Environment-mediated communication in open systems using tensor networks

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QICS Small Seminar

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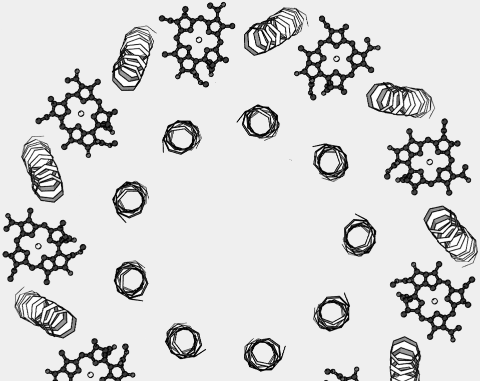
Quantum information center
SORBONNE UNIVERSITÉ



The Model

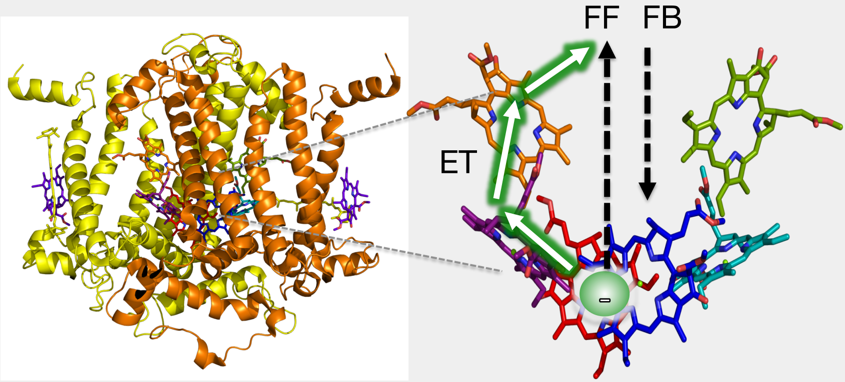
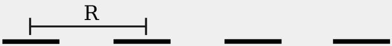
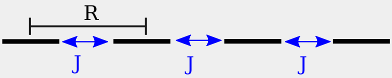


Figure: (Left) The protein structure of a nanoscale photosynthetic reaction centre. (Right) Molecules active in charge separation.

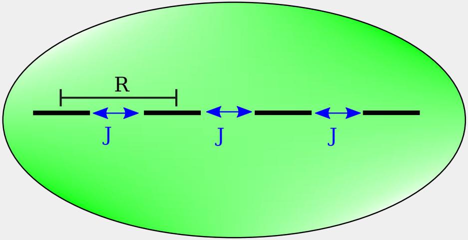
Hamiltonian



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

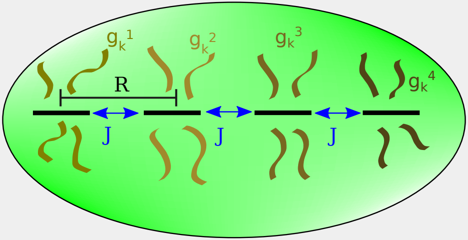


$$\hat{H} = \sum_{\alpha=1}^{N} E_{\alpha} |\alpha\rangle \langle\alpha| + \sum_{\alpha=1}^{N-1} J \left(|\alpha\rangle \langle\alpha + 1| + \text{h.c.} \right)$$



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

Hamiltonian



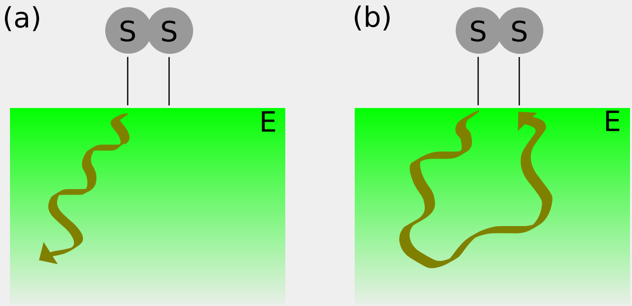
$$\hat{H} = \sum_{\alpha=1}^{N} E_\alpha |\alpha\rangle\langle\alpha| + \sum_{\alpha=1}^{N-1} J\left(|\alpha\rangle\langle\alpha+1| + \text{h.c.}\right) + \int_{-k_c}^{+k_c} \omega_k \hat{a}_k^\dagger \hat{a}_k \mathrm{d}k + \sum_\alpha |\alpha\rangle\langle\alpha| \int_{-k_c}^{+k_c} (g_k^\alpha \hat{a}_k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

