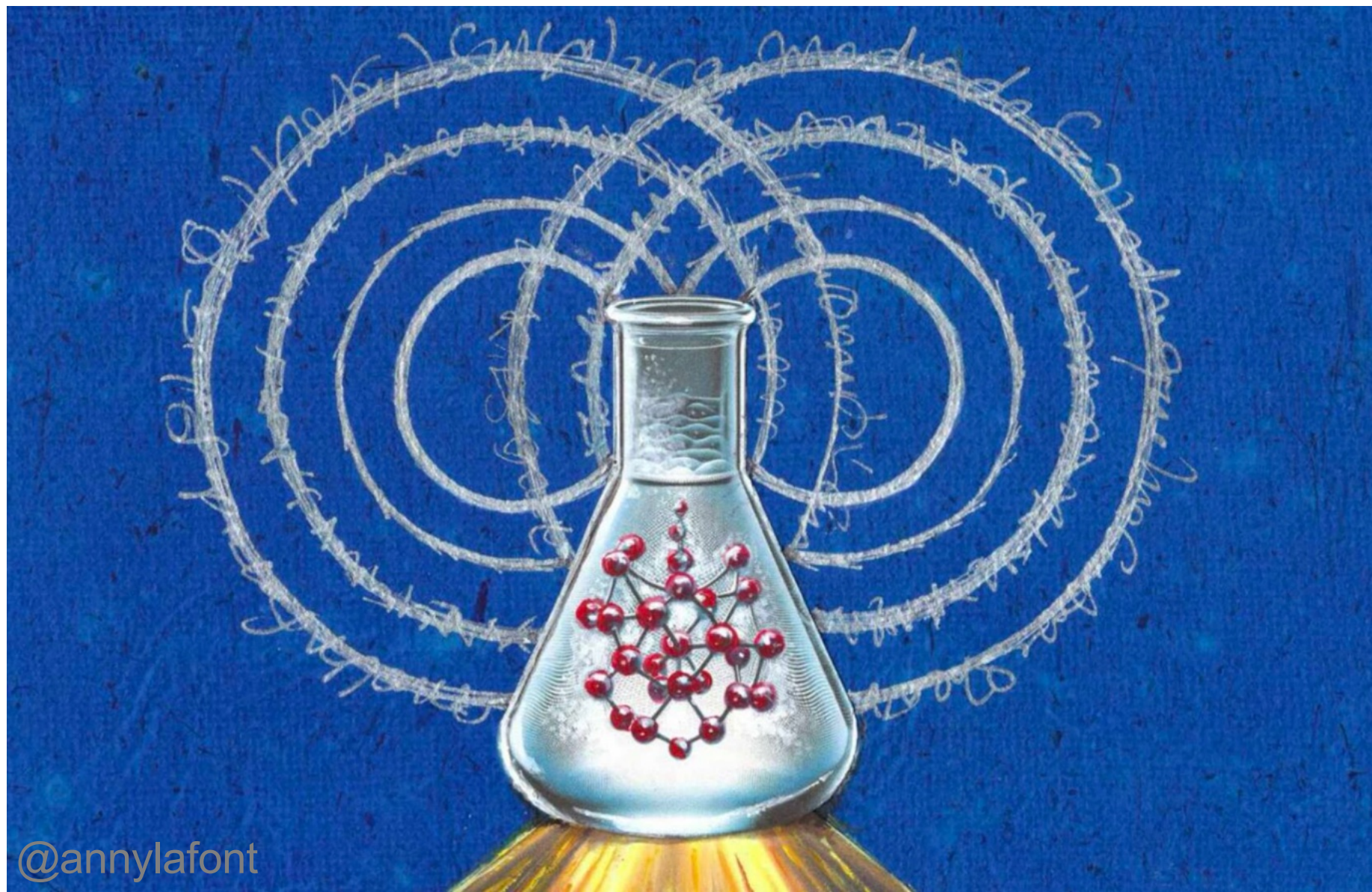
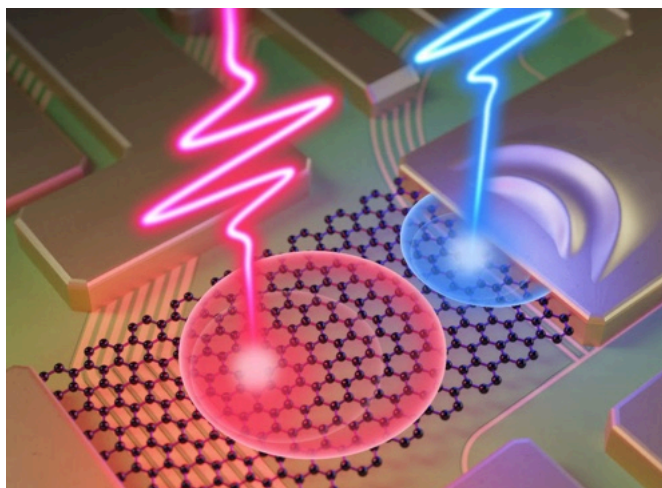




“Numerically Exact” Open Quantum Dynamics using Tensor Networks
Ignacio Franco, University of Rochester

CyberTraining: Modeling Quantum Dynamics of Excited States
July 10, 2026

Research in the Franco Group



Quantum Control of Matter at the Level of Electrons

e.g. Nature **605**, 251 (2022)
PRL **135**, 186901 (2025)



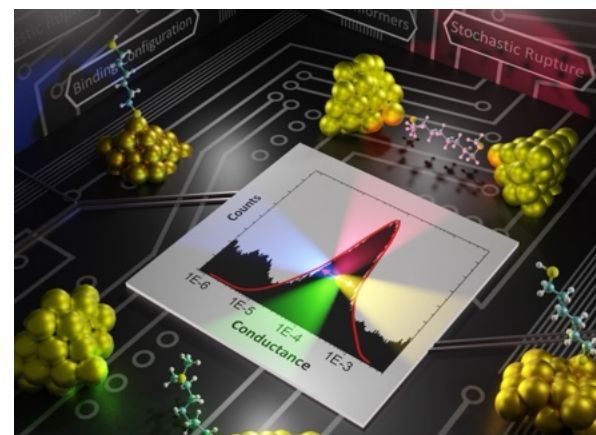
Quantum Coherence in Matter

e.g. PNAS **120**, e2309987120 (2023)
J. Chem. Phys. **163** 104109 (2025)



Quantum Simulation

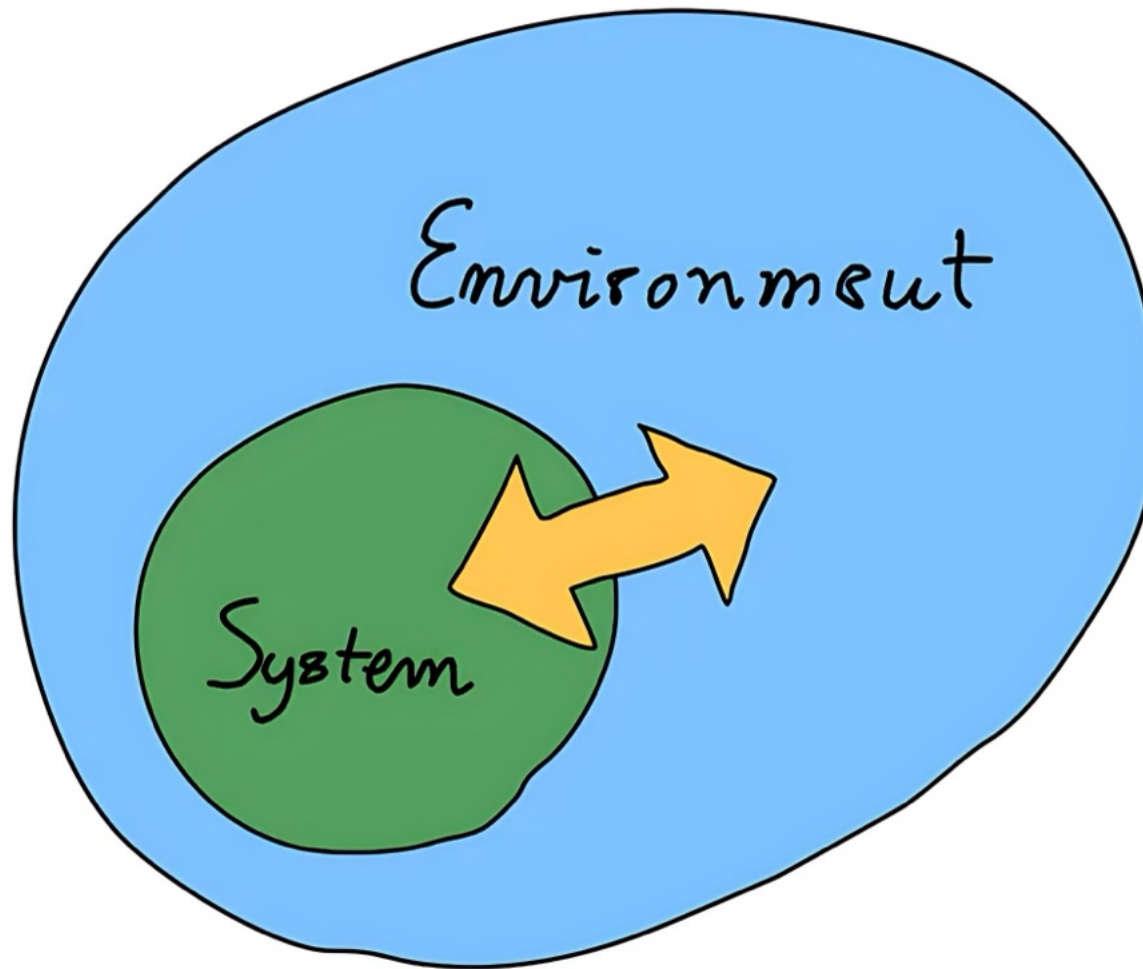
e.g. PRX Quantum **3**, 040308 (2022)



Quantum Transport

e.g. Nature Comm. **14**, 7646 (2023)
JACS **147**, 20310 (2025)

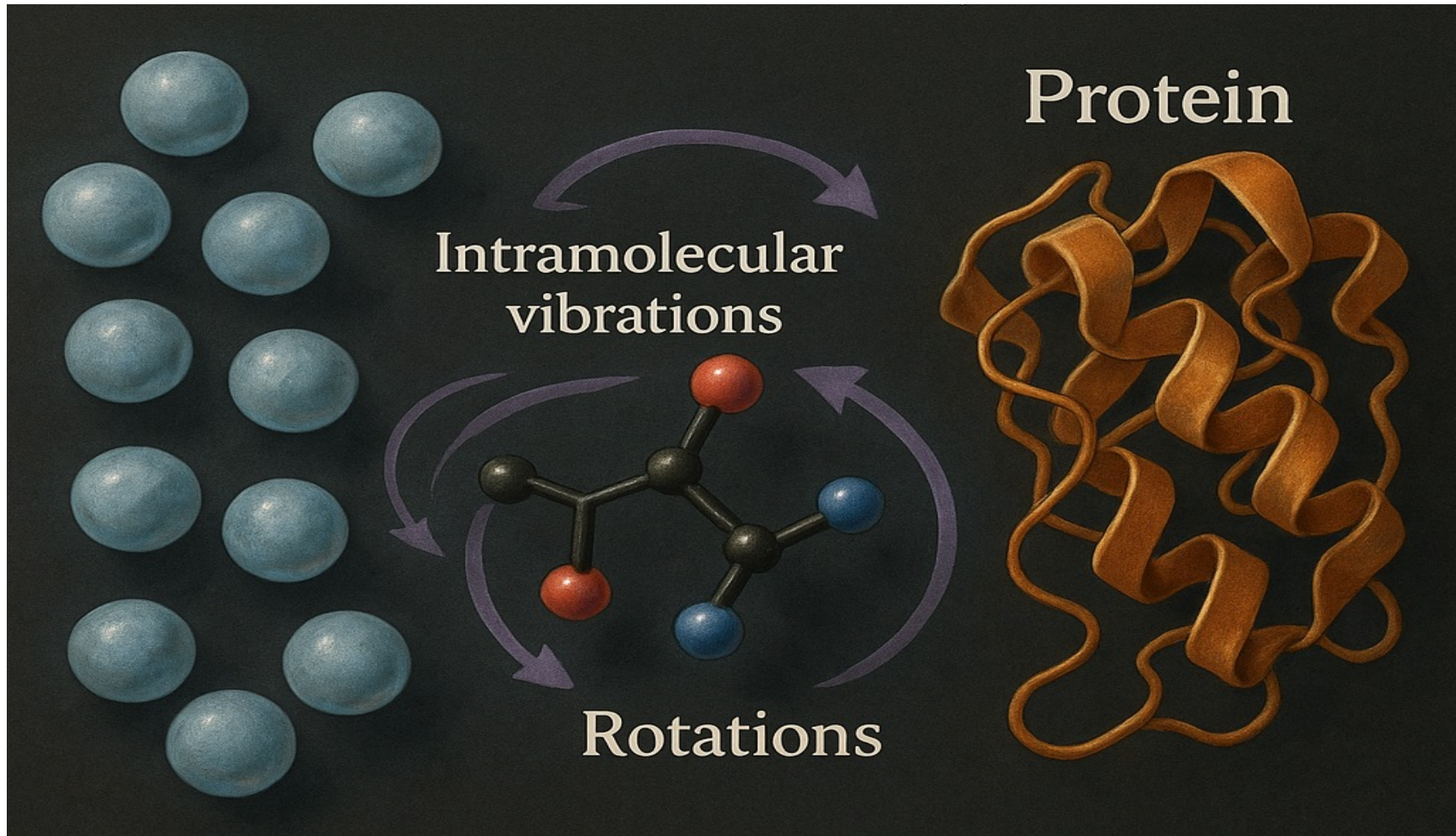
Open Quantum Dynamics



In Nature, nothing exists alone ...



