Studying Non-Markovian Signalling in Open Quantum Systems with Tensor Networks

Thibaut Lacroix

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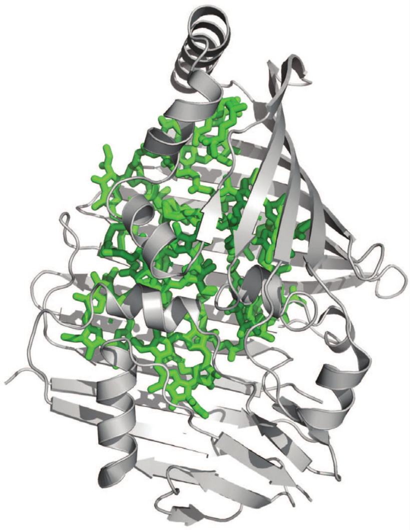
Polaron Day

01/09/2022

University of St Andrews

Motivation

Systems interacting with complex environments



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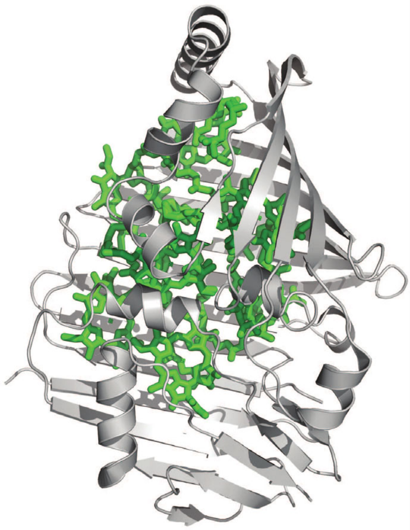

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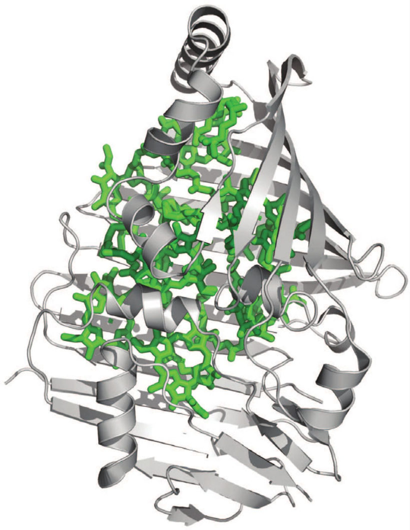

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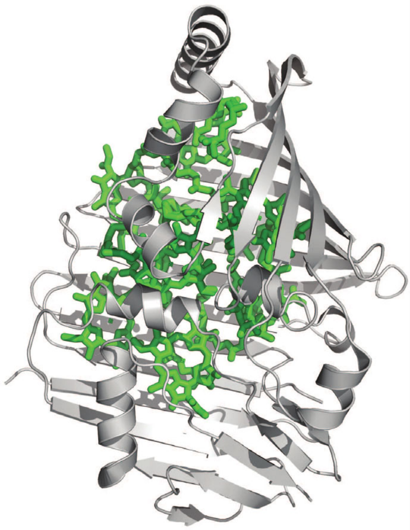
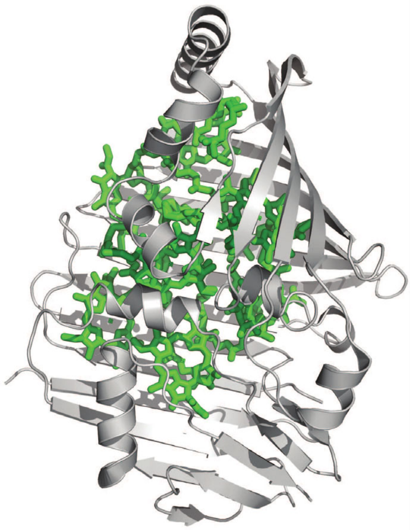


Motivation

Systems interacting with complex environments

- biological systems,
- chemical systems,
- etc.

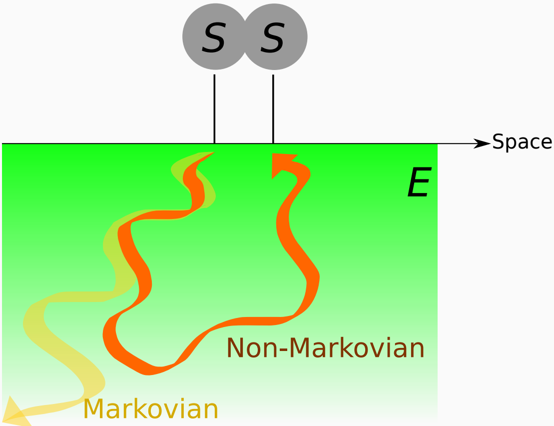
$\Longrightarrow$ Identify environment-mediated processes



Shared History Matters

Non-Markovian Environment

- $\tau_E \sim \tau_S$



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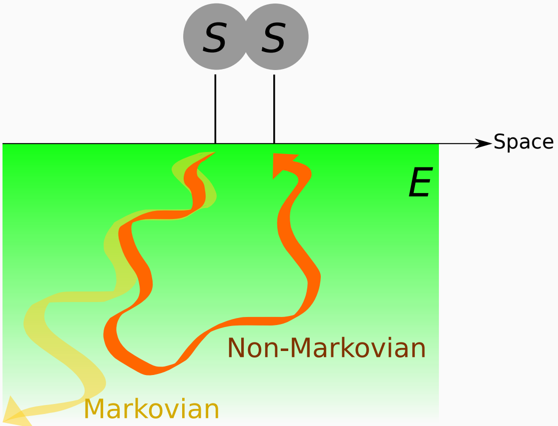

Shared History Matters

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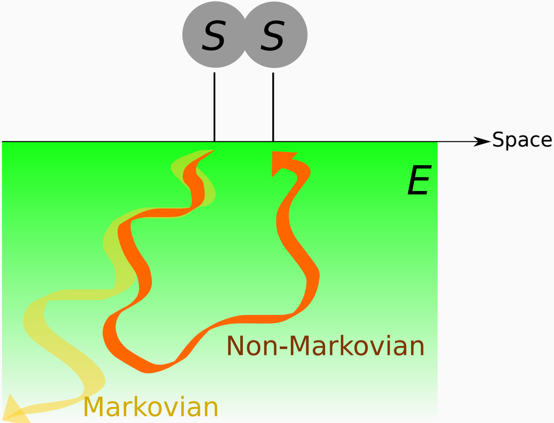
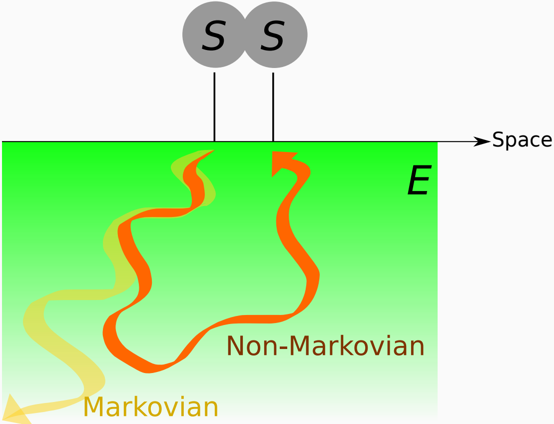
- Non time-local Master Equations



