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

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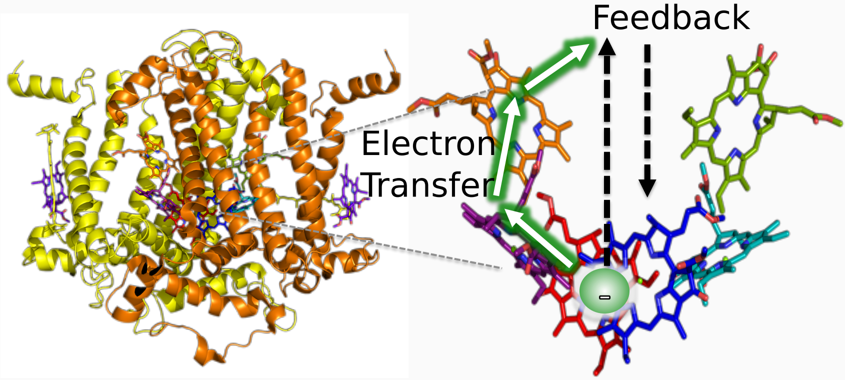
Light-matter Interactions from scratch

22/11/2021



Light-Harvesting Complexes

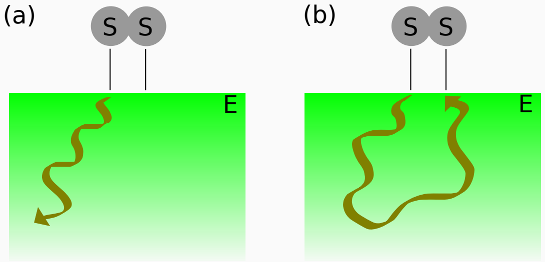
(Non-)Markovian Environment

Markovian

- $\tau_E << \tau_S$

Non-Markovian

- $\tau_E \sim \tau_S$



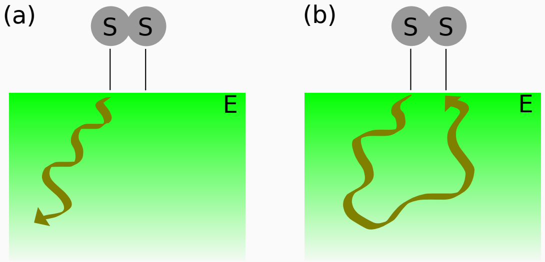
(Non-)Markovian Environment

Markovian

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

Non-Markovian

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



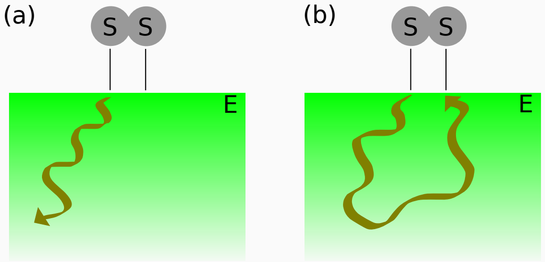
(Non-)Markovian Environment

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

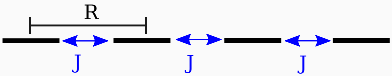


Simplified Model

Open Quantum System

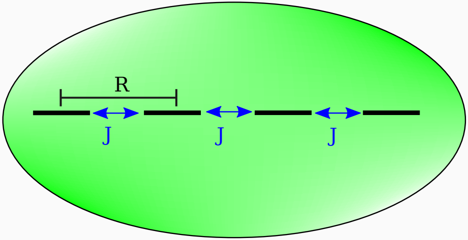
$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha \left|\alpha\right\rangle \left\langle\alpha\right|$$

Open Quantum System



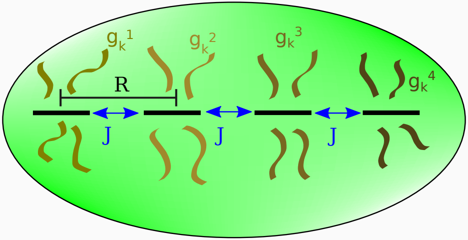
$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha |\alpha\rangle\langle\alpha| + \sum_{\alpha=1}^{N-1} J\left(|\alpha\rangle\langle\alpha+1| + \text{h.c.}\right)$$