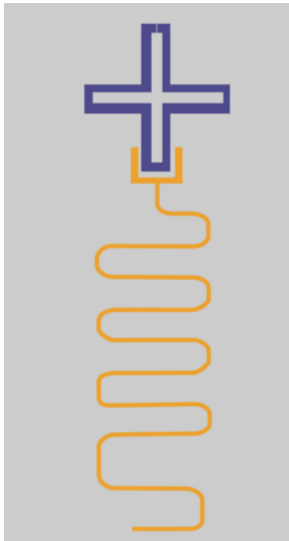
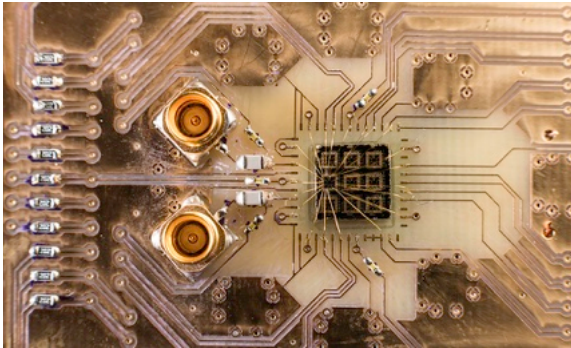
Open Quantum Dynamics



Environment changes the system's dynamics,
introduces dephasing and relaxation

What's the fuzz about quantum coherence

Coherence is the fuel behind all quantum technologies



**Quantum Control
Quantum Computation
Quantum Sensing**



Needed for matter to exhibit
interference/controlled entanglement
Needed for quantum unitary dynamics
Enhanced temporal coherence leads to
enhanced laser spectroscopy



The Chemistry of Quantum Decoherence

How molecular electronic decoherence studies look like right now:

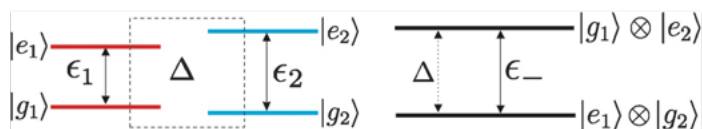


Figure 1. Left-hand side: The pair of interacting chromophores. Right-hand side: the effective light-harvesting two-level system formed from the pair of interacting chromophores.^{19,20}

The environment is fully characterized by the spectral density $J(\omega) = \sum_{\alpha} g_{\alpha}^2 \delta(\omega - \omega_{\alpha})$, being a quasi-continuous function for typical condensed-phase applications that determines all bath correlations that are relevant for the system.^{21,22} For Ohmic dissipation, $J(\omega) = 2K\omega e^{-\omega/\omega_c}$, where the dimensionless parameter K describes the damping strength and ω_c is the cutoff

e.g. J. Phys. Chem. Lett. **2**, 2728 (2011)

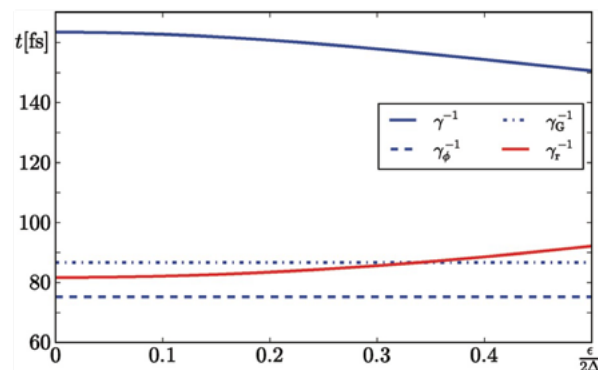
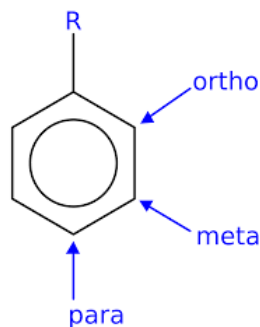


Figure 3. Relaxation time γ_r^{-1} (red line) and decoherence time γ^{-1} (continuous blue line) as functions of $\epsilon/2\Delta$ for fixed $\Delta = 35 \text{ cm}^{-1}$ and at $T = 77 \text{ K}$. The dashed blue line, $\gamma_{\phi} = 2\pi(k_B T/\hbar)\lambda/\hbar\omega_c$, denotes the dephasing rate used in refs 4, 7, and 10, and the dot-dashed blue line denotes the decoherence time $\tau_G = (\hbar^2/2\lambda k_B T)^{1/2}$ used in refs 3–5. Fixed parameters as in Table 1.

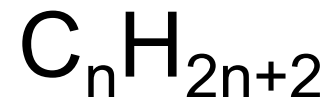
How I would like them to look like



How does chemical substitution change decoherence?

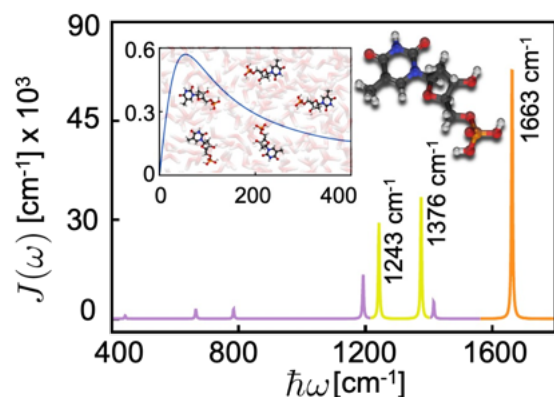


How does solvent polarity influence coherence loss?



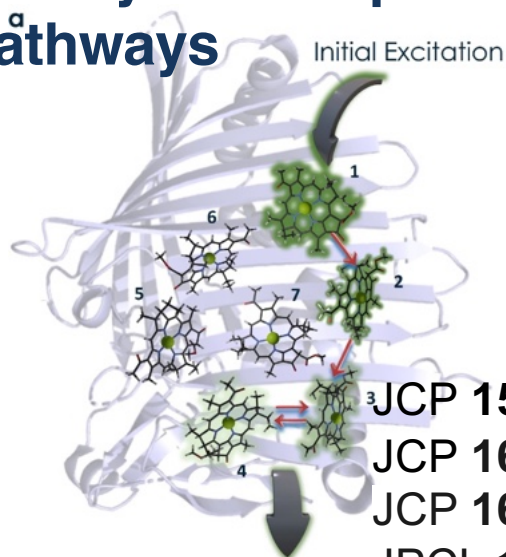
How does decoherence change along a homologous series?

Chemical Principles of Quantum Decoherence



PNAS **120**, e2309987120 (2023)

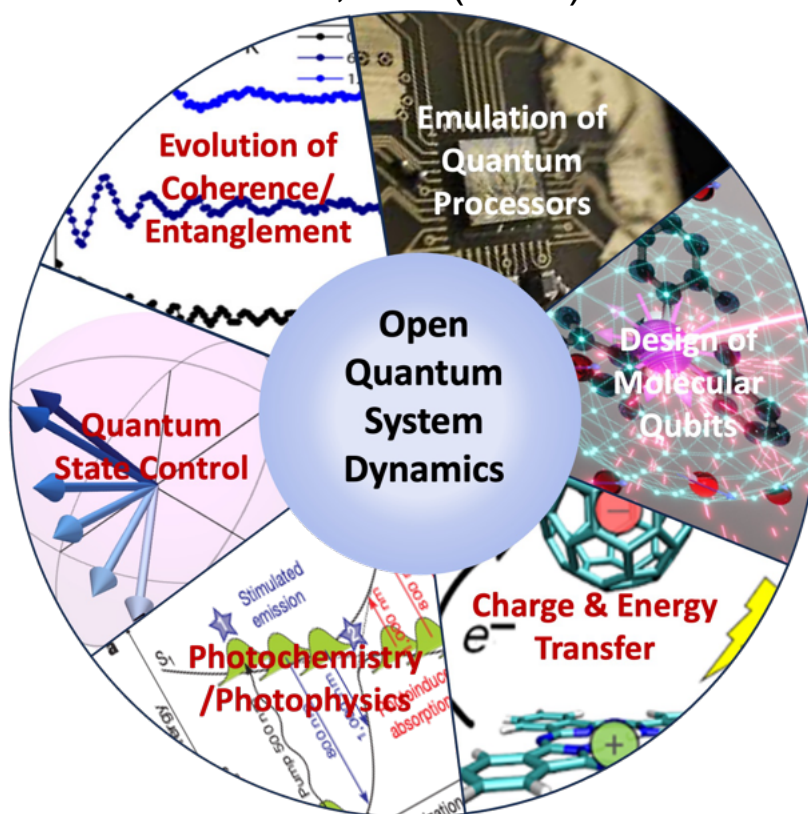
Theory of Dissipation Pathways



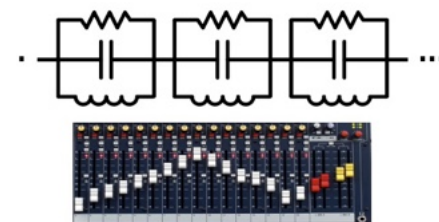
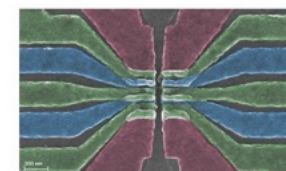
JCP **154**, 084103 (2021);
 JCP **160**, 214111 (2024);
 JCP **160**, 214112 (2024);
 JPCL **16**, 13093 (2025);
 JCP **164**, 034105 (2026)

Foundations of Decoherence

e.g. JCP **162**, 064106 (2025);
 JPCL **13**, 11503 (2022);
 JCP **151**, 014109 (2019);
 JCP, **148**, 134304 (2018);
 JPCL **9**, 773 (2018)

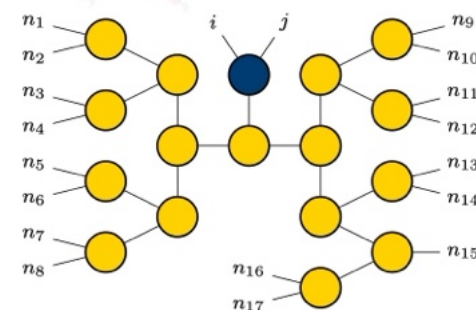


Quantum Simulation



PRX Quantum **3**, 040308 (2022); JPC A **129**, 15, 3587 (2025)

Tensor Network Strategies

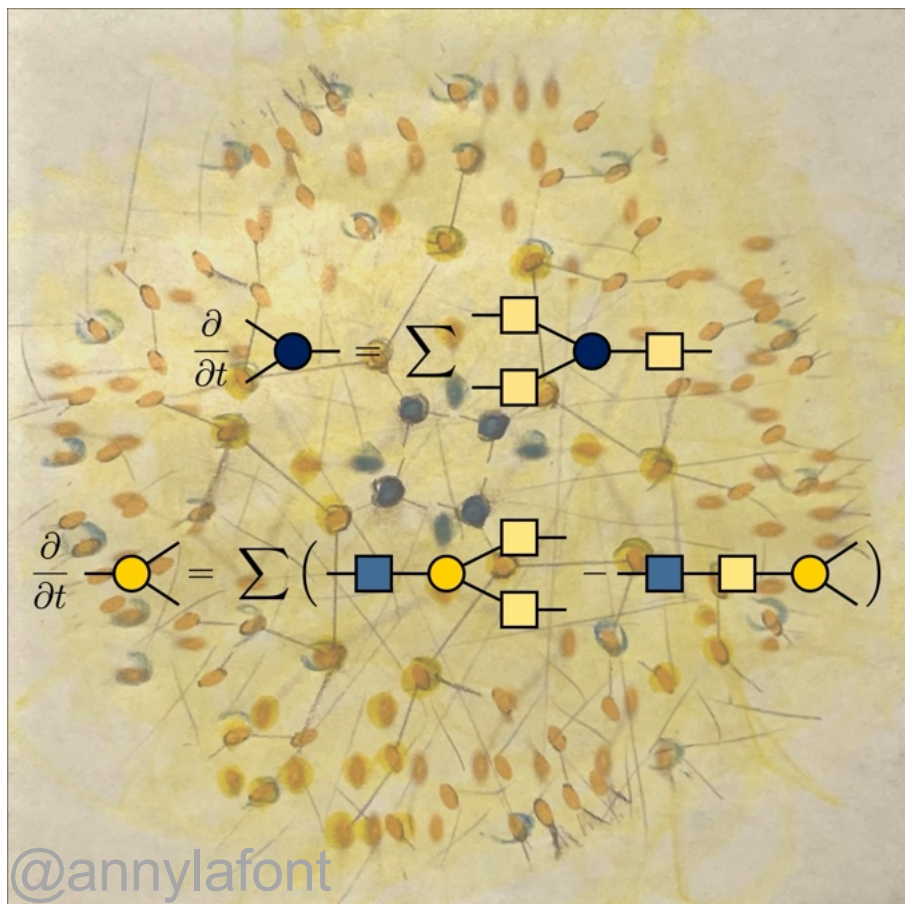


JCP **160**, 204116 (2024);
 JCP **163**, 104109 (2025);
 JCP **164**, 024112 (2026)

[arXiv:2603.17711](https://arxiv.org/abs/2603.17711)



Tree Tensor Network Decomposition of Open Quantum Dynamics for Efficient Simulation of Next-Generation Quantum Systems



Chen and IF J. Chem. Phys. **160**, 204116 (2024)

Chen and IF J. Chem. Phys. **163**, 104109 (2025)

Chen and IF J. Chem. Phys. **164**, 024112 (2026)

Rodriguez, Anderson, Niu, Chen, IF JCTC [arXiv:2603.17711](https://arxiv.org/abs/2603.17711)

Xinxian Chen

Michelle Anderson

Juan Camilo Rodriguez

Methods in Open Quantum Dynamics

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X. Zheng, J. Jin, S. Welack, M. Luo, and Y. Yan, The Journal of Chemical Physics 130, 164708 (2009).

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J. Hu, M. Luo, F. Jiang, R.-X. Xu, and Y. Yan, The Journal of Chemical Physics 134, 244106 (2011).

arXiv:1105.3230 [quant-ph] (2011).