Shared History Matters

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

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



Theory of Open Quantum Systems

$$\frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle = -\mathrm{i}\hat{H} |\psi(t)\rangle$$

where $|\psi\rangle \in \mathcal{S} \otimes \mathcal{E}$

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Curse of dimensionality

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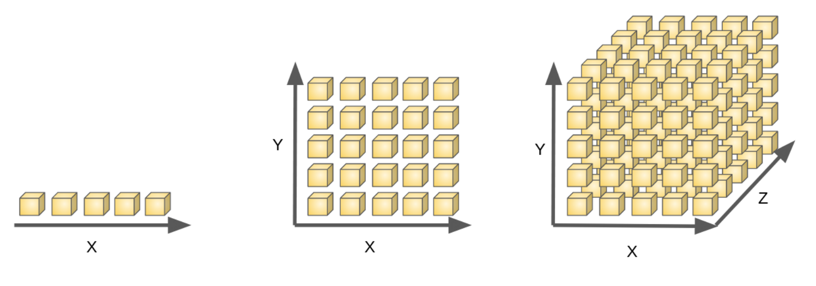
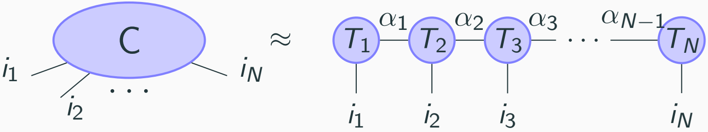


Working around the curse of dimensionality

Tensor Networks are wave-functions Ansätze

$$
\begin{aligned}
|\psi(t)\rangle &= \sum_{\{i\}} C_{i_1\, i_2 \ldots i_N} |\phi_{i_1} \ldots \phi_{i_N}\rangle \\
&\approx \sum_{\{i\}} \sum_{\{\alpha\}} T_{i_1}^{\alpha_1} T_{i_2}^{\alpha_1\ \alpha_2} T_{i_3}^{\alpha_2\ \alpha_3} \ldots T_{i_N}^{\alpha_{N-1}} |\phi_{i_1} \ldots \phi_{i_N}\rangle
\end{aligned}
$$



$\#$ elements $\simeq d^N$

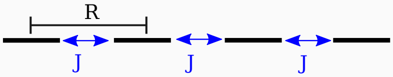
$\#$ elements $\simeq NdD^2$

Identifying Environmental Signalling

General Model

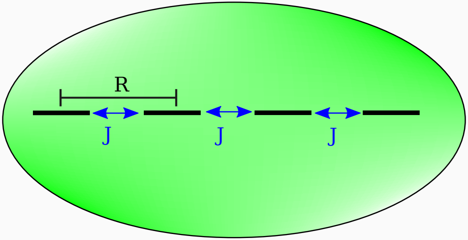
$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha \hat{P}_\alpha$$

General Model



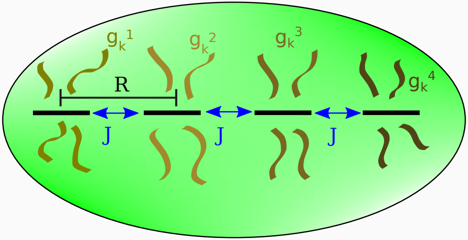
$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha \hat{P}_\alpha + \sum_{\alpha=1}^{N-1} J\left(|\alpha\rangle\langle\alpha+1| + \text{h.c.}\right)$$

General Model



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

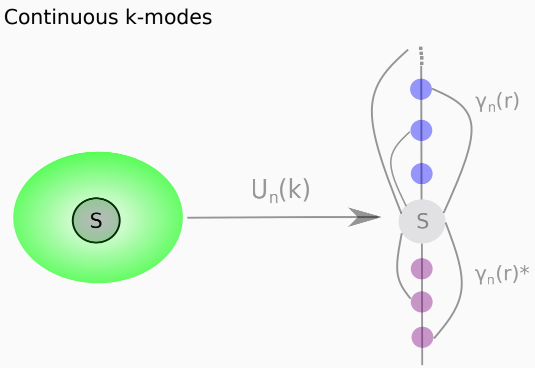
General Model



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

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

Environment - Chain Mapping



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

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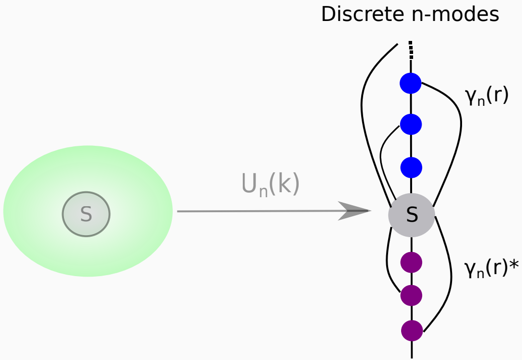
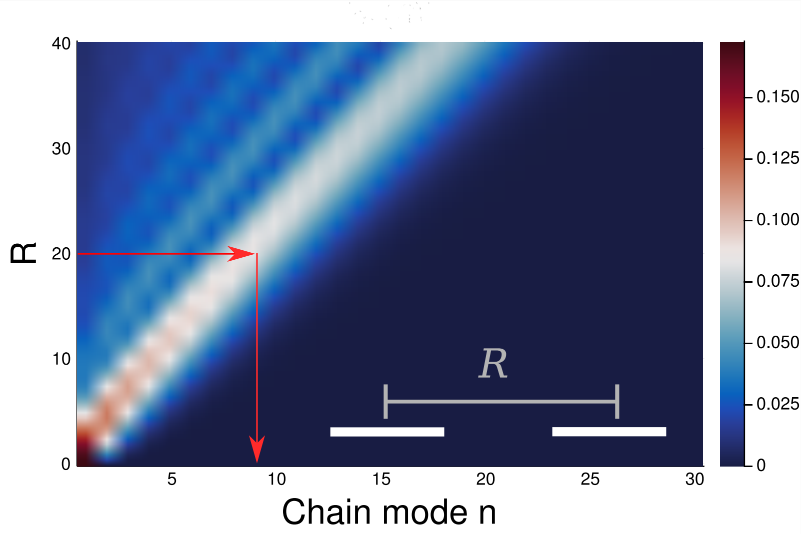


