Quantum model of allosteric signalling as a non-Markovian effect

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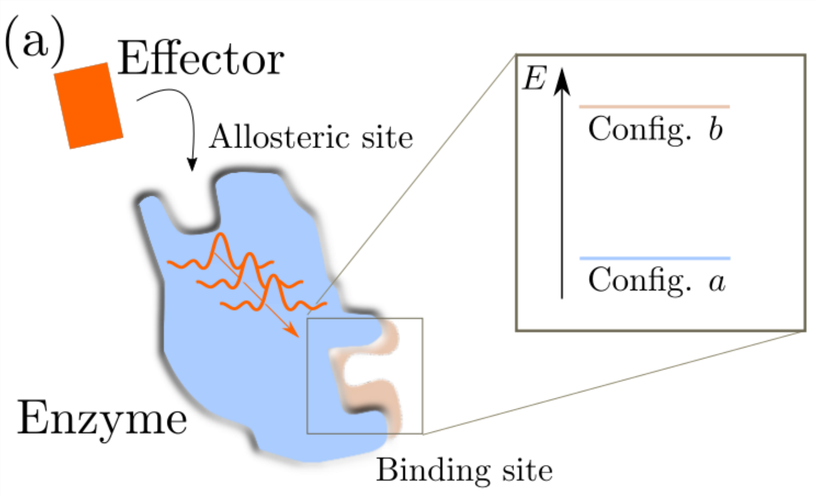
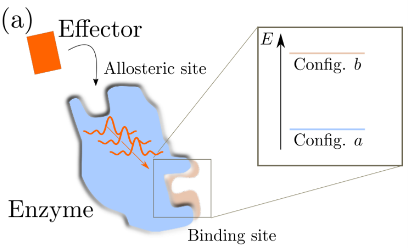
University of St Andrews

Allostery



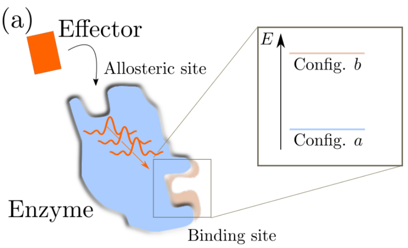
(a)
Effector
Allosteric site
Enzyme
Binding site
E
Config. b
Config. a

Allostery



Key Properties

Allostery



Key Properties

- At-a-distance influence

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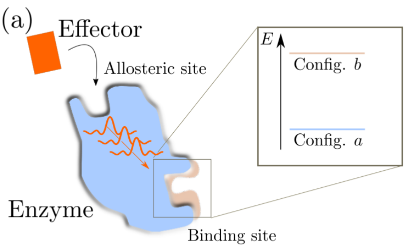

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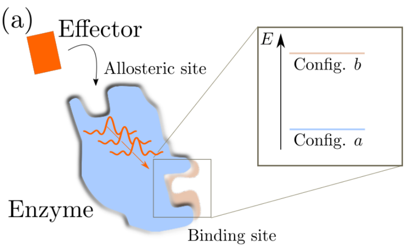
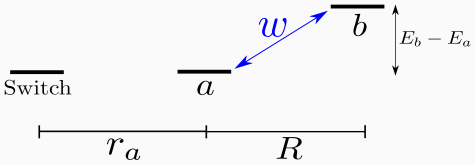


Key Properties

- At-a-distance influence
- Reversible
- Mechanical (?)

Simplified Model



$$\hat{H} = \sum_{\gamma=S,a,b} E_\gamma \hat{P}_\gamma + w \left(|a\rangle \langle b| + \text{h.c.} \right)$$

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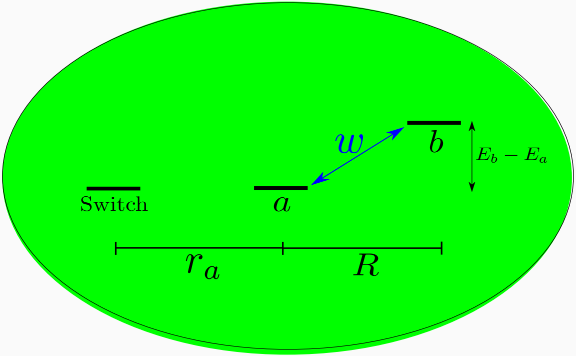

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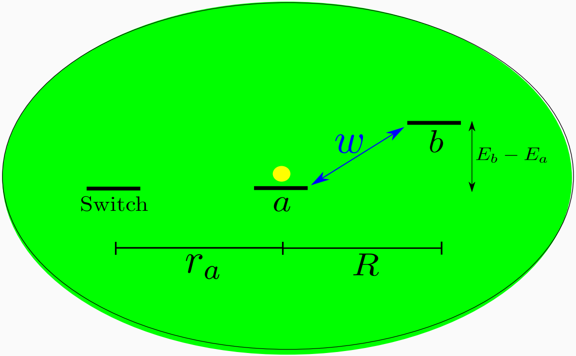

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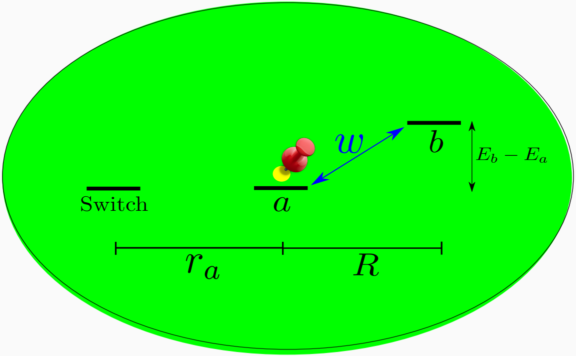

