History is the best guide to the future

Propagating non-Markovian memory effects across spacetime with long-range tensor network models for open quantum systems

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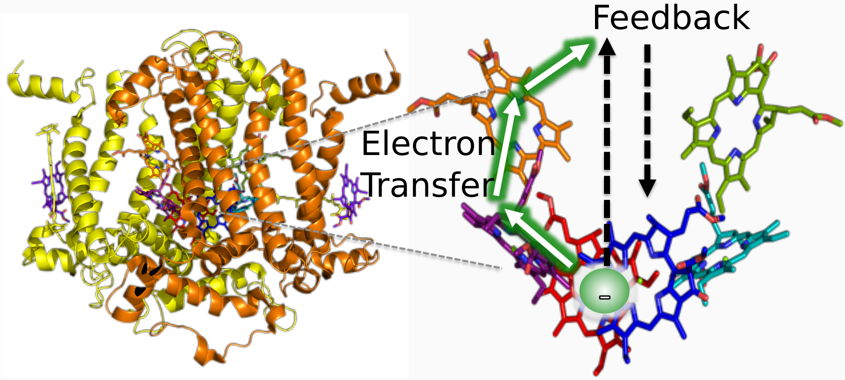
Biological Quantum Systems

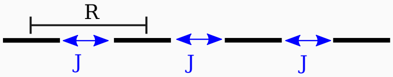


Light-Harvesting Complexes

Simplified Model

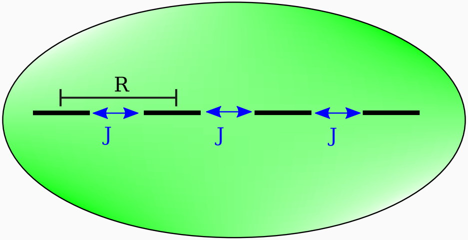
$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha \hat{P}_\alpha$$

Simplified Model



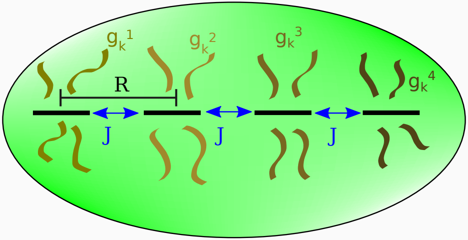
$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha \hat{P}_\alpha + \sum_{\alpha=1}^{N-1} J \left(|\alpha\rangle \langle \alpha + 1| + \text{h.c.} \right)$$

Simplified Model



$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha \hat{P}_\alpha + \sum_{\alpha=1}^{N-1} J \left(|\alpha\rangle \langle \alpha + 1| + \text{h.c.} \right)$$
$$+ \int_{-k_c}^{+k_c} \omega_k \hat{a}_k^\dagger \hat{a}_k \mathrm{d}k$$

Simplified Model



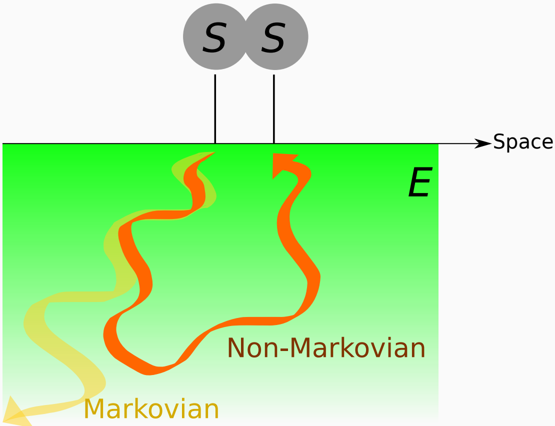
$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha \hat{P}_\alpha + \sum_{\alpha=1}^{N-1} J \left(|\alpha\rangle \langle \alpha + 1| + \text{h.c.} \right)$$

$$+ \int_{-k_c}^{+k_c} \omega_k \hat{a}_k^\dagger \hat{a}_k \mathrm{d}k + \sum_\alpha \hat{P}_\alpha \int_{-k_c}^{+k_c} (g_k \mathrm{e}^{\mathrm{i}kr_\alpha} \hat{a}_k + \text{h.c.}) \mathrm{d}k$$