Lindblad

QuAPI

HEOM

Redfield

Reaction Coordinate

Pseudo-mode



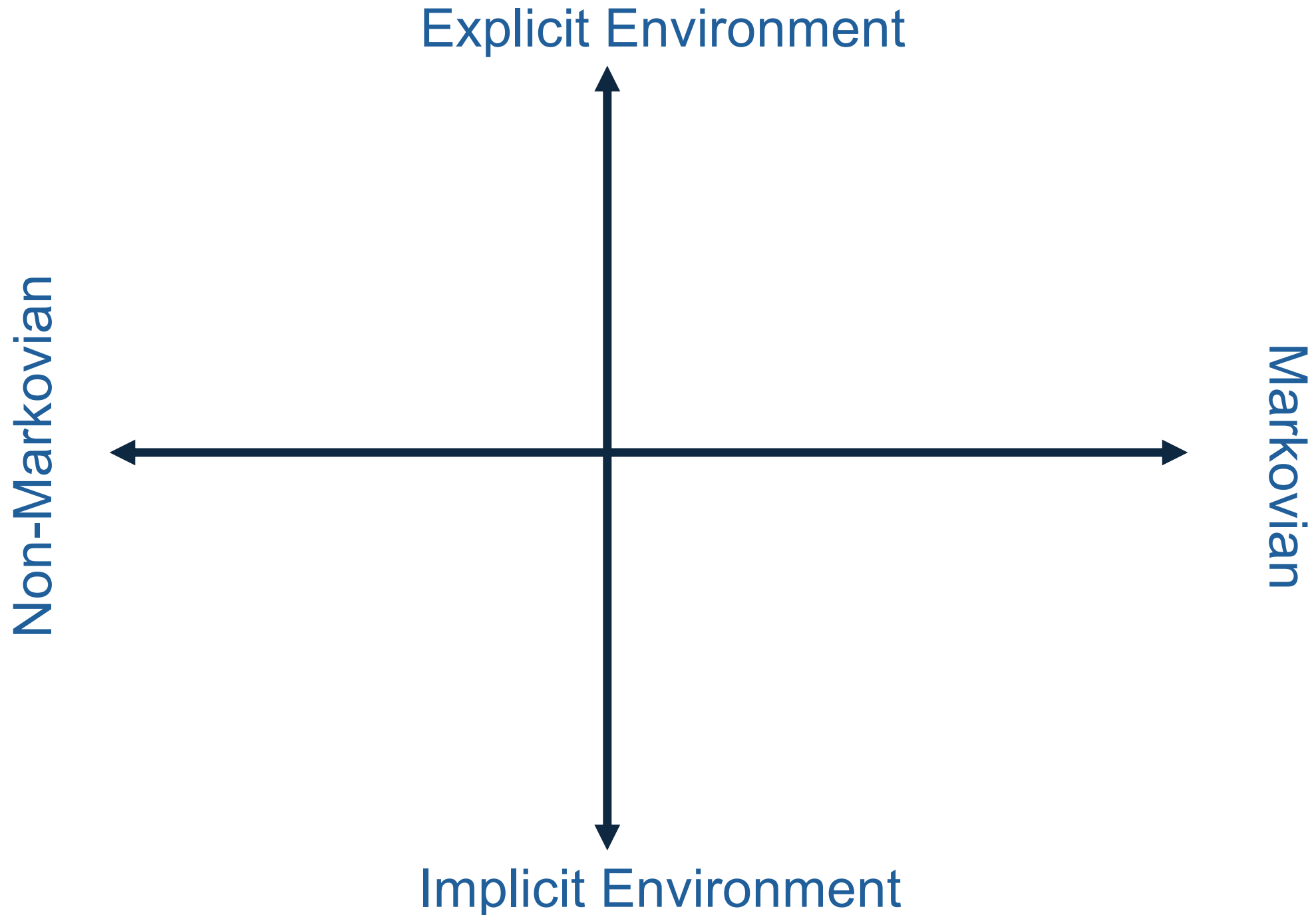
The Hierarchical Equation of Motion (HEOM)

- System agnostic
- Admits driven systems
- Numerically exact for harmonic environments
- Admits non-commuting system-bath interactions
- Goes beyond Lindblad/Redfield Markovian models
- Memory hungry
- Computational cost scales exponentially with size of system and complexity of the environment

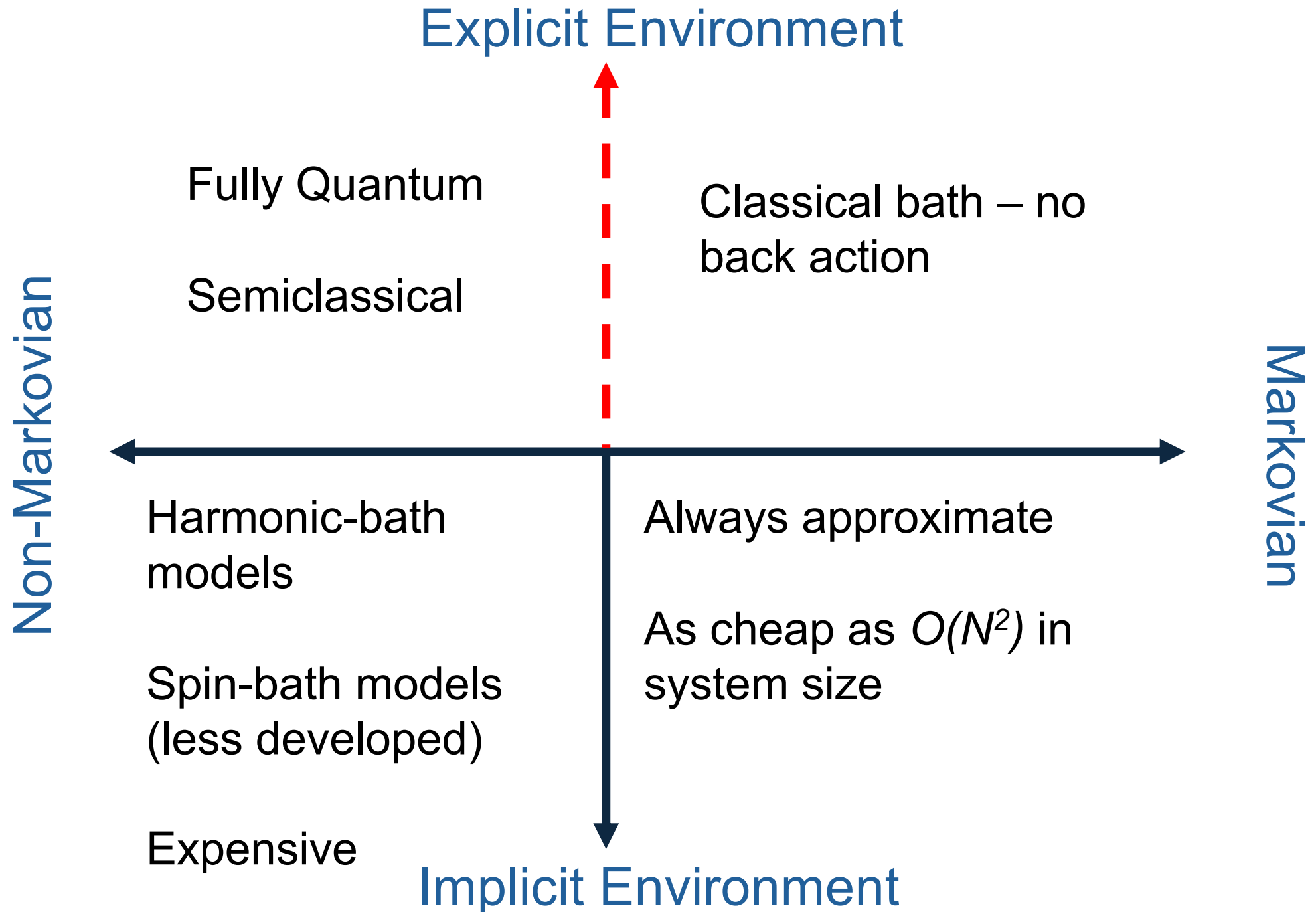
Ishizaki and Tanimura, JCP 125 084501 (2006)
Tanaka and Tanimura, JCP **132** 214502 (2010)
Tanimura JCP **141** 044114 (2014)
Ikeda and Scholes, JCP, **152**, 204101 (2020)
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Yan, Xu, Li, and Shi, JCP **154**, 194104 (2021)
Chen and Franco, JCP **160**, 204116 (2024)



How does the HEOM fits in Quantum Dynamics



How does the HEOM fits in Quantum Dynamics



How does the HEOM fits in Quantum Dynamics

Explicit Environment

MCTDH

Classical bath – no
back action

Surface hopping

ab initio multiple
spawning

HEOM

Redfield and Lindblad

Hierarchy of pure
states (HOPS)

TCL2 and other
perturbative methods

Quasi-adiabatic path
integral (QuAPI)

Implicit Environment

Non-Markovian

Markovian

Harmonic Environments

Useful model of the environment: Collection of harmonic oscillators

- Any environment can be mapped into an effective harmonic environment to second order in perturbation theory
- Dominant behavior in the thermodynamic limit
- The reason why the displaced harmonic oscillator model is so successful in spectroscopy

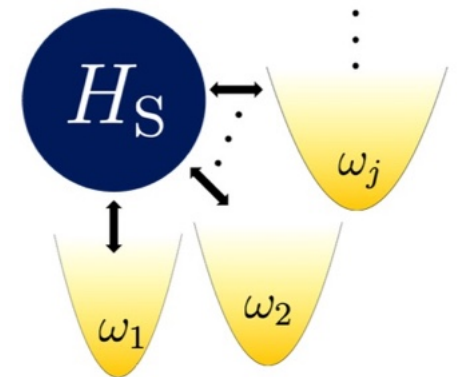
Hamiltonian

$$H = H_S + H_{SB} + H_B,$$

$$H_B = \sum_{j=1}^{\infty} \omega_j a_j^\dagger a_j$$

$$H_{SB} = Q_S \otimes X_B$$

$$X_B = \sum_{j=1}^{\infty} (g_j a_j^\dagger + g_j^* a_j)$$



Feynman and Vernon. Ann. Phys. 24 118–173 (1963)

Caldeira and Leggett. Ann. Phys. 149 374–456 (1983)

Suárez and Silbey, J Chem. Phys. 95, 9115 (1991)

Makri J. Phys. Chem. B 103, 2823-2829 (1999)

Dynamical Map for Harmonic Environments

Hamiltonian $H = H_S + H_{SB} + H_B,$

$$H_B = \sum_{j=1}^{\infty} \omega_j a_j^\dagger a_j \quad H_{SB} = Q_S \otimes X_B \quad X_B = \sum_{j=1}^{\infty} (g_j a_j^\dagger + g_j^* a_j)$$

Initially separable state $\rho(0) = \rho_S(0) \otimes \rho_B^{\text{eq}}$

Exact dynamical map in interaction picture

$$\tilde{\rho}_S(t) = \mathcal{T} \tilde{\mathcal{F}}(t, 0) \rho_S(0) \equiv \mathcal{T} \exp \left(- \int_0^t dt_2 \tilde{Q}_S^\times(t_2) \int_0^{t_2} dt_1 [\mathbf{C}(t_2 - t_1) \tilde{Q}_S(t_1)]^\times \right) \rho_S(0)$$

Notation $A^\times B = AB - BA^\dagger$

Correlation Function $C(t) = \langle X_B(t) X_B(0) \rangle_B.$

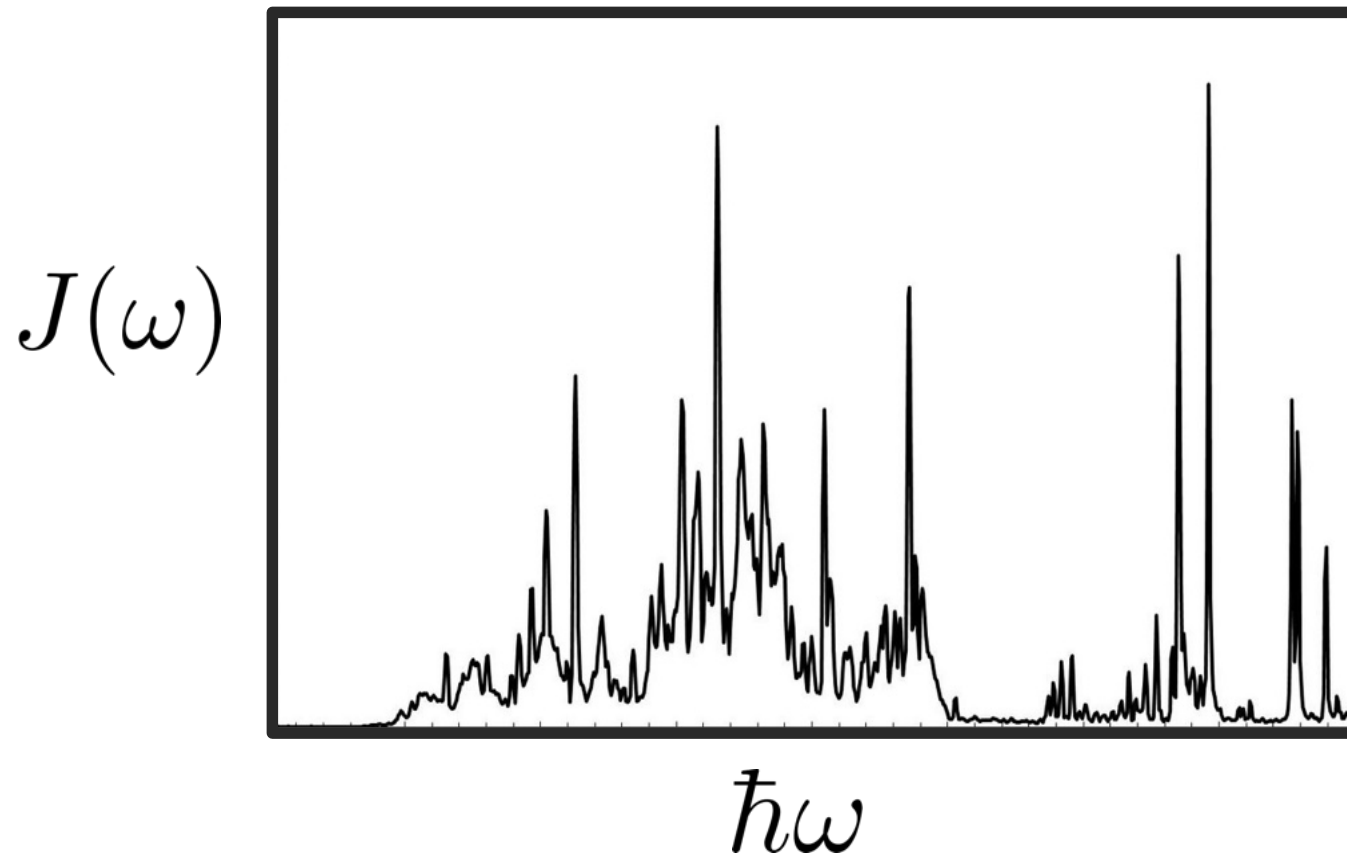
Spectral Density $C(t) = \int_{-\infty}^{\infty} \mathcal{J}(\omega) (1 + n_{\text{BE}}(\omega, T)) e^{-i\omega t} d\omega.$

$$J(\omega) = \sum_j |g_j|^2 \delta(\omega - \omega_j) \quad (\omega > 0)$$

$$\mathcal{J}(\omega) = J(\omega) - J(-\omega) \quad \text{odd extension}$$



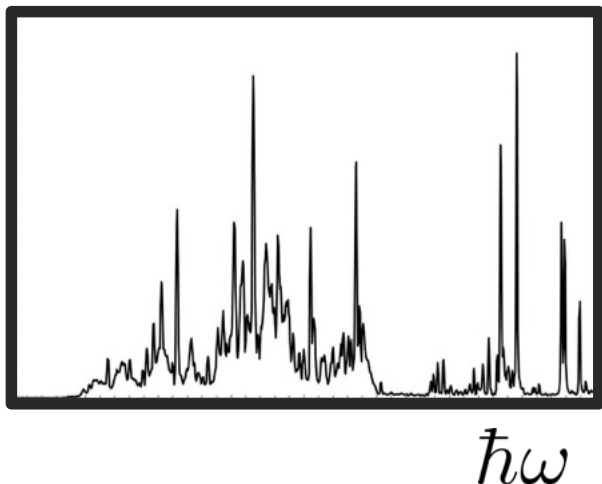
Spectral Density: characterizes system-bath interaction