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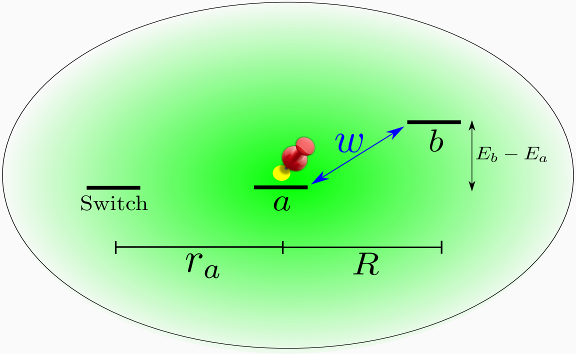

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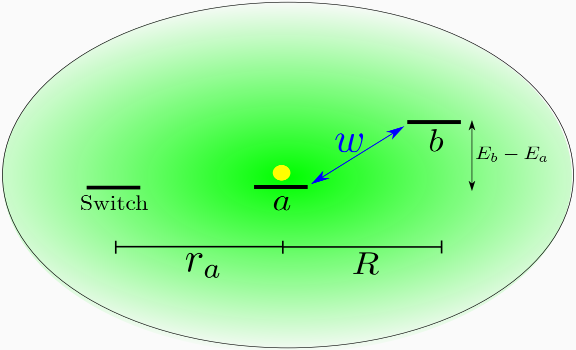

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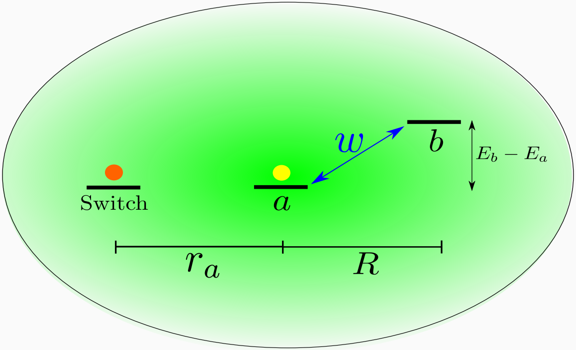

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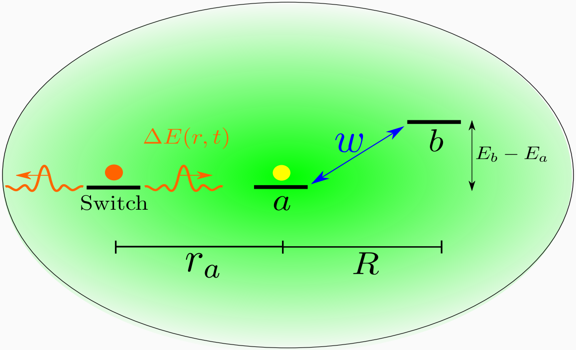

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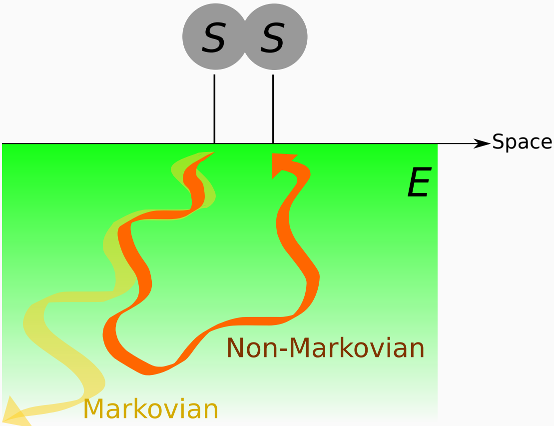
Shared History Matters

Non-Markovian Environment

- $\tau_E \sim \tau_S$



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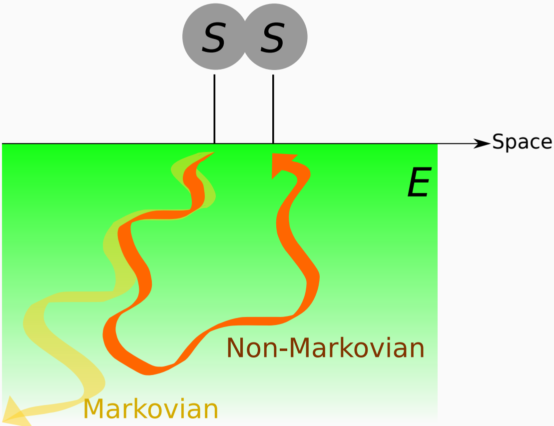

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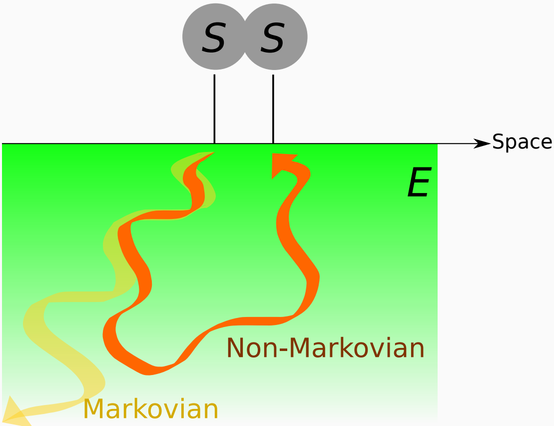