Markovian

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

Non-Markovian

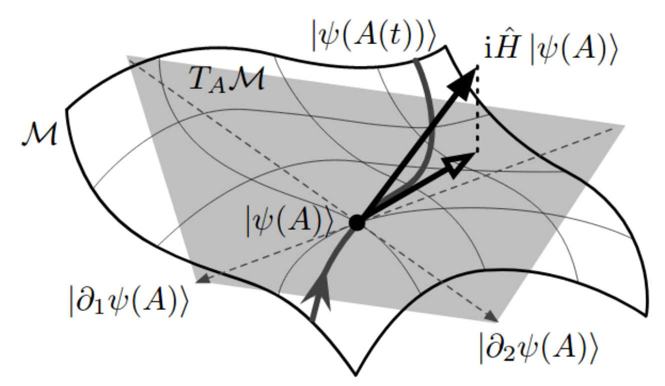
- $\tau_E \sim \tau_S$
- Strong Coupling
- Non time-local Master Equations



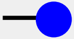
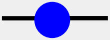
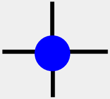
Methods

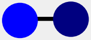
Time-Dependent Variational Principle

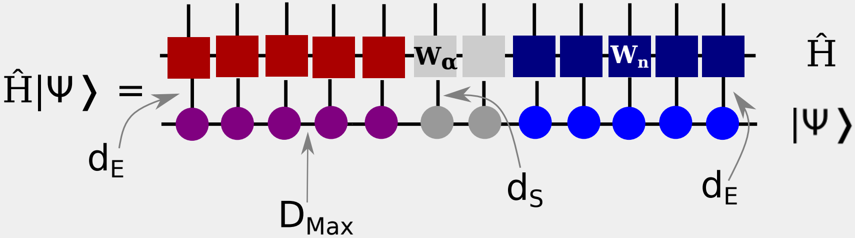
$$\frac{\partial}{\partial t}|\psi\rangle = -\mathrm{i}\hat{P}_{T_{|\psi\rangle}}\hat{H}|\psi\rangle$$



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



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

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

Time Evolving Density operator with Orthonormal Polynomials

Goal: transform a continuous environment into a discrete one.

$$\hat{H}_E + \hat{H}_{\text{int}} = \int_0^{+k_c} \mathrm{d}k \omega_k (\hat{a}_k^\dagger \hat{a}_k + \hat{b}_k^\dagger \hat{b}_k) + \sum_\alpha |\alpha\rangle \langle\alpha| \int_0^{+k_c} \mathrm{d}k g_k \left(\mathrm{e}^{\mathrm{i}kr_\alpha} (\hat{a}_k + \hat{b}_k^\dagger) + \text{h.c.} \right)$$

with $\hat{b}_k \overset{\text{def.}}{=} \hat{a}_{-k}$.

Orthonormal Polynomials

We define the polynomials with

$$\int_0^{+k_c} P_n(k)P_m(k)J(k)\mathrm{d}k = \delta_{n,m} \text{ where } J(k) = |g_k|^2.$$

And the unitary transformations

$$\hat{a}_{k\geq 0} = \sum_n U_n(k)\hat{c}_n \ ,$$
$$\hat{b}_{k\geq 0} = \sum_m V_m(k)\hat{d}_m$$

where the matrix elements are

$$U_n(k) = V_n(k) = \sqrt{J(k)}P_n(k) \ .$$

Chains' Hamiltonians

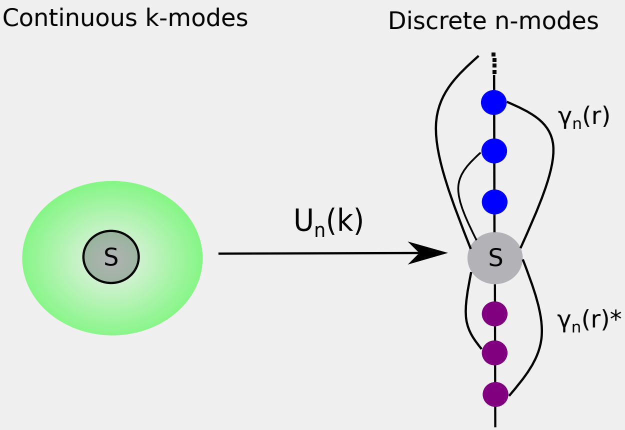
The bath and interaction Hamiltonians become

$$\hat{H}_E = \sum_n \omega_n (\hat{c}_n^\dagger \hat{c}_n + \hat{d}_n^\dagger \hat{d}_n) + t_n (\hat{c}_n^\dagger \hat{c}_{n+1} + \hat{c}_{n+1}^\dagger \hat{c}_n + \hat{d}_n^\dagger \hat{d}_{n+1} + \hat{d}_{n+1}^\dagger \hat{d}_n) \ ,$$