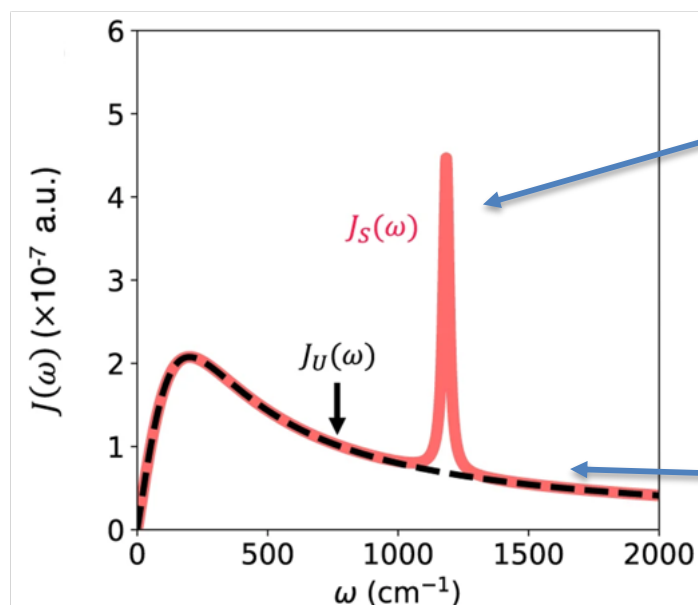
Summarizes frequencies of the bath and interaction strength with the system

Common Decomposition of the Spectral Density

$J(\omega)$



$$J(\omega) = \sum_{\alpha=0}^N J_{\alpha}(\omega)$$



$$J_{\alpha}(\omega) = \frac{2}{\pi} \lambda_{\alpha} \omega_{\alpha}^2 \frac{\omega \gamma_{\alpha}}{(\omega_{\alpha}^2 - \omega^2)^2 + \omega^2 \gamma_{\alpha}^2}$$

Brownian Oscillator: intramolecular vibrations

$$J_0(\omega) = \frac{2}{\pi} \lambda_0 \frac{\omega \Lambda}{\omega^2 + \Lambda^2}$$

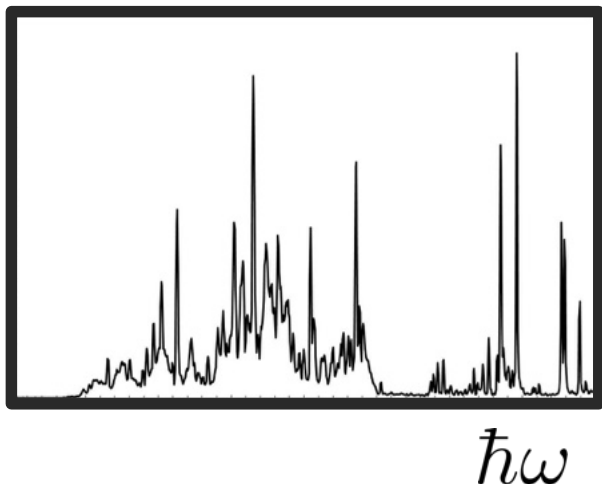
Drude-Lorentz: solvent

Other decompositions are possible



Common Decomposition of the Spectral Density

$J(\omega)$



$$J(\omega) = \sum_{\alpha=0}^N J_{\alpha}(\omega)$$

$$J_{\alpha}(\omega) = \frac{2}{\pi} \lambda_{\alpha} \omega_{\alpha}^2 \frac{\omega \gamma_{\alpha}}{(\omega_{\alpha}^2 - \omega^2)^2 + \omega^2 \gamma_{\alpha}^2}$$

Reorganization energy

Oscillator frequency

width

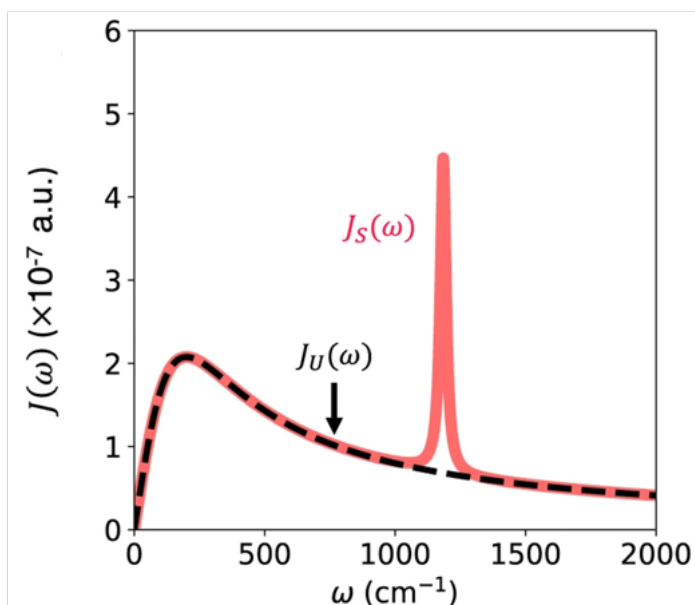
Brownian Oscillator: intramolecular vibrations

$$J_0(\omega) = \frac{2}{\pi} \lambda_0 \frac{\omega \Lambda}{\omega^2 + \Lambda^2}$$

Reorganization energy

Cutoff frequency

Drude-Lorentz: solvent



Other decompositions are possible



The HEOM way

Spectral Density

$$C(t) = \int_{-\infty}^{\infty} \mathcal{J}(\omega)(1 + n_{\text{BE}}(\omega, T))e^{-i\omega t}d\omega.$$

Decomposition the BCF into complex exponentials or features

$$C^*(t) = \sum_{k=1}^K \bar{c}_k e^{\gamma_k t}. \quad C(t) = \sum_{k=1}^K c_k e^{\gamma_k t}$$



The HEOM way

Spectral Density

$$C(t) = \int_{-\infty}^{\infty} \mathcal{J}(\omega)(1 + n_{\text{BE}}(\omega, T))e^{-i\omega t} d\omega.$$

Decomposition the BCF into complex exponentials or features

$$C^*(t) = \sum_{k=1}^K \bar{c}_k e^{\gamma_k t}, \quad C(t) = \sum_{k=1}^K c_k e^{\gamma_k t}$$

From residue theorem/Padé or Matsubara expansions

$$C(t) = -2\pi i \sum_i \text{Res}[\mathcal{J}(z)] f_{\text{BE}}(\beta \zeta_i) e^{-i\zeta_i t} - 2\pi i \sum_j \text{Res}[f_{\text{BE}}(z)] \mathcal{J}(\xi_j/\beta) e^{-i(\xi_j/\beta)t},$$

Complexity of the spectral density

Low temperature corrections

$\{\zeta_i\}$ First order poles of $\mathcal{J}(\omega)$ in the lower half
 $\{\xi_i/\beta\}$ $f_{\text{BE}}(\beta\omega) = (1 - e^{-\beta\omega})^{-1}$
complex plane (guarantees that $C(t) \rightarrow 0$ as $t \rightarrow \infty$)

Several available methods:

JCP 130, 164708 (2009)

JCP 133, 101106 (2010)

JCP 151, 024110 (2019)

JCP 152, 064107 (2020)

PRL 129, 230601 (2022)

JCP 160, 204105 (2024)



The HEOM way

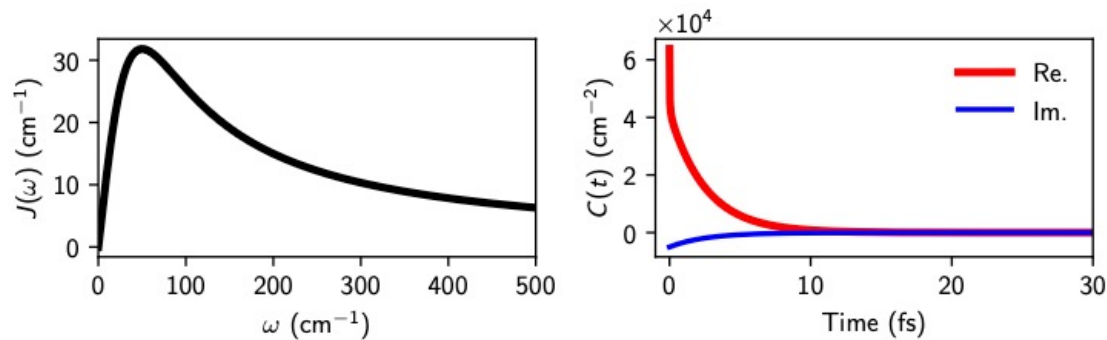
Spectral Density

$$C(t) = \int_{-\infty}^{\infty} \mathcal{J}(\omega)(1 + n_{\text{BE}}(\omega, T))e^{-i\omega t}d\omega.$$

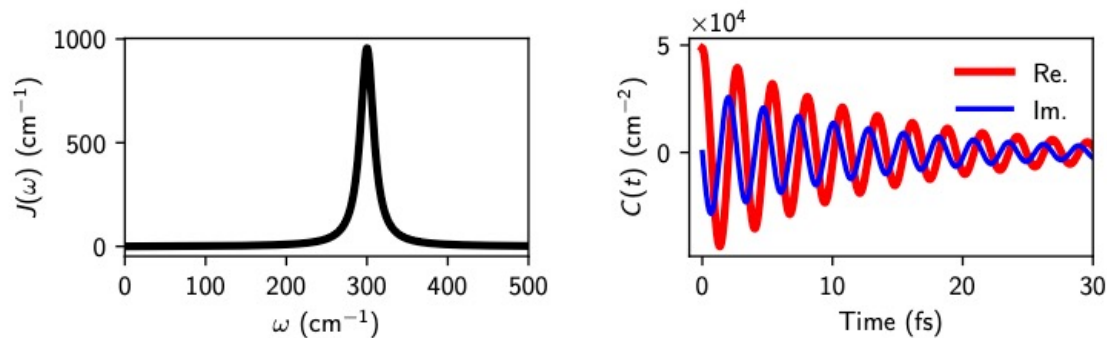
Decomposition the BCF into complex exponentials or features

$$C^*(t) = \sum_{k=1}^K \bar{c}_k e^{\gamma_k t}. \quad C(t) = \sum_{k=1}^K c_k e^{\gamma_k t}$$

- Solvent: Drude–Lorentz model



- Intramolecular vibrations: Brownian oscillators



The HEOM way

BCF decomposition

$$C^*(t) = \sum_{k=1}^K \bar{c}_k e^{\gamma_k t}.$$

$$C(t) = \sum_{k=1}^K c_k e^{\gamma_k t}$$

Common Cases

Drude-Lorentz

$$J(\omega) = \frac{2}{\pi} \frac{\lambda \omega \omega_c}{\omega_c^2 + \omega^2}$$

- leads to one decaying real exponential with characteristic rate ω_c (one feature)

Brownian

$$J(\omega) = \frac{4}{\pi} \lambda_b \omega_b^2 \frac{\omega \gamma_b}{(\omega^2 - \omega_b^2)^2 + 4\omega^2 \gamma_b^2}$$

- leads to two oscillatory decaying exponentials (two features)

Low temperature corrections

- Poles of thermal factor are purely imaginary

- Each leads to a decaying exponentials (one feature per correction)



The HEOM way

Decomposition the BCF into complex exponentials or features is exact

$$C^*(t) = \sum_{k=1}^K \bar{c}_k e^{\gamma_k t}, \quad C(t) = \sum_{k=1}^K c_k e^{\gamma_k t}$$

From residue theorem/Padé or Matsubara expansions

$$C(t) = -2\pi i \sum_i \operatorname{Res}_{z=\zeta_i} [\mathcal{J}(z)] f_{\text{BE}}(\beta \zeta_i) e^{-i\zeta_i t} - 2\pi i \sum_j \operatorname{Res}_{z=\xi_j} [f_{\text{BE}}(z)] \mathcal{J}(\xi_j/\beta) e^{-i(\xi_j/\beta)t},$$

Use this decomposition to decompose the dynamical map

Introduce auxiliary density matrix (ADM) to keep bath information

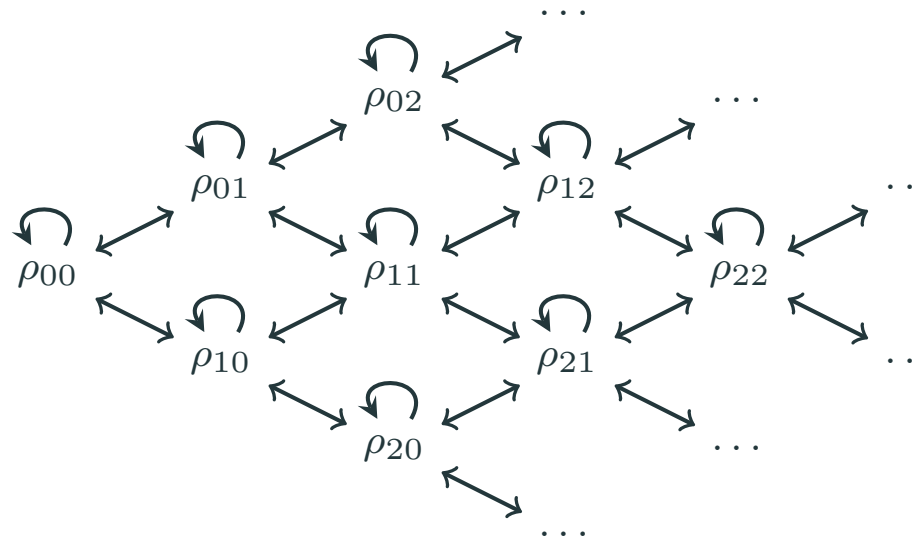
$$\rho_{\vec{n}} = \rho_{n_1, \dots, n_K} \quad n_k = 0, 1, 2, \dots, N$$

N is the depth of the HEOM



The HEOM way

$$\frac{\partial}{\partial t} \rho_{\vec{n}}(t) = -iH_S^\times + \sum_k \left(n_k \gamma_k \rho_{\vec{n}}(t) - i n_k (c_k q_S^> - \bar{c}_k q_S^<) \rho_{\vec{n}-\hat{1}_k}(t) - i q_S^\times \rho_{\vec{n}+\hat{1}_k}(t) \right)$$



Curse of dimensionality: The hierarchy generate an infinite K-dimensional grid

Tanimura and Kubo. J. Phys. Soc. Jpn. **58**, 101–114 (1989)

Tanimura. J. Chem. Phys. **153**, 020901 (2020)



Bexcitonic generalization of the HEOM

X. Chen and I. Franco, J. Chem. Phys. **160**, 204116 (2024)

Decomposition of the BCF into K features

$$C(t) = \sum_{k=1}^K c_k \psi_k(t) \quad C^*(t) = \sum_{k=1}^K \bar{c}_k \psi_k(t) \quad \frac{d}{dt} \psi_k(t) = \sum_{k'=1}^K \gamma_{kk'} \psi_{k'}(t)$$

$$\psi_k(0) = 1$$

$$\tilde{\rho}_S(t) = \mathcal{T} \tilde{\mathcal{F}}(t, 0) \rho_S(0) \equiv \mathcal{T} \exp \left(- \int_0^t dt_2 \tilde{Q}_S^\times(t_2) \int_0^{t_2} dt_1 [\mathbf{C}(t_2 - t_1) \tilde{Q}_S(t_1)]^\times \right) \rho_S(0)$$

