

# Efficient non-Markovian quantum dynamics using time-**e**volving matrix product operators

Jonathan Keeling

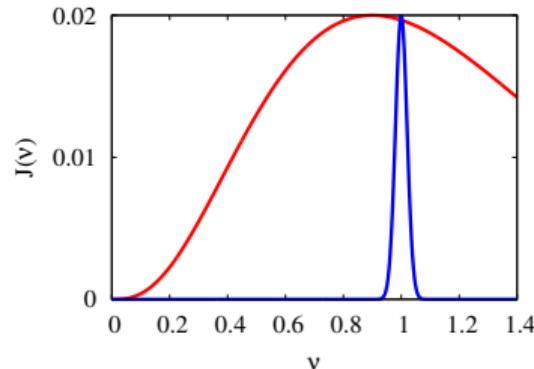


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Charge and Energy Transfer Processes: Open Problems in Open Quantum Systems

# Why non-Markovian master equations?



→ Why non-Markovian?

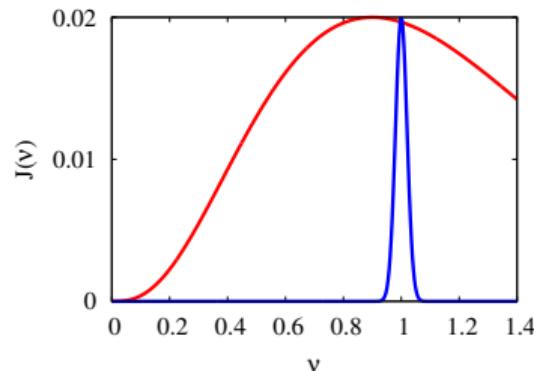
→ Non-time-local equations

- 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

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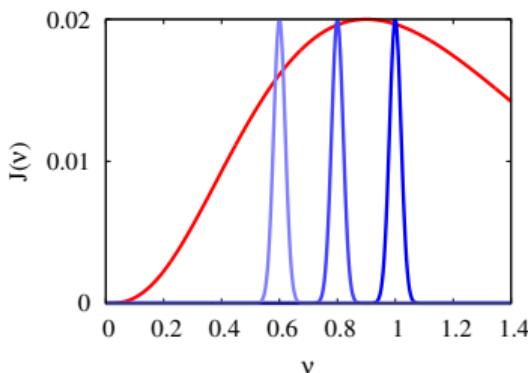
→ Can still be time local (non-secular, non-positive)  $\partial_t \rho = \sum_i X_i X_i^\dagger J(E - E_i) \rho (i \neq k) / i + \dots$

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# Why non-Markovian master equations?



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- ▶ Strong energy shifts

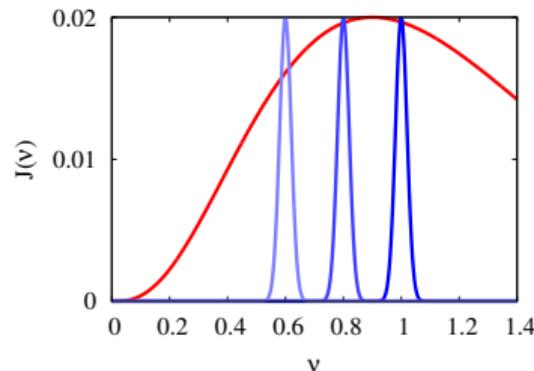
→ Non-time-local (non-secular, non-Markovian) terms:  
$$\sum_{i,j} X_i X_j J(E - E_i) \rho_j (j, i) K(i) + \dots$$

- Born + Markov + Secular  
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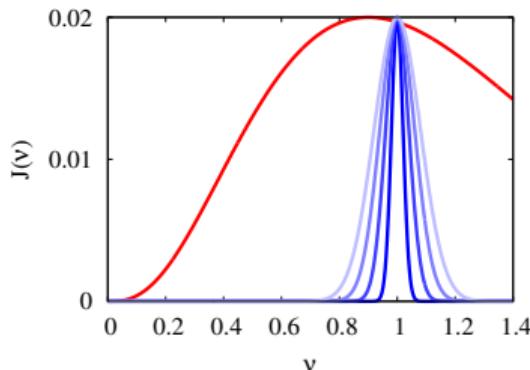
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- Non-time-local equations

- ▶ Strong coupling to bath

→ Strong energy shifts (Karlsson and Garuccio, PRA '06)

