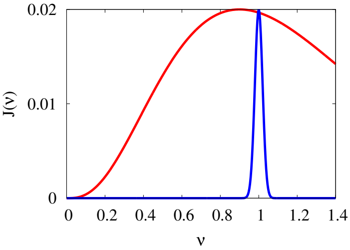
Efficient non-Markovian quantum dynamics using time-evolving matrix product operators

Jonathan Keeling

Charge and Energy Transfer Processes: Open Problems in Open Quantum Systems

Why non-Markovian master equations?

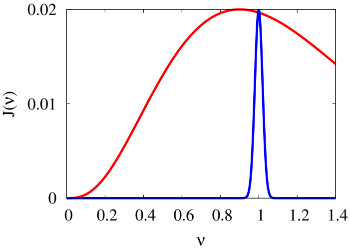


- Born + Markov + Secular
  $\rightarrow$ Lindblad Master equation:

$$\partial_t \rho = \sum_i \kappa_i \mathcal{L}[X_i], \quad \mathcal{L}[X] = X\rho X^\dagger - \frac{1}{2}[X^\dagger X, \rho]_+$$

- Markov good at optical frequencies

Why non-Markovian master equations?



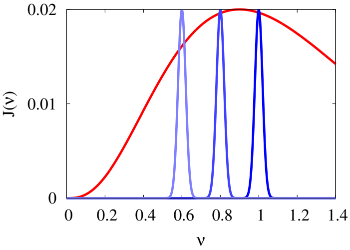
- Why non-Markovian?
  - Strong energy shifts
  - Can still be time local (non-secular, non-positive): $\partial_t \rho = \sum_{ijkl} X_{ij} X_{kl} J(E_i - E_j) |i\rangle\langle j|\rho|k\rangle\langle l| + \ldots$
- Non-time-local equations

- Born + Markov + Secular
  $\rightarrow$ Lindblad Master equation:

$$\partial_t \rho = \sum_i \kappa_i \mathcal{L}[X_i], \quad \mathcal{L}[X] = X \rho X^\dagger - \frac{1}{2}[X^\dagger X, \rho]_+$$

- Markov good at optical frequencies

Why non-Markovian master equations?



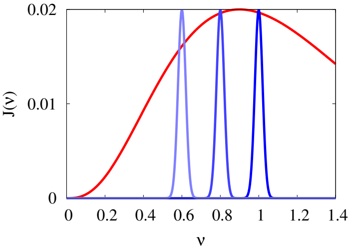
- Why non-Markovian?
  - Strong energy shifts
  - Can still be time local (non-secular, non-positive): $\partial_t \rho = \sum_{ijkl} X_{ij} X_{kl} J(E_i - E_j) |i\rangle\langle j|\rho|k\rangle\langle l| + \ldots$
- Non-time-local equations

- Born + Markov + Secular
  $\rightarrow$ Lindblad Master equation:

$$\partial_t \rho = \sum_i \kappa_i \mathcal{L}[X_i], \quad \mathcal{L}[X] = X \rho X^\dagger - \frac{1}{2}[X^\dagger X, \rho]_+$$

- Markov good at optical frequencies

Why non-Markovian master equations?



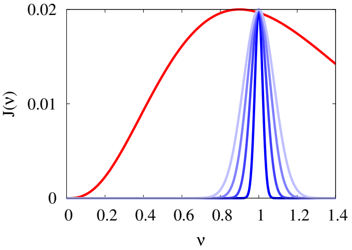
- Why non-Markovian?
  - Strong energy shifts
  - Can still be time local (non-secular, non-positive): $\partial_t \rho = \sum_{ijkl} X_{ij} X_{kl} J(E_i - E_j) |i\rangle\langle j|\rho|k\rangle\langle l| + \ldots$
- Non-time-local equations

- Born + Markov + Secular
  $\rightarrow$ Lindblad Master equation:

$$\partial_t \rho = \sum_i \kappa_i \mathcal{L}[X_i], \quad \mathcal{L}[X] = X\rho X^\dagger - \frac{1}{2}[X^\dagger X, \rho]_+$$

- Markov good at optical frequencies

Why non-Markovian master equations?



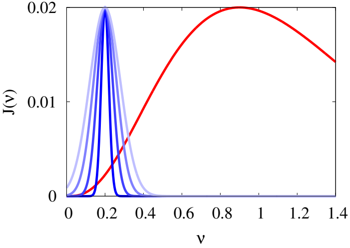
- Born + Markov + Secular
  $\rightarrow$ Lindblad Master equation:

$$\partial_t \rho = \sum_i \kappa_i \mathcal{L}[X_i], \quad \mathcal{L}[X] = X\rho X^\dagger - \frac{1}{2}[X^\dagger X, \rho]_+$$

- Markov good at optical frequencies

- Why non-Markovian?
  - Strong energy shifts
  - Can still be time local (non-secular, non-positive): $\partial_t \rho = \sum_{ijkl} X_{ij} X_{kl} J(E_i - E_j)|i\rangle\langle j|\rho|k\rangle\langle l| + \ldots$
- Non-time-local equations
  - Strong coupling to bath
  - Ultra-strong coupling: need $J(\omega < 0) = 0$ e.g. [Ciuti and Carusotto, PRA '06]
  - Structured baths
    - Vibrational resonances
    - Spatial structure
  - Information return from bath
  - Unknown system eigenstates

Why non-Markovian master equations?



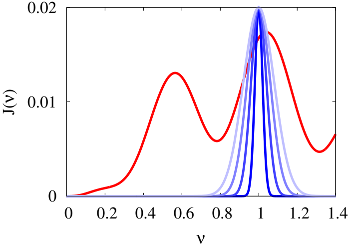
- Born + Markov + Secular
  $\rightarrow$ Lindblad Master equation:

$$\partial_t \rho = \sum_i \kappa_i \mathcal{L}[X_i], \quad \mathcal{L}[X] = X \rho X^\dagger - \frac{1}{2}[X^\dagger X, \rho]_+$$

- Markov good at optical frequencies

- Why non-Markovian?
  - Strong energy shifts
  - Can still be time local (non-secular, non-positive): $\partial_t \rho = \sum_{ijkl} X_{ij} X_{kl} J(E_i - E_j) |i\rangle\langle j|\rho|k\rangle\langle l| + \ldots$
- Non-time-local equations
  - Strong coupling to bath
  - Ultra-strong coupling: need $J(\omega < 0) = 0$ e.g. [Ciuti and Carusotto, PRA '06]
  - Structured baths
    - Vibrational resonances
    - Spatial structure
  - Information return from bath
  - Unknown system eigenstates

Why non-Markovian master equations?



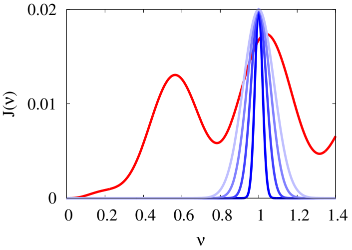
- Born + Markov + Secular
  $\rightarrow$ Lindblad Master equation:

$$\partial_t \rho = \sum_i \kappa_i \mathcal{L}[X_i], \quad \mathcal{L}[X] = X\rho X^\dagger - \frac{1}{2}[X^\dagger X, \rho]_+$$

- Markov good at optical frequencies

- Why non-Markovian?
  - Strong energy shifts
  - Can still be time local (non-secular, non-positive): $\partial_t \rho = \sum_{ijkl} X_{ij} X_{kl} J(E_i - E_j) |i\rangle\langle j|\rho|k\rangle\langle l| + \ldots$
- Non-time-local equations
  - Strong coupling to bath
  - Ultra-strong coupling: need $J(\omega < 0) = 0$ e.g. [Ciuti and Carusotto, PRA '06]
  - Structured baths
    - Vibrational resonances
    - Spatial structure
  - Information return from bath
  - Unknown system eigenstates

Why non-Markovian master equations?



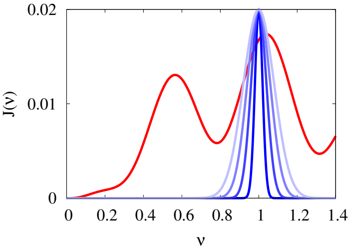
- Born + Markov + Secular
  $\rightarrow$ Lindblad Master equation:

$$\partial_t \rho = \sum_i \kappa_i \mathcal{L}[X_i], \quad \mathcal{L}[X] = X\rho X^\dagger - \frac{1}{2}[X^\dagger X, \rho]_+$$

- Markov good at optical frequencies

- Why non-Markovian?
  - Strong energy shifts
  - Can still be time local (non-secular, non-positive): $\partial_t \rho = \sum_{ijkl} X_{ij} X_{kl} J(E_i - E_j)|i\rangle\langle j|\rho|k\rangle\langle l| + \ldots$
- Non-time-local equations
  - Strong coupling to bath
  - Ultra-strong coupling: need $J(\omega < 0) = 0$ e.g. [Ciuti and Carusotto, PRA '06]
  - Structured baths
    - Vibrational resonances
    - Spatial structure
  - Information return from bath
  - Unknown system eigenstates

Why non-Markovian master equations?