Shared History Matters

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

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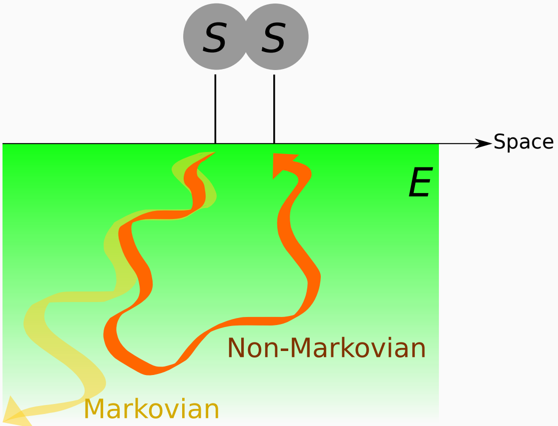
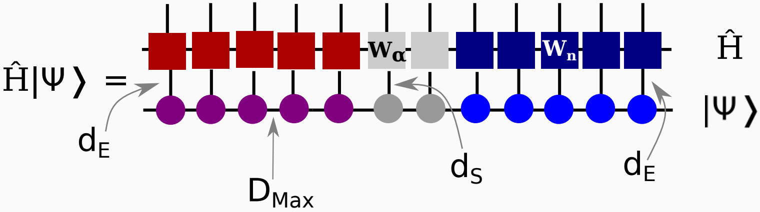


Matrix Product State Ansatz for the system-environment wave-function



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

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

Results

Reorganization Dynamics

Pedagogical case: separable state

Reorganization Dynamics

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Trace out the bath d.o.f

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

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

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

Reorganization Dynamics

For a bath with a hard cut-off Ohmic spectral density

$$J(\omega) = 2\alpha\omega H(\omega_c - \omega)$$

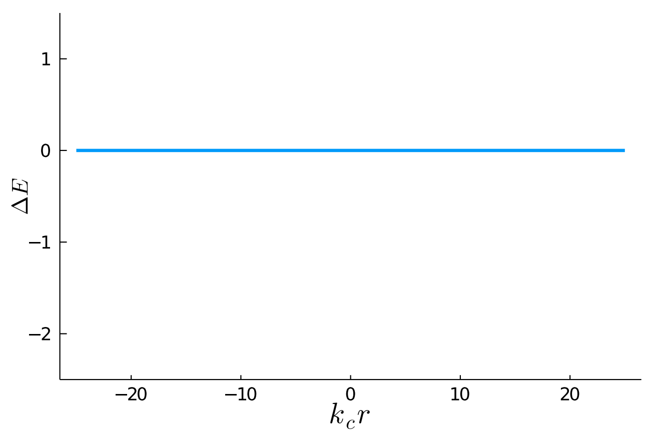
the energy shift takes the form

$$\Delta E(r_\gamma, t) = \frac{-\varsigma_\gamma 2\lambda \sin(k_c r_\gamma)}{k_c r_\gamma} + \varsigma_\gamma \sum_{\xi=\pm 1} \frac{\lambda \sin(k_c(r_\gamma - \xi ct))}{k_c(r_\gamma - \xi ct)} \ .$$

With the reorganisation energy $\lambda = \int_{\mathbb{R}} \frac{J(\omega)}{\omega} \mathrm{d}\omega = 4\alpha\omega_c$.

Reorganization Dynamics

$$\Delta E(r_\gamma, t) = \frac{-2\lambda \sin(k_c r_\gamma)}{k_c r_\gamma} + \frac{\lambda \sin(k_c(r_\gamma - ct))}{k_c(r_\gamma - ct)} + \frac{\lambda \sin(k_c(r_\gamma + ct))}{k_c(r_\gamma + ct)}$$



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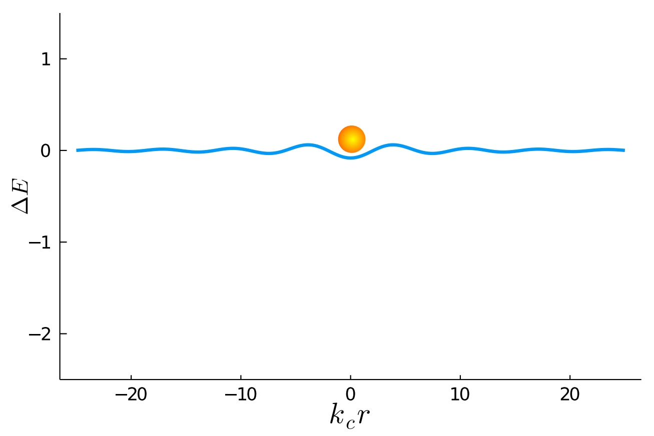

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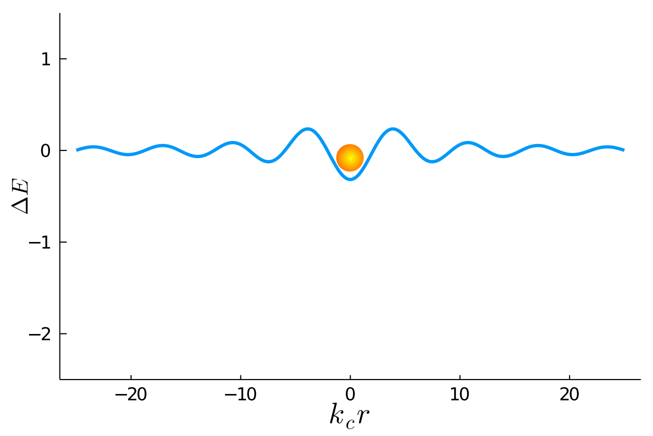