Define Auxiliary Density Matrices (ADMs)

$$\tilde{\rho}_{\vec{n}}(t) \equiv \mathcal{T} \left(\prod_{k=1}^K \frac{\tilde{f}_k^{n_k}(t, 0)}{Z_k(n_k) \sqrt{n_k!}} \right) \tilde{\mathcal{F}}(t, 0) \rho_S(0) \quad \vec{n} \equiv (n_1, \dots, n_K)$$

$$\tilde{f}_k(t, 0) = c_k \tilde{\theta}_k^>(t, 0) - \bar{c}_k \tilde{\theta}_k^<(t, 0) \quad \tilde{\theta}_k(s, 0) = \int_0^s \tilde{Q}_S(u) \psi_k(s - u) du$$

Z_k is a non-zero c-number: metric



Bexcitonic generalization of the HEOM

X. Chen and I. Franco, J. Chem. Phys. **160**, 204116 (2024)

Put all the ADMs in a vector

$$|\Omega(t)\rangle \equiv \sum_{\vec{n}} \varrho_{\vec{n}}(t) |\vec{n}\rangle$$

$$|\vec{n}\rangle \equiv |n_1\rangle \otimes \cdots \otimes |n_k\rangle$$

Equations of motion

$$\frac{d}{dt} |\Omega(t)\rangle = \left(-iH_S^\times(t) + \sum_{k=1}^K \mathcal{D}_k \right) |\Omega(t)\rangle \quad |\Omega(0)\rangle = \rho_S(0) |0\rangle \otimes \cdots \otimes |0\rangle$$

$$\mathcal{D}_k = \gamma_{kk} \hat{n}_k + \sum_{k' \neq k} \gamma_{kk'} \hat{z}_k^{-1} \hat{\alpha}_k^\dagger \hat{\alpha}_{k'} \hat{z}_{k'} + (c_k Q_S^> - \bar{c}_k Q_S^<) \hat{z}_k^{-1} \hat{\alpha}_k^\dagger - Q_S^\times \hat{\alpha}_k \hat{z}_k$$

$$\hat{\alpha}_k^\dagger |n_k\rangle = \sqrt{n_k + 1} |n_k + 1\rangle \quad \hat{\alpha}_k |n_k\rangle = \sqrt{n_k} |n_k - 1\rangle$$

$$\hat{n}_k = \hat{\alpha}_k^\dagger \hat{\alpha}_k$$

$\hat{z}_k$ metric operator (needs to commute with n_k)

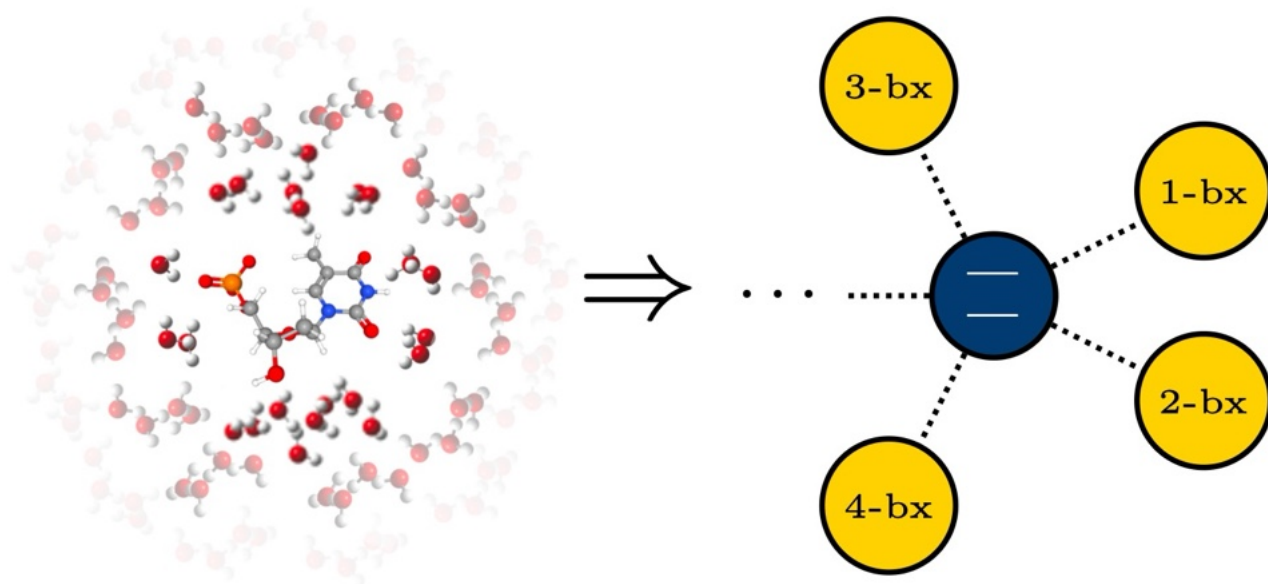
Bexciton
raising/lowering
operators

Varying BCF decomposition, metric, representation leads to various HEOM variants



Bexcitonic picture

X. Chen and I. Franco, J. Chem. Phys. **160**, 204116 (2024)



$$\frac{d}{dt}|\Omega(t)\rangle = \left(-iH_S^\times(t) + \sum_{k=1}^K \mathcal{D}_k \right) |\Omega(t)\rangle$$

$$\mathcal{D}_k = \gamma_{kk} \hat{n}_k + \sum_{k' \neq k} \gamma_{kk'} \hat{z}_k^{-1} \hat{\alpha}_k^\dagger \hat{\alpha}_{k'} \hat{z}_{k'} + (c_k Q_S^> - \bar{c}_k Q_S^<) \hat{z}_k^{-1} \hat{\alpha}_k^\dagger - Q_S^\times \hat{\alpha}_k \hat{z}_k$$

Open Quantum Dynamics = Dynamics of the System + Bexcitons
(fictitious bosonic quasiparticles)

Depth of HEOM N = Number of bexcitonic levels



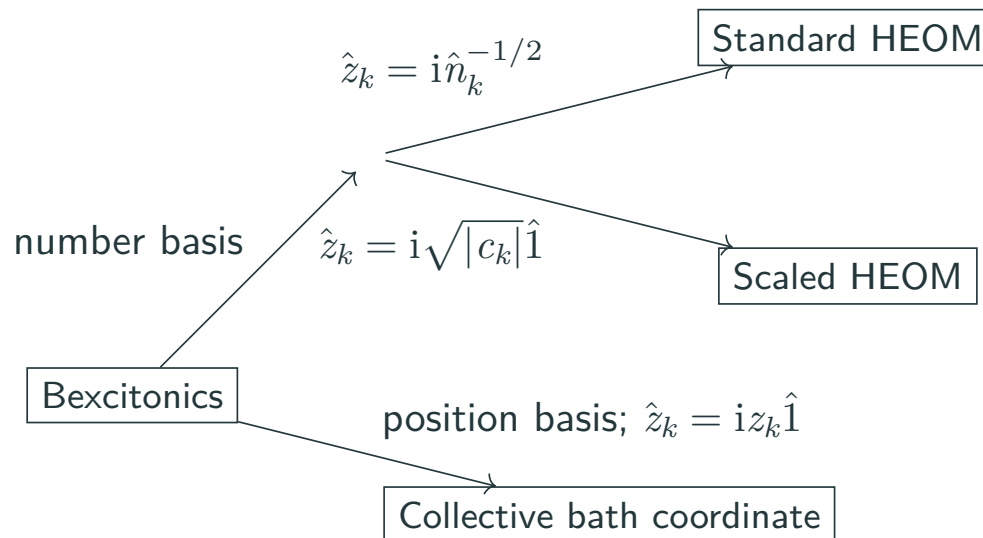
Develop many HEOM variants

$$\frac{d}{dt}|\Omega(t)\rangle = \left(-iH_S^\times(t) + \sum_{k=1}^K \mathcal{D}_k \right) |\Omega(t)\rangle$$

$$\mathcal{D}_k = \gamma_{kk} \hat{n}_k + \sum_{k' \neq k} \gamma_{kk'} \hat{z}_k^{-1} \hat{a}_k^\dagger \hat{a}_{k'} \hat{z}_{k'} + (c_k Q_S^> - \bar{c}_k Q_S^<) \hat{z}_k^{-1} \hat{a}_k^\dagger - Q_S^\times \hat{a}_k \hat{z}_k$$

Flexibility:

- Varying BCF decomposition
- Bexciton representation: position, momentum, number, etc
- Metric

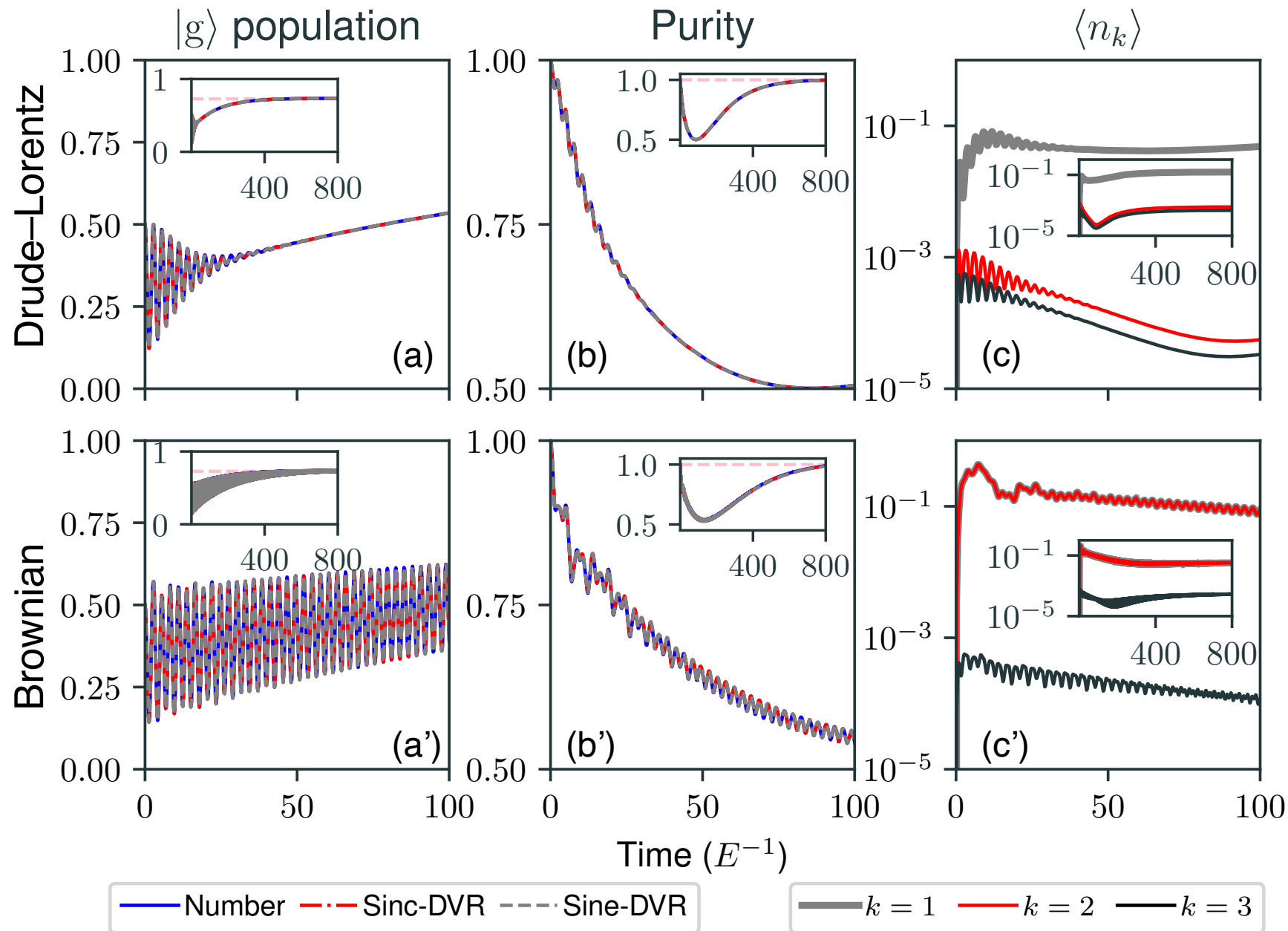


Q. Shi, et al., J. Chem. Phys. **130**, 84105 (2009)

T. Ikeda and A. Nakayama, J. Chem. Phys. **156**, 104104 (2022)



Anatomy of the Decoherence

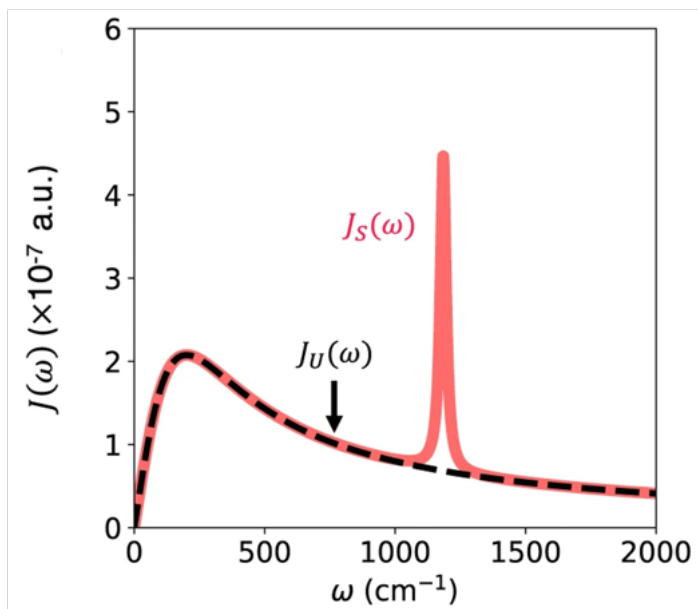


The curse of dimensionality in HEOM

Memory needs grow exponentially with number of features

$$\mathcal{O}(N^K)$$

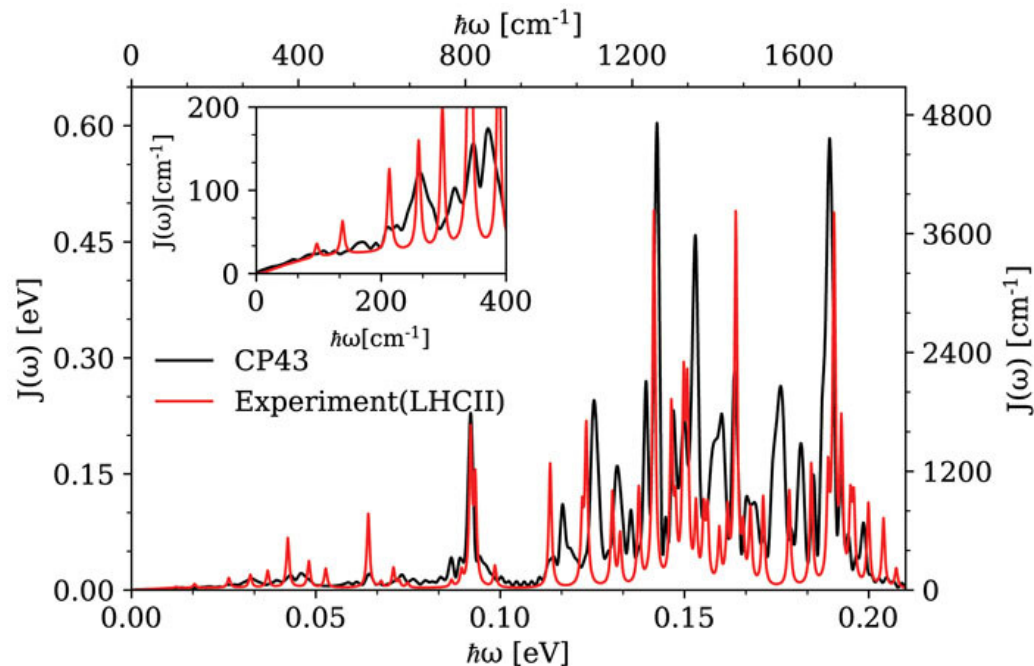
Model spectral density



L. P. Lindoy, et al., *Nat. Commun.* 14, 2733 (2023)

K : typically $1 \sim 5$.