- Born + Markov + Secular
  → Lindblad Master equation:

$$\partial_t \rho = \sum_i \kappa_i \mathcal{L}[X_i], \quad \mathcal{L}[X] = X\rho X^\dagger - \frac{1}{2}[X^\dagger X, \rho]_+$$

- Markov good at optical frequencies

- Why non-Markovian?
  - Strong energy shifts
  - Can still be time local (non-secular, non-positive): $\partial_t \rho = \sum_{ijkl} X_{ij} X_{kl} J(E_i - E_j)|i\rangle\langle j|\rho|k\rangle\langle l| + \ldots$
- Non-time-local equations
  - Strong coupling to bath
  - Ultra-strong coupling: need $J(\omega < 0) = 0$ e.g. [Ciuti and Carusotto, PRA '06]
  - Structured baths
    - ★ Vibrational resonances
    - ★ Spatial structure
  - Information return from bath
  - Unknown system eigenstates

non-Markovian master equations: How: See [de Vega & Alonso, RMP '17]

- Exactly soluble problems . . .
  - e.g. Bosonic: $H = \psi_i^\dagger M_{ij}\psi_j + \sum_{i,k} \xi_{i,k}(\psi_i + \psi_i^\dagger)(b_k^\dagger + b_k) + H_{\text{bath}}$
  - Independent Boson model, $H = \sigma_z(A + \sum_k \xi_k(b_k^\dagger + b_k)) + H_{\text{bath}}$
- Polaron master equation

  $$H \to e^{-V} H e^{V}, \qquad V = \sum_k \xi_k (b_k - b_k^\dagger) X_{\text{sys}}$$

  - Renormalize system parameters
  - Perturbative remaining coupling

  [Jang, J. Chem. Phys '09, McCutcheon *et al.* PRB '11, Roy and Hughes PRB '12]
- Re-sum perturbation theory: [Chen *et al.* J. Chem. Phys. '17]

non-Markovian master equations: How: See [de Vega & Alonso, RMP '17]

- Exactly soluble problems . . .
  - e.g. Bosonic: $H = \Psi_i^\dagger M_{ij} \Psi_j + \sum_{i,k} \xi_{i,k} (\psi_i + \psi_i^\dagger)(b_k^\dagger + b_k) + H_{\text{bath}}$,
  - Independent Boson model, $H = \sigma_z (A + \sum_k \xi_k (b_k^\dagger + b_k)) + H_{\text{bath}}$
- Polaron master equation

  $H \to e^{-V} H e^{V}, \quad V = \sum_k \xi_k (b_k - b_k^\dagger) X_{\text{sys}}$

  - Renormalize system parameters
  - Perturbative remaining coupling

  [Jang, J. Chem. Phys '09, McCutcheon *et al.* PRB '11, Roy and Hughes PRB '12]
- Re-sum perturbation theory: [Chen *et al.* J. Chem. Phys. '17]

non-Markovian master equations: How: See [de Vega & Alonso, RMP '17]

- Exactly soluble problems ...
  - e.g. Bosonic: $H = \Psi_i^\dagger M_{ij} \Psi_j + \sum_{i,k} \xi_{i,k}(\psi_i + \psi_i^\dagger)(b_k^\dagger + b_k) + H_{\text{bath}}$,
  - Independent Boson model, $H = \sigma_z(A + \sum_k \xi_k(b_k^\dagger + b_k)) + H_{\text{bath}}$
- Polaron master equation

$$H \to e^{-V} H e^{V}, \quad V = \sum_k \xi_k (b_k - b_k^\dagger) X_{\text{sys}}$$

  - Renormalize system parameters
  - Perturbative remaining coupling

  [Jang, J. Chem. Phys '09, McCutcheon *et al.* PRB '11, Roy and Hughes PRB '12]
- Re-sum perturbation theory: [Chen *et al.* J. Chem. Phys. '17]

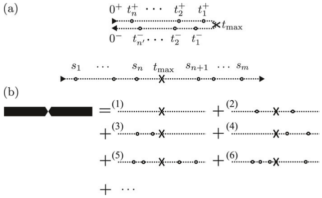
non-Markovian master equations: How: See [de Vega & Alonso, RMP '17]

- Exactly soluble problems ...
  - e.g. Bosonic: $H = \Psi_i^\dagger M_{ij} \Psi_j + \sum_{i,k} \xi_{i,k}(\psi_i + \psi_i^\dagger)(b_k^\dagger + b_k) + H_{\text{bath}}$,
  - Independent Boson model, $H = \sigma_z(A + \sum_k \xi_k(b_k^\dagger + b_k)) + H_{\text{bath}}$
- Polaron master equation

$$H \rightarrow e^{-V} H e^{V}, \qquad V = \sum_k \xi_k (b_k - b_k^\dagger) X_{\text{sys}}$$

  - Renormalize system parameters
  - Perturbative remaining coupling

  [Jang, J. Chem. Phys '09, McCutcheon *et al.* PRB '11, Roy and Hughes PRB '12]
- Re-sum perturbation theory: [Chen *et al.* J. Chem. Phys. '17]



non-Markovian master equations: augmentation

- Increase no. coupled EOM
  [Tanimura & Kubo, JPSJ '89]
- Increase system — include resonant modes

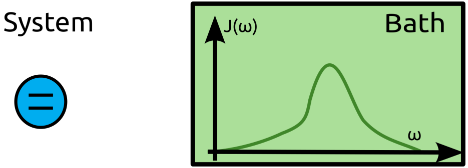
  [Garraway PRA '97, Iles-Smith *et al.* PRA '14, Schröder *et al.* '17]

- Augment state space/history: QUAPI
  [Makri and Makarov, J. Chem Phys '95]

non-Markovian master equations: augmentation

- Increase no. coupled EOM

  [Tanimura & Kubo, JPSJ '89]
- Increase system — include resonant modes



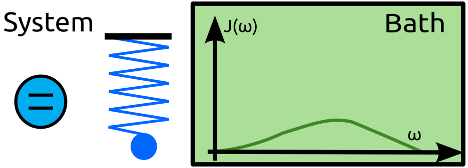
  [Garraway PRA '97, Iles-Smith *et al.* PRA '14, Schröder *et al.* '17]
  - Include bath → chain mapping (TEDOPA — previous talk)

    [Woods *et al.* , J. Math. Phys. '14]
- Augment state space/history: QUAPI

  [Makri and Makarov, J. Chem Phys '95]

non-Markovian master equations: augmentation

- Increase no. coupled EOM
  [Tanimura & Kubo, JPSJ '89]
- Increase system — include resonant modes



[Garraway PRA '97, Iles-Smith *et al.* PRA '14, Schröder *et al.* '17]

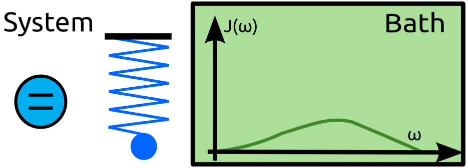
- Include bath → chain mapping (TEDOPA — previous talk)

  [Woods *et al.* , J. Math. Phys. '14]
- Augment state space/history: QUAPI
  [Makri and Makarov, J. Chem Phys '95]

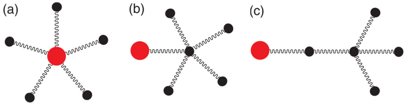
non-Markovian master equations: augmentation

- Increase no. coupled EOM

  [Tanimura & Kubo, JPSJ ’89]
- Increase system — include resonant modes



  [Garraway PRA ’97, Iles-Smith *et al.* PRA ’14, Schröder *et al.* ’17]
  - Include bath $\rightarrow$ chain mapping (TEDOPA — previous talk)



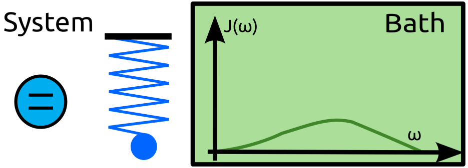
[Woods *et al.* , J. Math. Phys. ’14]

- Augment state space/history: QUAPI

  [Makri and Makarov, J. Chem Phys ’95]

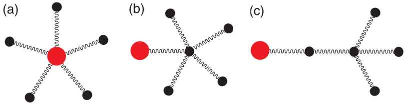
non-Markovian master equations: augmentation

- Increase no. coupled EOM
  [Tanimura & Kubo, JPSJ '89]
- Increase system — include resonant modes



[Garraway PRA '97, Iles-Smith *et al.* PRA '14, Schröder *et al.* '17]

  - Include bath $\rightarrow$ chain mapping (TEDOPA — previous talk)



[Woods *et al.* , J. Math. Phys. '14]

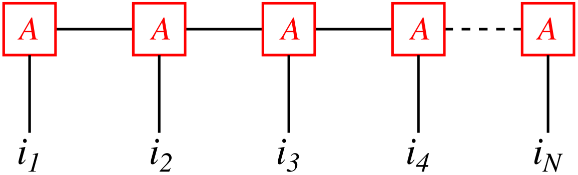
- Augment state space/history: QUAPI
  [Makri and Makarov, J. Chem Phys '95]