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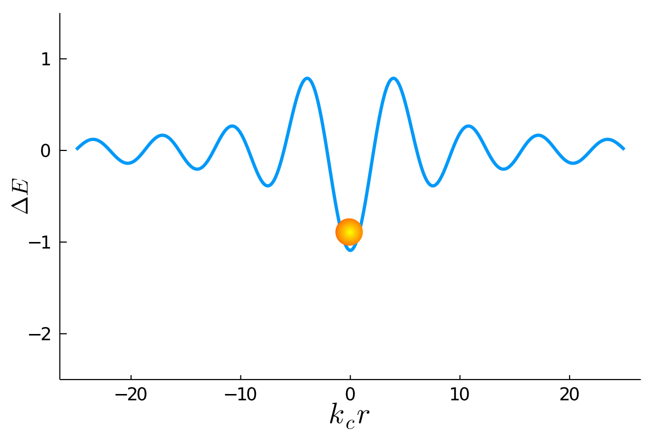

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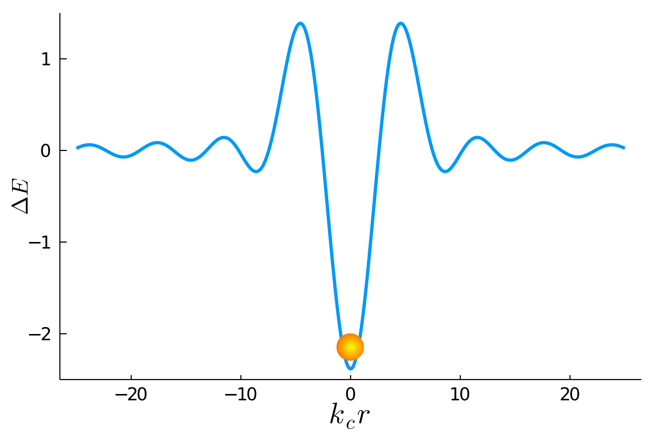

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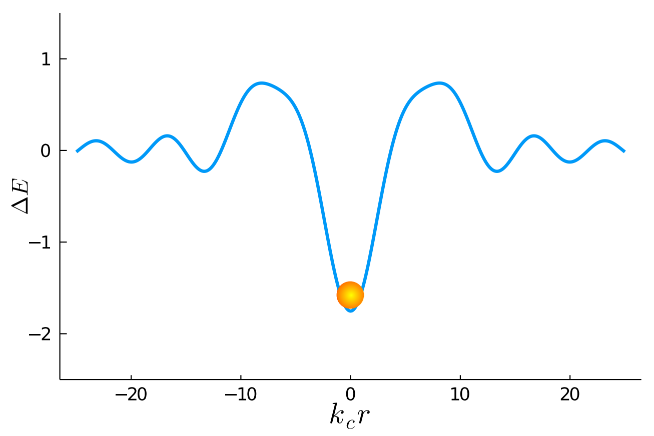

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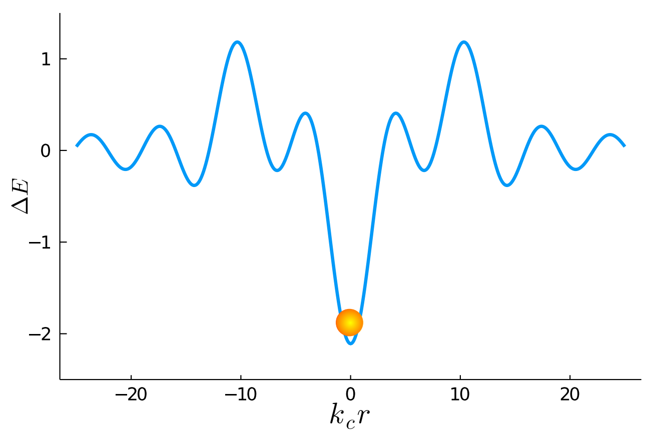

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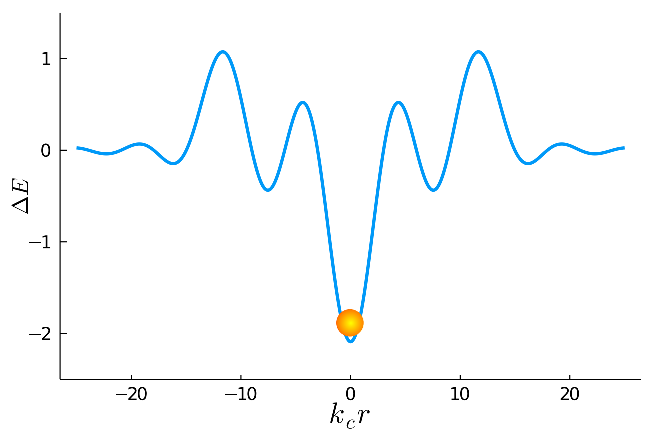