Open Quantum System



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

Open Quantum System

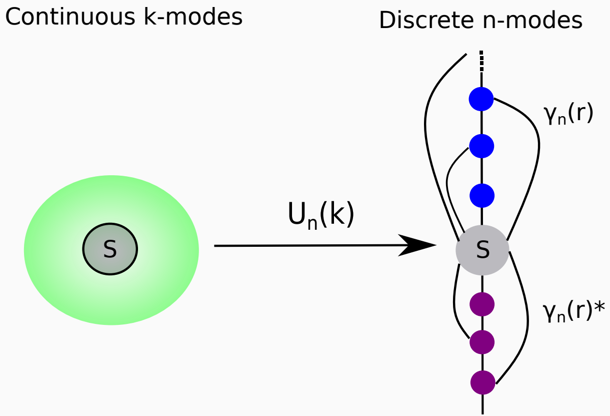


$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha |\alpha\rangle\langle\alpha| + \sum_{\alpha=1}^{N-1} J\left(|\alpha\rangle\langle\alpha+1| + \text{h.c.}\right)$$

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

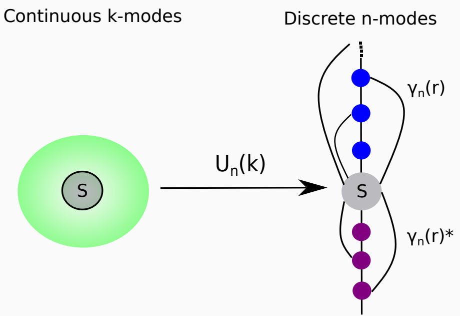
Methods

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)

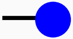
Environment-Chain Mapping

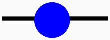


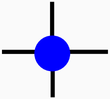
$$\hat{H}_B + \hat{H}_{\text{int}} = \sum_n \omega_n(\hat{c}_n^\dagger \hat{c}_n + \hat{d}_n^\dagger \hat{d}_n)$$
$$+ t_n(\hat{c}_n^\dagger \hat{c}_{n+1} + \hat{c}_{n+1}^\dagger \hat{c}_n + \hat{d}_n^\dagger \hat{d}_{n+1} + \hat{d}_{n+1}^\dagger \hat{d}_n)$$
$$+ \sum_\alpha |\alpha\rangle\langle\alpha|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