1. Why Non-Markovian problems
2. Introduction to MPS
3. QUAPI and TEMPO algorithm
4. Applications
   - Spin-Boson problem
   - Information backflow: Revivals

Introduction to matrix product states

- Matrix product state:

$$T_{i_1,i_2,i_3,\ldots} = \sum_{\{\alpha_j\}} A^{[1]i_1}_{1,\alpha_1} A^{[2]i_2}_{\alpha_1,\alpha_2} \ldots A^{[N-1]i_{N-1}}_{\alpha_{N-2},\alpha_{N-1}} A^{[N]i_N}_{\alpha_{N-1},1}$$

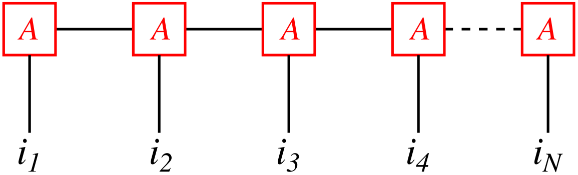


  - Local dimension: $i_1 = 1 \ldots d$, Bond dimension $\alpha_1 = 1 \ldots \chi_1$.
  - Size $\sum_i d\chi_i^2$ vs d^N
- Uses:
  - Wavefunction: $|\Psi\rangle = \sum_{\{i_j\}} T_{i_1,i_2,i_3,\ldots} |i_1\rangle \otimes |i_2\rangle \ldots$
  - Density matrix $\langle \sigma_1, \sigma_2, \ldots |\rho| \sigma_1', \sigma_2' \ldots \rangle = \sum_{\{i_j\}} T_{i_1,i_2,i_3,\ldots} T^{1,i_1}_{\sigma_1,\sigma_1'} T^{1,i_2}_{\sigma_2,\sigma_2'}$
  - Classical probabilities

Introduction to matrix product states

- Matrix product state:

$$T_{i_1,i_2,i_3,\ldots} = \sum_{\{\alpha_j\}} A^{[1]i_1}_{1,\alpha_1} A^{[2]i_2}_{\alpha_1,\alpha_2} \ldots A^{[N-1]i_{N-1}}_{\alpha_{N-2},\alpha_{N-1}} A^{[N]i_N}_{\alpha_{N-1},1}$$



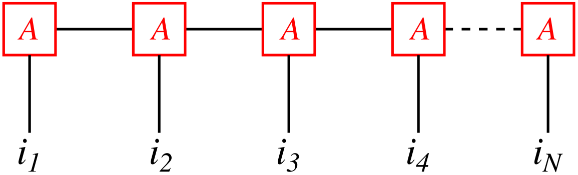
  - Local dimension: $i_1 = 1 \ldots d$, Bond dimension $\alpha_1 = 1 \ldots \chi_1$.
  - Size $\sum_i d\chi_i^2$ vs d^N

- Uses:
  - Wavefunction: $|\Psi\rangle = \sum_{\{i_j\}} T_{i_1,i_2,i_3,\ldots} |i_1\rangle \otimes |i_2\rangle \ldots$
  - Density matrix $\langle \sigma_1, \sigma_2, \ldots |\rho| \sigma_1', \sigma_2' \ldots \rangle = \sum_{\{i_j\}} T_{i_1,i_2,i_3,\ldots} T^{1,i_1}_{\sigma_1,\sigma_1'} T^{1,i_2}_{\sigma_2,\sigma_2'}$
  - Classical probabilities

Introduction to matrix product states

- Matrix product state:

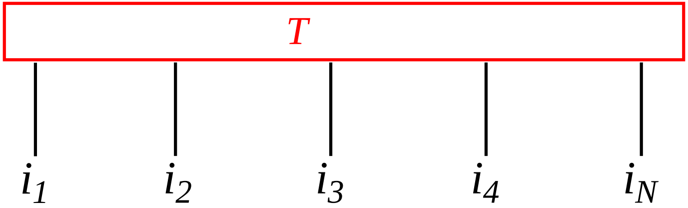
$$T_{i_1,i_2,i_3,\dots} = \sum_{\{\alpha_j\}} A^{[1]i_1}_{1,\alpha_1} A^{[2]i_2}_{\alpha_1,\alpha_2} \dots A^{[N-1]i_{N-1}}_{\alpha_{N-2},\alpha_{N-1}} A^{[N]i_N}_{\alpha_{N-1},1}$$



  - Local dimension: $i_1 = 1 \dots d$, Bond dimension $\alpha_1 = 1 \dots \chi_1$.
  - Size $\sum_i d\chi_i^2$ vs d^N
- Uses:
  - Wavefunction: $|\Psi\rangle = \sum_{\{i_j\}} T_{i_1,i_2,i_3,\dots}|i_1\rangle \otimes |i_2\rangle \dots$
  - Density matrix $\langle\sigma_1,\sigma_2,\dots|\rho|\sigma'_1,\sigma'_2\dots\rangle = \sum_{\{i_j\}} T_{i_1,i_2,i_3,\dots}\tau^{1,i_1}_{\sigma_1,\sigma'_1}\tau^{1,i_2}_{\sigma_2,\sigma'_2}$
  - Classical probabilities

Manipulating matrix product states

- Singular value decomposition

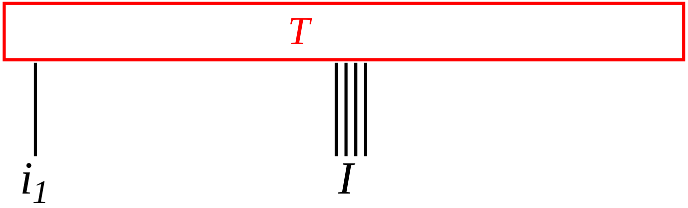


$T_{i_1,\ldots i_N}$

  - Repeat on each leg
  - Truncation: Keep $|\lambda| > \lambda_c$ or $|\alpha_i| < \chi$
  - Bond dimension χ_n: Storage $Nd\chi^2$ vs d^N

Manipulating matrix product states

- Singular value decomposition

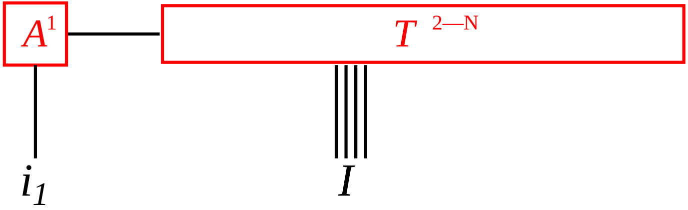


$$T_{i_1,\ldots i_N} = T_{i_1,I}$$

- Repeat on each leg
- Truncation: Keep $|\lambda| > \lambda_c$ or $|\alpha| < \chi$
- Bond dimension χ_n: Storage $Nd\chi^2$ vs d^N

Manipulating matrix product states

- Singular value decomposition



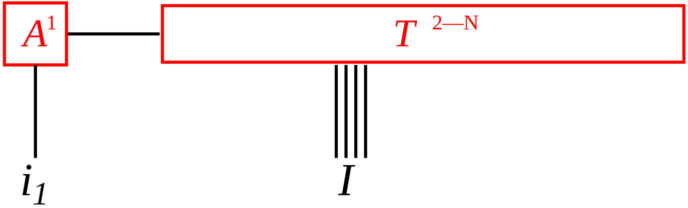
$$T_{i_1,\ldots i_N} = T_{i_1,I} = U^{(1)}_{i_1,\alpha_1} \lambda^{(1)}_{\alpha_1} [V^{(1)\dagger}]_{\alpha_1,I}.$$

$$TT^\dagger = U\Lambda^2 U^\dagger, \qquad T^\dagger T = V\Lambda^2 V^\dagger$$

- Repeat on each leg
- Truncation: Keep $|\lambda| > \lambda_c$ or $|\alpha_i| < \chi$
- Bond dimension χ_n: Storage $Nd\chi^2$ vs d^N

Manipulating matrix product states

- Singular value decomposition



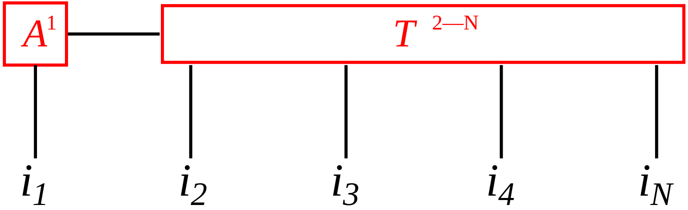
$$T_{i_1,\ldots i_N} = T_{i_1,I} = U^{(1)}_{i_1,\alpha_1} \lambda^{(1)}_{\alpha_1} [V^{(1)\dagger}]_{\alpha_1,I}.$$

$$TT^\dagger = U\Lambda^2 U^\dagger, \qquad T^\dagger T = V\Lambda^2 V^\dagger \quad \text{Get: } A^{1,i_1}_{\alpha_1} = U^{(1)}_{i_1,\alpha_1}\sqrt{\lambda^{(1)}_{\alpha_1}}$$

- Repeat on each leg
- Truncation: Keep $|\lambda| > \lambda_c$ or $|\alpha| < \chi$
- Bond dimension χ_n: Storage $Nd\chi^2$ vs d^N