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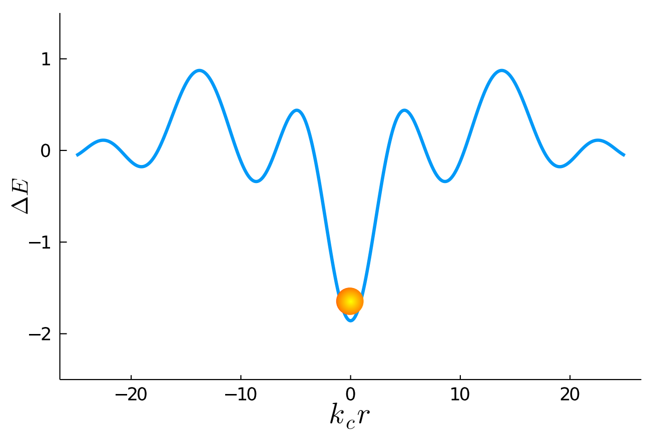

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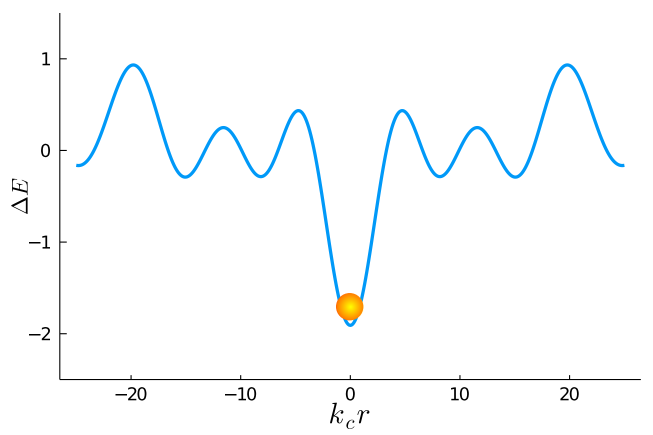

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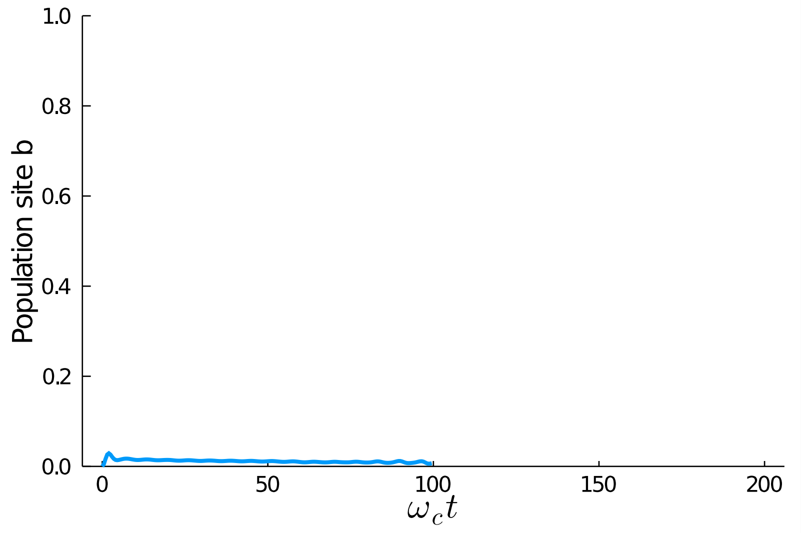

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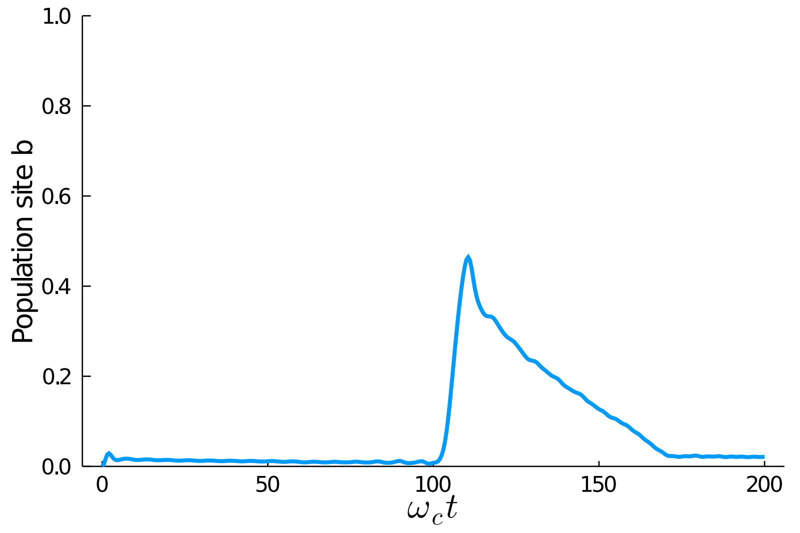

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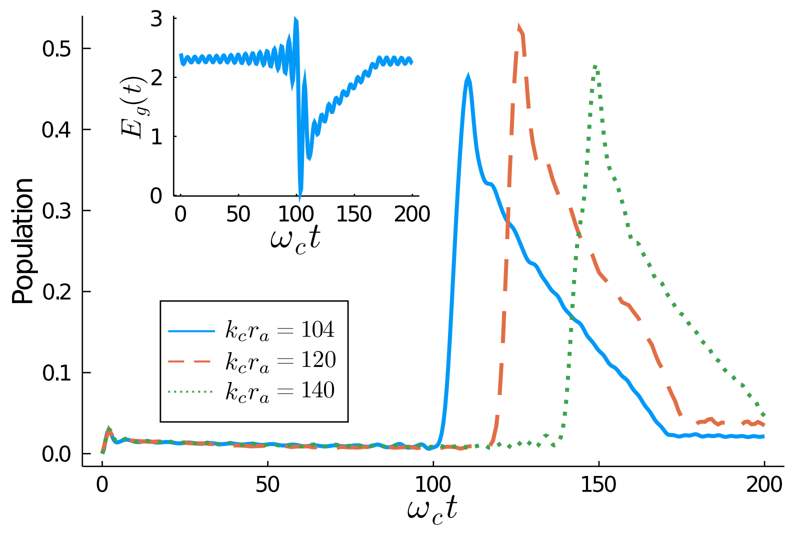