→ Structured baths

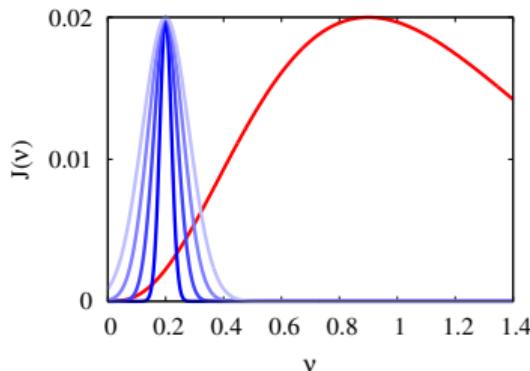
→ Vibrational resonances

→ Spatial structure

→ Information return from bath

→ Unknockable states

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- ▶ Ultra-strong coupling:  
need  $J(\omega < 0) = 0$  e.g. [Ciuti and Carusotto, PRA '06]

↳ Dissipation channels

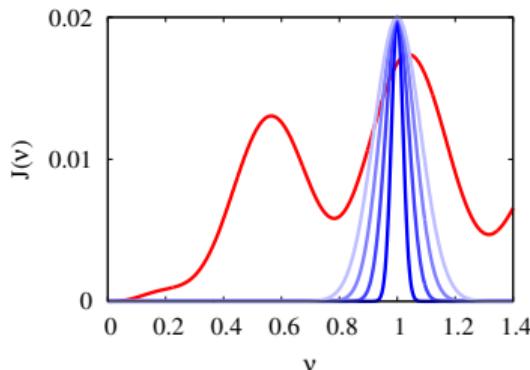
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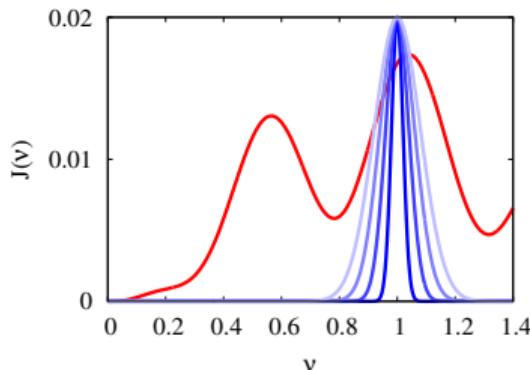
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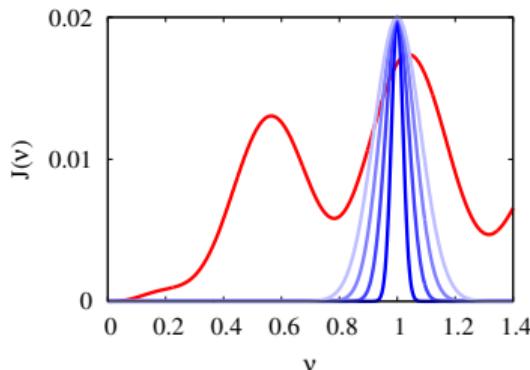
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- ▶ Information return from bath
- ▶ Unknown system eigenstates

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

- Exactly soluble problems ...

- e.g. Bosonic:  $H = \hat{V}^\dagger M_j \hat{V} + \sum_k \epsilon_{jk} (a_j + a_k^\dagger) (a_j^\dagger + a_k) + H_{\text{int}}$

- Independent Boson model,  $H = \mu_s (A + \sum_k \epsilon_k (b_k^\dagger + b_k)) + H_{\text{int}}$

- Polaron master equation

- $H \rightarrow e^{-V} H e^V, \quad V = \sum_k \epsilon_k (b_k - b_k^\dagger) X_{\text{sys}}$        $\Rightarrow$  Renormalize system parameters  
[Jang, J. Chem. Phys '09, McCutcheon et al PRB '11, Roy and Hughes PRB '12]
  - $\Rightarrow$  Perturbative remaining coupling

- Re-sum perturbation theory:

- [Chen et al. J. Chem. Phys. '17]

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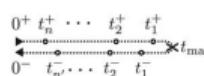
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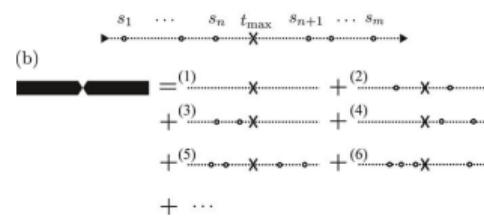
- Re-sum perturbation theory:

(a)



[Chen *et al.* J. Chem. Phys. '17]

(b)



# non-Markovian master equations: augmentation

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

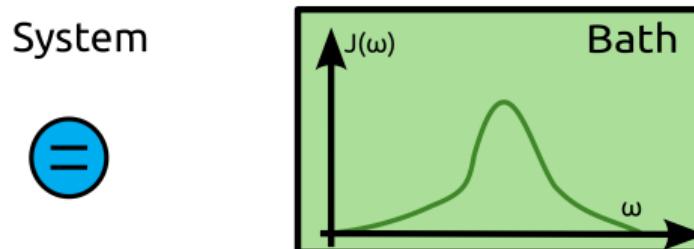
[Garraway PRA '97, Iles-Smith et al. PRA '14, Schröder et al. '17]

## AUGMENTABLE SPECTROSCOPY: QUAPI

Non-Markovian Chem Phys '95

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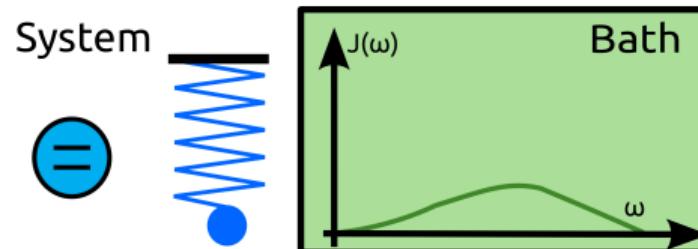
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AUGMENTED MARKOVIANITY, QUAPI

Non-Markovian Chem. Phys. '95

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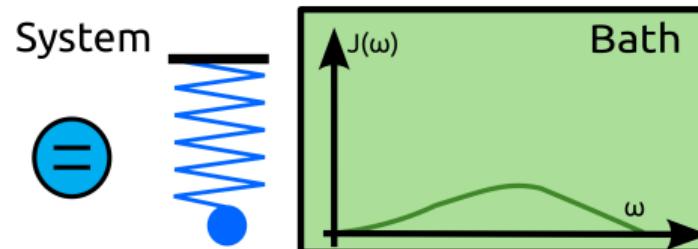
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AUGMENTED SYSTEM/BATH (TEMPO) → QUAPI

Non-Markovian Chem. Phys. '95

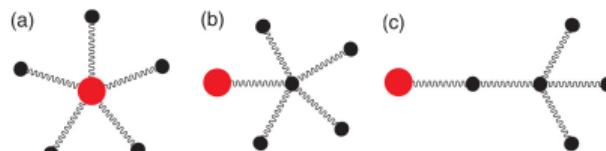
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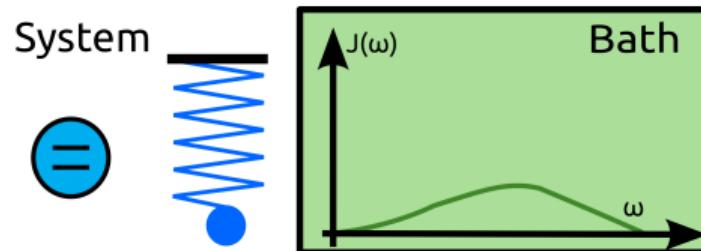
- ▶ Include bath  $\rightarrow$  chain mapping (TEDOPA — previous talk)



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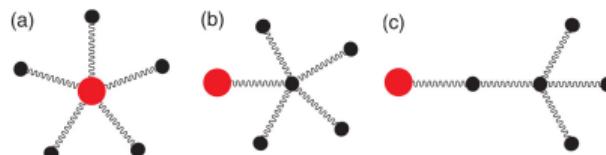
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[Woods *et al.* , J. Math. Phys. '14]

- 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

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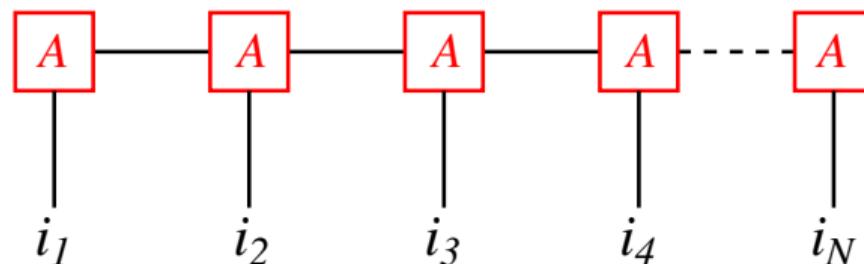
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# Introduction to matrix product states

- Matrix product state:

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



- Local dimension:  $i_1 = 1 \dots d$ , Bond dimension  $\alpha_1 = 1 \dots \chi_1$ .