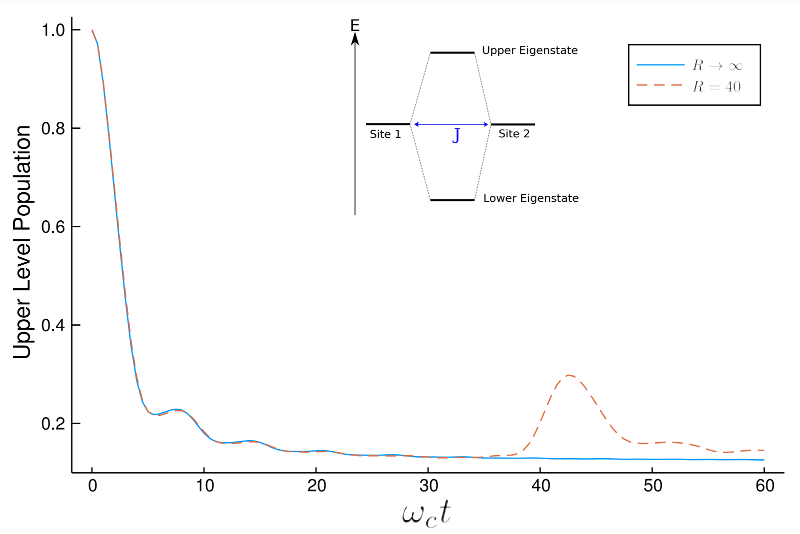
$$\hat{H}_B + \hat{H}_{\text{int}} = \sum_n \omega_n(\hat{c}_n^\dagger \hat{c}_n + \hat{d}_n^\dagger \hat{d}_n) + t_n(\hat{c}_n^\dagger \hat{c}_{n+1} + \hat{d}_n^\dagger \hat{d}_{n+1} + \text{h.c.})$$
$$+ \sum_\alpha \hat{P}_\alpha \sum_n \left(\gamma_n(r_\alpha)(\hat{c}_n + \hat{d}_n^\dagger) + \text{h.c.}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

Couplings $\gamma_n(R)$ at Zero Temperature



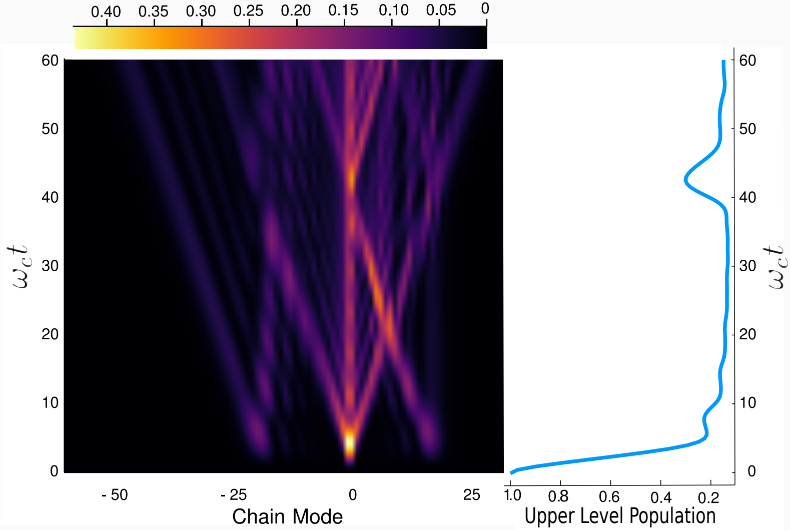
Ohmic spectral density: $J(k) = 2\alpha k c^2 H(k_c - k)$

Non-Markovian Population Revivals



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

Environment Feedback



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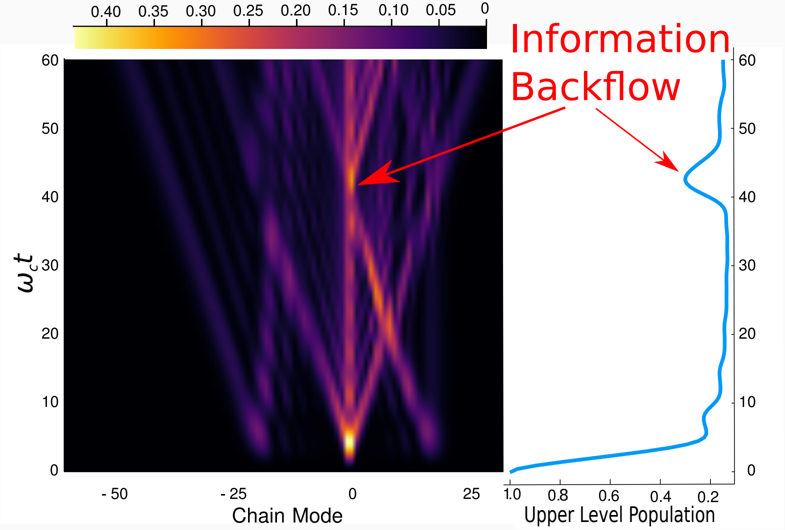
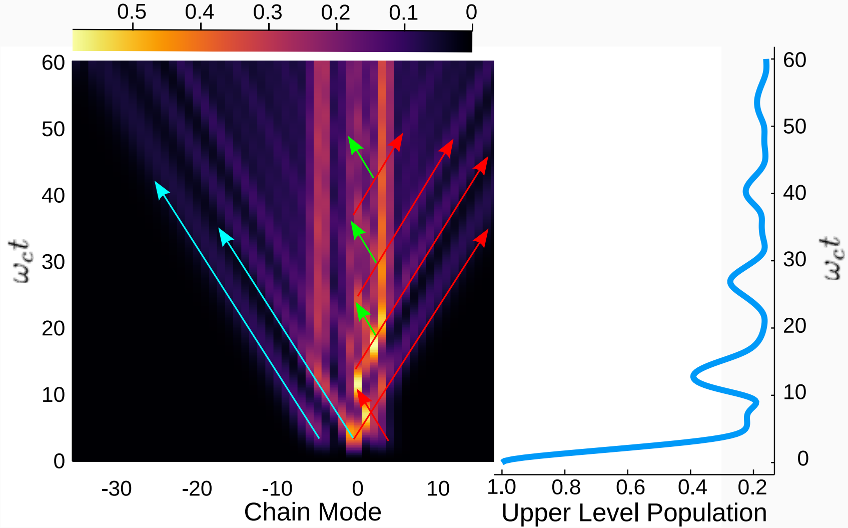
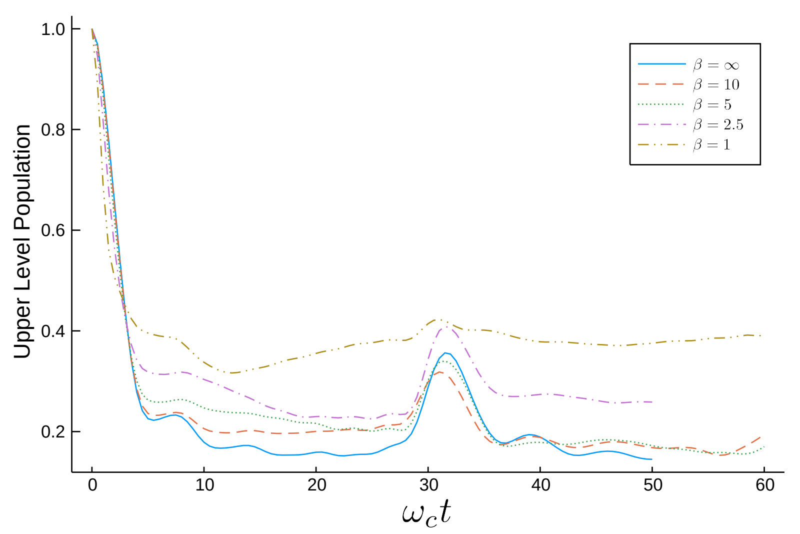