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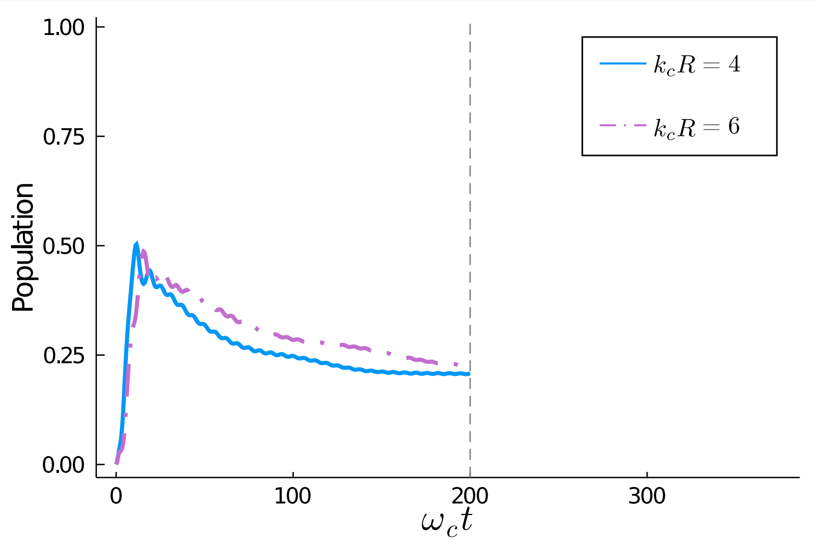

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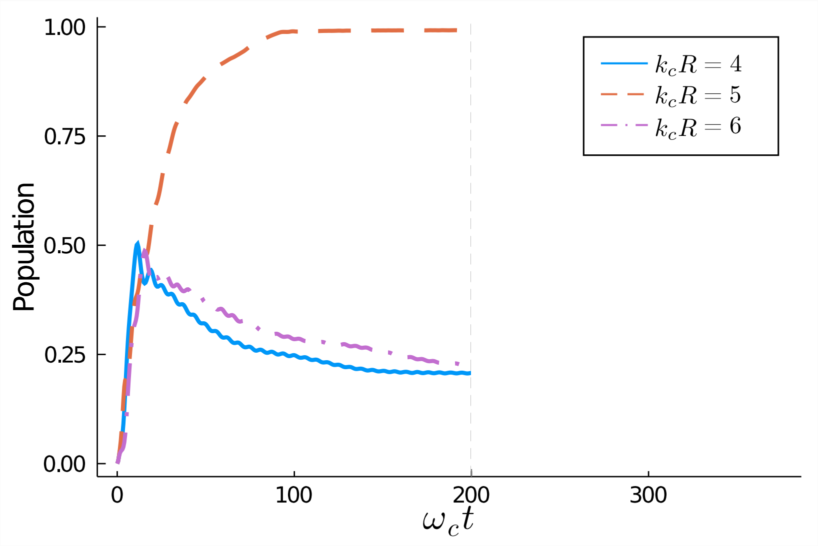

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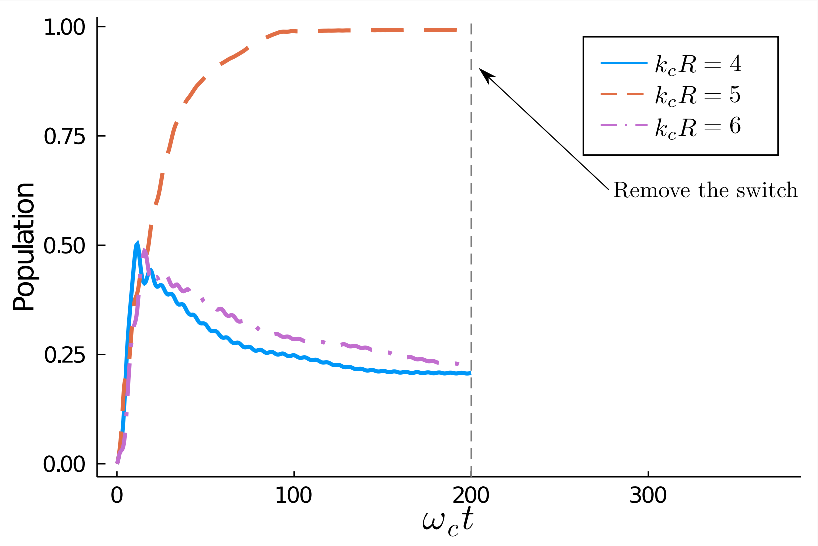