Tensor network

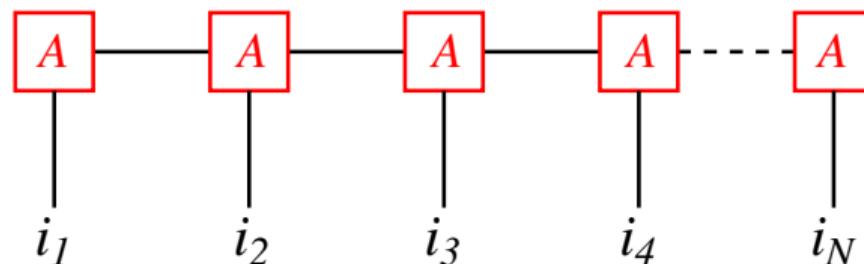
Uses

- Wavefunctions:  $|i\rangle = \sum_{i_1} T_{i, i_1, \dots, i_N} |i_1\rangle \otimes |i_2\rangle \dots$
- Density matrix:  $\langle m_1, m_2, \dots, m_N | n_1, n_2, \dots \rangle = \sum_{i_1} T_{i, i_1, \dots, i_N} \langle m_1 | i_1 \rangle \langle i_2 | m_2 \rangle \dots$
- Classical probabilities

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- Size  $\sum_i d \chi_i^2$  vs  $d^N$

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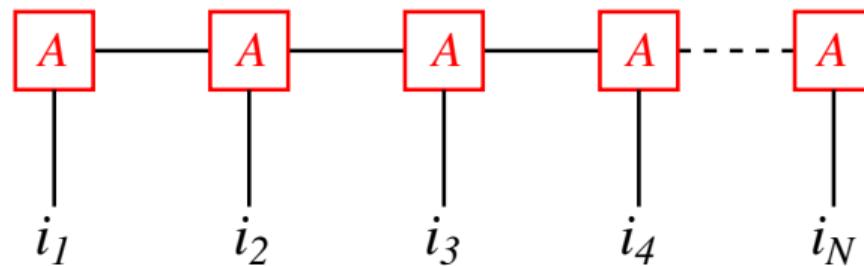
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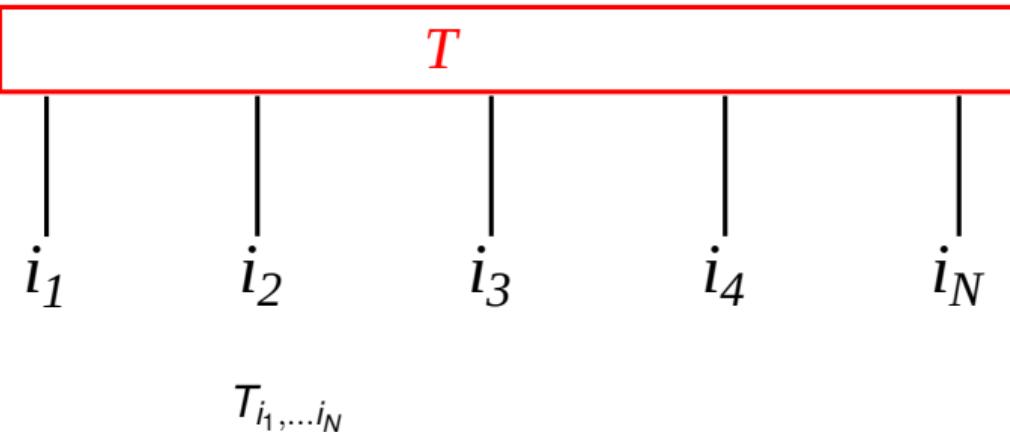
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- Density matrix  $\langle \sigma_1, \sigma_2, \dots | \rho | \sigma'_1, \sigma'_2 \dots \rangle = \sum_{\{i_j\}} T_{i_1, i_2, i_3, \dots} \tau_{\sigma_1, \sigma'_1}^{1, i_1} \tau_{\sigma_2, \sigma'_2}^{1, i_2}$
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# Manipulating matrix product states