Shared History Matters

Non-Markovian Environment

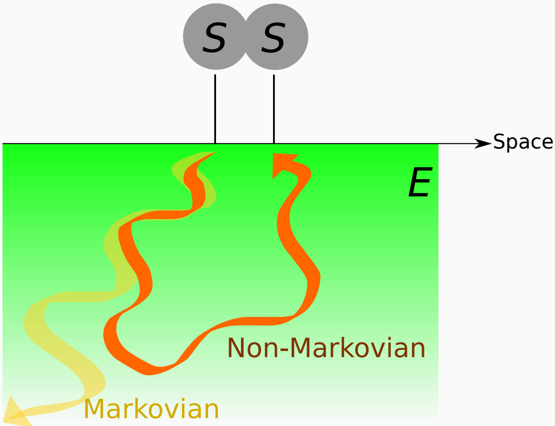
- $\tau_E \sim \tau_S$



Shared History Matters

Non-Markovian Environment

- $\tau_E \sim \tau_S$
- Strong Coupling



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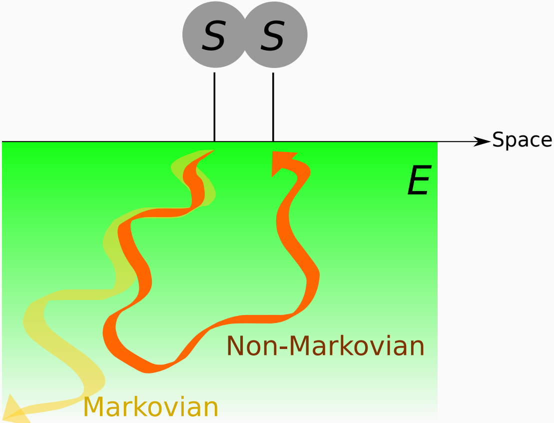
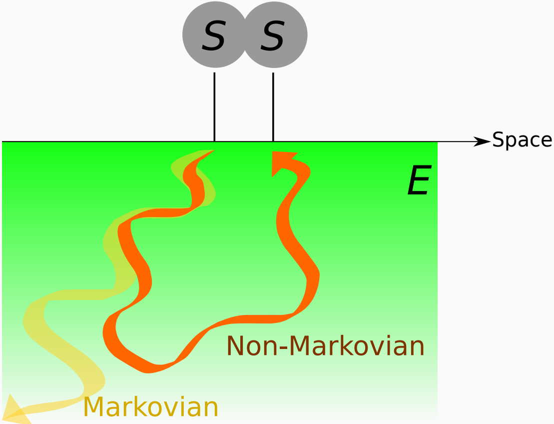
- Non time-local Master Equations



Shared History Matters

Non-Markovian Environment **is hard to study!**

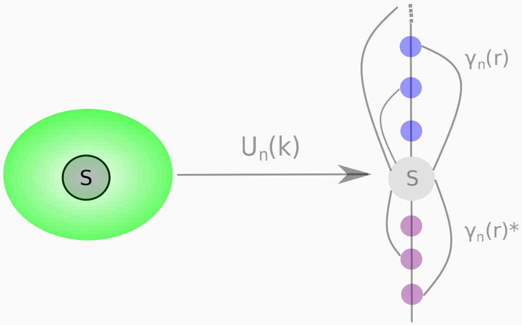
- $\tau_E \sim \tau_S$
- Strong Coupling
- Non time-local Master Equations



Methods

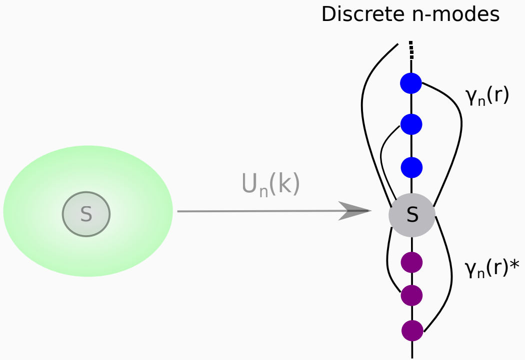
Environment-Chain Mapping

Continuous k-modes



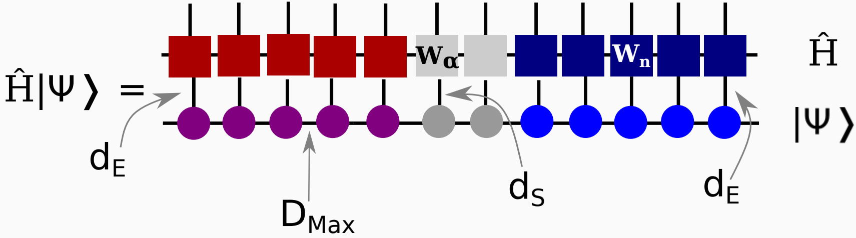
$$\hat{H}_B + \hat{H}_{\text{int}} = \int_{-k_c}^{+k_c} \omega_k \hat{a}_k^\dagger \hat{a}_k \mathrm{d}k + \sum_\alpha \hat{P}_\alpha \int_{-k_c}^{+k_c} (g_k \mathrm{e}^{\mathrm{i}kr_\alpha} \hat{a}_k + \text{h.c.}) \mathrm{d}k$$

Environment-Chain Mapping



$$\hat{H}_B + \hat{H}_{\text{int}} = \sum_n \omega_n(\hat{c}_n^\dagger \hat{c}_n + \hat{d}_n^\dagger \hat{d}_n) + t_n(\hat{c}_n^\dagger \hat{c}_{n+1} + \hat{d}_n^\dagger \hat{d}_{n+1} + \text{h.c.})$$
$$+ \sum_\alpha \hat{P}_\alpha \sum_n \left(\gamma_n(r_\alpha)(\hat{c}_n + \hat{d}_n^\dagger) + \text{h.c.} \right)$$