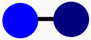
Diagrammatic Notation

a  Scalar

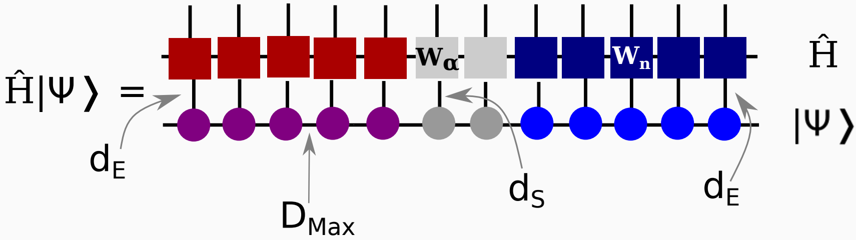
a_i  Vector

a_{ij}  Matrix

a_{ijkl}  Rank-4 Tensor

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

$M\mathbf{a}$  Vector

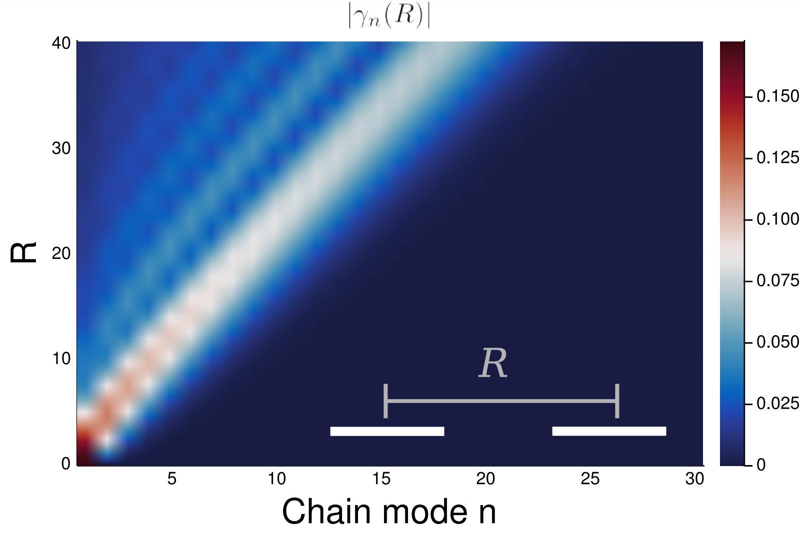


$$|\psi\rangle = \sum_{\{i_k\}} \sum_{\{\alpha\}} T_{i_1}^{\alpha_1} T_{i_2}^{\alpha_1 \ \alpha_2} T_{i_3}^{\alpha_2 \ \alpha_3} \dots T_{i_N}^{\alpha_{N-1}} |\phi_{i_1} \dots \phi_{i_N}\rangle$$

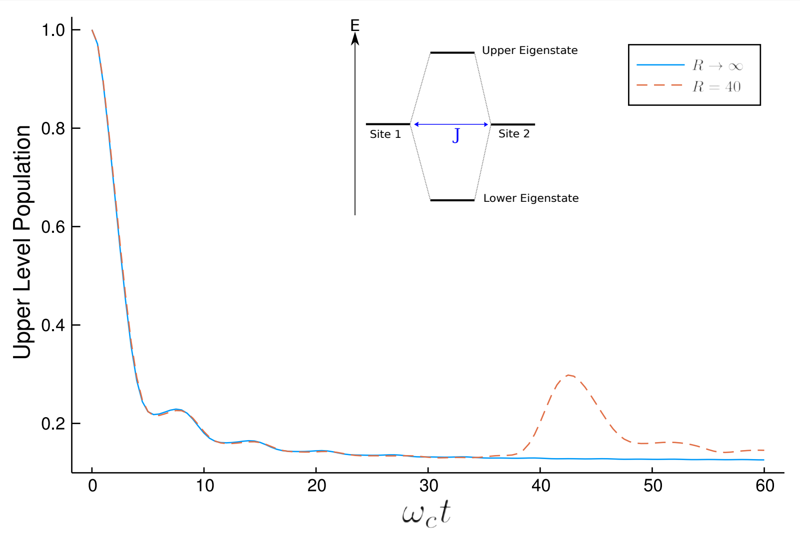
$$\hat{H} = \sum_{\{\sigma\},\{\sigma'\},\{w\}} W_{1 \ w_1}^{\sigma_1 \sigma_1'} W_{2 \ w_1 w_2}^{\sigma_2 \sigma_2'} \dots W_{N \ w_{N-1}}^{\sigma_N \sigma_N'} |\sigma_1 \dots \sigma_N\rangle \langle \sigma_1' \dots \sigma_N'| \ .$$