Manipulating matrix product states

- Singular value decomposition



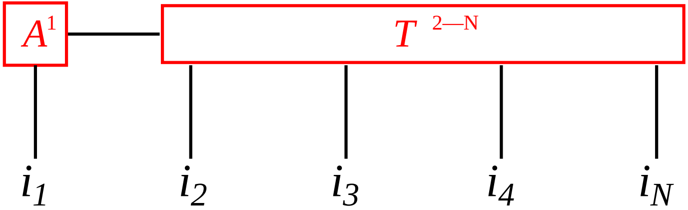
$$T_{i_1,\dots i_N} = T_{i_1,I} = U^{(1)}_{i_1,\alpha_1}\lambda^{(1)}_{\alpha_1}[V^{(1)\dagger}]_{\alpha_1,I}.$$

$TT^\dagger = U\Lambda^2 U^\dagger, \qquad T^\dagger T = V\Lambda^2 V^\dagger$ Get: $A^{1,i_1}_{\alpha_1} = U^{(1)}_{i_1,\alpha_1}\sqrt{\lambda^{(1)}_{\alpha_1}}$

  - Repeat on each leg
  - Truncation: Keep $|\lambda| > \lambda_c$ or $|\alpha| < \chi$
  - Bond dimension χ_n: Storage $Nd\chi^2$ vs d^N

Manipulating matrix product states

- Singular value decomposition



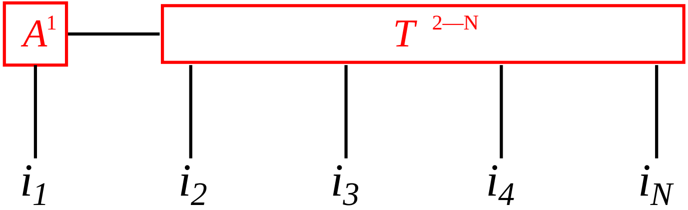
$$T_{i_1,\ldots i_N} = T_{i_1,I} = U^{(1)}_{i_1,\alpha_1}\lambda^{(1)}_{\alpha_1}[V^{(1)\dagger}]_{\alpha_1,I}.$$

$$TT^\dagger = U\Lambda^2U^\dagger, \qquad T^\dagger T = V\Lambda^2V^\dagger \text{ Get: } A^{1,i_1}_{\alpha_1} = U^{(1)}_{i_1,\alpha_1}\sqrt{\lambda^{(1)}_{\alpha_1}}$$

  - Repeat on each leg
  - Truncation: Keep $|\lambda| > \lambda_c$ or $|\alpha_i| < \chi$
  - Bond dimension χ_n: Storage $Nd\chi^2$ vs d^N

Manipulating matrix product states

- Singular value decomposition



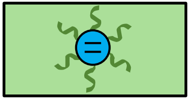
$$T_{i_1,\ldots i_N} = T_{i_1,I} = U^{(1)}_{i_1,\alpha_1} \lambda^{(1)}_{\alpha_1} [V^{(1)\dagger}]_{\alpha_1,I}.$$

$TT^\dagger = U\Lambda^2 U^\dagger, \qquad T^\dagger T = V\Lambda^2 V^\dagger$ Get: $A^{1,i_1}_{\alpha_1} = U^{(1)}_{i_1,\alpha_1} \sqrt{\lambda^{(1)}_{\alpha_1}}$

- Repeat on each leg
- Truncation: Keep $|\lambda| > \lambda_c$ or $|\alpha_i| < \chi$
- Bond dimension χ_n: Storage $Nd\chi^2$ vs d^N

QUAPI [Makri and Makarov, J. Chem Phys '95]

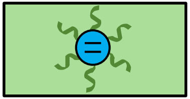
- System + harmonic bath



$$H = H_S + O\sum_k \xi_k(b_k^\dagger + b_k) + H_B$$

QUAPI [Makri and Makarov, J. Chem Phys '95]

- System + harmonic bath



$$H = H_S + O \sum_k \xi_k (b_k^\dagger + b_k) + H_B$$

- Write $\rho_j(t)$ as path sum/integral
  - Discrete sum for system
    $$\mathbb{1} = \sum_j |j\rangle\langle j|$$
  - Coordinate path integral for bath
    $$\mathbb{1} = \int dx_n |x_n\rangle\langle x_n|$$
  - Discretize times, $t_N = N\Delta$
- Integrate out bath.

- Path sum (doubled indices) $j = (j_f, j_b)$:

$$\rho_{j_N}(t_N) = \sum_{j_1 \ldots j_{N-1}} \left(\prod_{n=1}^{N} \prod_{k=0}^{n-1} I_k(j_n, j_{n-k}) \right) \rho_{j_1}(t_1)$$

- ADT: products $\to$ Growth.

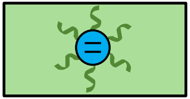
$$A^{j_4 j_3 j_2 j_1} = B^{j_4 j_3 j_2 j_1}_{j_3 j_2 j_1} A^{j_3 j_2 j_1}$$

$$B^{j_n j_{n-1} \ldots j_1}_{j_{n-1} \ldots j_1} = \left(\prod_{k=1}^{n-1} \delta^{j_{n-k}}_{j_{n-k}} \right) \prod_{k=0}^{n-1} I_k(j_n, j_{n-k}).$$

- Problem: n^{th} Tensor size $\sim d^{2n}$

QUAPI [Makri and Makarov, J. Chem Phys '95]

- System + harmonic bath



$$H = H_S + O \sum_k \xi_k (b_k^\dagger + b_k) + H_B$$

- Write $\rho_j(t)$ as path sum/integral
  - Discrete sum for system
    $$\mathbb{1} = \sum_j |j\rangle\langle j|$$
  - Coordinate path integral for bath
    $$\mathbb{1} = \int dx_n |x_n\rangle\langle x_n|$$
  - Discretize times, $t_N = N\Delta$
- Integrate out bath.

- Path sum (doubled indices) $j = (j_f, j_b)$:

$$\rho_{j_N}(t_N) = \sum_{j_1 \cdots j_{N-1}} \left(\prod_{n=1}^{N} \prod_{k=0}^{n-1} I_k(j_n, j_{n-k}) \right) \rho_{j_1}(t_1)$$

- ADT; products $\to$ Growth.

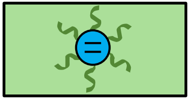
$$A^{j_4, j_3, j_2, j_1} = B^{j_4, j_3, j_2, j_1}_{j_3, j_2, j_1} A^{j_3, j_2, j_1}$$

$$B^{j_n, j_{n-1}, \ldots, j_1}_{i_{n-1}, \ldots, i_1} = \left(\prod_{k=1}^{n-1} \delta^{j_{n-k}}_{i_{n-k}} \right) \prod_{k=0}^{n-1} I_k(j_n, j_{n-k}).$$

- Problem: n^{th} Tensor size $\sim d^{2n}$

QUAPI [Makri and Makarov, J. Chem Phys '95]

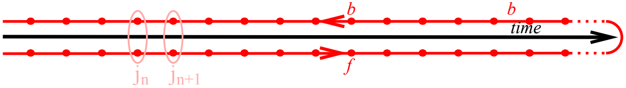
- System + harmonic bath



$$H = H_S + O \sum_k \xi_k (b_k^\dagger + b_k) + H_B$$

- Write $\rho_j(t)$ as path sum/integral
  - Discrete sum for system
    $$\mathbb{1} = \sum_j |j\rangle\langle j|$$
  - Coordinate path integral for bath
    $$\mathbb{1} = \int dx_n |x_n\rangle\langle x_n|$$
  - Discretize times, $t_N = N\Delta$
- Integrate out bath.

- Path sum (doubled indices) $j = (j_f, j_b)$:



$$\rho_{j_N}(t_N) = \sum_{j_1 \ldots j_{N-1}} \left(\prod_{n=1}^{N} \prod_{k=0}^{n-1} I_k(j_n, j_{n-k}) \right) \rho_{j_1}(t_1)$$

- ADT; products → Growth.

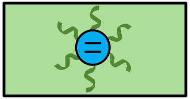
$$A^{j_4, j_3, j_2, j_1} = B^{j_4, j_3, j_2, j_1}_{i_3, i_2, i_1} A^{i_3, i_2, i_1}$$

$$B^{j_n, j_{n-1}, \ldots, j_1}_{i_{n-1}, \ldots, i_1} = \left(\prod_{k=1}^{n-1} \delta^{j_{n-k}}_{i_{n-k}} \right) \prod_{k=0}^{n-1} I_k(j_n, j_{n-k}).$$

- Problem: n^{th} Tensor size $\sim d^{2n}$

QUAPI [Makri and Makarov, J. Chem Phys '95]

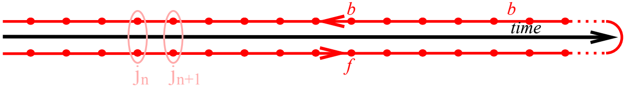
- System + harmonic bath



$$H = H_S + O \sum_k \xi_k (b_k^\dagger + b_k) + H_B$$

- Write $\rho_j(t)$ as path sum/integral
  - Discrete sum for system
    $$\mathbb{1} = \sum_j |j\rangle\langle j|$$
  - Coordinate path integral for bath
    $$\mathbb{1} = \int dx_n |x_n\rangle\langle x_n|$$
  - Discretize times, $t_N = N\Delta$
- Integrate out bath.