Tensor Networks

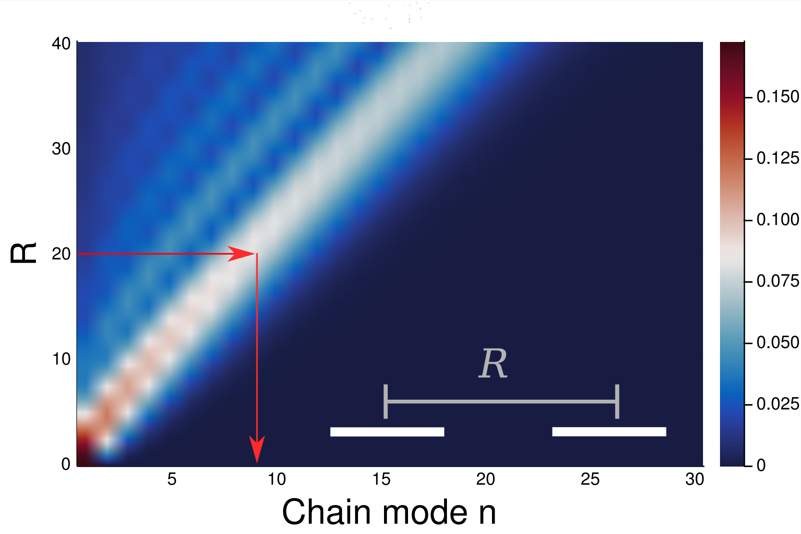


$$|\psi\rangle = \sum_{\{i_k\}} \sum_{\{\alpha\}} T^{\alpha_1}_{i_1} T^{\alpha_1\ \ \alpha_2}_{i_2} T^{\alpha_2\ \ \alpha_3}_{i_3} \dots T^{\alpha_{N-1}}_{i_N} |\phi_{i_1} \dots \phi_{i_N}\rangle$$

$$\hat{H} = \sum_{\{\sigma\},\{\sigma'\},\{w\}} W_{1\ \ w_1}^{\sigma_1\sigma_1'} W_{2\ \ w_1 w_2}^{\sigma_2\sigma_2'} \dots W_{N\ \ w_{N-1}}^{\sigma_N\sigma_N'} |\sigma_1 \dots \sigma_N\rangle \langle\sigma_1' \dots \sigma_N'| \ .$$

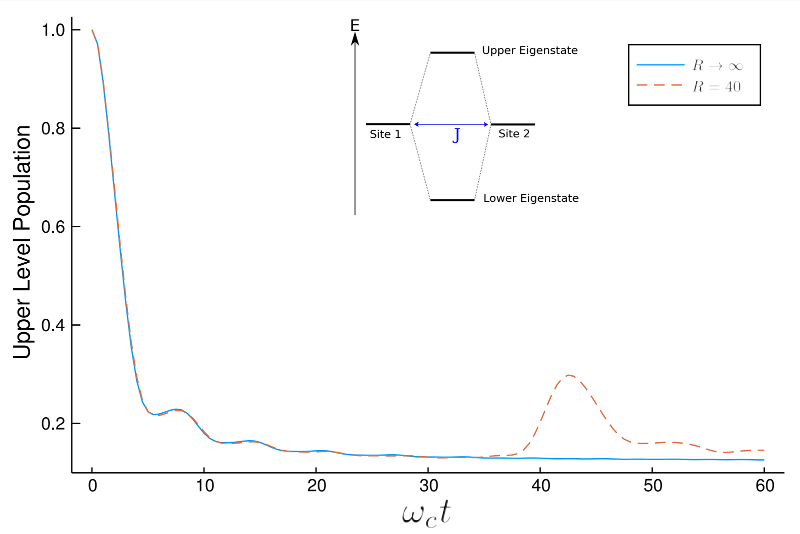
Results

Couplings $\gamma_n(R)$ at Zero Temperature



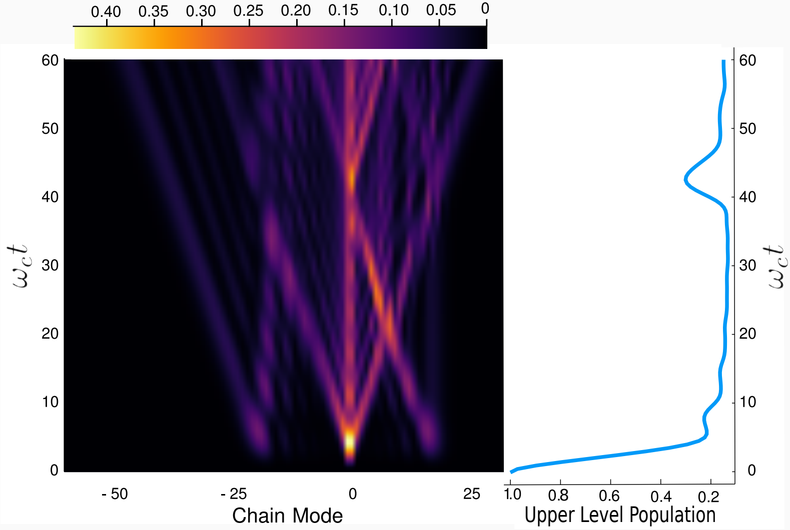
Ohmic spectral density: $J(k) = 2\alpha k H(k_c - k)$

Non-Markovian Revivals



Lacroix et al., Phys. Rev. A, 104(5), 052204 (2021)