0.5
0.4
0.3
0.2
0.1
0
60
50
40
30
20
10
0
$\omega_c t$
-30
-20
-10
0
10
Chain Mode
1.0
0.8
0.6
0.4
0.2
Upper Level Population

Finite Temperature



Origin of the Revivals?

Trace out the bath d.o.f

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

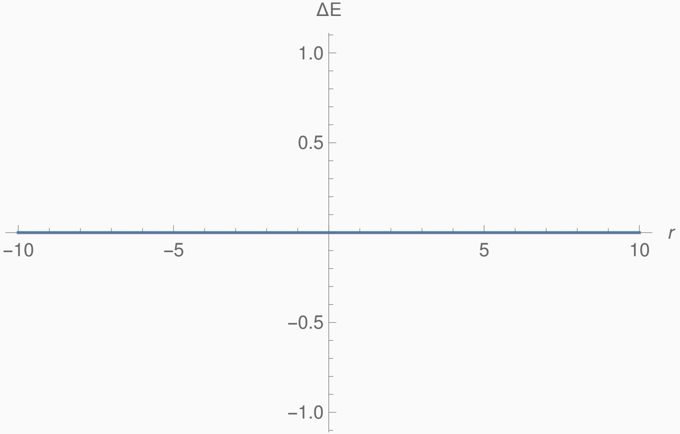
The interaction Hamiltonian becomes a shift term for the bare sites energies

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

Energy Shift

Skipping the details...

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



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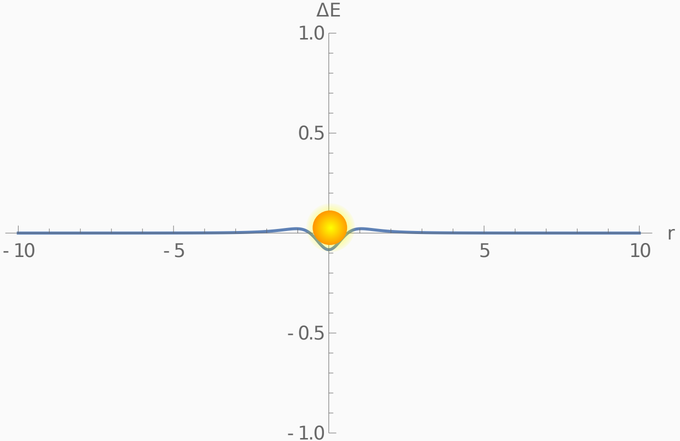

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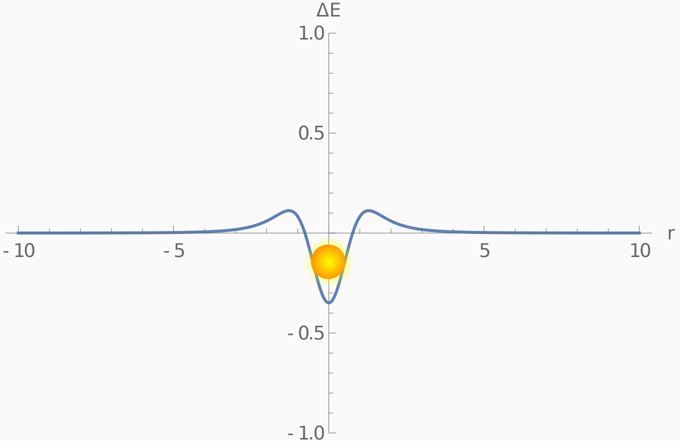

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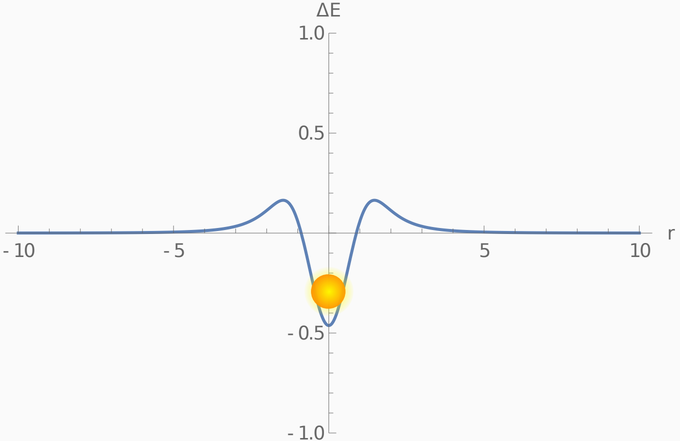