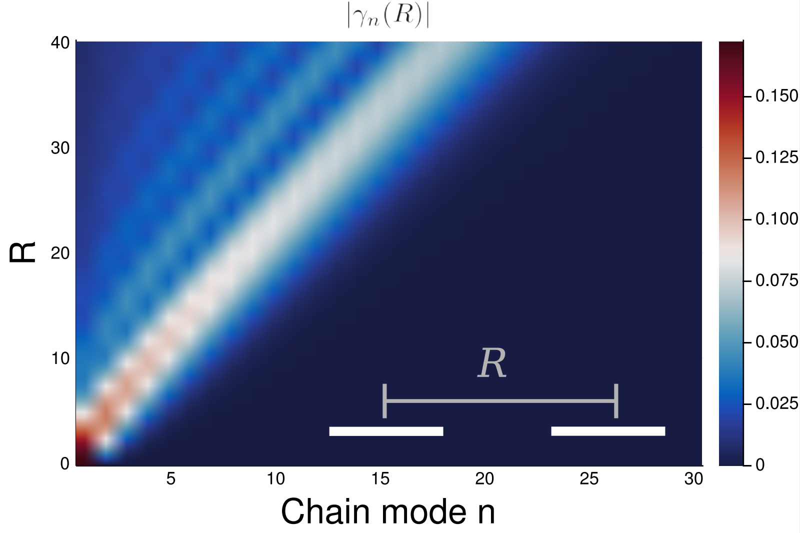
$$\hat{H}_{\text{int}} = \sum_\alpha |\alpha\rangle \langle\alpha| \sum_n \left(\gamma_n(r_\alpha)(\hat{c}_n + \hat{d}_n^\dagger) + \text{h.c.} \right) \ ,$$

where

$$\gamma_n(r_\alpha) = \int_0^{+k_c} \mathrm{d}k \, J(k) P_n(k) \mathrm{e}^{\mathrm{i}kr_\alpha} \ .$$