Environment Feedback



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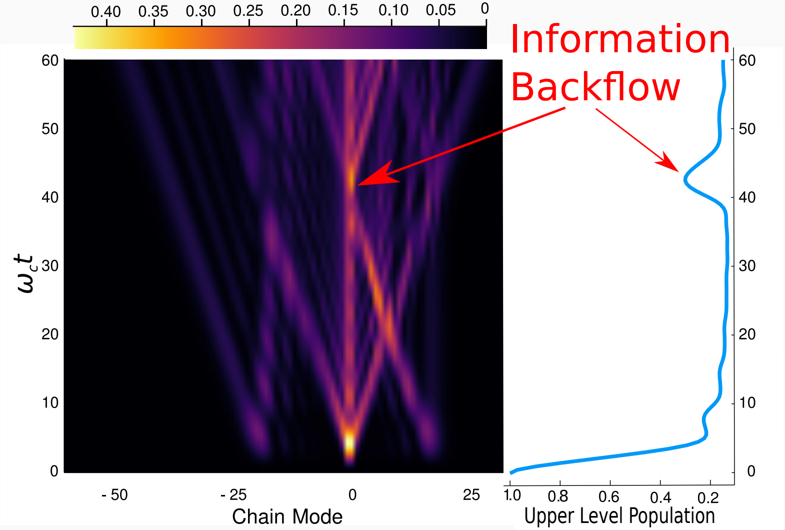
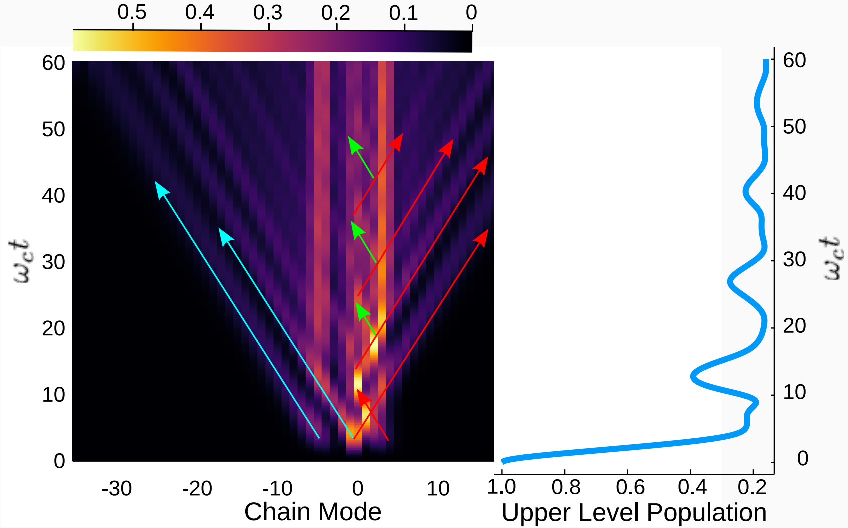
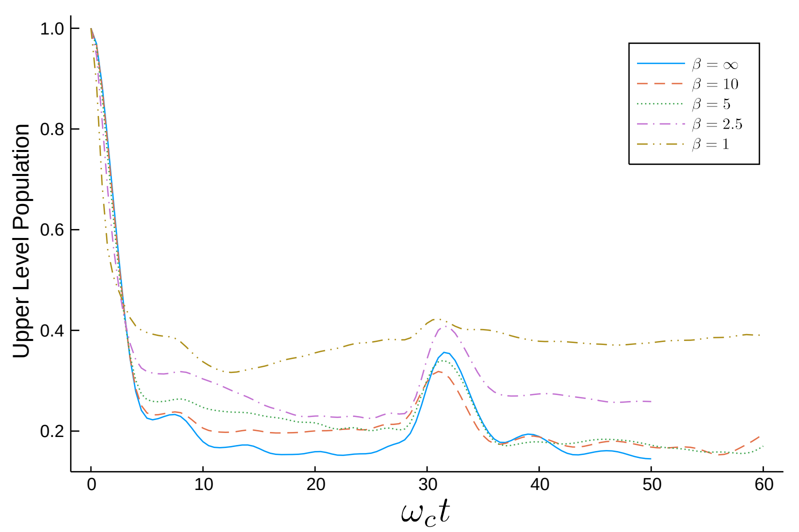


Environment Feedback II



Finite Temperature



Conclusion

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Take Away

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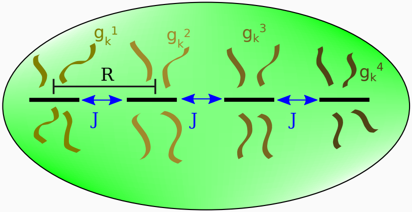
- Spatially extended system in a common environment



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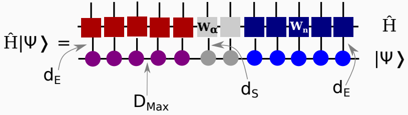
- MPS/MPO representation of $\{\text{System} + \text{Environment}\}$



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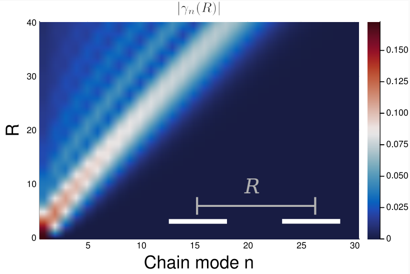

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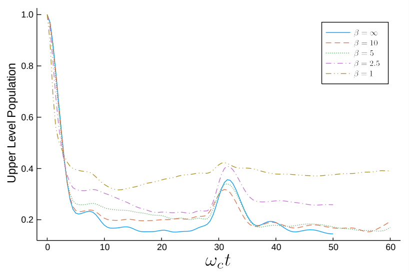

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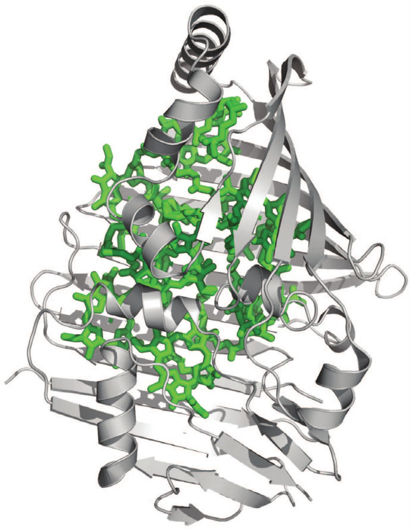
Stay Tuned!