- Path sum (doubled indices) $j = (j_f, j_b)$:



$$\rho_{j_N}(t_N) = \sum_{j_1 \cdots j_{N-1}} A^{j_N, j_{N-1}, \ldots, j_1}$$

- ADT; products $\to$ Growth.

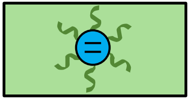
$$A^{j_4,j_3,j_2,j_1} = B^{j_4,j_3,j_2,j_1}_{i_3,i_2,i_1} A^{i_3,i_2,i_1}$$

$$B^{j_n,j_{n-1},\ldots,j_1}_{i_{n-1},\ldots,i_1} = \left(\prod_{k=1}^{n-1} \delta^{j_{n-k}}_{i_{n-k}} \right) \prod_{k=0}^{n-1} I_k(j_n, j_{n-k}).$$

- Problem: n^{th} Tensor size $\sim d^{2n}$

QUAPI [Makri and Makarov, J. Chem Phys ’95]

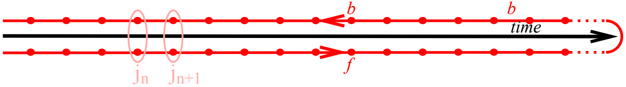
- System + harmonic bath



$$H = H_S + O\sum_k \xi_k(b_k^\dagger + b_k) + H_B$$

- Write $\rho_j(t)$ as path sum/integral
  - Discrete sum for system
    $$\mathbb{1} = \sum_j |j\rangle\langle j|$$
  - Coordinate path integral for bath
    $$\mathbb{1} = \int dx_n |x_n\rangle\langle x_n|$$
  - Discretize times, $t_N = N\Delta$
- Integrate out bath.

- Path sum (doubled indices) $j = (j_f, j_b)$:



$$\rho_{j_N}(t_N) = \sum_{j_1 \cdots j_{N-1}} A^{j_N, j_{N-1}, \ldots, j_1}$$

- ADT; products $\rightarrow$ Growth.

$$A^{j_4,j_3,j_2,j_1} = B^{j_4,j_3,j_2,j_1}_{i_3,i_2,i_1} A^{i_3,i_2,i_1}$$

$$B^{j_n,j_{n-1},\ldots,j_1}_{i_{n-1},\ldots,i_1} = \left(\prod_{k=1}^{n-1} \delta^{j_{n-k}}_{i_{n-k}}\right) \prod_{k=0}^{n-1} I_k(j_n, j_{n-k}).$$

- Problem: $\mathrm{n^{th}}$ Tensor size $\sim d^{2n}$

QUAPI as tensor network: TEMPO

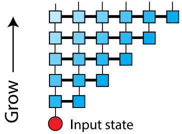
So far . . . : $$\rho_{j_N}(t_N) = \sum_{j_1 \cdots j_{N-1}} A^{j_N, j_{N-1}, \ldots, j_1} \rho_{j_1}(t_1), \qquad \mathbb{A} \to \mathbb{B} \cdot \mathbb{A}$$

- B is tensor network: $B^{j_n, j_{n-1}, \ldots, j_1}_{i_{n-1}, \ldots, i_1} = [b_0]^{j_n}_{\alpha_1} \left(\prod_{k=1}^{n-2} [b_k]^{\alpha_k, j_{n-k}}_{\alpha_{k+1}, i_{n-k}} \right) [b_{n-1}]^{\alpha_{n-1}, j_1}_{i_1}$
- Finite memory approx — neglect correlations K steps ago

QUAPI as tensor network: TEMPO

So far . . . : $$\rho_{j_N}(t_N) = \sum_{j_1 \ldots j_{N-1}} A^{j_N, j_{N-1}, \ldots, j_1} \rho_{j_1}(t_1), \qquad \mathbb{A} \to \mathbb{B} \cdot \mathbb{A}$$

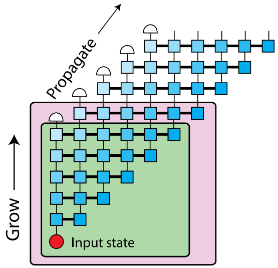
- B is tensor network: $B^{j_n, j_{n-1}, \ldots, j_1}_{i_{n-1}, \ldots, i_1} = [b_0]^{j_n}_{\alpha_1} \left(\prod_{k=1}^{n-2} [b_k]^{\alpha_k, \; j_{n-k}}_{\alpha_{k+1}, i_{n-k}} \right) [b_{n-1}]^{\alpha_{n-1}, j_1}_{i_1}$,
- Finite memory approx — neglect correlations K steps ago



QUAPI as tensor network: TEMPO

$$\text{So far}\ldots: \quad \rho_{j_N}(t_N) = \sum_{j_1 \ldots j_{N-1}} A^{j_N, j_{N-1}, \ldots, j_1} \rho_{j_1}(t_1), \qquad \mathbb{A} \to \mathbb{B} \cdot \mathbb{A}$$

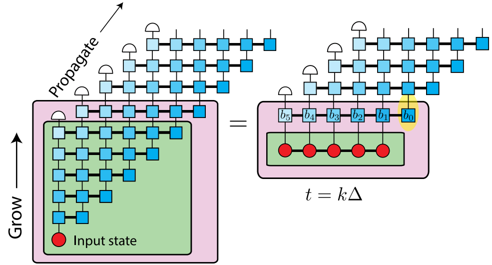
- B is tensor network: $B^{j_n, j_{n-1}, \ldots, j_1}_{i_{n-1}, \ldots, i_1} = [b_0]^{j_n}_{\alpha_1} \left(\prod_{k=1}^{n-2} [b_k]^{\alpha_k, \ j_{n-k}}_{\alpha_{k+1}, i_{n-k}} \right) [b_{n-1}]^{\alpha_{n-1}, j_1}_{i_1},$
- Finite memory approx — neglect correlations K steps ago



QUAPI as tensor network: TEMPO

So far ... : $\rho_{j_N}(t_N) = \sum_{j_1 \cdots j_{N-1}} A^{j_N, j_{N-1}, \ldots, j_1} \rho_{j_1}(t_1)$, $\mathbb{A} \to \mathbb{B} \cdot \mathbb{A}$

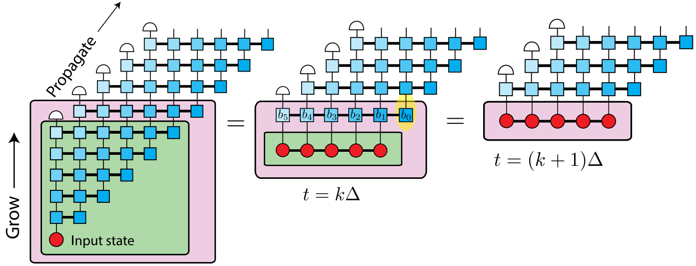
- B is tensor network: $B^{j_n, j_{n-1}, \ldots, j_1}_{i_{n-1}, \ldots, i_1} = [b_0]^{j_n}_{\alpha_1} \left(\prod_{k=1}^{n-2} [b_k]^{\alpha_k, \; j_{n-k}}_{\alpha_{k+1}, i_{n-k}} \right) [b_{n-1}]^{\alpha_{n-1}, j_1}_{i_1}$,
- Finite memory approx — neglect correlations K steps ago



QUAPI as tensor network: TEMPO

So far . . . : $\rho_{j_N}(t_N) = \sum_{j_1 \cdots j_{N-1}} A^{j_N, j_{N-1}, \ldots, j_1} \rho_{j_1}(t_1), \qquad \mathbb{A} \to \mathbb{B} \cdot \mathbb{A}$

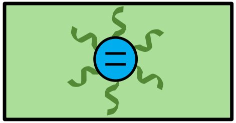
- B is tensor network: $B^{j_n, j_{n-1}, \ldots, j_1}_{i_{n-1}, \ldots, i_1} = [b_0]^{j_n}_{\alpha_1} \left(\prod_{k=1}^{n-2} [b_k]^{\alpha_k, \quad j_{n-k}}_{\alpha_{k+1}, i_{n-k}} \right) [b_{n-1}]^{\alpha_{n-1}, j_1}_{i_1},$
- Finite memory approx — neglect correlations K steps ago



1. Why Non-Markovian problems
2. Introduction to MPS
3. QUAPI and TEMPO algorithm
4. Applications
   - Spin-Boson problem
   - Information backflow: Revivals

spin Boson model

- Archetypal non-Markovian model:



$$H = \Omega S_x + \sum_i S_z(g_i a_i + g_i^* a_i^\dagger) + \omega_i a_i^\dagger a_i,$$

- Ohmic Bath density of states:

$$J(\omega) = \sum_i |g_i|^2 \delta(\omega - \omega_i) = 2\alpha\omega \exp(-\omega/\omega_c)$$