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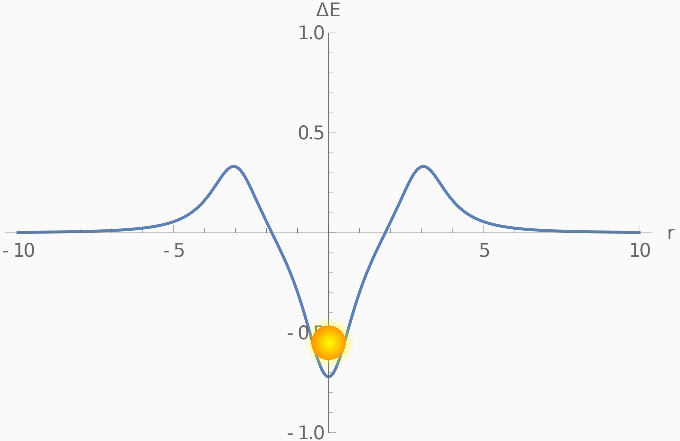

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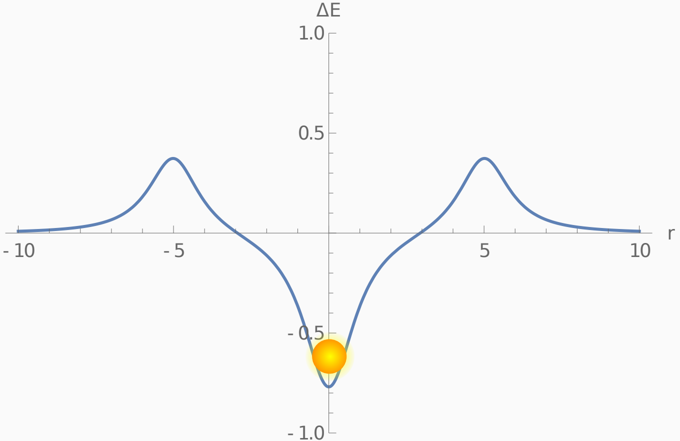

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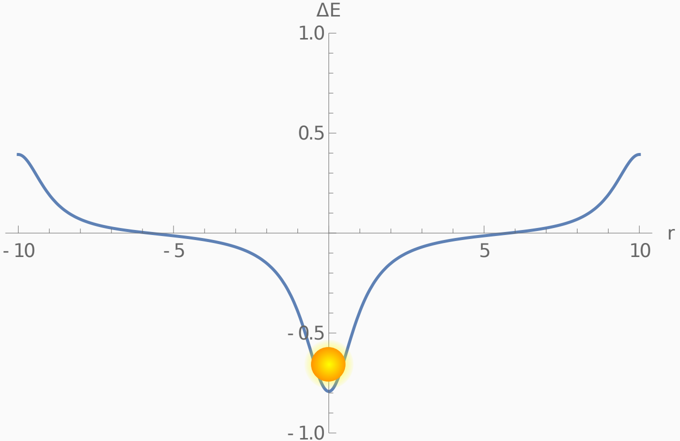
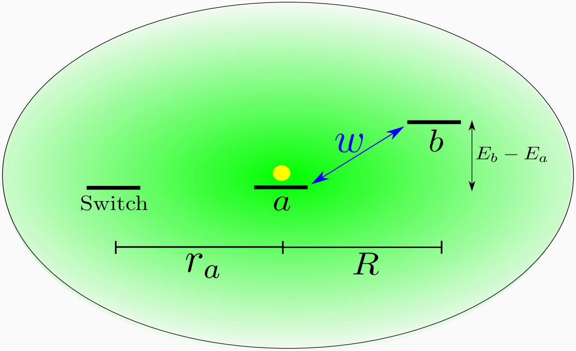


Leveraging Environmental Signalling

Switch Model



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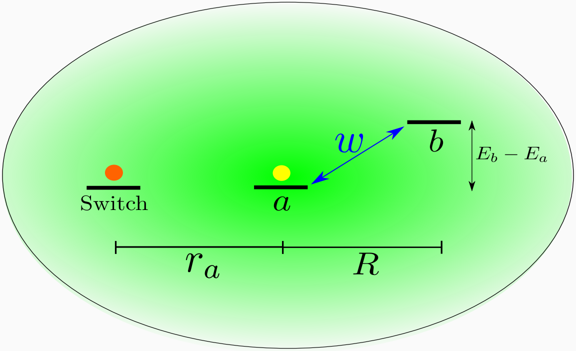

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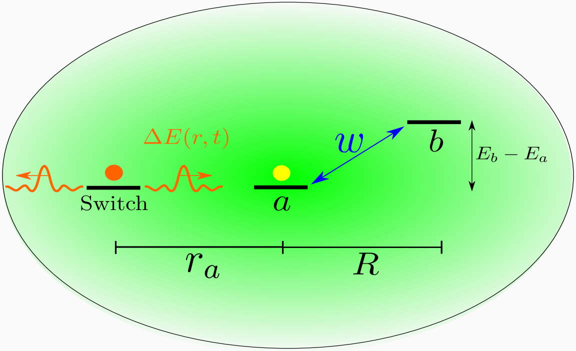
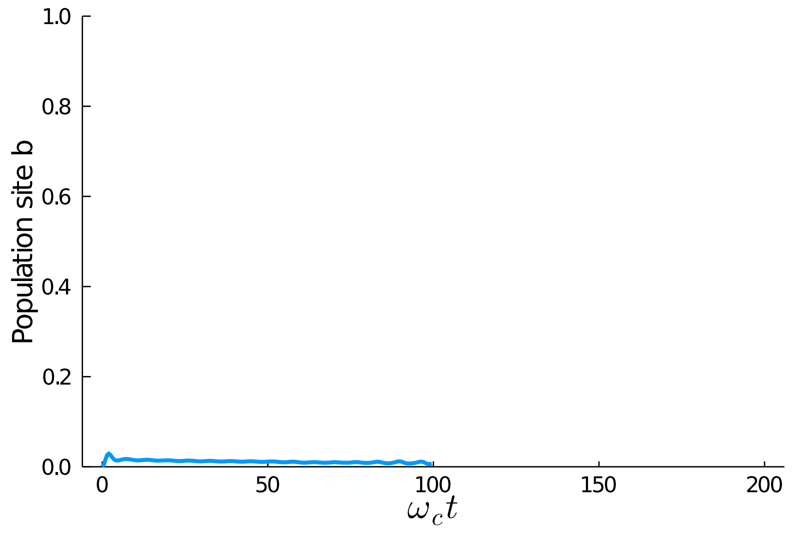