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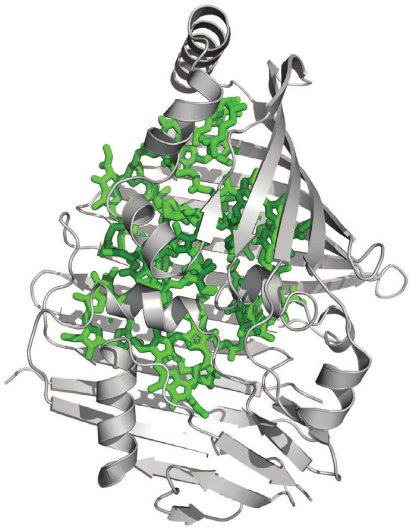
⚠ Multi-sites dynamics & different topologies



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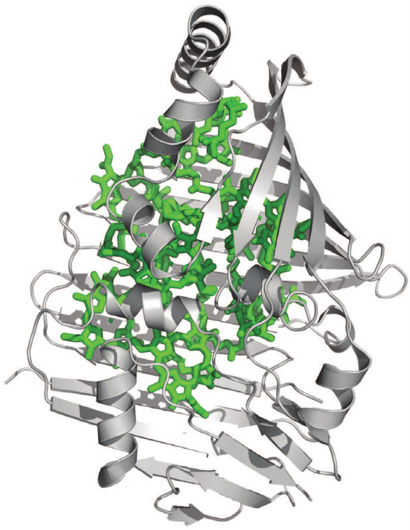
Stay Tuned!

- ⚠ Multi-sites dynamics & different topologies
- ⚠ Allostery & other biological processes



Conclusion

Thank you for your attention!

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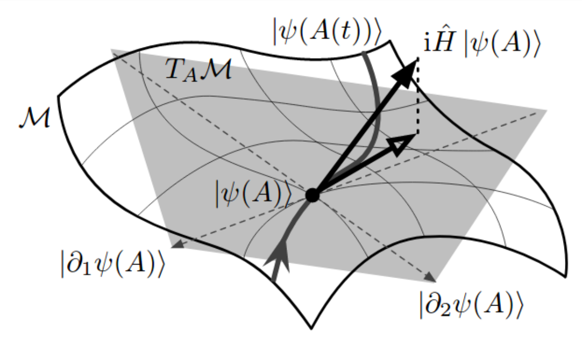
SCAN ME

Lacroix et al., Phys. Rev. A, 104(5), 052204 (2021)

You want to know more?

Time-Dependent Variational Principle

$$\frac{\partial}{\partial t} |\psi\rangle = -\mathrm{i}\hat{P}_{T_{|\psi\rangle}} \hat{H} |\psi\rangle$$



Haegeman et al., Phys. Rev. Lett. 107(7), 070601 (2011)

Dunnet, *MPSDynamics.jl*, `github.com/angusdunnett/MPSDynamics/`

Matrix Product Operator I

The matrices W_k define the Hamiltonian MPO

$$\hat{H} = \sum_{\{\sigma\},\{\sigma'\},\{w\}} W_{1\ w_1}^{\sigma_1\sigma_1'} W_{2\ w_1 w_2}^{\sigma_2\sigma_2'} \dots W_{N\ w_{N-1}}^{\sigma_N\sigma_N'} \left|\sigma_1 \dots \sigma_N\right\rangle \left\langle\sigma_1' \dots \sigma_N'\right| \ .$$

with, for the system

$$W_{1<\alpha\leq N} =$$

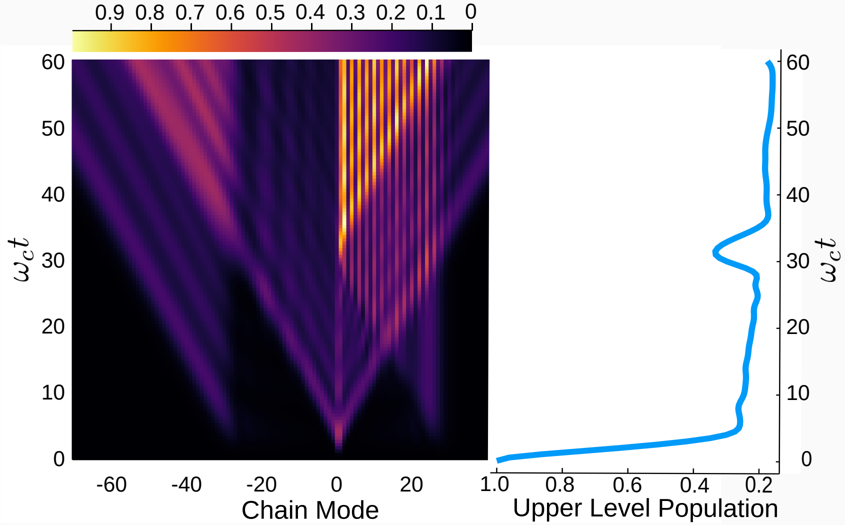
$$\begin{pmatrix}
\hat{\mathbb{1}} & J\,\hat{f}_\alpha & J\,\hat{f}_\alpha^\dagger & 0 & 0 & \overbrace{\dots}^{2(\alpha-2)} & \left|\alpha\right\rangle\left\langle\alpha\right| & \left|\alpha\right\rangle\left\langle\alpha\right| & E_\alpha \hat{P}_\alpha \\
 & & & 0 & & & & & \hat{f}_\alpha^\dagger \\
 & & & 0 & & & & & \hat{f}_\alpha \\
 & & & \hat{\mathbb{1}} & & & & & 0 \\
 & & & & \hat{\mathbb{1}} & & & & 0 \\
 & & & & & \ddots & & & \vdots \\
 & & & & & & 0 & 0 & 0 \\
 & & & & & & & & \hat{\mathbb{1}}
\end{pmatrix}$$