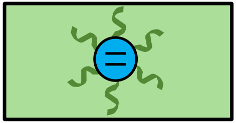
- Known behaviour, initially excited [Leggett *et al.* RMP '87] for $\omega_c \gg \Omega$:

$$\begin{array}{lllll} 0 & < & \alpha & < & 1/2 & \text{Decaying oscillations, } \langle S_z \rangle \sim e^{i\omega t - \gamma t} \\ 1/2 & < & \alpha & < & 1 & \text{Overdamped decay, } \langle S_z \rangle \sim e^{-\gamma t} \\ 1 & < & \alpha & & & \text{Localization, } \langle S_z \rangle \text{ finite at } t \to \infty. \end{array}$$

- Challenge for QUAPI — finite $K = \tau_c/\Delta \to$ non-zero γ for $\forall \alpha$

spin Boson model

- Archetypal non-Markovian model:



$$H = \Omega S_x + \sum_i S_z(g_i a_i + g_i^* a_i^\dagger) + \omega_i a_i^\dagger a_i,$$

- Ohmic Bath density of states:

$$J(\omega) = \sum_i |g_i|^2 \delta(\omega - \omega_i) \equiv 2\alpha\omega \exp(-\omega/\omega_c)$$

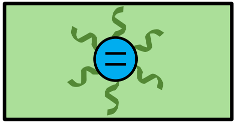
- Known behaviour, initially excited [Leggett *et al.* RMP '87] for $\omega_c \gg \Omega$:

0	$<$	α	$< 1/2$	Decaying oscillations, $\langle S_z \rangle \sim e^{i\omega t - \gamma t}$
$1/2$	$<$	α	< 1	Overdamped decay, $\langle S_z \rangle \sim e^{-\gamma t}$
1	$<$	α		Localization, $\langle S_z \rangle$ finite at $t \to \infty$.

- Challenge for QUAPI — finite $K = \tau_c/\Delta \to$ non-zero γ for $\forall \alpha$

spin Boson model

- Archetypal non-Markovian model:



$$H = \Omega S_x + \sum_i S_z(g_i a_i + g_i^* a_i^\dagger) + \omega_i a_i^\dagger a_i,$$

- Ohmic Bath density of states:

$$J(\omega) = \sum_i |g_i|^2 \delta(\omega - \omega_i) \equiv 2\alpha\omega \exp(-\omega/\omega_c)$$

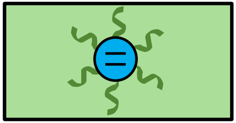
- Known behaviour, initially excited [Leggett *et al.* RMP '87] for $\omega_c \gg \Omega$:

0	$<$	α	$<$	$1/2$	Decaying oscillations, $\langle S_z \rangle \sim e^{i\omega t - \gamma t}$
$1/2$	$<$	α	$<$	1	Overdamped decay, $\langle S_z \rangle \sim e^{-\gamma t}$
1	$<$	α			Localization, $\langle S_z \rangle$ finite at $t \to \infty$.

- Challenge for QUAPI — finite $K = \tau_c/\Delta \to$ non-zero γ for $\forall\alpha$

spin Boson model

- Archetypal non-Markovian model:



$$H = \Omega S_x + \sum_i S_z(g_i a_i + g_i^* a_i^\dagger) + \omega_i a_i^\dagger a_i,$$

- Ohmic Bath density of states:

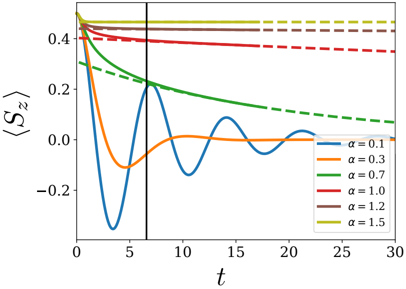
$$J(\omega) = \sum_i |g_i|^2 \delta(\omega - \omega_i) \equiv 2\alpha\omega \exp(-\omega/\omega_c)$$

- Known behaviour, initially excited [Leggett *et al.* RMP '87] for $\omega_c \gg \Omega$:

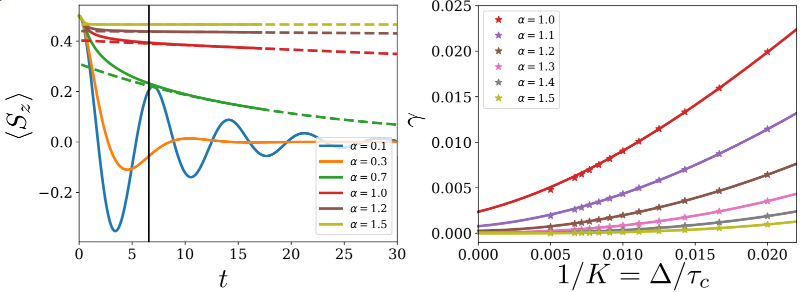
$$\begin{array}{lllll} 0 & < & \alpha & < & 1/2 \quad \text{Decaying oscillations, } \langle S_z \rangle \sim e^{i\omega t - \gamma t} \\ 1/2 & < & \alpha & < & 1 \quad \text{Overdamped decay, } \langle S_z \rangle \sim e^{-\gamma t} \\ 1 & < & \alpha & & \quad \text{Localization, } \langle S_z \rangle \text{ finite at } t \to \infty. \end{array}$$

- Challenge for QUAPI — finite $K = \tau_c/\Delta \to$ non-zero γ for $\forall\alpha$

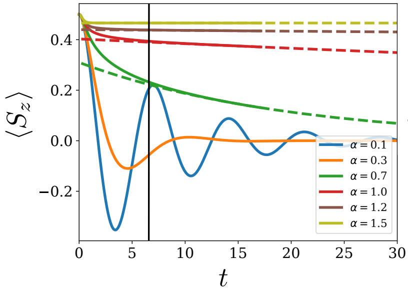
TEMPO spin Boson results

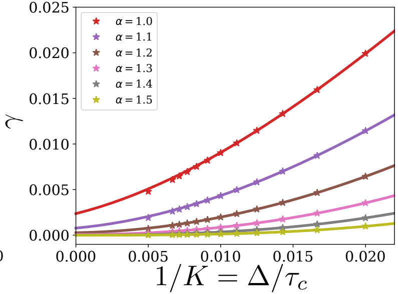


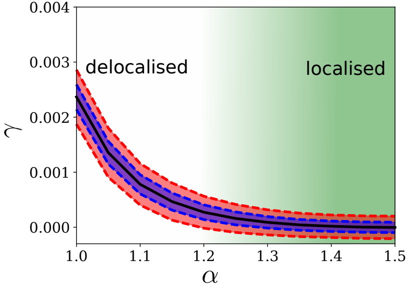
TEMPO spin Boson results



TEMPO spin Boson results



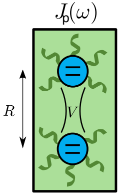




Environment induced revivals

- Two spins in common environment

$$H = \Omega \mathbf{S}_a \cdot \mathbf{S}_b + \sum_i \omega_i a_i^\dagger a_i + \sum_{\nu=a,b} \sum_i S_{z,\nu}(g_{i,\nu} a_i + g_{i,\nu}^* a_i^\dagger)$$

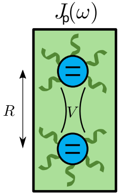


- Phase factors, $g_{i,\nu} = g_i e^{-i\mathbf{k}_i \cdot \mathbf{r}_\nu}$, $\omega_i = |\mathbf{k}_i|$
- Propagation: revivals at $t = R, 2R, \ldots$
- Spin Boson, $J(\omega) = J_p(\omega)(1 - \cos(\omega R))$

Environment induced revivals

- Two spins in common environment

$$H = \Omega \mathbf{S}_a \cdot \mathbf{S}_b + \sum_i \omega_i a_i^\dagger a_i + \sum_{\nu=a,b} \sum_i S_{z,\nu}(g_{i,\nu} a_i + g_{i,\nu}^* a_i^\dagger)$$

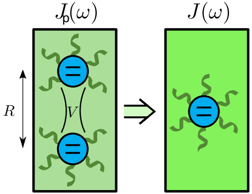


- Phase factors, $g_{i,\nu} = g_i e^{-i\mathbf{k}_i \cdot \mathbf{r}_\nu}$, $\omega_i = |\mathbf{k}_i|$
- Propagation: revivals at $t = R, 2R, \ldots$
- Spin Boson, $J(\omega) = J_p(\omega)(1 - \cos(\omega R))$

Environment induced revivals

- Two spins in common environment

$$H = \Omega \mathbf{S}_a \cdot \mathbf{S}_b + \sum_i \omega_i a_i^\dagger a_i + \sum_{\nu=a,b} \sum_i S_{z,\nu}(g_{i,\nu} a_i + g_{i,\nu}^* a_i^\dagger)$$



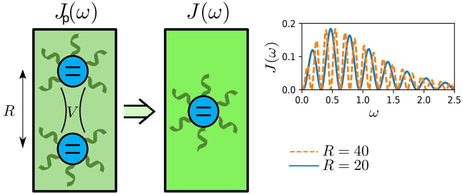
- Phase factors, $g_{i,\nu} = g_i e^{-i\mathbf{k}_i \cdot \mathbf{r}_\nu}$, $\omega_i = |\mathbf{k}_i|$
- Propagation: revivals at $t = R, 2R, \ldots$
- Spin Boson, $J(\omega) = J_p(\omega)(1 - \cos(\omega R))$