Results

Couplings $\gamma_n(R)$ at Zero Temperature

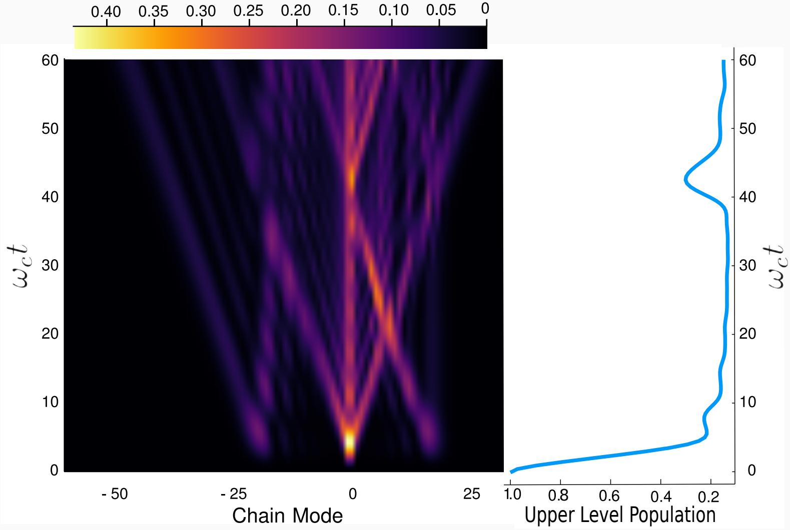


Non-Markovian Dynamics

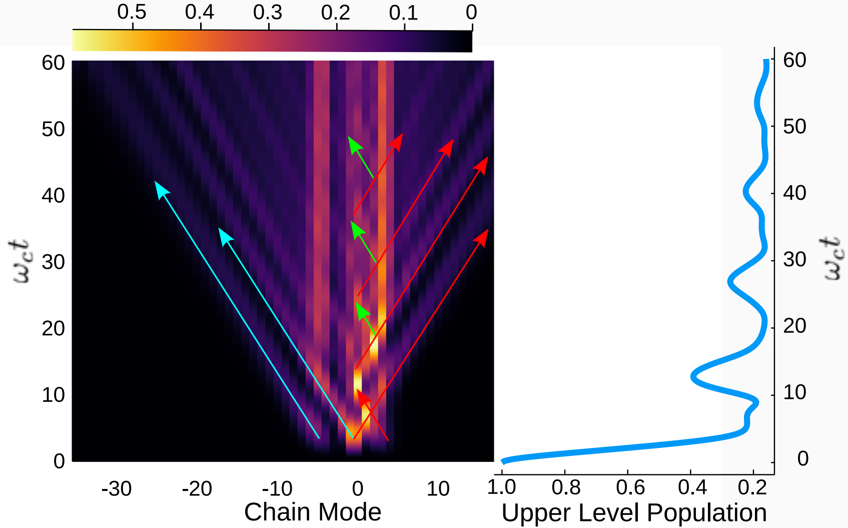


Lacroix et al., Phys. Rev. A, 104(5), 052204 (2021)