Matrix Product Operator II

And for the environment

$$
W_{1\leq n\leq N_m} = \begin{pmatrix}
\hat{\mathbb{1}} & t_n\hat{c}_n^\dagger & t_n\hat{c}_n & 0 & 0 & \dots & 0 & \omega_n\hat{c}_n^\dagger\hat{c}_n \\
 & & & 0 & & & & \hat{c}_n \\
 & & & 0 & & & & \hat{c}_n^\dagger \\
 & & & \hat{\mathbb{1}} & & & & \gamma_n^1\hat{c}_n \\
 & & & & \hat{\mathbb{1}} & & & \gamma_n^{1*}\hat{c}_n^\dagger \\
 & & & & & \ddots & & \vdots \\
 & & & & & & \hat{\mathbb{1}} & \gamma_n^{N*}\hat{c}_n^\dagger \\
 & & & & & & & \hat{\mathbb{1}}
\end{pmatrix}
$$

Finite Temperature



Bath Spectral density

For an interaction Hamiltonian

$$\hat{H}_{\text{int}} = \hat{O} \sum_k (g_k \hat{a}_k + \text{h.c.}) \ ,$$

the *Bath Spectral Density* is defined as

$$J(\omega) = \sum_k |g_k|^2 \delta(\omega - \omega_k) \ .$$

Ohmic spectral density: $J(\omega) = 2\alpha\omega H(\omega_c - \omega)$

Origin of the Revivals?

Trace out the bath d.o.f

$$\left\langle \hat{H}_{\text{int}} \right\rangle_B = \sum_\alpha \hat{P}_\alpha \left\langle \int_{\mathbb{R}} g_k (\hat{a}_k e^{ikr_\alpha} + \text{h.c.}) \mathrm{d}k \right\rangle_B = \sum_\alpha \hat{P}_\alpha \Delta E(r_\alpha, t) \; .$$

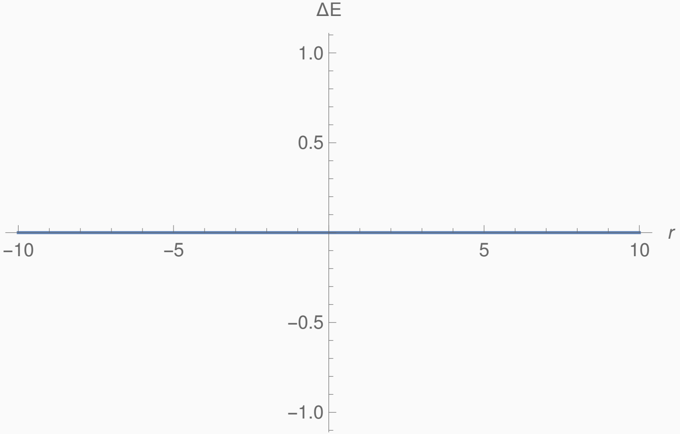
The interaction Hamiltonian becomes a shift term for the bare sites energies

$$\begin{aligned} \hat{H}_S + \left\langle \hat{H}_{\text{int}} \right\rangle_B &= \sum_\alpha E_\alpha \hat{P}_\alpha + J(|\alpha\rangle\langle\alpha+1| + \text{h.c.}) + \sum_\alpha \Delta E(r_\alpha, t) \hat{P}_\alpha \\ &= \sum_\alpha \left(E_\alpha + \Delta E(r_\alpha, t)\right) \hat{P}_\alpha + J(|\alpha\rangle\langle\alpha+1| + \text{h.c.}) \; . \end{aligned}$$

Energy Shift

Skipping the details...

$$\Delta E(r,t) = \lambda\left(\frac{-2}{1+(k_c r)^2} + \frac{1}{1+k_c^2(r-ct)^2} + \frac{1}{1+k_c^2(r+ct)^2} \right)$$



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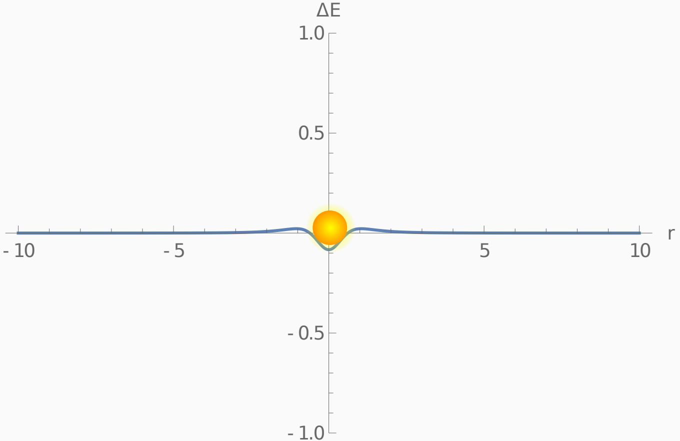