Environment induced revivals

- Two spins in common environment

$$H = \Omega \mathbf{S}_a \cdot \mathbf{S}_b + \sum_i \omega_i a_i^\dagger a_i + \sum_{\nu=a,b} \sum_i S_{z,\nu}(g_{i,\nu} a_i + g_{i,\nu}^* a_i^\dagger)$$

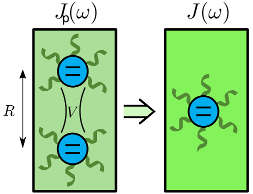
- Phase factors, $g_{i,\nu} = g_i e^{-i\mathbf{k}_i \cdot \mathbf{r}_\nu}$, $\omega_i = |\mathbf{k}_i|$
- Propagation: revivals at $t = R, 2R, \ldots$
- Spin Boson, $J(\omega) = J_p(\omega)(1 - \cos(\omega R))$

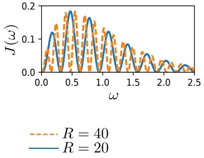


Environment induced revivals

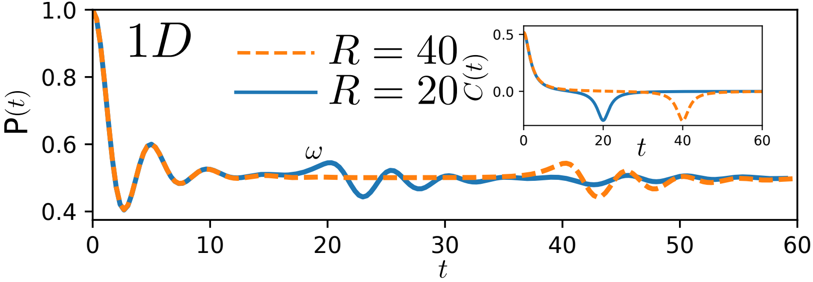
- Two spins in common environment

$$H = \Omega \mathbf{S}_a \cdot \mathbf{S}_b + \sum_i \omega_i a_i^\dagger a_i + \sum_{\nu=a,b} \sum_i S_{z,\nu}(g_{i,\nu} a_i + g_{i,\nu}^* a_i^\dagger)$$

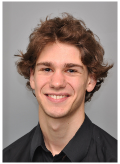




- Phase factors, $g_{i,\nu} = g_i e^{-i\mathbf{k}_i \cdot \mathbf{r}_\nu}$, $\omega_i = |\mathbf{k}_i|$
- Propagation: revivals at $t = R, 2R, \ldots$
- Spin Boson, $J(\omega) = J_p(\omega)(1 - \cos(\omega R))$



Acknowledgements

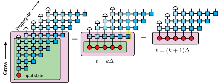
FUNDING:

EPSRC
Engineering and Physical Sciences
Research Council

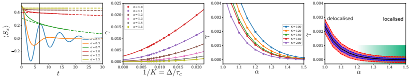
Hybrid
Polaritonics

Summary

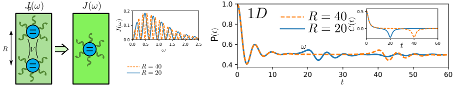
- TEMPO Algorithm for general non-Markovian problems



- Captures localisation transition of spin Boson model



- Capable to handling oscillating DoS.



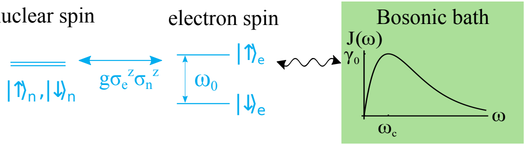
- Code publicly available at DOI:10.5281/zenodo.1322407

[Strathearn, Kirton, Kilda, Keeling & Lovett, Nat. Comm. (2018)]

5 Protected coherence

Protected coherence: Two coupled spins

- Coupled electron + nucleus

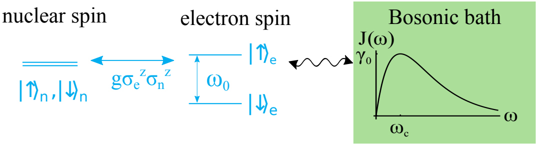


$$H = \frac{\omega_0}{2}\sigma_e^z + g\sigma_e^z\sigma_n^z + \sum_k \xi_k\left(\sigma_e^+ b_k + \text{H.c.}\right) + H_B$$

[Cammack *et al.* PRA ’18]

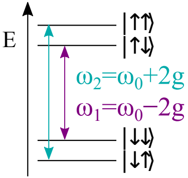
Protected coherence: Two coupled spins

- Coupled electron + nucleus



$$H = \frac{\omega_0}{2}\sigma_e^z + g\sigma_e^z\sigma_n^z + \sum_k \xi_k \left(\sigma_e^+ b_k + \text{H.c.}\right) + H_B$$

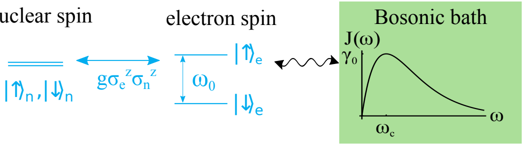
- Electron spin flip – effect on nuclear coherence



[Cammack *et al.* PRA '18]

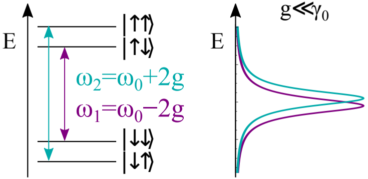
Protected coherence: Two coupled spins

- Coupled electron + nucleus



$$H = \frac{\omega_0}{2}\sigma_e^z + g\sigma_e^z\sigma_n^z + \sum_k \xi_k \left(\sigma_e^+ b_k + \text{H.c.}\right) + H_B$$

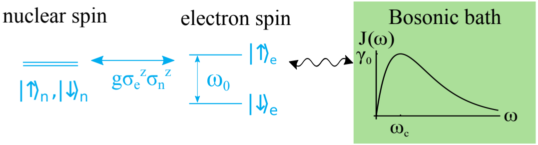
- Electron spin flip – effect on nuclear coherence



[Cammack *et al.* PRA ’18]

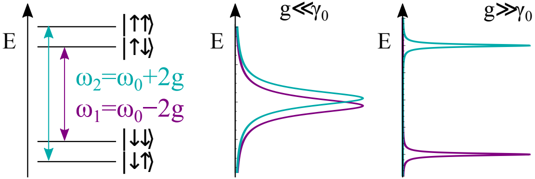
Protected coherence: Two coupled spins

- Coupled electron + nucleus



$$H = \frac{\omega_0}{2}\sigma_e^z + g\sigma_e^z\sigma_n^z + \sum_k \xi_k \left(\sigma_e^+ b_k + \text{H.c.}\right) + H_B$$

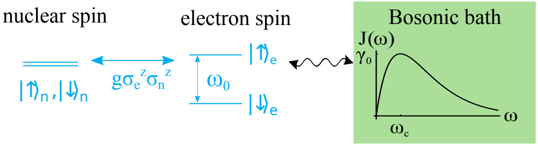
- Electron spin flip – effect on nuclear coherence



[Cammack *et al.* PRA '18]

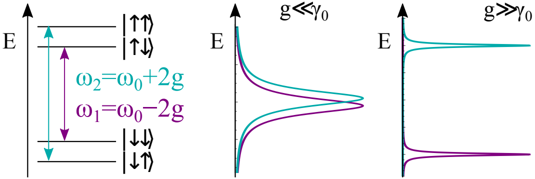
Protected coherence: Two coupled spins

- Coupled electron + nucleus



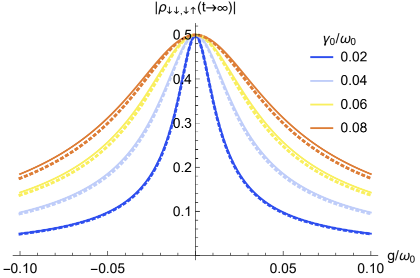
$$H = \frac{\omega_0}{2}\sigma^z_e + g\sigma^z_e\sigma^z_n + \sum_k \xi_k\left(\sigma^+_e b_k + \text{H.c.}\right) + H_B$$

- Electron spin flip – effect on nuclear coherence



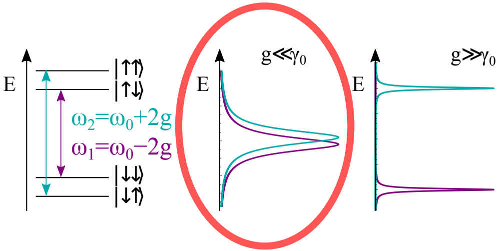
[Cammack *et al.* PRA '18]

- $T = 0$ — single emission, final coherence:



Protected coherence: Finite temperature

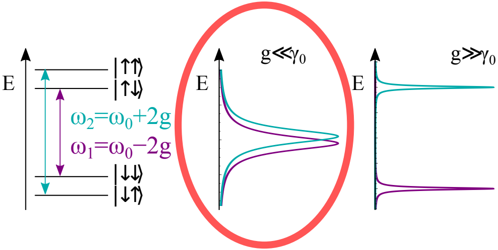
- $T > 0$, Born-Markov approx



[Cammack *et al.* PRA ’18]

Protected coherence: Finite temperature

- $T > 0$, Born-Markov approx
- Separation of timescales, Decay rates $\kappa_{\pm}$.
- For $1/\kappa_{-} \gg t \gg 1/\kappa_{+}$, quasi-steady state $\rho = r$.