Realistic spectral density



K : 10s to 100s.



Approaches to curb the curse of dimensionality

More efficient BCF decomposition schemes, e.g.

Dé, Jaouadi, Mangaud, Chin and Desouter-Lecomte,
JCP **160**, 244102 (2024)

Filter out near-zero ADMs

Q. Shi, L. Chen, G. Nan, R.-X. Xu, and Y. Yan,
JCP **130**, 084105 (2009)



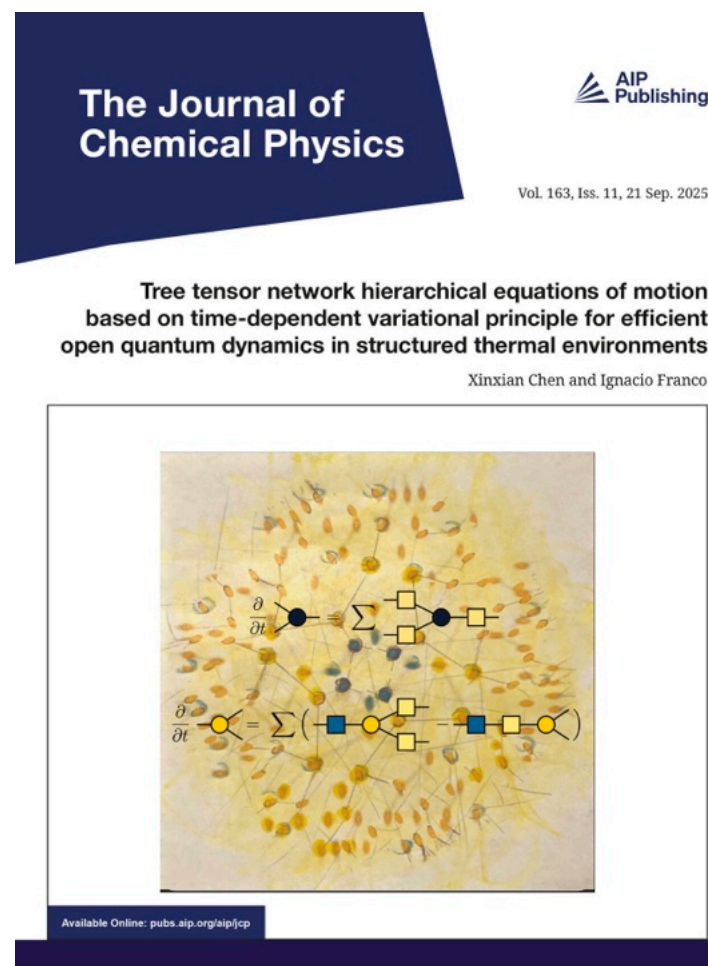
Tree Tensor Network HEOM and TENSO

Chen and Franco *J. Chem. Phys.* **163**, 104109 (2025)
Rodriguez, Anderson, Niu, Chen, IF [arXiv:2603.1771](https://arxiv.org/abs/2603.1771)

Editor's Pick!
Cover Article!

<https://github.com/ifgroup/pytenso>

- Enables HEOM computations with highly structured environments
- Implements tensor trains and tensor trees
- Three propagation strategies (Direct, PS1 and PS2)
- Fixed and variable rank propagation strategies
- Allows for time-dependent driving and non-commuting fluctuations
- Open-source code TENSO



Other HEOM Tensor Network Efforts

Tensor Train Y. Yan, M. Xu, T. Li, and Q. Shi, JCP **154**, 194104 (2021)

Tensor Tree Y. Ke, R. Borrelli, and M. Thoss, JCP **156**, 194102 (2022)

Y. Ke JCP **158**, 211102 (2023)

Fixed Rank + Propagator based on Trotter Splitting

No need for master equations for core tensors

Our Work Chen and Franco JCP **163**, 104109 (2025)

Tensor Trees + Trains

Master equation for core tensors

Arbitrary Tree Geometry

Arbitrary Order for Tensors

Fixed and Variable Rank

Three Propagation Strategies



Singular Value Decomposition (SVD)

$$A_{ij} = \sum_{k=1}^R U_{ik} s_k V_{jk}^*$$

$$U^\dagger U = V^\dagger V = \hat{1}$$

semi-unitary matrices

s_k : singular values ($s_1 \geq s_2 \geq s_K \geq 0$)

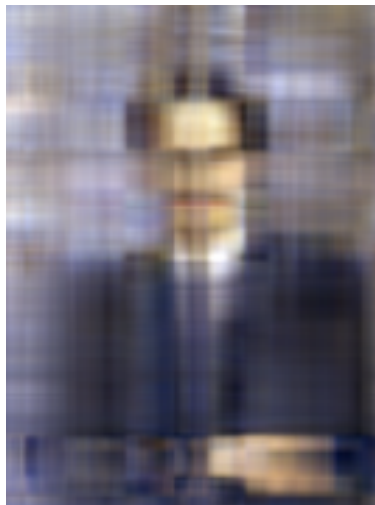
Keep the R largest singular values to compress redundant information in an array

R is called the “rank” or “bond dimension”

Raw ($R = 587$)



$R = 5$



$R = 10$



$R = 20$



$R = 50$

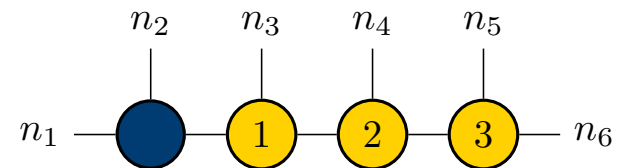


From SVD to Tree Tensor Network (TTN)

TTN: repeated SVDs of a high-order tensor

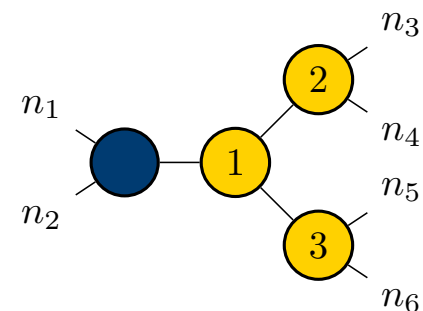
Tensor Train

$$A_{n_1 \dots n_6} = \sum_{a_1 a_2 a_3} C_{n_1 n_2 a_1} U_{a_2 n_3 a_1}^{(1)} U_{a_3 n_4 a_2}^{(2)} U_{n_5 n_6 a_3}^{(3)}.$$



Tensor Tree

$$A_{n_1 \dots n_6} = \sum_{a_1 a_2 a_3} C_{n_1 n_2 a_1} U_{a_2 a_3 a_1}^{(1)} U_{n_3 n_4 a_2}^{(2)} U_{n_5 n_6 a_3}^{(3)}$$



Root Tensor

Semi-Unitary Tensors

$$\sum_{\alpha\beta} U_{\alpha\beta\gamma}^* U_{\alpha\beta\gamma'} = \delta_{\gamma\gamma'}$$



TTN decomposition of the extended density operator

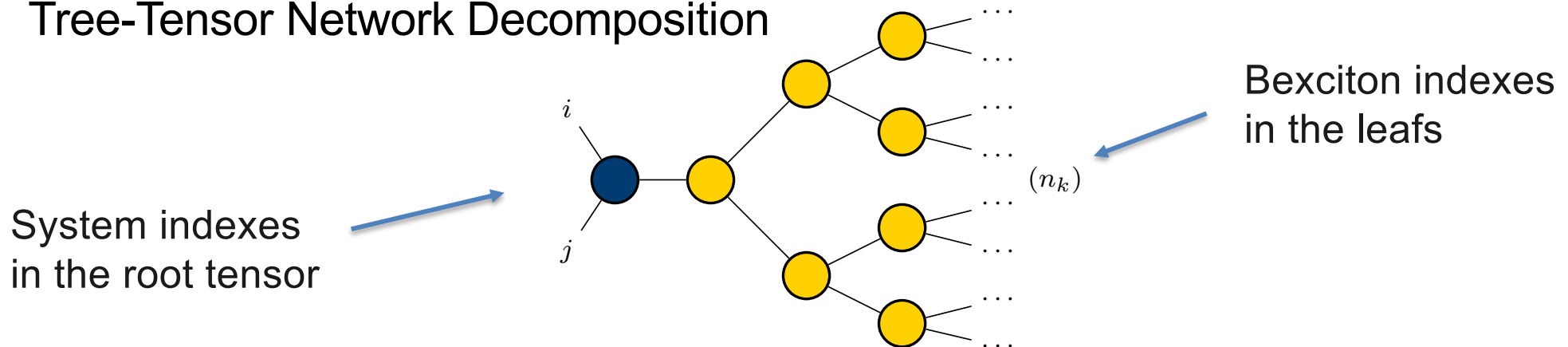
Hypothesis: There is significant redundancy in the bexcitonic space that can be compressed

Extended Density Operator $|\Omega(t)\rangle \equiv \sum_{\vec{n}} \varrho_{\vec{n}}(t) |\vec{n}\rangle$

Put all ADMs in a high-order tensor

$$\Omega_{ij n_1 \dots n_K} = (\rho_{\vec{n}})_{ij}$$

Tree-Tensor Network Decomposition



Polynomial space complexity with K (!)

$$\mathcal{O}((M^2 + N^2)R + KR^2N)$$



Sum of product form for the generator of the dynamics

$$\frac{d}{dt}\Omega(t) = \mathcal{L}(t)\Omega(t)$$

$$\mathcal{L}(t) = -iH_S^\times(t) + \sum_{k=1}^K \mathcal{D}_k = \sum_m h_m^>(t) \otimes h_m^<(t) \otimes h_m^{(1)} \otimes \dots \otimes h_m^{(K)}.$$

m	$h_m^>(t)$	$h_m^<(t)$	$h_m^{(k)}$
1	$-iH_S(t)$	$\hat{1}$	$\hat{1}$
2	$\hat{1}$	$iH_S(t)$	$\hat{1}$
$5k-2$	$\hat{1}$	$\hat{1}$	$\gamma_{kk}\hat{n}_k$
$5k-1$	$c_k Q_S$	$\hat{1}$	$\hat{z}_k^{-1} \hat{\alpha}_k^\dagger$
$5k$	$\hat{1}$	$-\bar{c}_k Q_S$	$\hat{z}_k^{-1} \hat{\alpha}_k^\dagger$
$5k+1$	$-Q_S$	$\hat{1}$	$\hat{\alpha}_k \hat{z}_k$
$5k+2$	$\hat{1}$	Q_S	$\hat{\alpha}_k \hat{z}_k$

Parallel to Multi-configurational time-dependent Hartree

H. Wang and M. Thoss, JCP **119**, 1289 (2003)



Master Equation for Core Tensors

Time Dependent Variational Principle

$$\sum_{ijn_1 \cdots n_K} [\delta\Omega(t)]_{ijn_1 \cdots n_K}^* \left[\left(\mathcal{L} - \frac{d}{dt} \right) \Omega(t) \right]_{ijn_1 \cdots n_K} = 0$$

Root Tensor – Simpler Dynamics

$$\left[\frac{\partial}{\partial t} \begin{array}{c} i \\ \bullet \\ j \end{array} \begin{array}{c} a_1 \end{array} \right] = \sum_m \begin{array}{c} i \text{---} \boxed{h_m^>} \\ j \text{---} \boxed{h_m^<} \end{array} \bullet \begin{array}{c} \boxed{f_m^{(1)}} \end{array} \begin{array}{c} a_1 \end{array}$$

$$\frac{\partial}{\partial t} A_{i'j'a'_1}^{(0)} = \sum_m \sum_{ija_1} [h_m^>]_{i'i} [h_m^<]_{j'j} [f_m^{(1)}]_{a'_1 a_1} A_{ija_1}^{(0)}$$

Non-Root Tensors – Requires Regularization

$$\frac{\partial}{\partial t} U_{a''_s \beta' \gamma'}^{(s)} = \sum_m \sum_{a'_s a_s \beta \gamma} [\mathcal{C}_m^{(s)}]_{a'_s a''_s} \left([f_m^{(\beta)}]_{\beta' \beta} [f_m^{(\gamma)}]_{\gamma' \gamma} U_{a'_s \beta \gamma}^{(s)} - U_{a_s \beta' \gamma'}^{(s)} [f_m^{(s)}]_{a_s a'_s} \right)$$

$$\left[\frac{\partial}{\partial t} \begin{array}{c} \beta \\ \bullet \\ \gamma \end{array} \begin{array}{c} a_s \end{array} \right] = \sum_m \left(\begin{array}{c} \beta \\ \bullet \\ \gamma \end{array} \begin{array}{c} \boxed{f_m^{(\beta)}} \\ \boxed{f_m^{(\gamma)}} \end{array} \begin{array}{c} a_s \text{---} \boxed{\mathcal{C}_m^{(s)}} \end{array} - \begin{array}{c} \beta \\ \bullet \\ \gamma \end{array} \begin{array}{c} \boxed{f_m^{(s)}} \end{array} \begin{array}{c} a_s \text{---} \boxed{\mathcal{C}_m^{(s)}} \end{array} \right)$$



Propagation Strategies

Adapt propagation strategies from MCTDH to the TTN-HEOM

Projector Splitting 1

- Trotterization algorithm. Errors determined by split time step
- Challenging to parallelize
- Fixed rank

Projector Splitting 2

- Similar features to PS1
- Two-site algorithm
- Adaptive rank

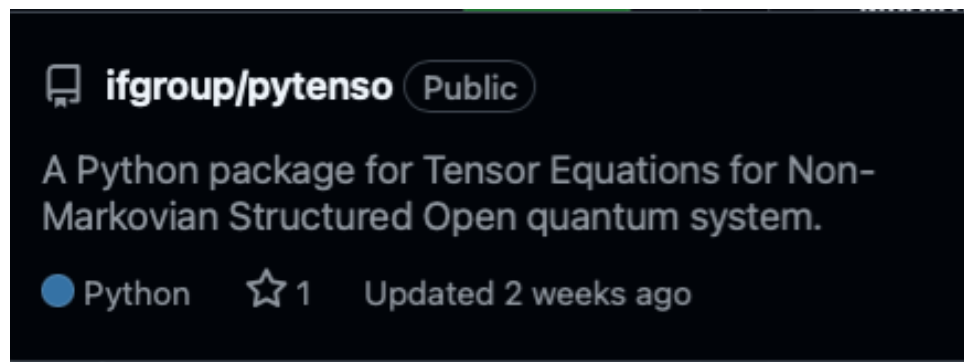
Direct Propagation of Master Equation for Core Tensors