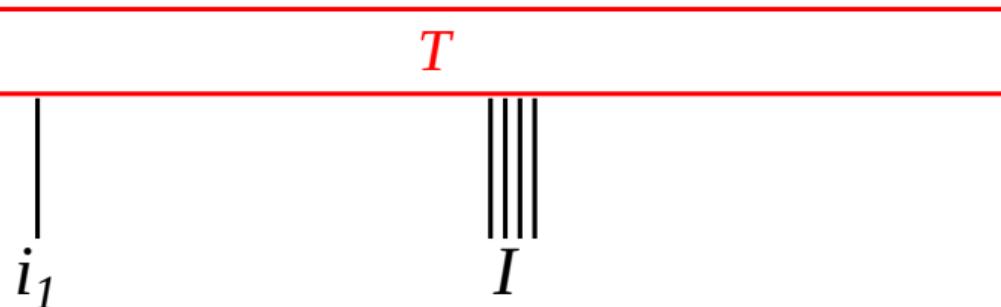
- Singular value decomposition



- Repeat on each leg
- Truncation: Keep  $|\lambda| > \lambda_c$  or  $|\alpha_j| < \epsilon$
- Bond dimension  $\gamma_m$ , Storage  $N \propto \gamma_m^2$

# Manipulating matrix product states

- Singular value decomposition

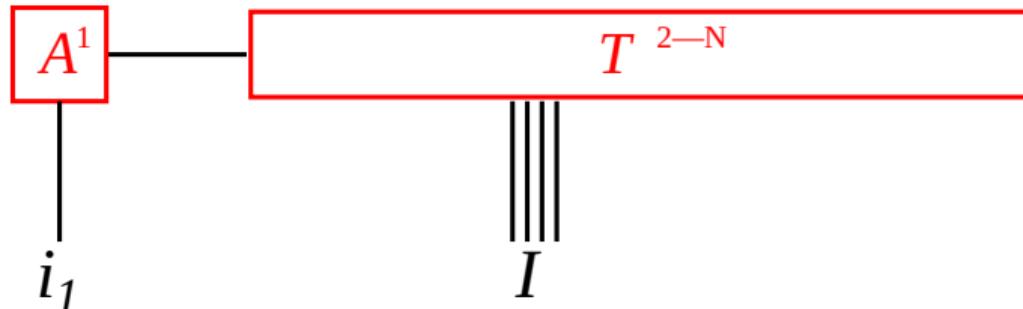


$$T_{i_1, \dots, i_N} = T_{i_1, I}$$

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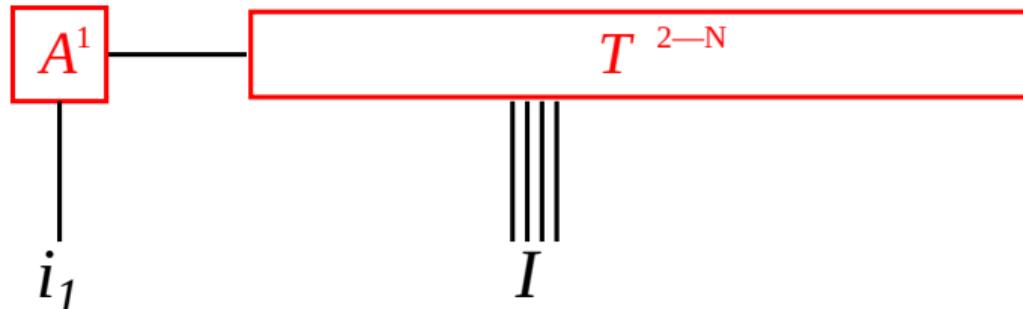
$$T_{i_1, \dots, i_N} = T_{i_1, I} = U_{i_1, \alpha_1}^{(1)} \lambda_{\alpha_1}^{(1)} [V^{(1)\dagger}]_{\alpha_1, I}.$$

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

- Repeat on each leg
- Truncation: Keep  $|\lambda| > \lambda_c$  or  $|\lambda| < \epsilon$
- Bond dimension  $\gamma_n$ : Storage  $N \propto \gamma_n^{2d}$