Transient Activation

TLS Gap $\gg$ coherent tunneling



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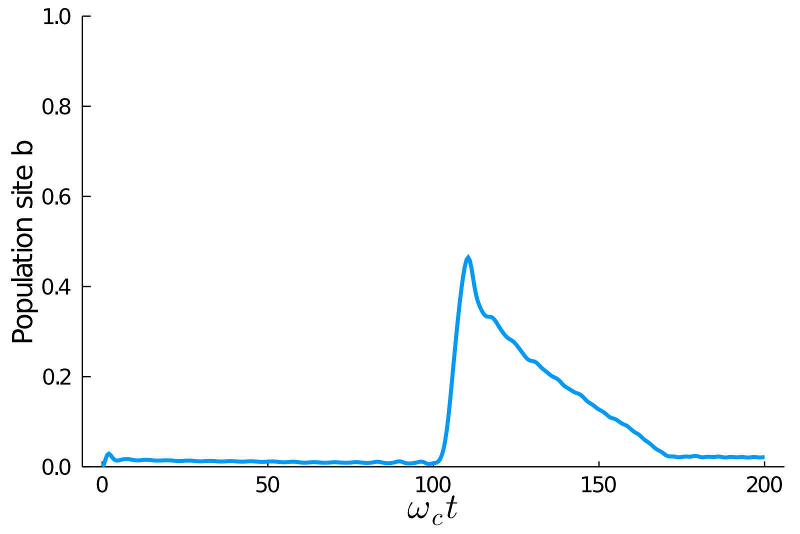

Conclusion

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Take Home

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- At zero and finite temperature
- Identify Information Back-Flow
- Associated with environment-performed work

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- Permanent switch-induced transition
- Sensing and Control
- Connection with allostery

Conclusion

Thank you for your attention!

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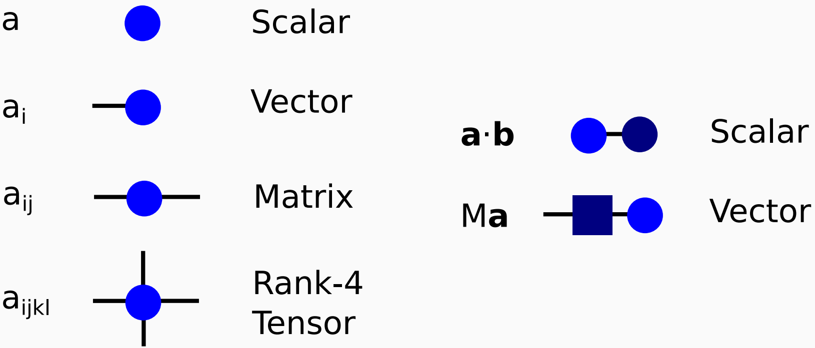
This work is supported by dstl.

SCAN ME

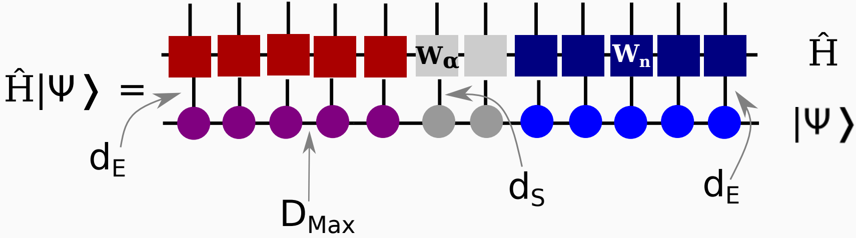
https://arxiv.org/abs/2205.11247

You want to know more?

Diagrammatic Notation



Tensor Networks



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

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

Matrix Product Operator I

The matrices W_k define the Hamiltonian MPO

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

with, for the system

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

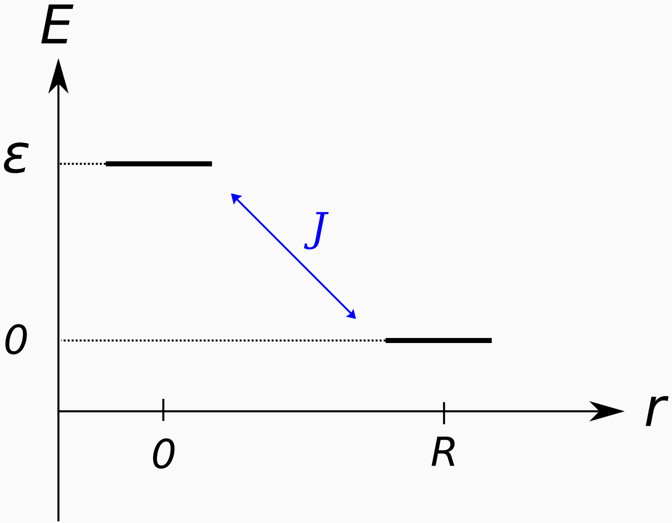
$$\begin{pmatrix}
\hat{\mathbb{1}} & J\,\hat{f}_\alpha & J\,\hat{f}_\alpha^\dagger & 0 & 0 & \overbrace{\ldots}^{2(\alpha-2)} & \left|\alpha\right\rangle\left\langle\alpha\right| & \left|\alpha\right\rangle\left\langle\alpha\right| & E_\alpha \hat{P}_\alpha \\
 & & & 0 & & & & & \hat{f}_\alpha^\dagger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

Matrix Product Operator II

And for the environment

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

Cartoonish Explanation



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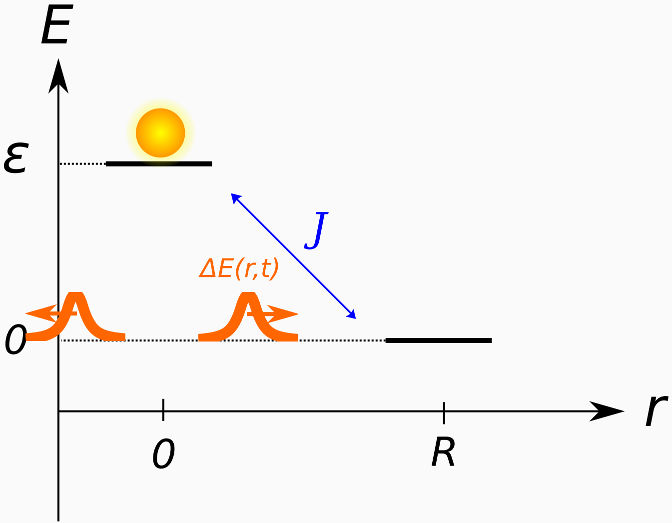