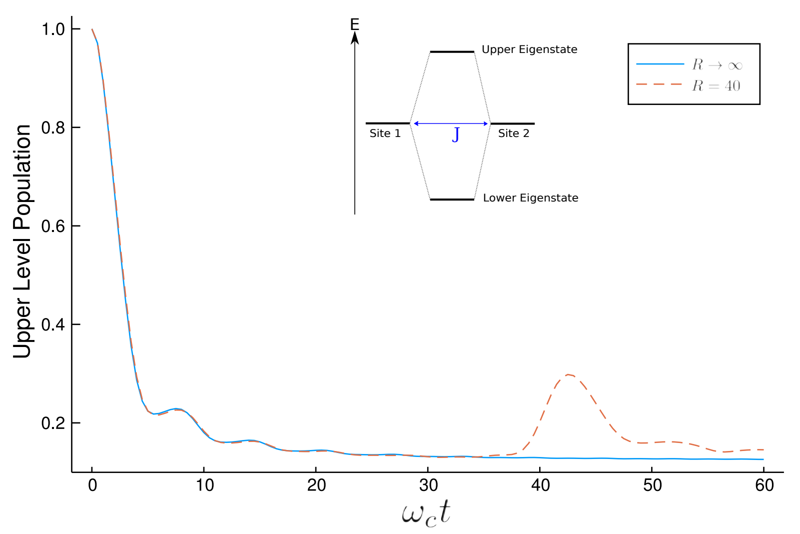

Continuous k-modes
Discrete n-modes
S
Uₙ(k)
S
γₙ(r)
γₙ(r)*

Long Range Couplings

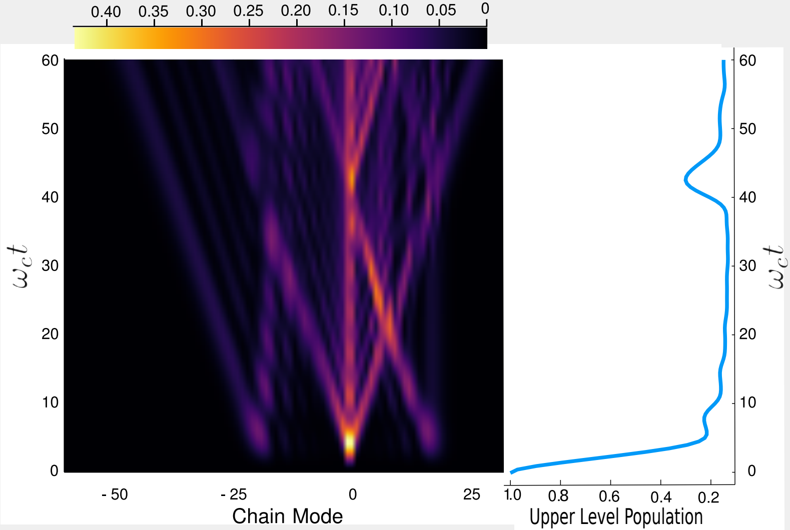


Results

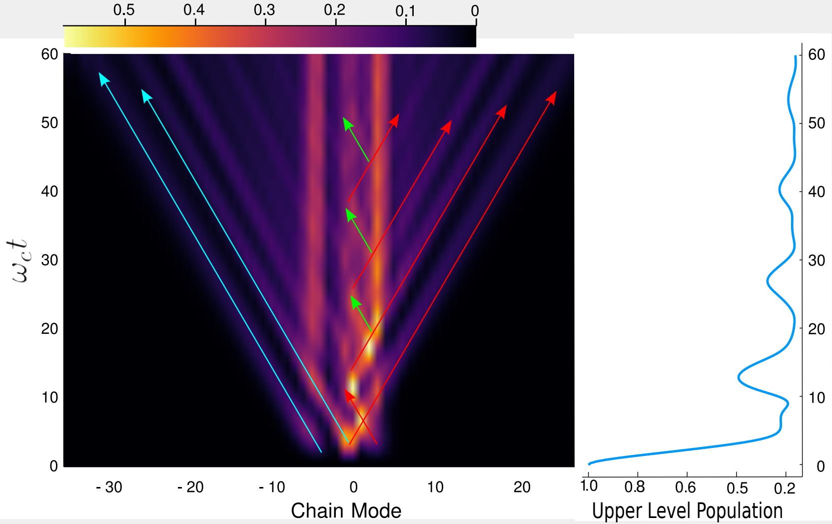
Eigen-Population Revivals



Bath Dynamics

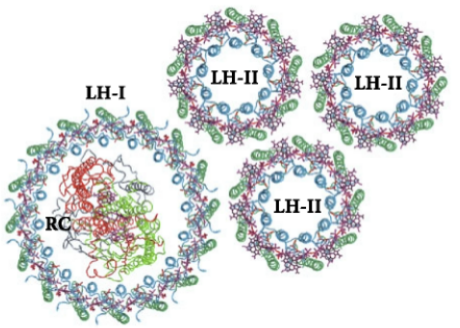


Multiple Revivals



Outlook

- Works at finite T ✓
- Multi-site dynamics ⚠
- More complex relations between modes and the spatial structure
- Different topologies ⚠



Thank you for listening!

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INSP Institut des Nanosciences de Paris

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

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

Bath Spectral density

For an interaction Hamiltonian

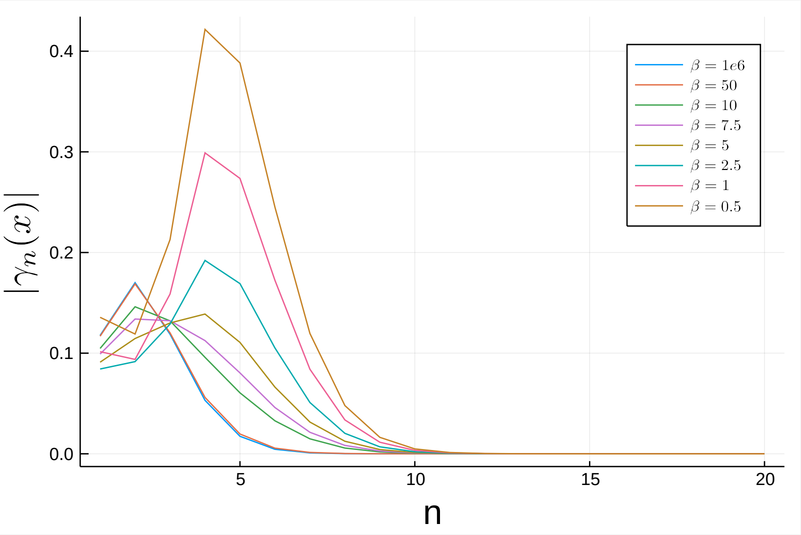
$$\hat{H}_{\text{int}} = \hat{O} \sum_k (g_k \hat{a}_k + \text{h.c.}) \ ,$$