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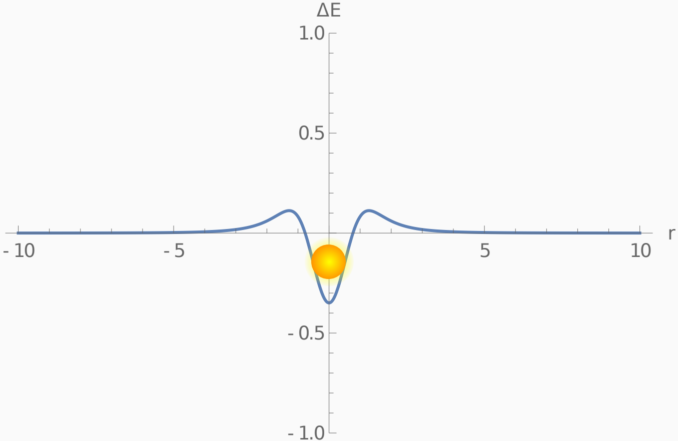

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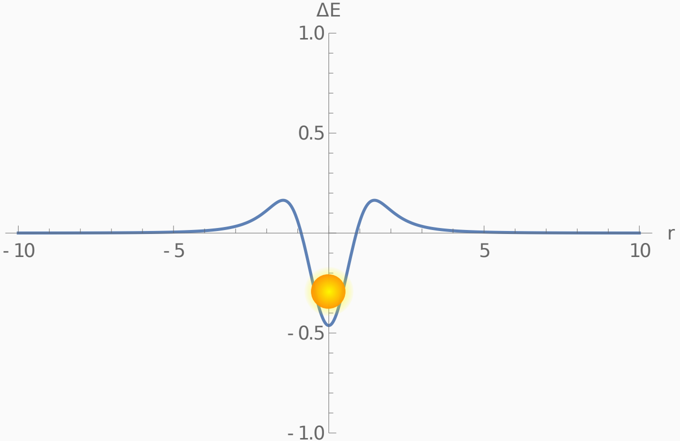

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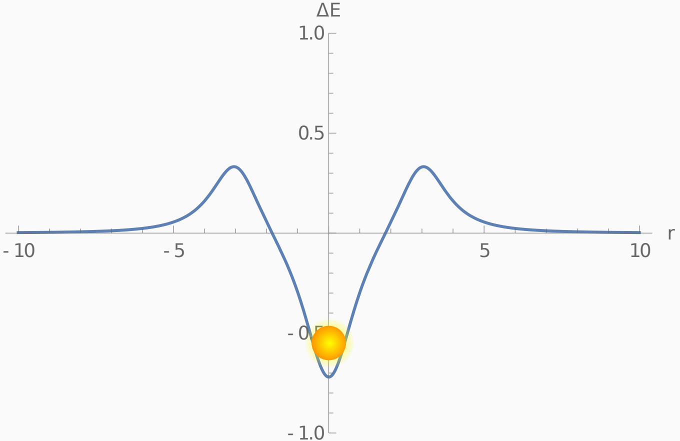

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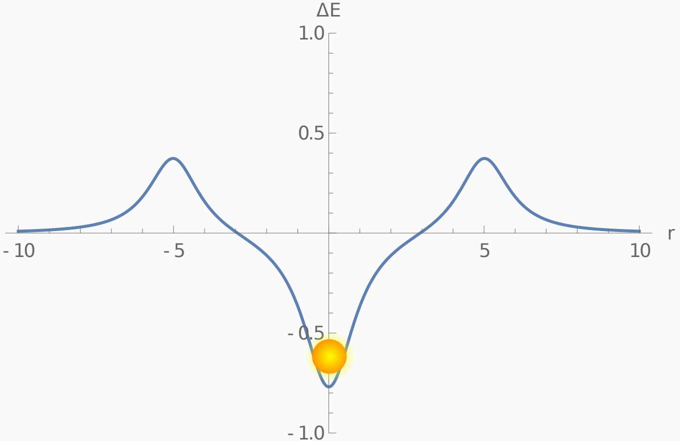

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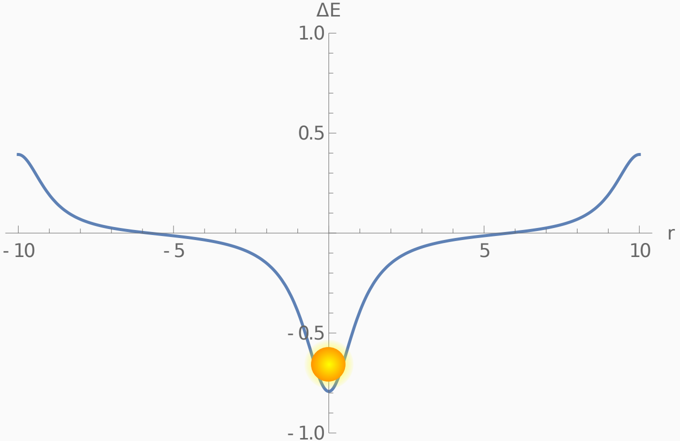
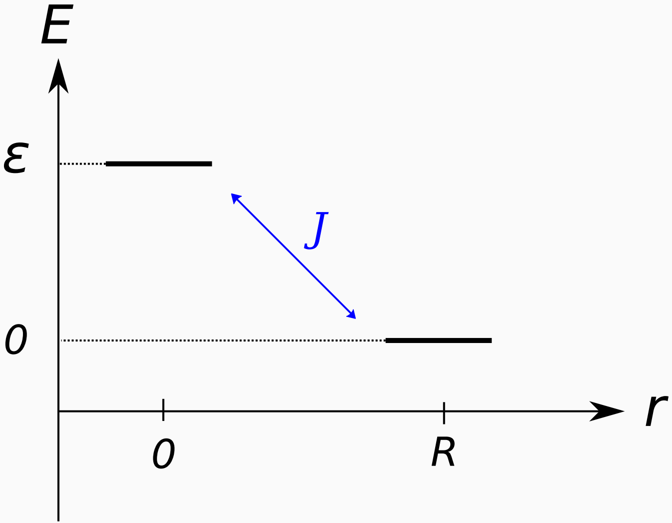