- Admits high-order numerical propagation schemes (e.g. Runge-Kutta) and their parallelization
- Requires regularization like in MCTDH (specially at early times)
- Fixed rank



TENSO

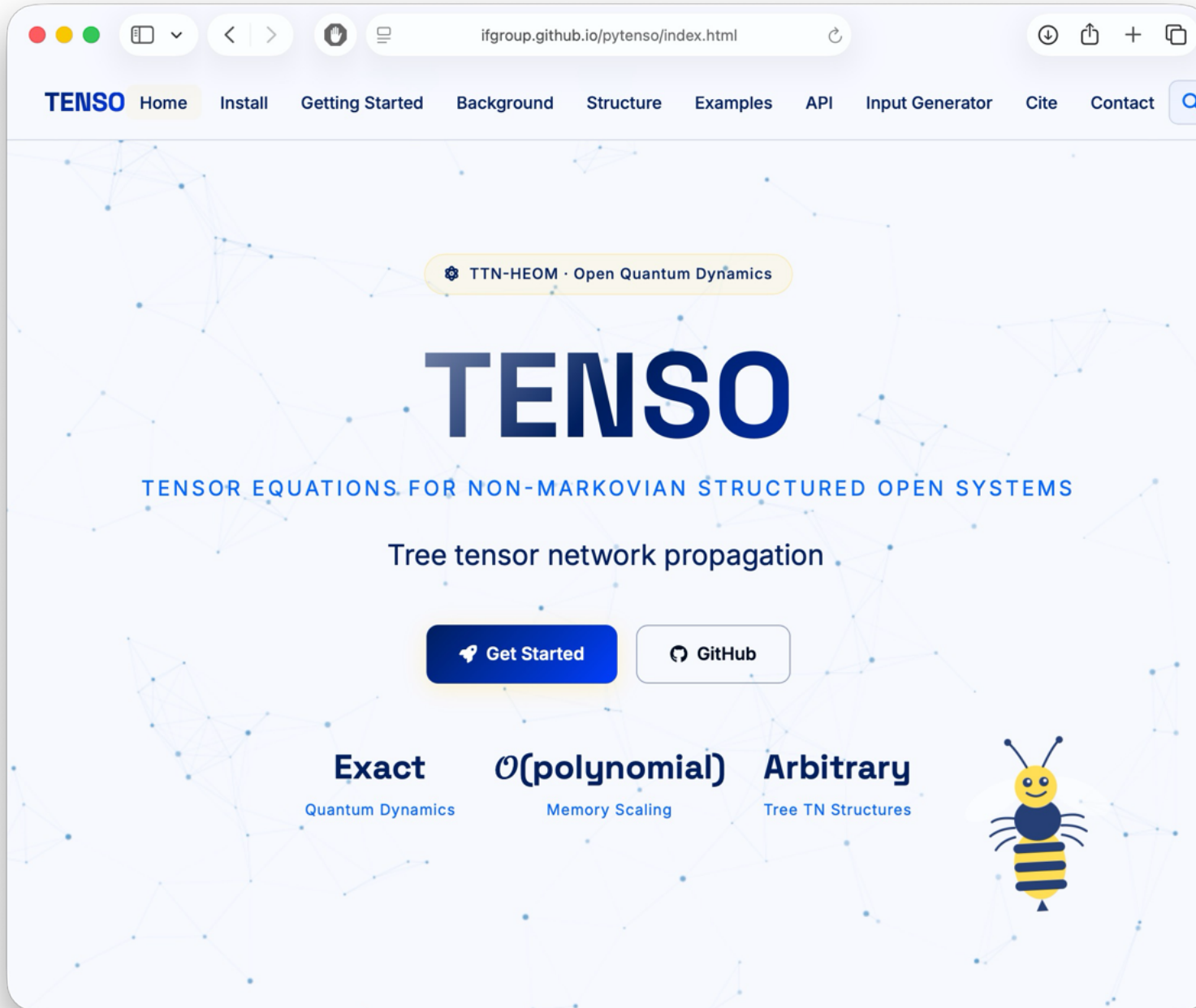
- Implemented in Python with NumPy and PyTorch
- Supports HEOM/ML-MCDTH/etc in a unified framework
- Supports direct integration, PS1, PS2 and mixed strategies for propagation
- Can handle structured baths for molecular systems
- Arbitrary tensor trees and tensor order
- User friendly, open source and available on GitHub



<https://github.com/ifgroup/pytenso>



TENSO



gies for



<https://github.com/ifgroup/pytenso>

TTN-HEOM vs HEOM

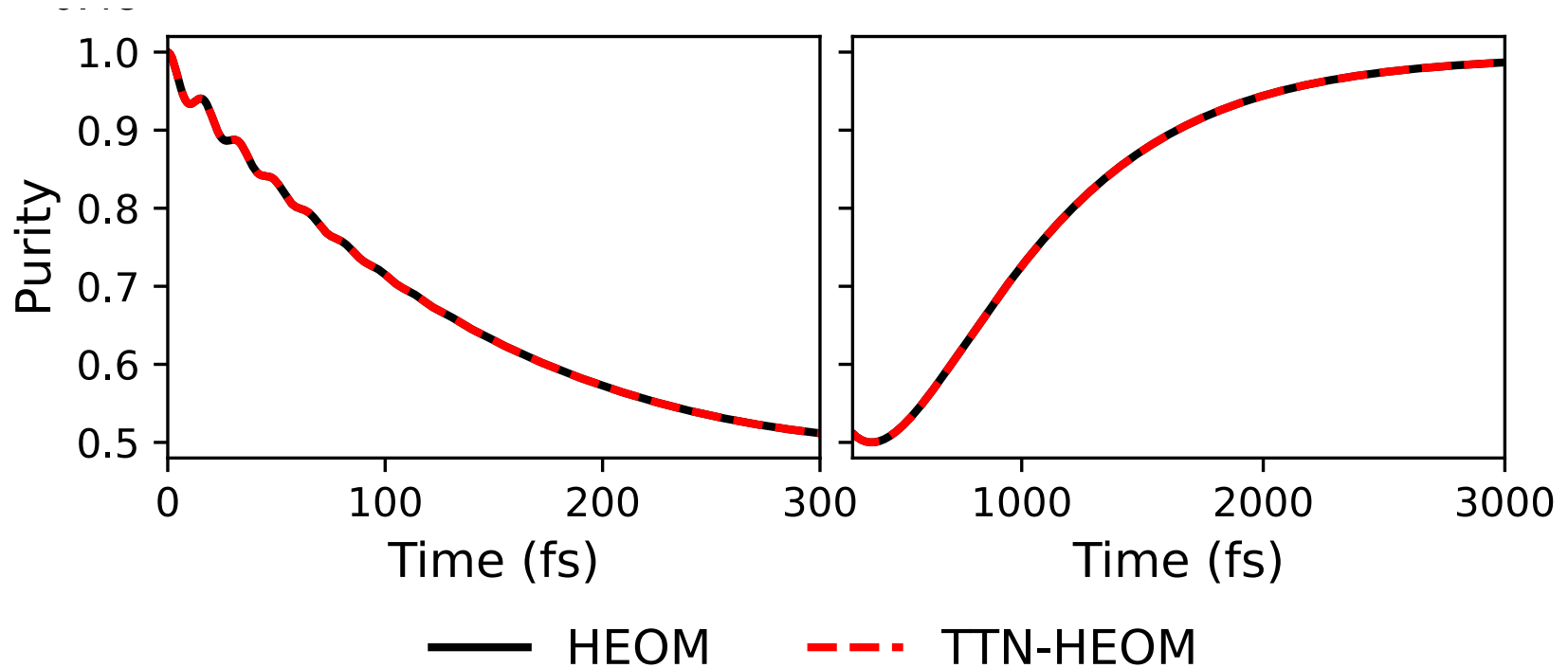
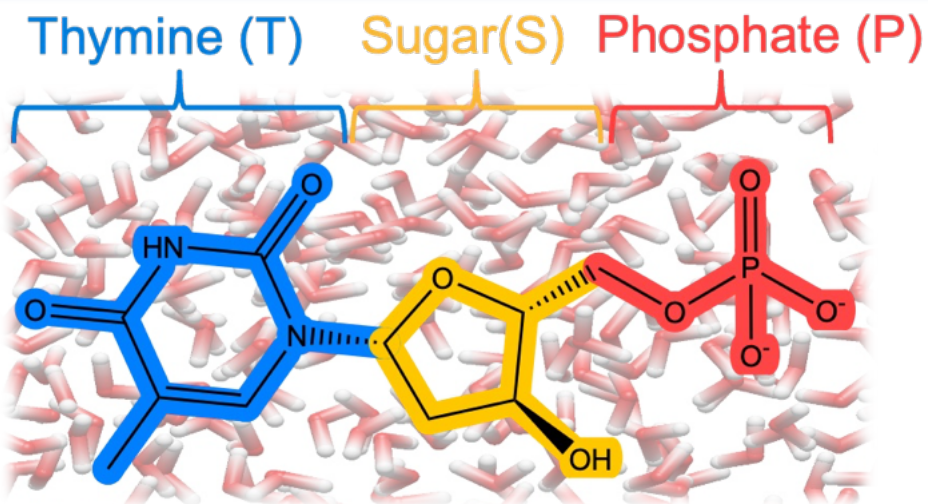
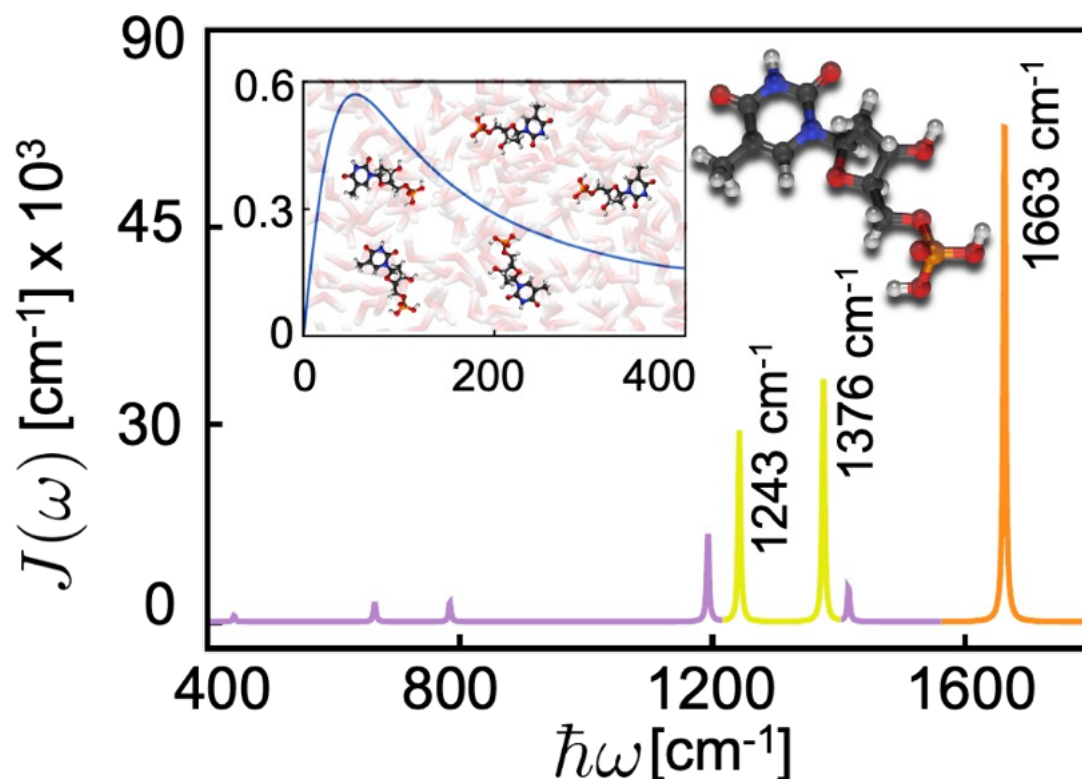


Figure 4.3 Comparison between the HEOM and the TTN-HEOM for a two-level system $\{|0\rangle, |1\rangle\}$ interacting with a Drude-Lorentz bath. The plots show the population and purity dynamics for the system $H_S = V\sigma_x$ with $V = 1000 \text{ cm}^{-1}$ coupled to a Drude-Lorentz bath with $\lambda_0 = 200 \text{ cm}^{-1}$ and $\gamma_0 = 100 \text{ cm}^{-1}$. The system operator Q_S is chosen as $\sigma_z/2$ such that $[H_S, H_{SB}] \neq 0$. The initial system is a pure one as $|\psi_S(t=0)\rangle = (|0\rangle + |1\rangle)/2$. As to the HEOM parameters, $N_k = 10$ is chosen for each bexciton to guarantee the convergence in depth, and the direct integration with a rank of 10 is used for TTN-HEOM.

