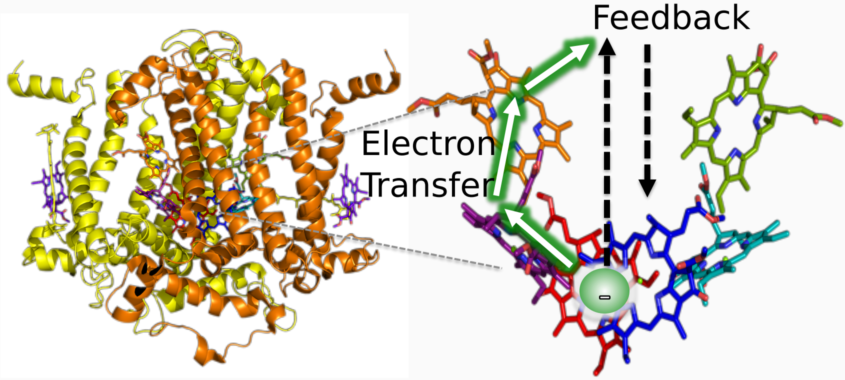
Propagating non-Markovian memory effects across spacetime with long-range tensor network models for open quantum systems

Thibaut Lacroix
tfml1@st-andrews.ac.uk

CDT Science Conference
21/01/2022

QM-CDT

University of St Andrews



Light-Harvesting Complexes

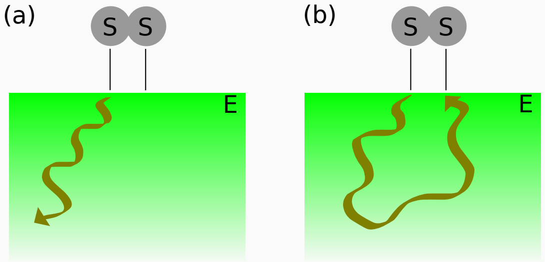
(Non-)Markovian Environment

Markovian

- $\tau_E << \tau_S$

Non-Markovian

- $\tau_E \sim \tau_S$



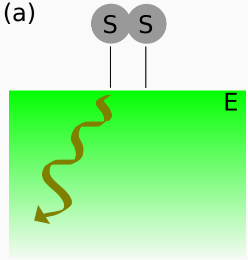
(Non-)Markovian Environment

Markovian

- $\tau_E << \tau_S$
- Weak Coupling

Non-Markovian

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



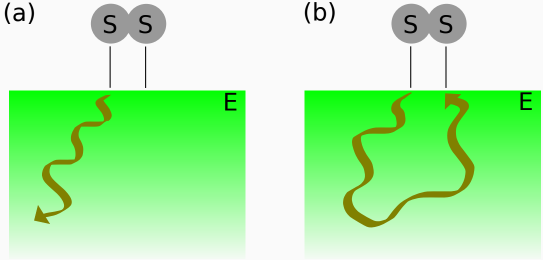
(Non-)Markovian Environment

Markovian

- $\tau_E << \tau_S$
- Weak Coupling
- Time-Local Master Equations (*e.g.* Lindblad)

Non-Markovian

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

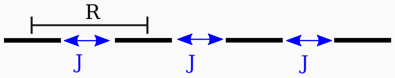


Simplified Model

Open Quantum System

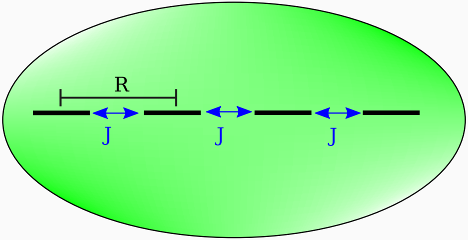
$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha \hat{P}_\alpha$$

Open Quantum System



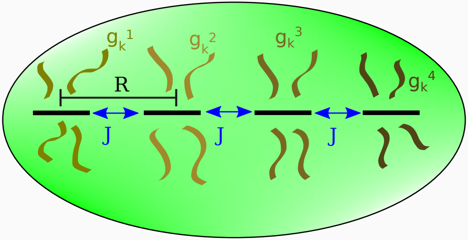
$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha \hat{P}_\alpha + \sum_{\alpha=1}^{N-1} J \left(|\alpha\rangle \langle\alpha+1| + \text{h.c.} \right)$$