Cartoonish Explanation



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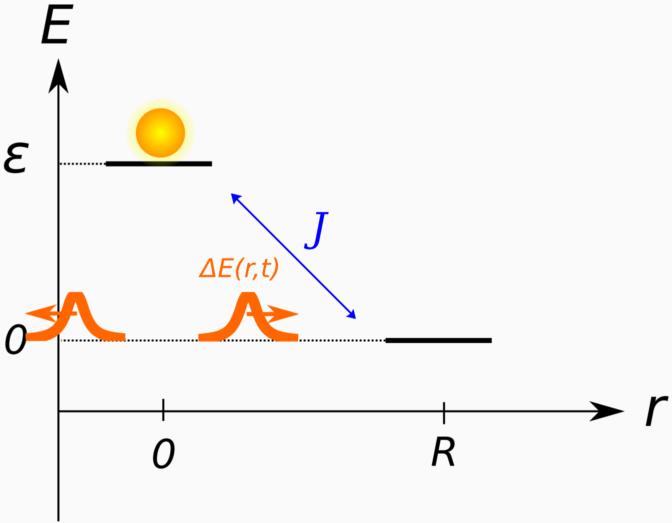

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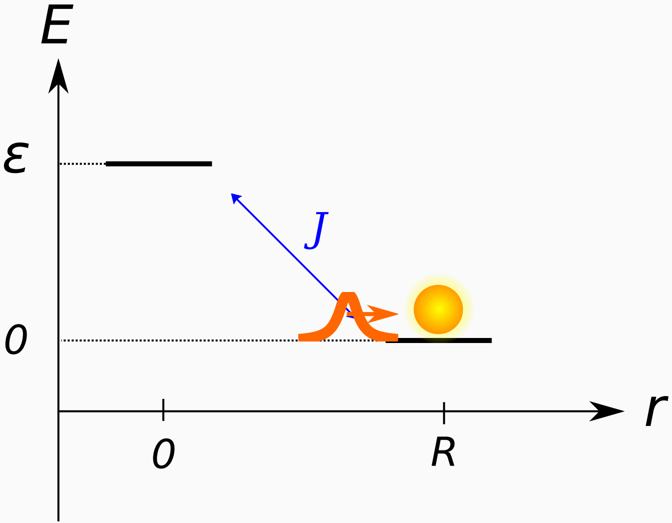

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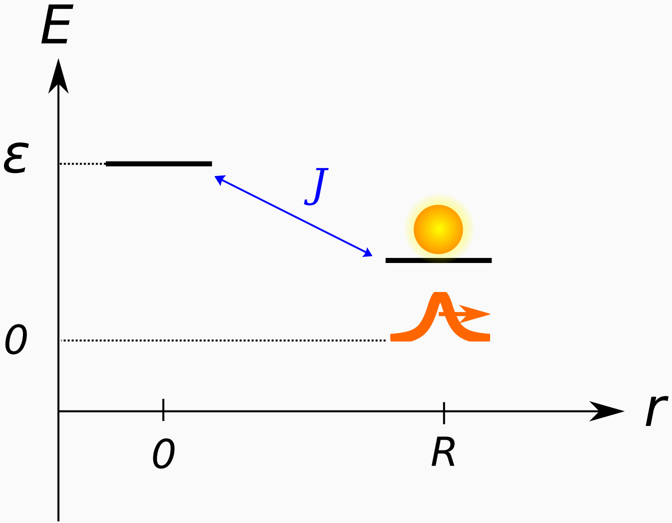

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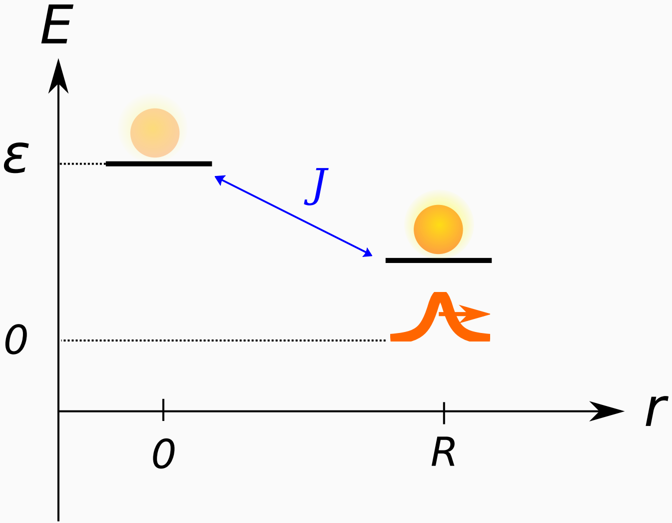

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