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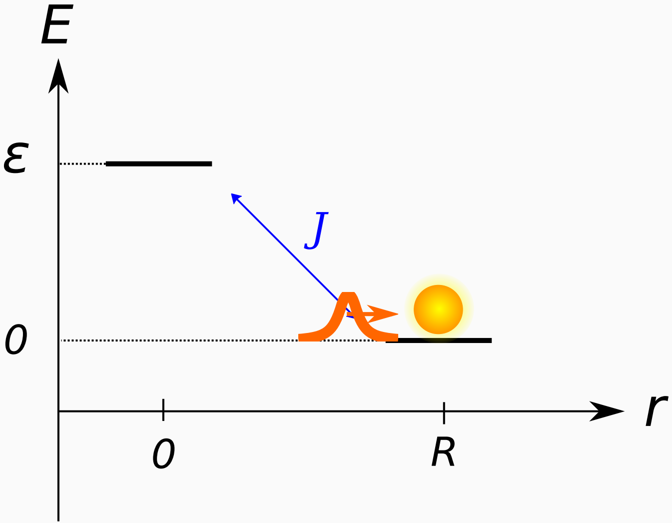

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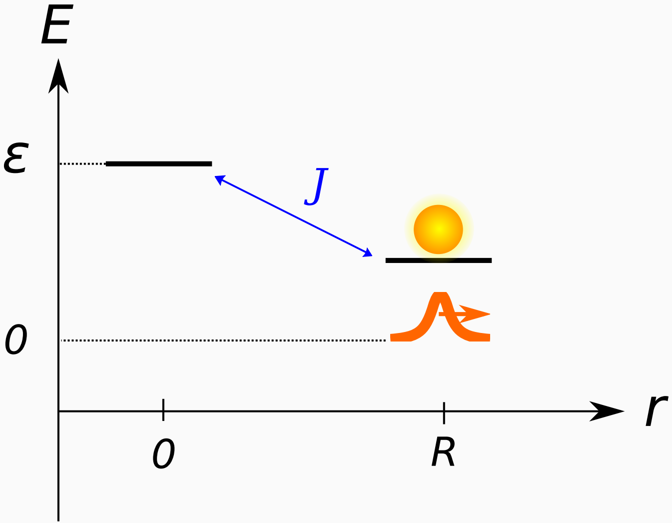

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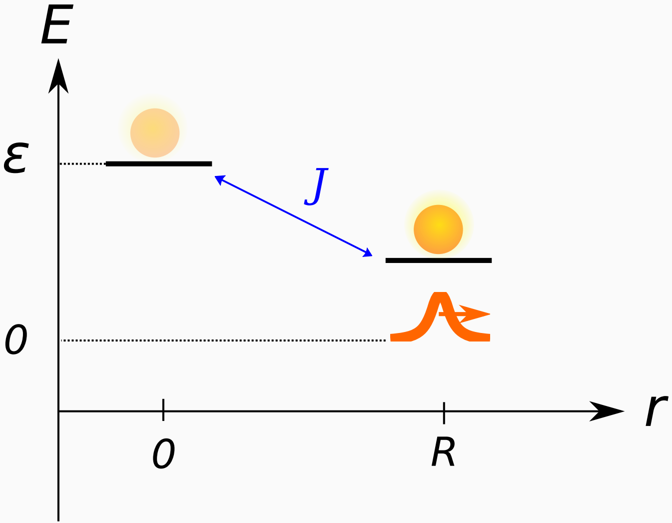
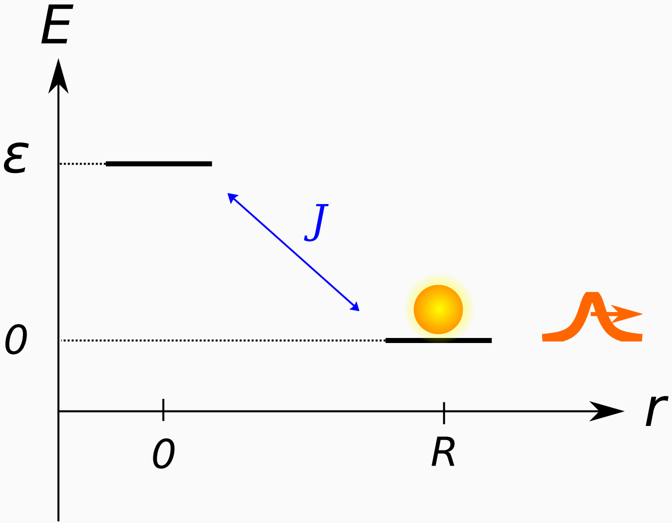
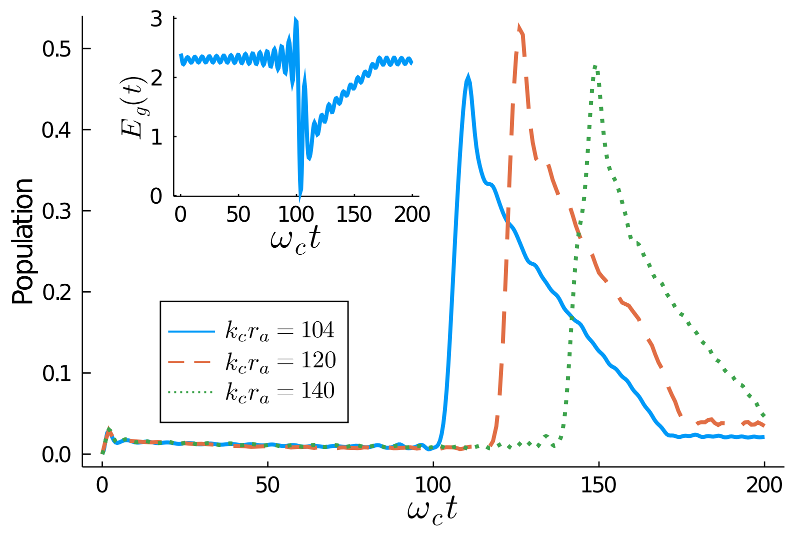