Open Quantum System



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

Open Quantum System

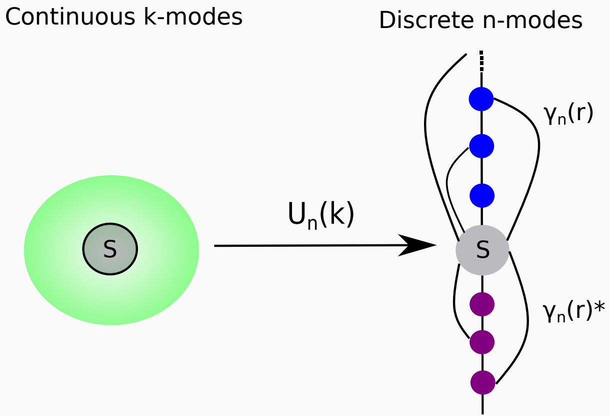


$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha \hat{P}_\alpha + \sum_{\alpha=1}^{N-1} J \left(|\alpha\rangle \langle \alpha+1| + \text{h.c.} \right)$$

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

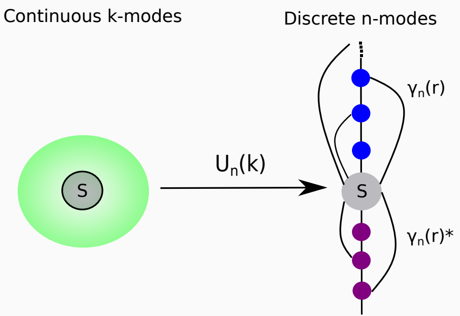
Methods

Environment-Chain Mapping



Chin et al., J. of Math. Phys. 51(9), 092109 (2010)
Tamascelli, et al., Phys. Rev. Lett., 123(9), 090402 (2019)
Lacroix et al., Phys. Rev. A, 104(5), 052204 (2021)

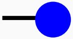
Environment-Chain Mapping

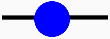


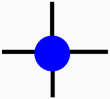
$$
\begin{aligned}
\hat{H}_B + \hat{H}_{\text{int}} = \sum_n \omega_n(\hat{c}_n^\dagger \hat{c}_n + \hat{d}_n^\dagger \hat{d}_n) \\
+ t_n(\hat{c}_n^\dagger \hat{c}_{n+1} + \hat{c}_{n+1}^\dagger \hat{c}_n + \hat{d}_n^\dagger \hat{d}_{n+1} + \hat{d}_{n+1}^\dagger \hat{d}_n) \\
+ \sum_\alpha |\alpha\rangle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

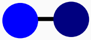
Diagrammatic Notation

a  Scalar

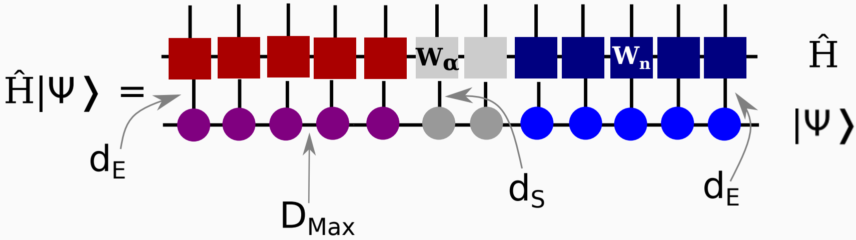
a_i  Vector

a_{ij}  Matrix

a_{ijkl}  Rank-4 Tensor

$\mathbf{a} \cdot \mathbf{b}$  Scalar

$M\mathbf{a}$  Vector

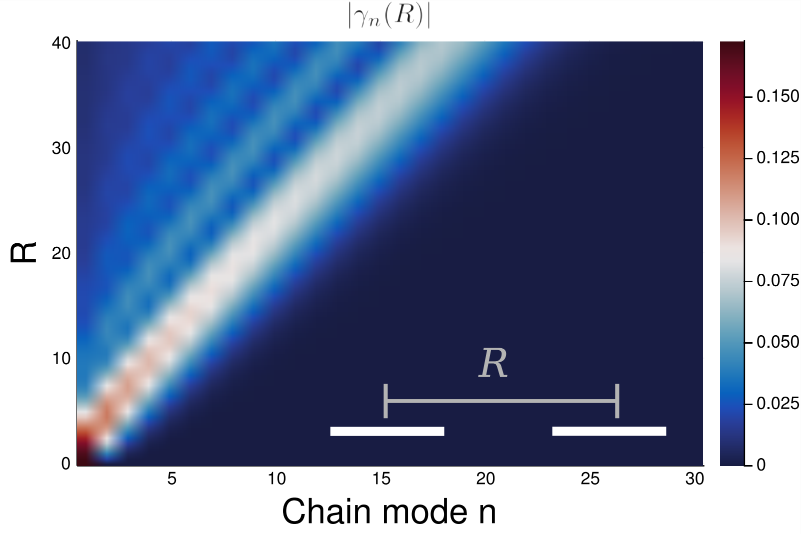


$$|\psi\rangle = \sum_{\{i_k\}} \sum_{\{\alpha\}} T^{\alpha_1}_{i_1} T^{\alpha_1 \ \alpha_2}_{i_2} T^{\alpha_2 \ \alpha_3}_{i_3} \dots T^{\alpha_{N-1}}_{i_N} |\phi_{i_1} \dots \phi_{i_N}\rangle$$