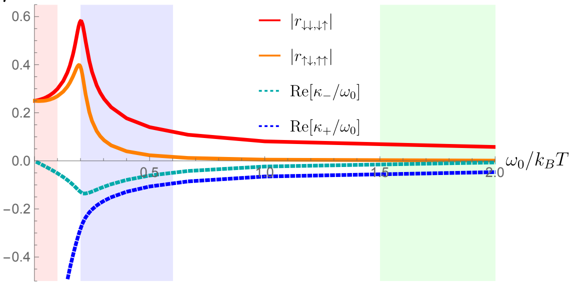


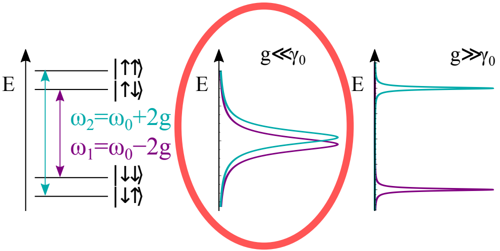
- High T: Large ratio of timescales
- High T protects coherence for longer!
- **But: Born-Markov invalid at high T**

[Cammack *et al.* PRA '18]

Protected coherence: Finite temperature

- $T > 0$, Born-Markov approx
- Separation of timescales, Decay rates $\kappa_\pm$.
- For $1/\kappa_- \gg t \gg 1/\kappa_+$, quasi-steady state $\rho = r$.



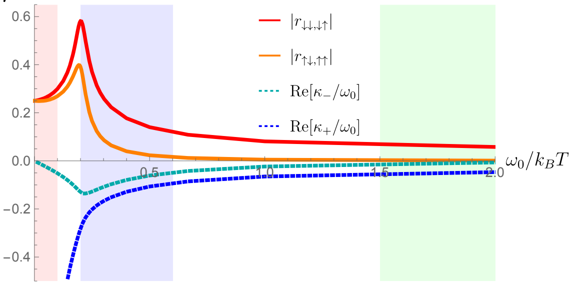


- High T: Large ratio of timescales
- High T protects coherence for longer!
- **But: Born-Markov invalid at high T**

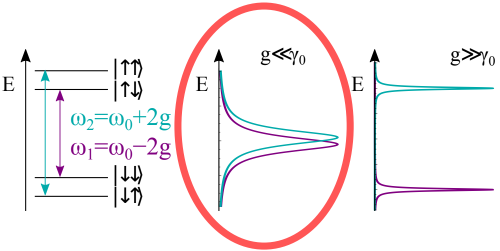
[Cammack *et al.* PRA '18]

Protected coherence: Finite temperature

- $T > 0$, Born-Markov approx
- Separation of timescales, Decay rates $\kappa_\pm$.
- For $1/\kappa_- \gg t \gg 1/\kappa_+$, quasi-steady state $\rho = r$.



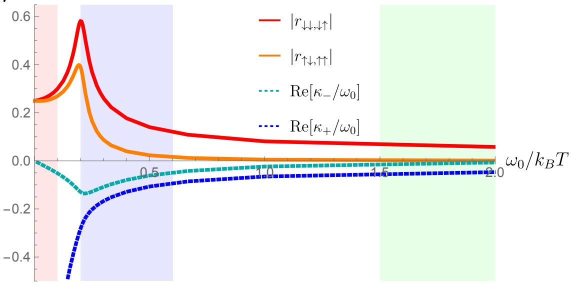
[Cammack *et al.* PRA '18]



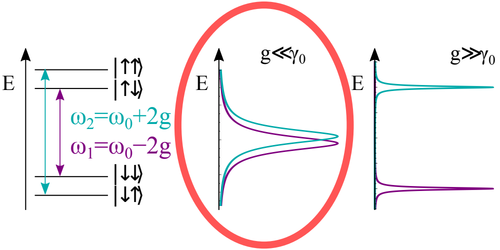
- High T: Large ratio of timescales
- High T protects coherence for longer!
- **But: Born-Markov invalid at high T**

Protected coherence: Finite temperature

- $T > 0$, Born-Markov approx
- Separation of timescales, Decay rates $\kappa_\pm$.
- For $1/\kappa_- \gg t \gg 1/\kappa_+$, quasi-steady state $\rho = r$.



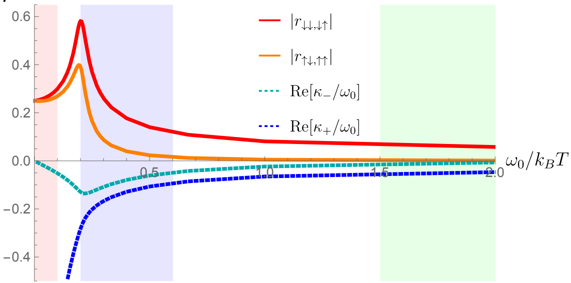
[Cammack *et al.* PRA '18]

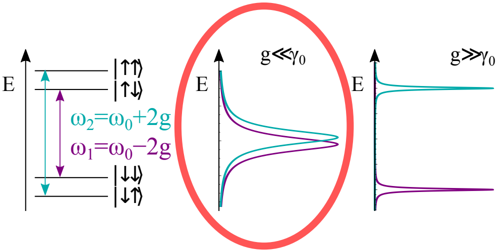


- High T: Large ratio of timescales
- High T protects coherence for longer!
- But: Born-Markov invalid at high T

Protected coherence: Finite temperature

- $T > 0$, Born-Markov approx
- Separation of timescales, Decay rates $\kappa_\pm$.
- For $1/\kappa_- \gg t \gg 1/\kappa_+$, quasi-steady state $\rho = r$.





[Cammack *et al.* PRA '18]

- High T: Large ratio of timescales
- High T protects coherence for longer!
- **But: Born-Markov invalid at high T**

Protected coherence: High temperature TEMPO

- Modify coupling for TEMPO form: $H = \frac{\omega_0}{2}\sigma^z_e + g\sigma^z_e\sigma^z_n + \sum_k \xi_k \sigma^x_e (b_k + b^\dagger_k) + H_B$

- Populations — see Markov breakdown
- Longer coherence at high T

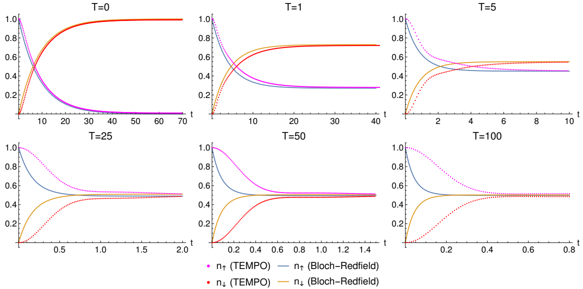
[Work by A. Dunnett]

Protected coherence: High temperature TEMPO

- Modify coupling for TEMPO form: $H = \frac{\omega_0}{2}\sigma_e^z + g\sigma_e^z\sigma_n^z + \sum_k \xi_k \sigma_e^x (b_k + b_k^\dagger) + H_B$

- Populations — see Markov breakdown

- Longer coherence at high T

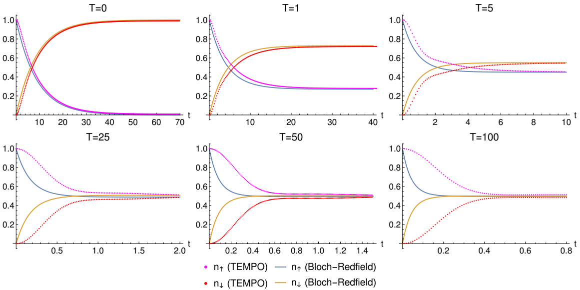


[Work by A. Dunnett]

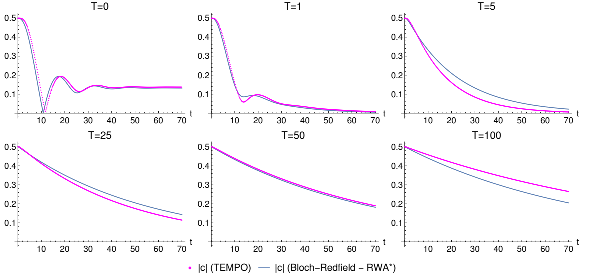
Protected coherence: High temperature TEMPO

- Modify coupling for TEMPO form: $H = \frac{\omega_0}{2}\sigma_e^z + g\sigma_e^z\sigma_n^z + \sum_k \xi_k \sigma_e^x (b_k + b_k^\dagger) + H_B$

- Populations — see Markov breakdown



- Longer coherence at high T



[Work by A. Dunnett]