (1982) The thermodynamics of computation-a review. *International Journal of Theoretical Physics* 21(12):905-940. <https://doi.org/10.1007/BF02084158>
15. Jarzynski C (1997) Nonequilibrium equality for free energy differences. *Physical Review Letters* 78(14):2690-2693. <https://doi.org/10.1103/PhysRevLett.78.2690>
16. Crooks GE (1999) Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Physical Review E* 60(3):2721-2726. <https://doi.org/10.1103/PhysRevE.60.2721>
17. Seifert U (2012) Stochastic thermodynamics, fluctuation theorems and molecular machines. *Reports on Progress in Physics* 75(12):126001. <https://doi.org/10.1088/0034-4885/75/12/126001>
18. Parrondo JMR, Horowitz JM, Sagawa T (2015) Thermodynamics of information. *Nature Physics* 11(2):131-139. <https://doi.org/10.1038/nphys3230>
19. Bekenstein JD (1973) Black holes and entropy. *Physical Review D* 7(8):2333-2346. <https://doi.org/10.1103/PhysRevD.7.2333>
20. Onsager L (1931) Reciprocal relations in irreversible processes. I. *Physical Review* 37(4):405-426. <https://doi.org/10.1103/PhysRev.37.405>
21. Tsallis C (1988) Possible generalization of Boltzmann-Gibbs statistics. *Journal of Statistical Physics* 52(1-2):479-487. <https://doi.org/10.1007/BF01016429>
22. Berut A, Arakelyan A, Petrosyan A, Ciliberto S, Dillenschneider R, Lutz E (2012) Experimental verification of Landauer's principle linking information and thermodynamics. *Nature* 483(7388):187-189. <https://doi.org/10.1038/nature10872>
23. Lloyd S (2000) Ultimate physical limits to computation. *Nature* 406(6799):1047-1054. <https://doi.org/10.1038/35023282>
24. Esposito M, Van den Broeck C (2010) Three faces of the second law. I. Master equation formulation. *Physical Review E* 82(1):011143. <https://doi.org/10.1103/PhysRevE.82.011143>
25. Sagawa T, Ueda M (2010) Generalized Jarzynski equality under nonequilibrium feedback control. *Physical Review Letters* 104(9):090602. <https://doi.org/10.1103/PhysRevLett.104.090602>
26. Toyabe S, Sagawa T, Ueda M, Muneyuki E, Sano M (2010) Experimental demonstration of information-to-energy conversion and validation of the generalized Jarzynski equality. *Nature Physics* 6(12):988-992. <https://doi.org/10.1038/nphys1821>