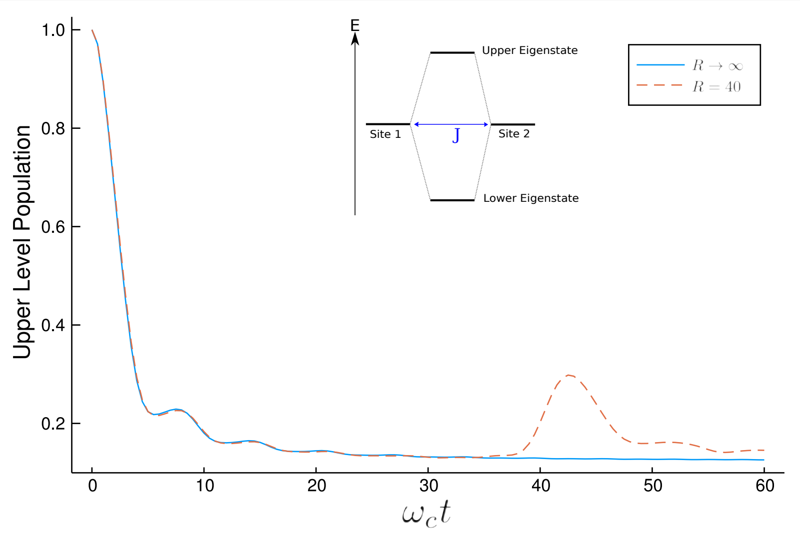
$$\hat{H} = \sum_{\{\sigma\},\{\sigma'\},\{w\}} W_{1\ \ w_1}^{\sigma_1 \sigma_1'} W_{2\ \ w_1 w_2}^{\sigma_2 \sigma_2'} \dots W_{N\ \ w_{N-1}}^{\sigma_N \sigma_N'} |\sigma_1 \dots \sigma_N\rangle \langle \sigma_1' \dots \sigma_N'| \ .$$

Results

Couplings $\gamma_n(R)$ at Zero Temperature

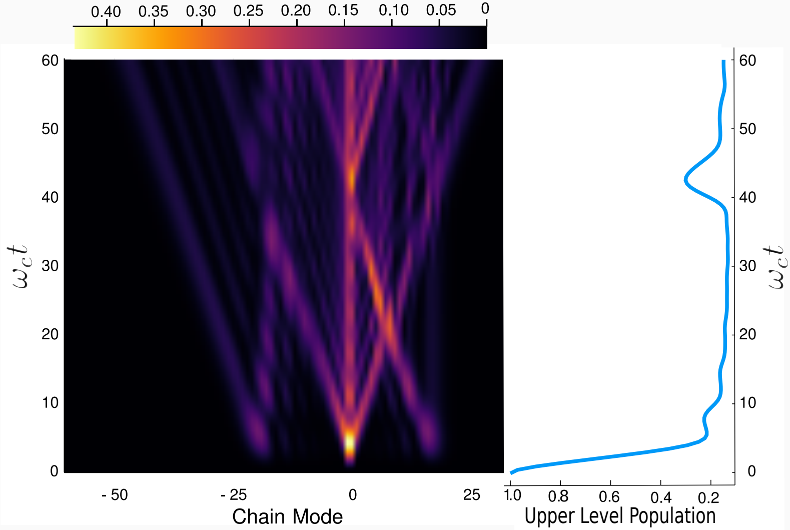


Non-Markovian Dynamics

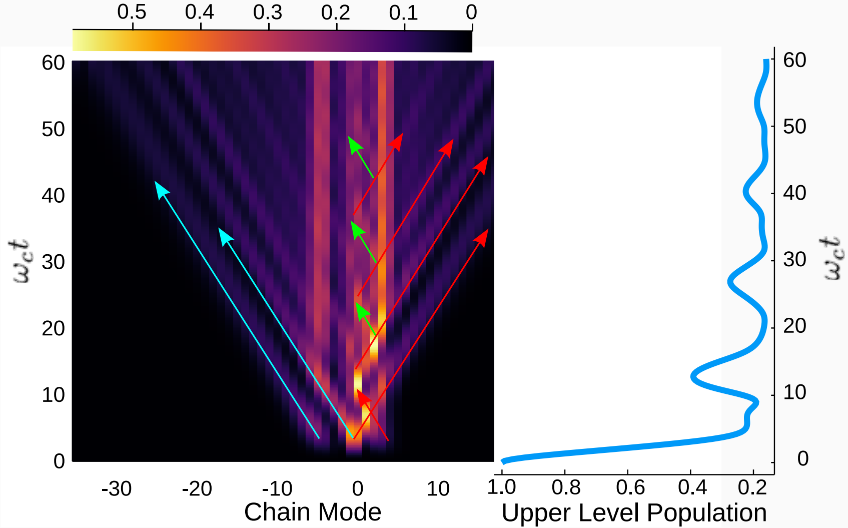


Lacroix et al., Phys. Rev. A, 104(5), 052204 (2021)