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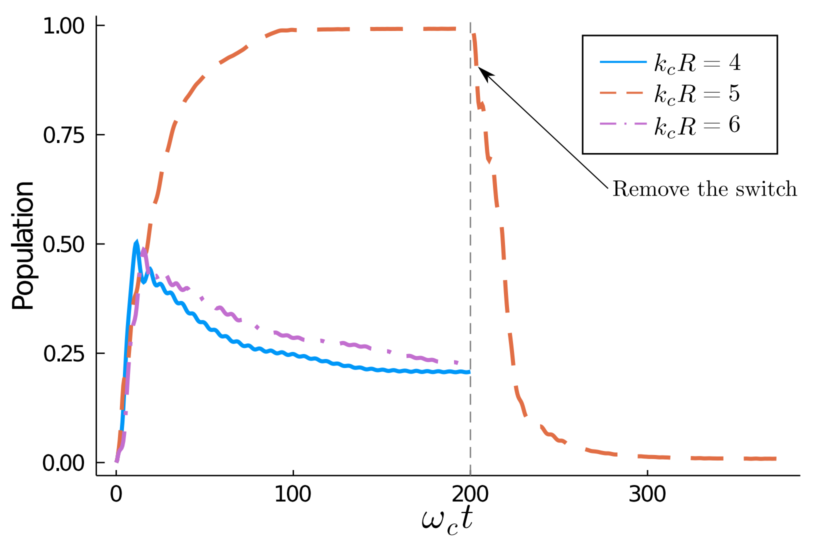
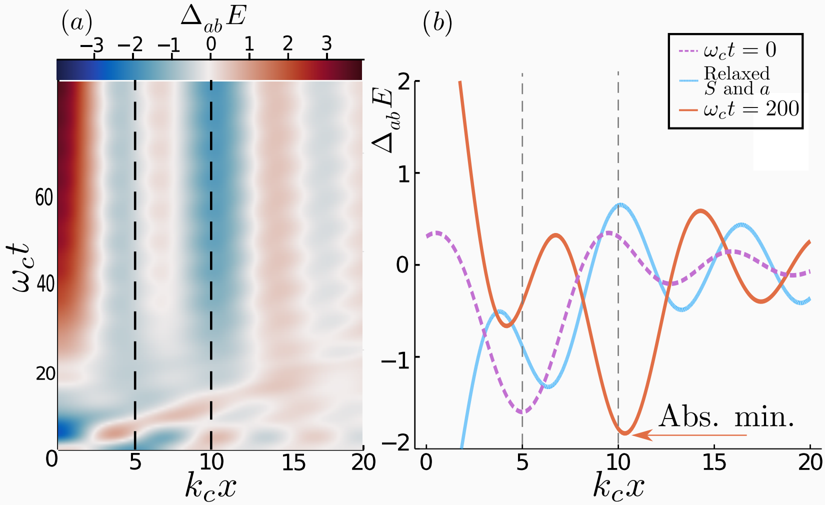


Reorganization Energy Landscape



Conclusion

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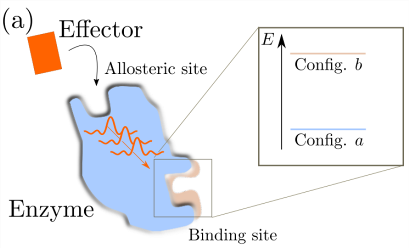

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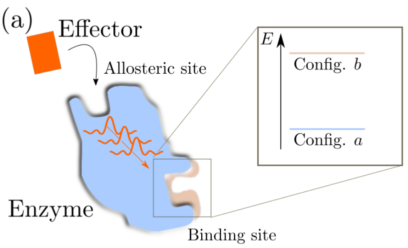

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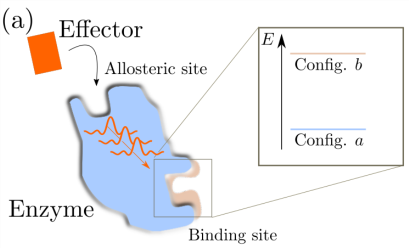

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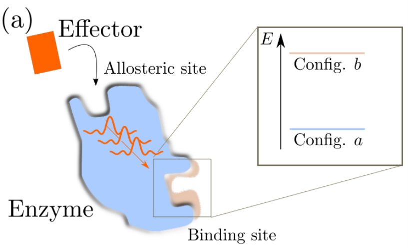

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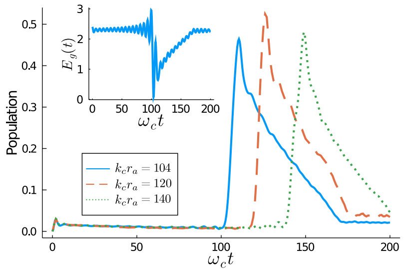

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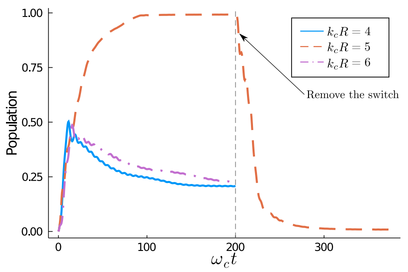
  - ◇ Transient Activation
  - ◇ Conformal Activation



Conclusion

Take Away

- OQS model of environmentally mediated signalling
- Common features with allosteric regulation
- Two types of processes

Outlook

Conclusion

Take Away

- OQS model of environmentally mediated signalling
- Common features with allosteric regulation
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Outlook

⚠ Purely Quantum Effects?

Conclusion

Take Away

- OQS model of environmentally mediated signalling
- Common features with allosteric regulation
- Two types of processes

Outlook

- ⚠ Purely Quantum Effects?
- ⚠ Sensing and Control?