Finally! Decoherence in realistic chemical systems



Spectral densities extracted from resonance Raman experiments



Example: Two-surface molecule

$$H_S = \frac{E}{2}\sigma_z + V\sigma_x \quad Q_S = \sigma_z \quad |\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

Spectral density for thymine in 300 K water

Bath Features $K = 20$

1 from Drude-Lorentz solvent

16 from Brownian Oscillators

3 from low temperature corrections (Padé)

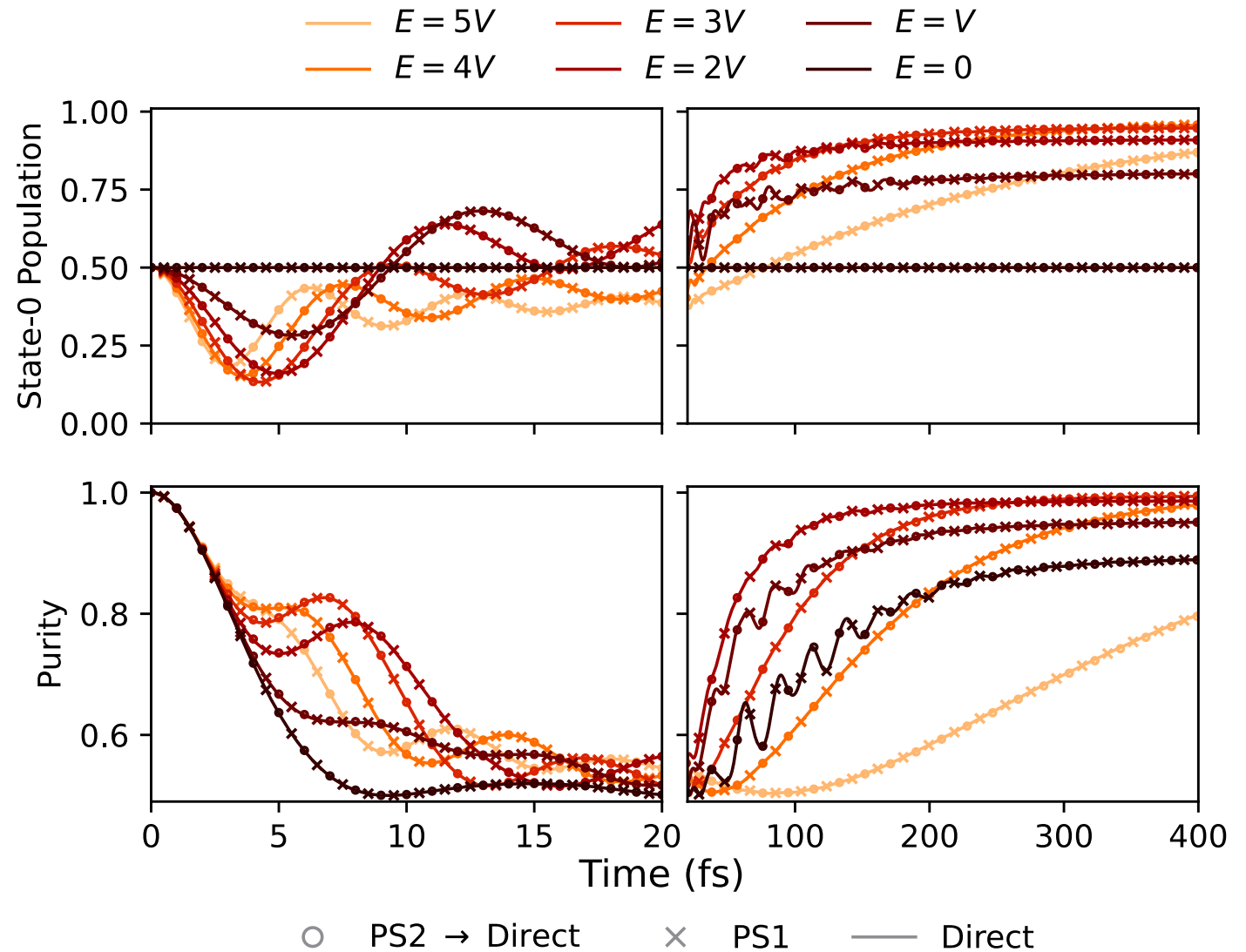
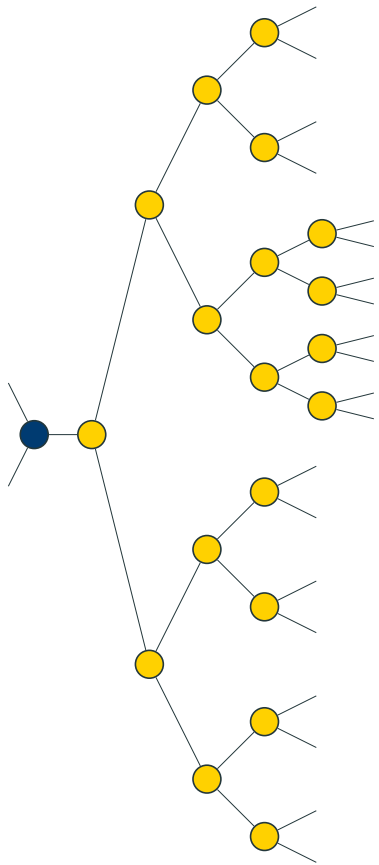
Impossible for other HEOM implementations

	Balanced Tree			Train			Dense HEOM
Rank	40	60	80	40	60	80	—
Size ($\times 10^6$)	0.7	2.2	4.9	0.6	1.3	2.3	4.2×10^{20}

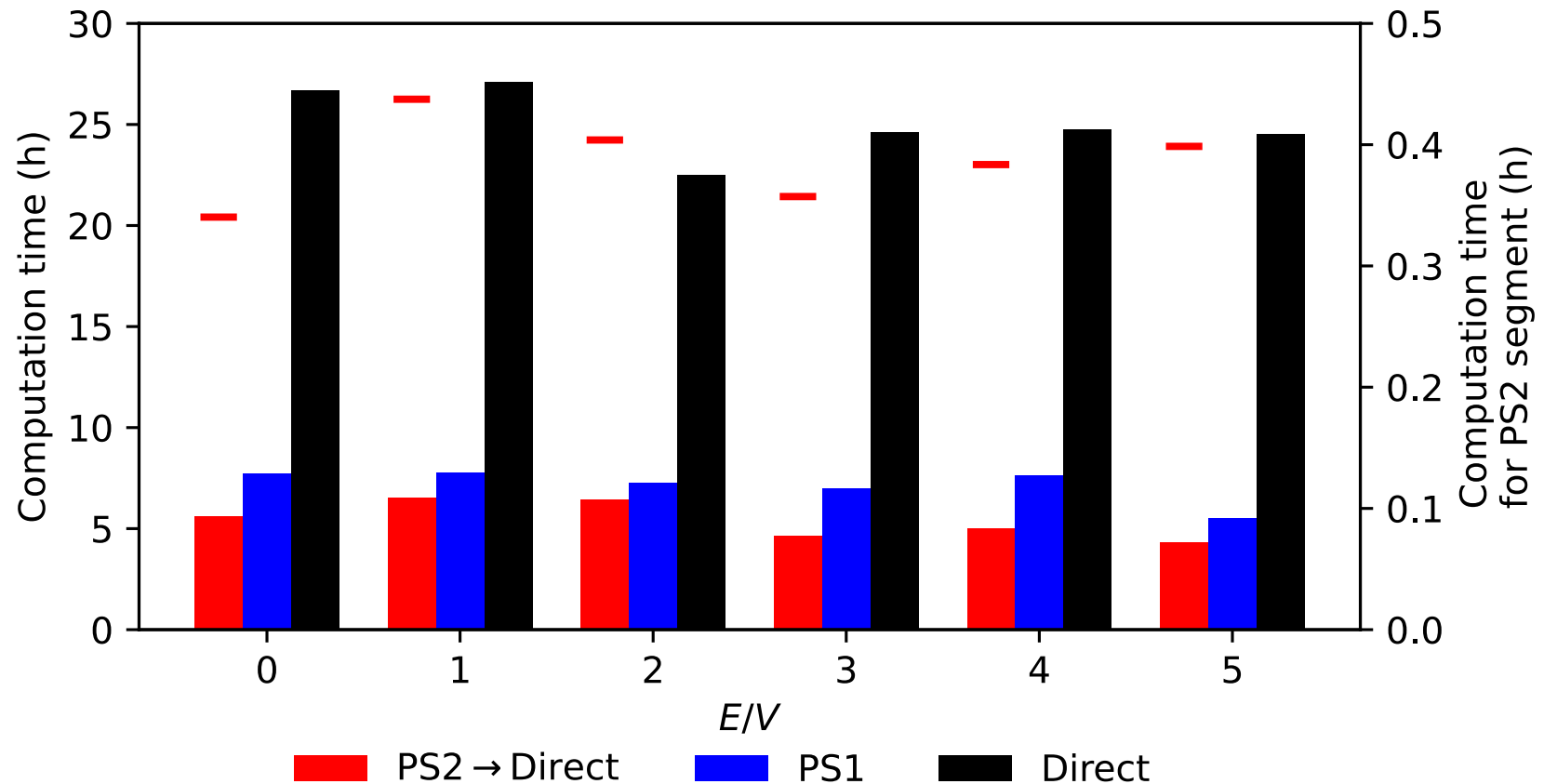
Table 4.2 The size (overall number of core tensor elements) of TTN for a bath described by 20 features and a depth of 20 for each N_k . The memory usage of a dense high-order EDO tensor in HEOM is also showed for comparison.



Consistency between propagation strategies



Performance differences

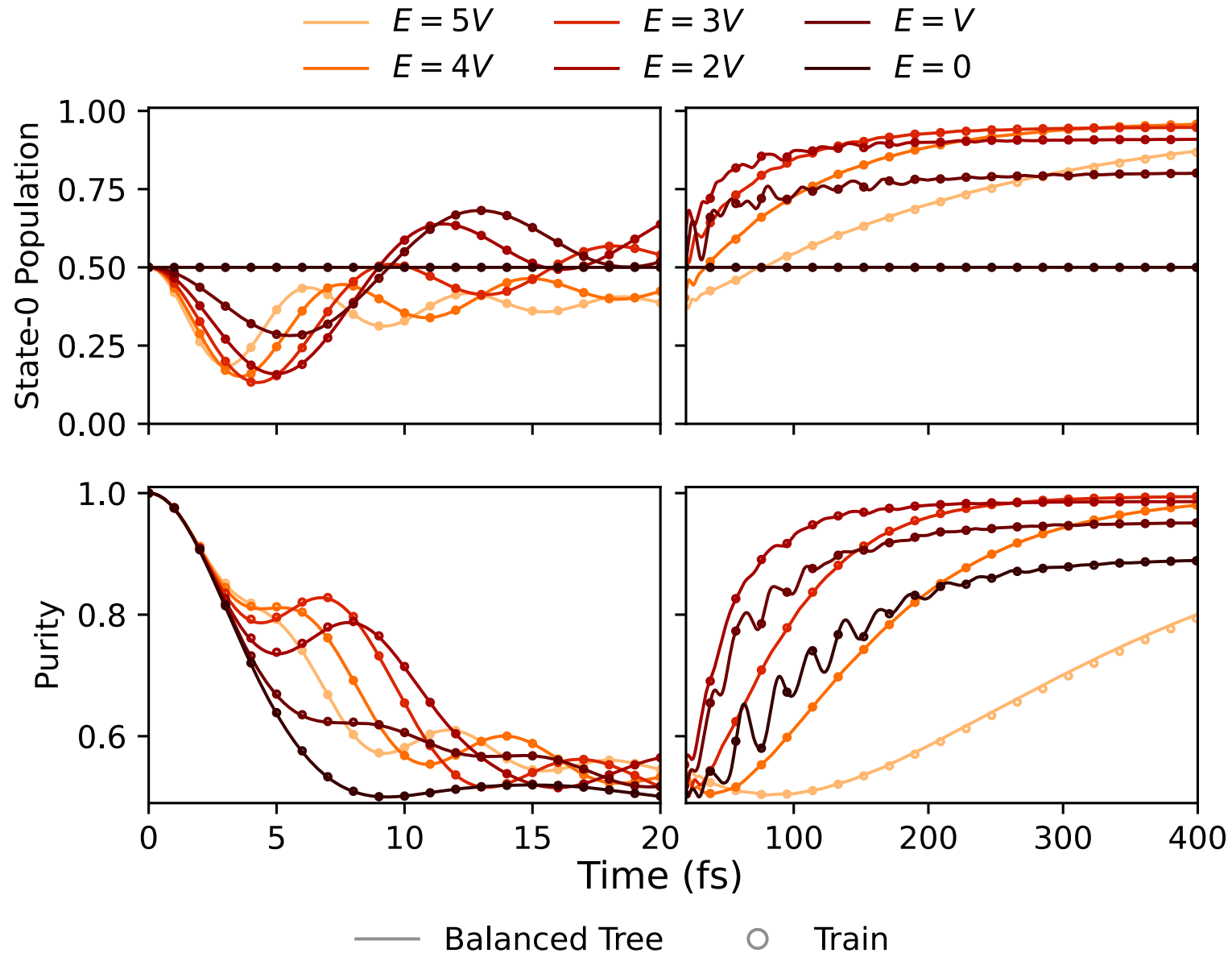


Mixed strategy (PS2 to Direct) is the fastest

PS2 determines the ranks from initial-time dynamics
Direct propagation is efficient (after very early times)



Trees vs. Trains



PS2 to Direct



TENSO Tutorial

Rodríguez, Anderson, Niu, Chen and Franco

<https://doi.org/10.48550/arXiv.2603.17711>

JCTC (in press)

<https://github.com/ifgroup/pytenso>

- Driven Qubits
- Non-Commuting Fluctuators
- FMO Complex
- Molecules in Cavities
- Entanglement Sudden Death
- Advanced Features



Tree Tensor Network HEOM and TENS0

Chen and Franco *J. Chem. Phys.* **163**, 104109 (2025)
Anderson, Rodriguez, Niu, Chen, IF [arXiv:2603.1771](https://arxiv.org/abs/2603.1771)

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- Implements tensor trains and tensor trees
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- Fixed and variable rank propagation strategies
- Allows for time-dependent driving and non-commuting fluctuations
- Open-source code TENS0
- **Awesome tool for molecular QIS research**



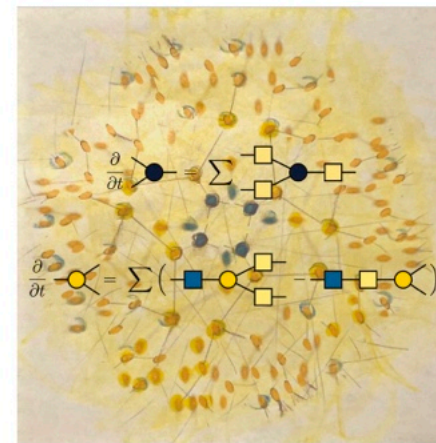
The Journal of
Chemical Physics

AIP
Publishing

Vol. 163, Iss. 11, 21 Sep. 2025

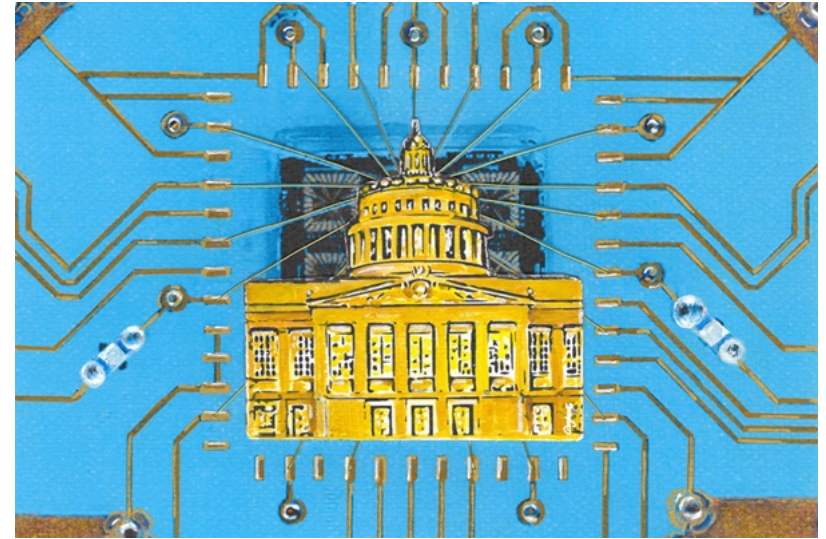
Tree tensor network hierarchical equations of motion
based on time-dependent variational principle for efficient
open quantum dynamics in structured thermal environments

Xinxian Chen and Ignacio Franco



Available Online: pubs.aip.org/aip/jcp

Thanks!



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