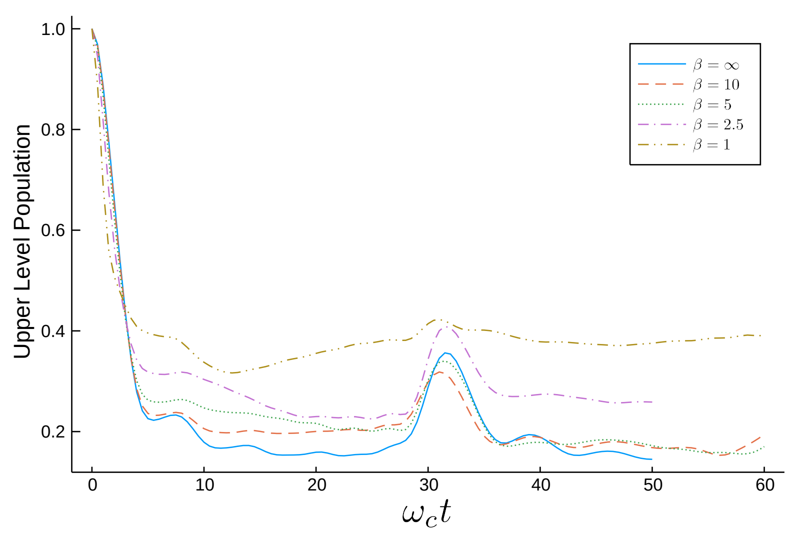
Environment Feedback



Environment Feedback II



Finite Temperature



Origin of the Revivals?

Trace out the bath d.o.f

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

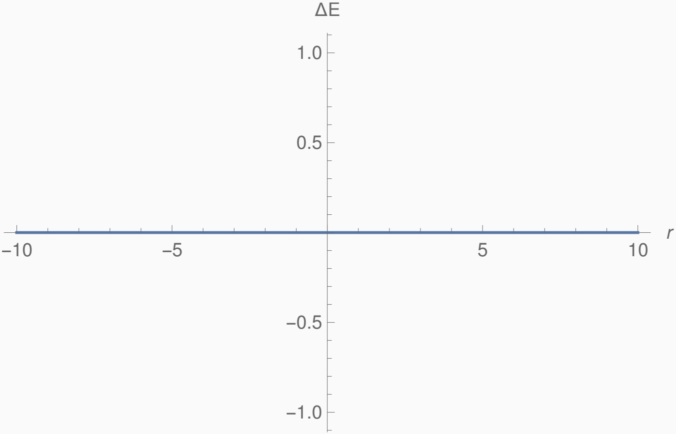
The interaction Hamiltonian becomes a shift term for the bare sites energies

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

Energy Shift

Skipping the details...

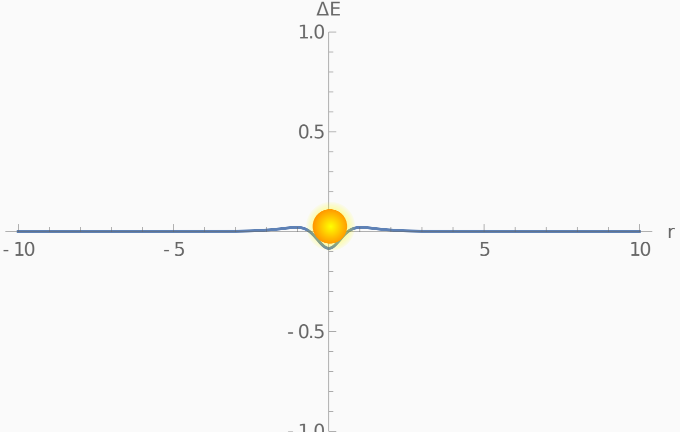
$$\Delta E(r,t) = \underbrace{4\alpha\omega_c}_{\lambda}\left(\frac{-2}{1+(k_c r)^2} + \frac{1}{1+k_c^2(r-ct)^2} + \frac{1}{1+k_c^2(r+ct)^2} \right)$$



Energy Shift

Skipping the details...