Conclusion

Thank you for your attention!

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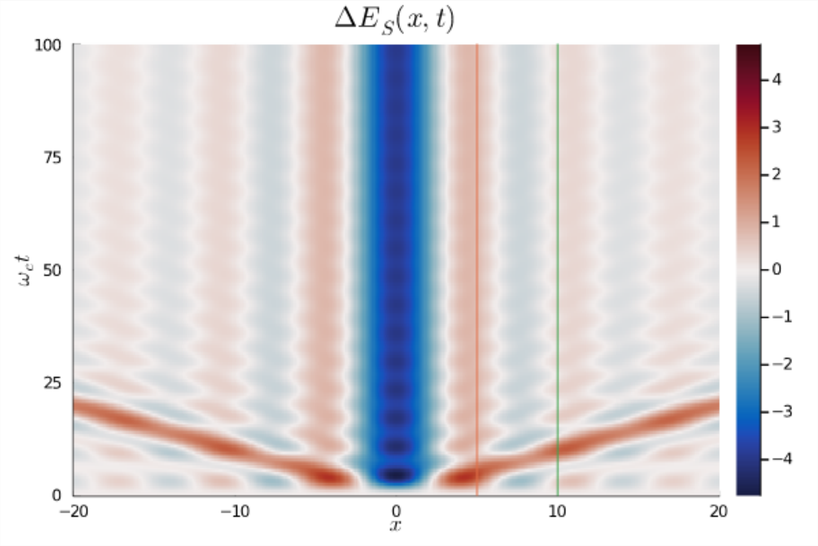
SCAN ME

https://arxiv.org/abs/2205.11247

You want to know more?

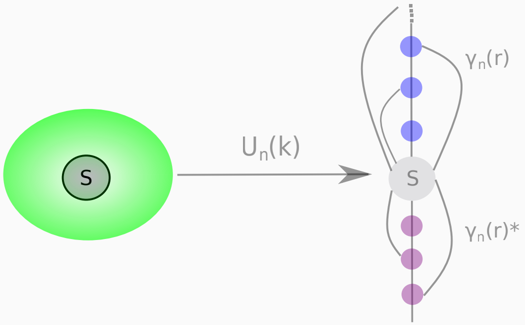
Switch Energy Landscape



Methods

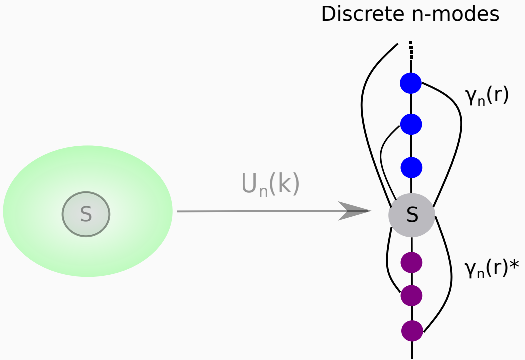
Environment-Chain Mapping

Continuous k-modes



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

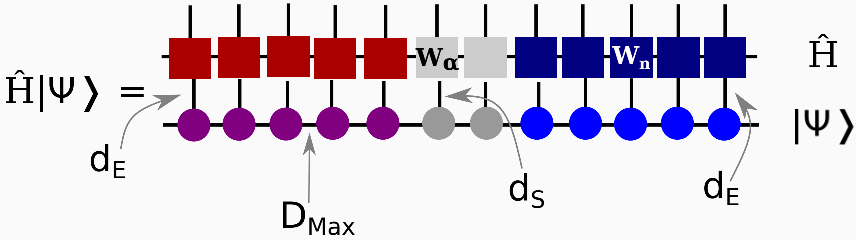
Environment-Chain Mapping



$$\hat{H}_B + \hat{H}_{\text{int}} = \sum_n \omega_n(\hat{c}_n^\dagger \hat{c}_n + \hat{d}_n^\dagger \hat{d}_n) + t_n(\hat{c}_n^\dagger \hat{c}_{n+1} + \hat{d}_n^\dagger \hat{d}_{n+1} + \text{h.c.})$$

$$+ \sum_\alpha \hat{P}_\alpha \sum_n \left(\gamma_n(r_\alpha)(\hat{c}_n + \hat{d}_n^\dagger) + \text{h.c.}\right)$$

Tensor Networks

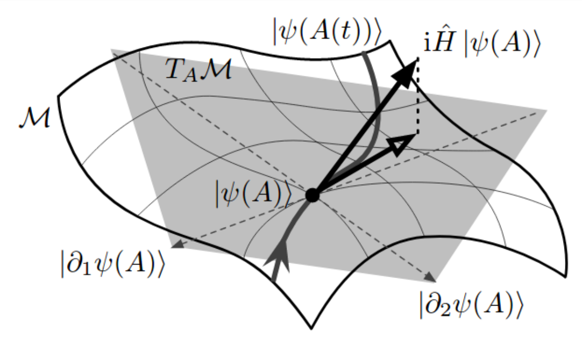


$$|\psi\rangle = \sum_{\{i_k\}} \sum_{\{\alpha\}} T_{i_1}^{\alpha_1} T_{i_2}^{\alpha_1 \; \alpha_2} T_{i_3}^{\alpha_2 \; \alpha_3} \dots T_{i_N}^{\alpha_{N-1}} |\phi_{i_1} \dots \phi_{i_N}\rangle$$

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

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

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