the *Bath Spectral Density* is defined as

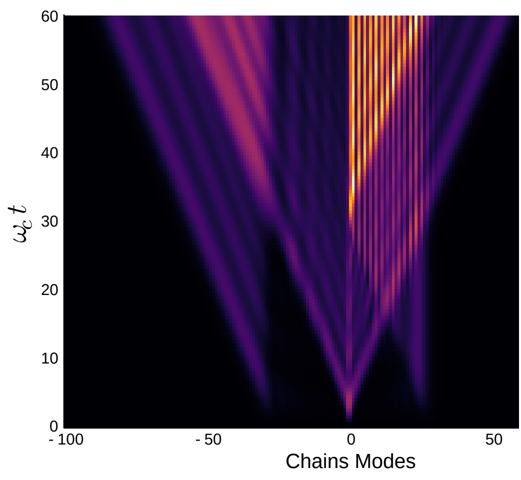
$$J(\omega) = \sum_k |g_k|^2 \delta(\omega - \omega_k) \ .$$

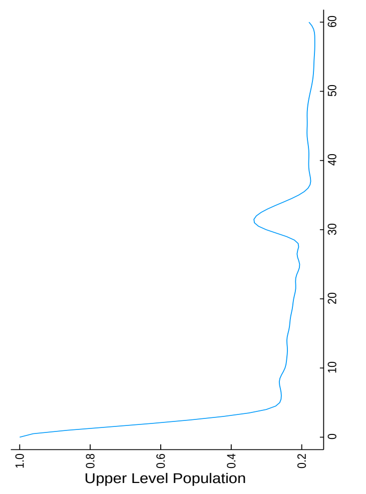
Ohmic spectral density: $J(\omega) = 2\alpha\omega H(\omega_c - \omega)$

Long Range Couplings - Finite T

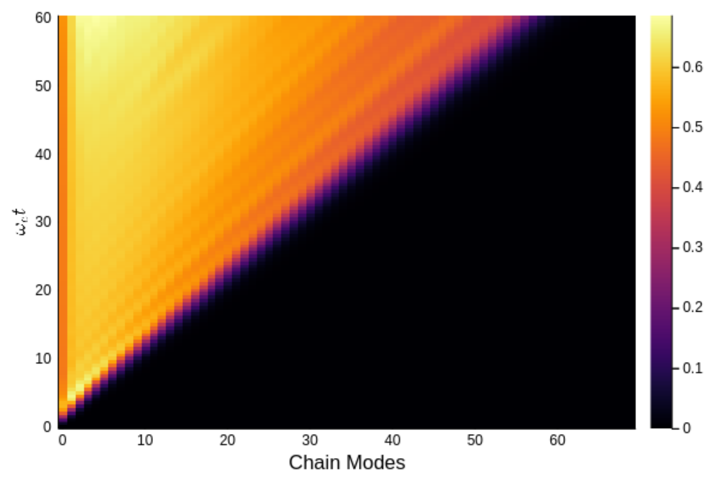


Finite Temperature $\beta = 5$

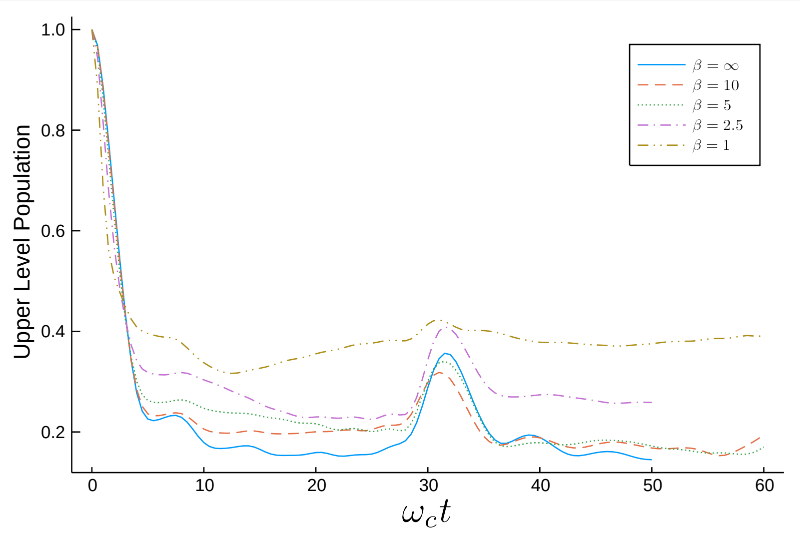




Finite Temperature $\beta = 0.5$ - SBM



Evolution of the Revivals with T



Incoherent Mechanism