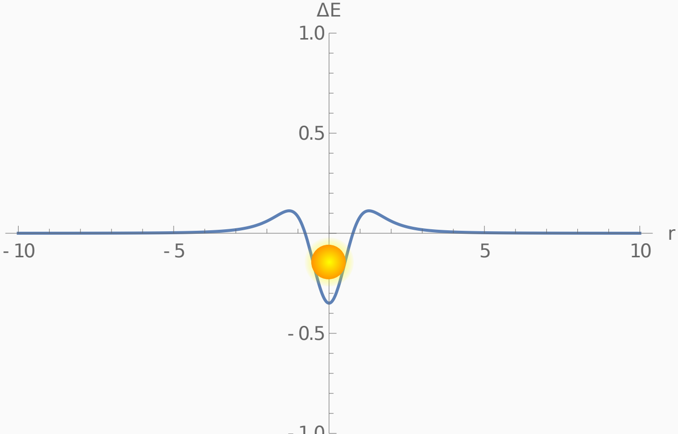
$$\Delta E(r,t) = \underbrace{4\alpha\omega_c}_{\lambda}\left(\frac{-2}{1+(k_c r)^2} + \frac{1}{1+k_c^2(r-ct)^2} + \frac{1}{1+k_c^2(r+ct)^2}\right)$$



Energy Shift

Skipping the details...

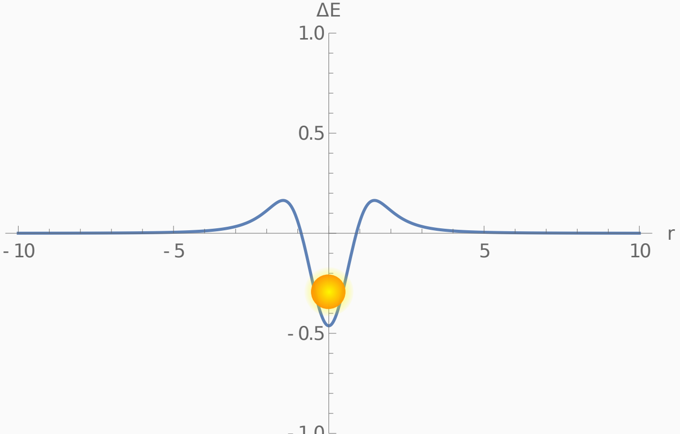
$$\Delta E(r,t) = \underbrace{4\alpha\omega_c}_{\lambda}\left(\frac{-2}{1+(k_c r)^2} + \frac{1}{1+k_c^2(r-ct)^2} + \frac{1}{1+k_c^2(r+ct)^2} \right)$$



Energy Shift

Skipping the details...

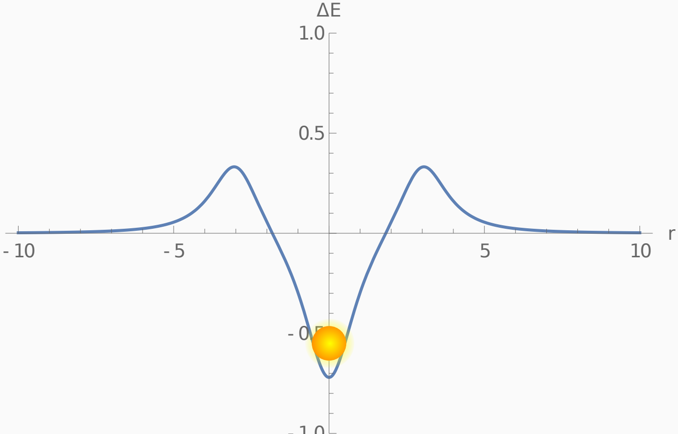
$$\Delta E(r,t) = \underbrace{4\alpha\omega_c}_{\lambda}\left(\frac{-2}{1+(k_c r)^2} + \frac{1}{1+k_c^2(r-ct)^2} + \frac{1}{1+k_c^2(r+ct)^2} \right)$$



Energy Shift

Skipping the details...

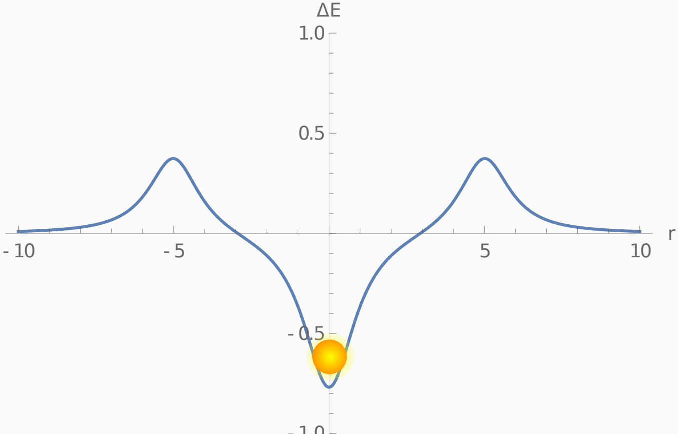
$$\Delta E(r,t) = \underbrace{4\alpha\omega_c}_{\lambda}\left(\frac{-2}{1+(k_c r)^2} + \frac{1}{1+k_c^2(r-ct)^2} + \frac{1}{1+k_c^2(r+ct)^2} \right)$$



Energy Shift

Skipping the details...