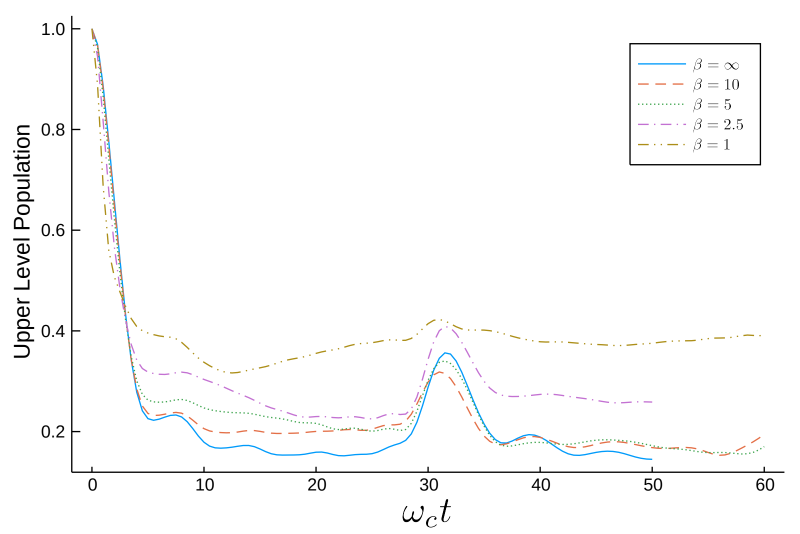
Environment Feedback



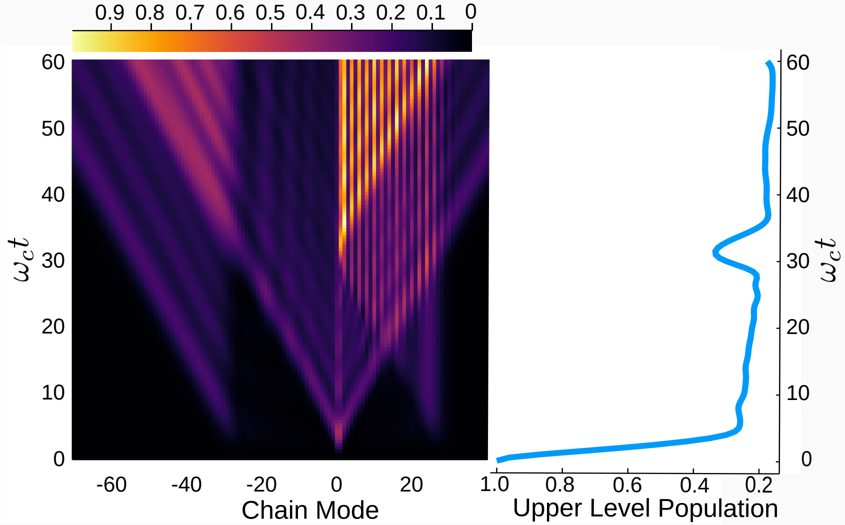
Environment Feedback II



Finite Temperature



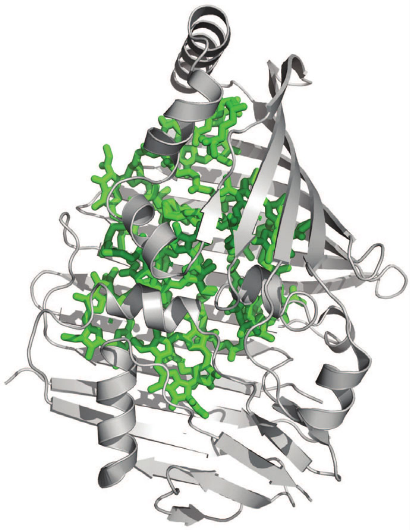
Finite Temperature II



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!

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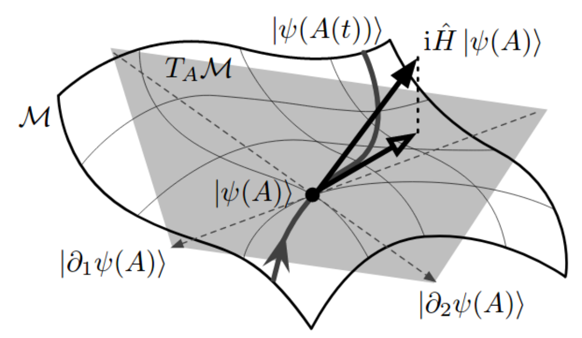
You want to know more?

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

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

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

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

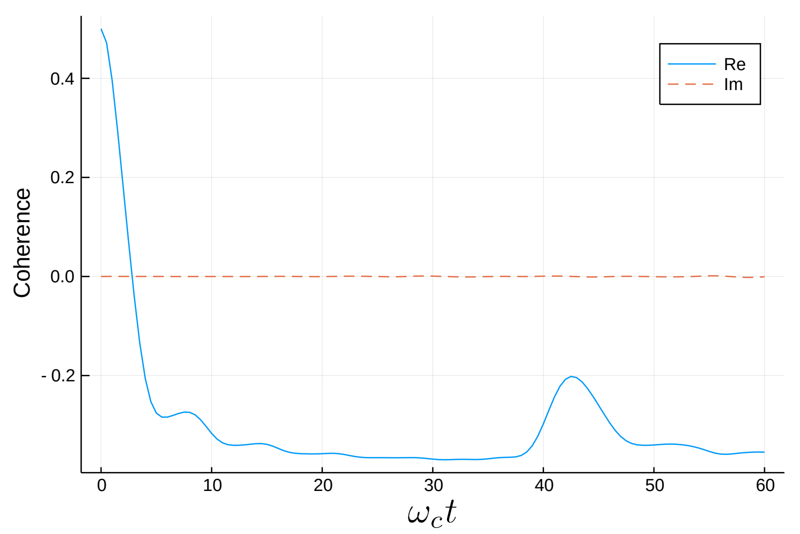
$$\hat{H}_{\text{int}} = \hat{O} \sum_k (g_k \hat{a}_k + \text{h.c.}) \ ,$$

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