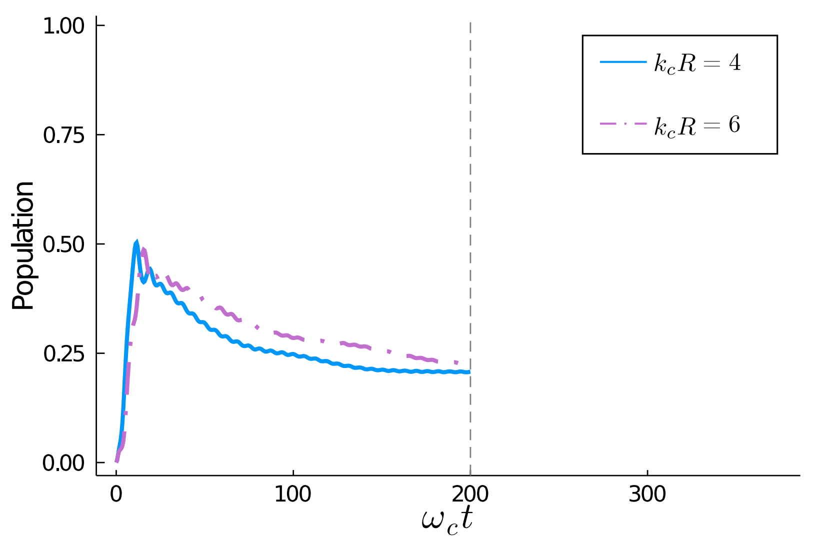
Cartoonish Explanation



Transient Activation



Permanent Transition



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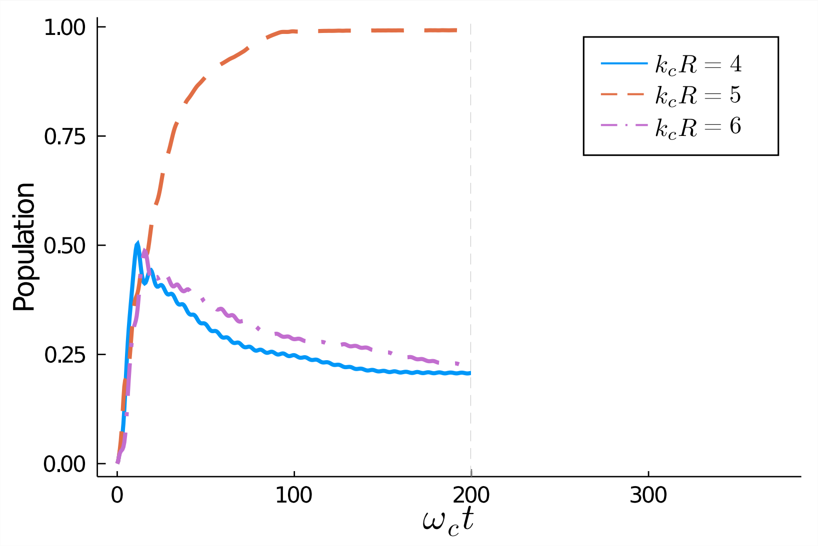

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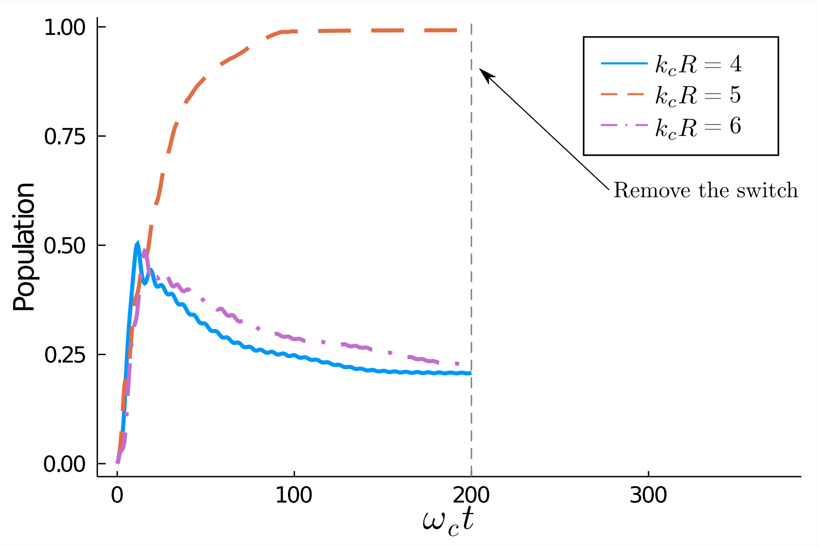

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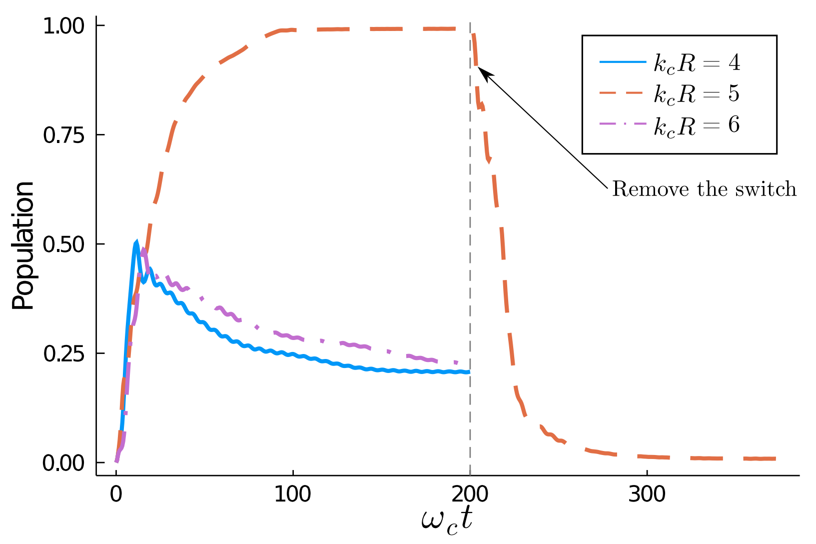
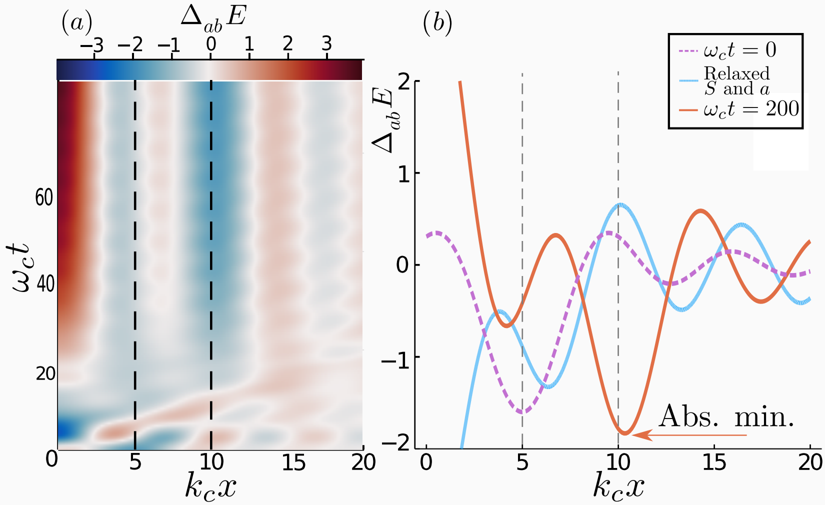


Reorganization Energy Landscape



Switch Energy Landscape