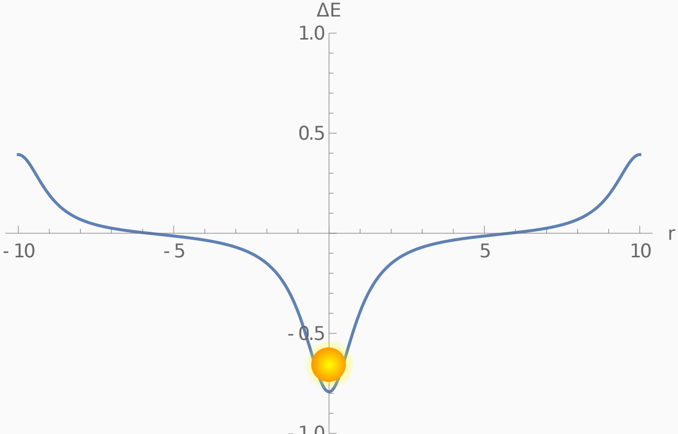
$$\Delta E(r,t) = \underbrace{4\alpha\omega_c}_{\lambda}\left(\frac{-2}{1+(k_c r)^2} + \frac{1}{1+k_c^2(r-ct)^2} + \frac{1}{1+k_c^2(r+ct)^2}\right)$$



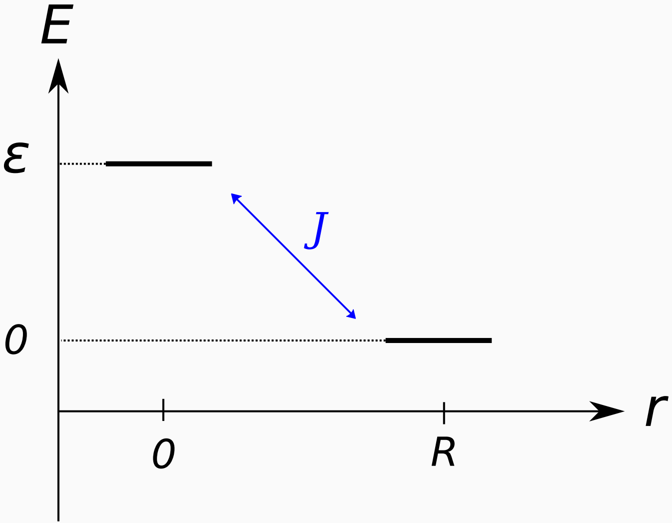
Energy Shift

Skipping the details...

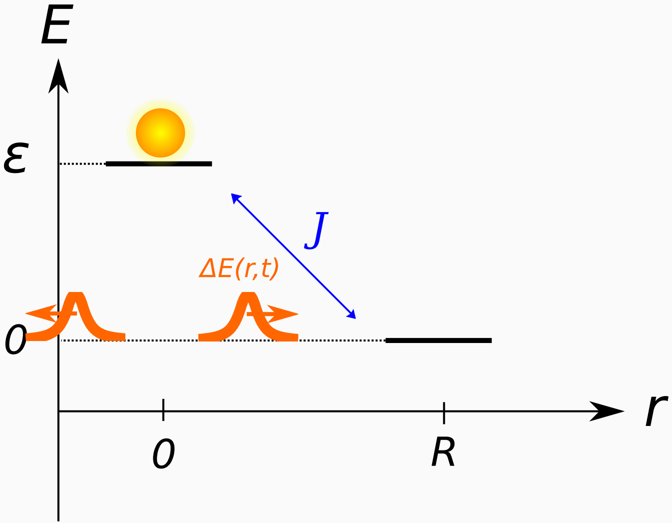
$$\Delta E(r,t) = \underbrace{4\alpha\omega_c}_{\lambda}\left(\frac{-2}{1+(k_c r)^2} + \frac{1}{1+k_c^2(r-ct)^2} + \frac{1}{1+k_c^2(r+ct)^2}\right)$$



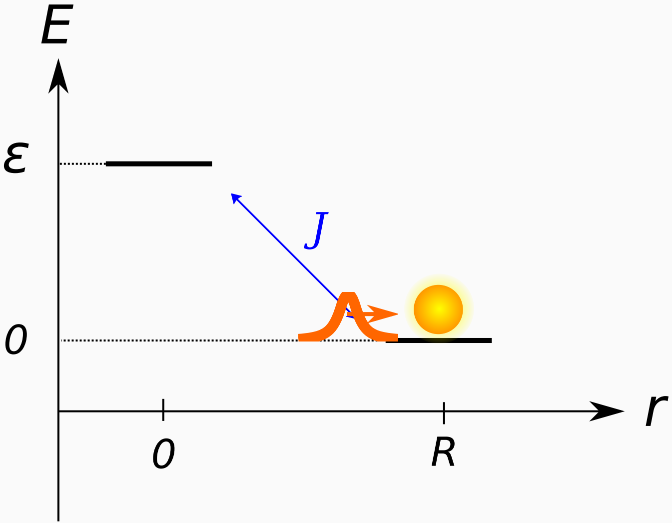
Cartoonish Explanation



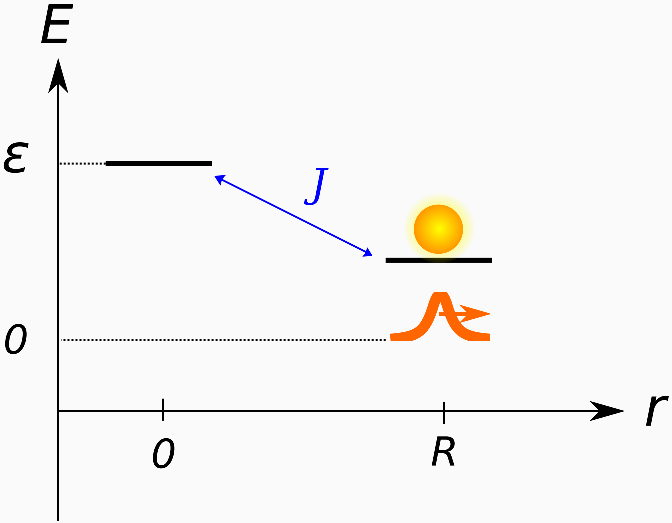
Cartoonish Explanation



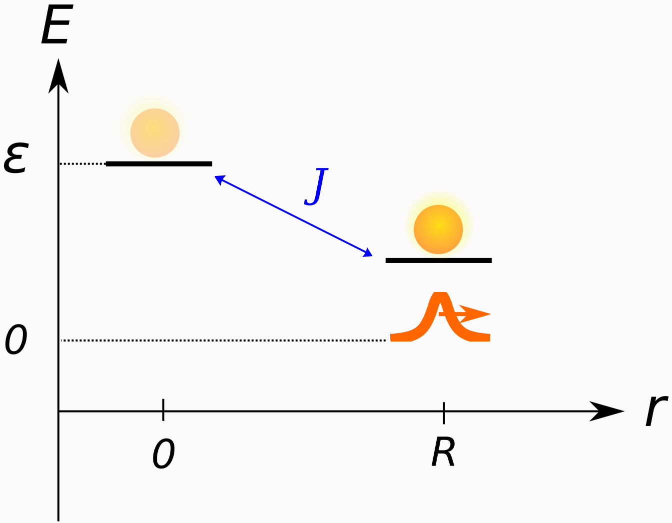
Cartoonish Explanation



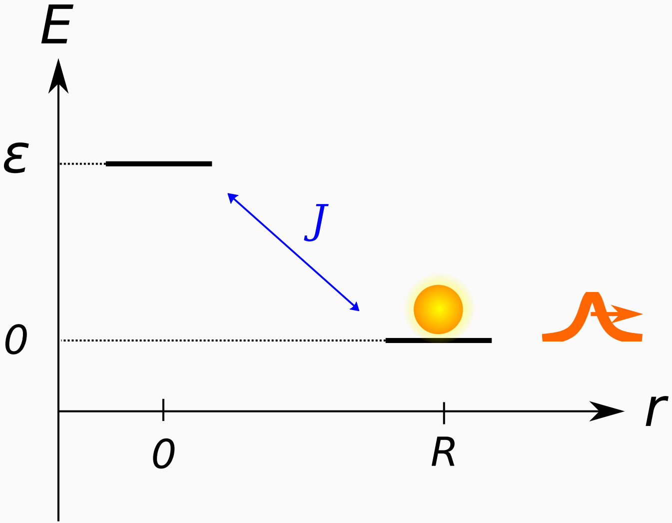
Cartoonish Explanation



Cartoonish Explanation



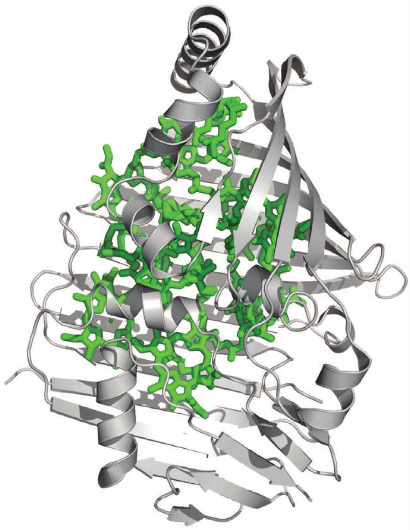
Cartoonish Explanation



Conclusion

Conclusion

- Spatially extended system in a common environment
- MPS/MPO representation of $\mathcal{S} = \{\text{system} + \text{environment}\}$
- Spatially correlated environment
- Zero- and finite-temperature
- ⚠ Multi-sites dynamics & different topologies
- ⚠ Allostery & other biological processes



Thank you for your attention!

tfml1@st-andrews.ac.uk

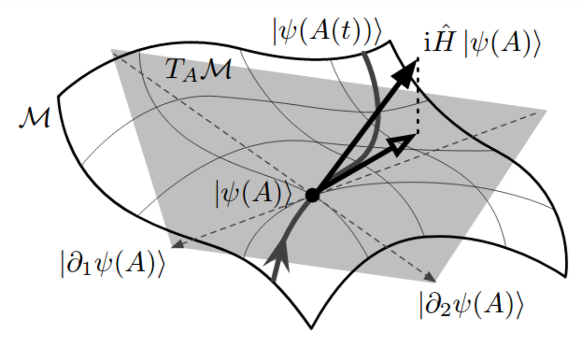
Acknowledgment: A. Dunnett (Sorbone U.), D. Gribben (St Andrews), B. Lovett (St Andrews) & A. Chin (Sorbonne U./CNRS).

This work is supported by dstl.

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

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

Bath Spectral density

For an interaction Hamiltonian

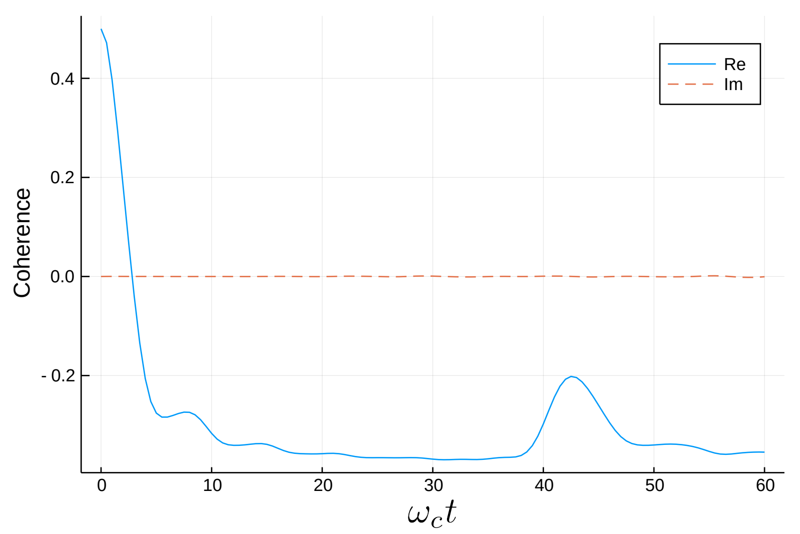
$$\hat{H}_{\text{int}} = \hat{O} \sum_k (g_k \hat{a}_k + \text{h.c.}) \ ,$$

the *Bath Spectral Density* is defined as

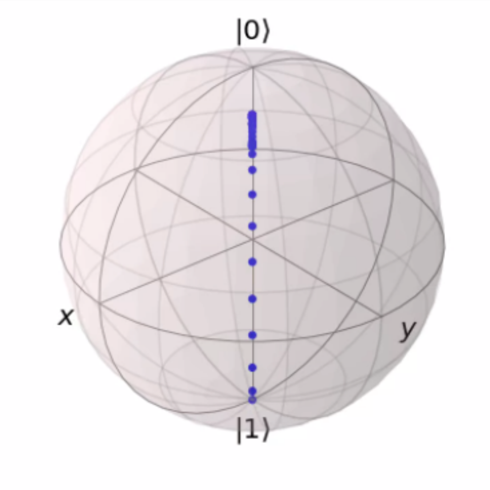
$$J(\omega) = \sum_k |g_k|^2 \delta(\omega - \omega_k) \ .$$

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

Incoherent Process



Incoherent Process II



Finite Temperature