# Manipulating matrix product states

- Singular value decomposition



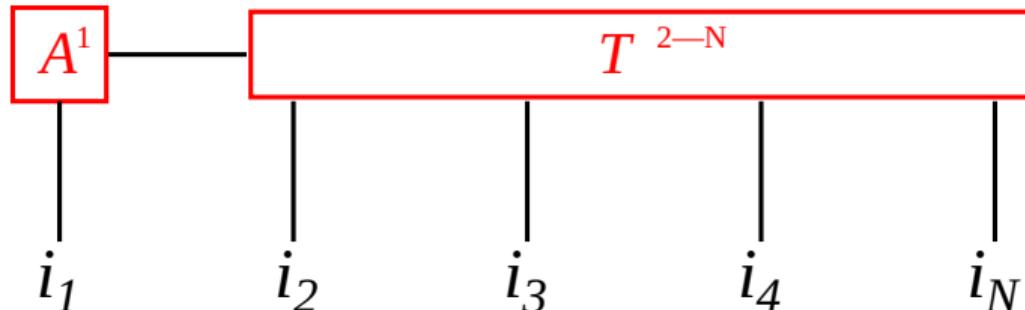
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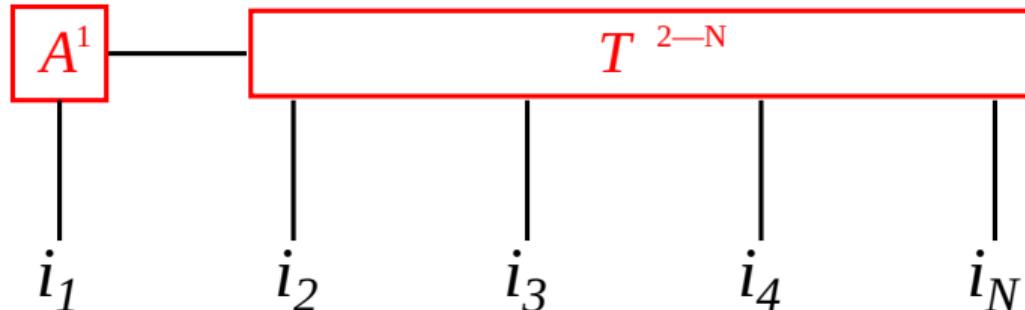
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- ▶ Repeat on each leg

→ Dimension of legs  $\geq \lambda_0$  or  $|\lambda| \leq \lambda_0$   
→ Bond dimension  $\gamma_0$ , Storage No.  $\gamma_0^2$

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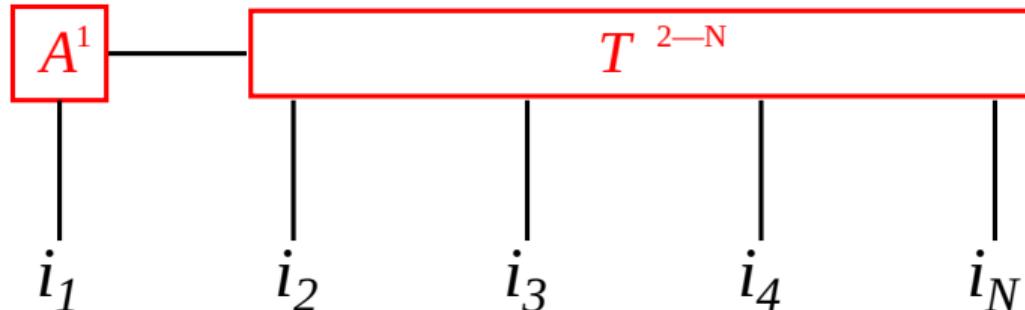
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- ▶ Truncation: Keep  $|\lambda| > \lambda_c$  or  $|\alpha_i| < \chi$

Bond dimension  $\gamma_n$ , Storage  $N \propto \gamma_n^2$

# Manipulating matrix product states

- Singular value decomposition



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

$$TT^\dagger = U\Lambda^2 U^\dagger, \quad T^\dagger T = V\Lambda^2 V^\dagger \quad \text{Get: } A_{\alpha_1}^{1, i_1} = U_{i_1, \alpha_1}^{(1)} \sqrt{\lambda_{\alpha_1}^{(1)}}$$

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

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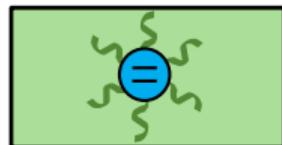
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# QUAPI [Makri and Makarov, J. Chem Phys '95]

- System + harmonic bath



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

→ Path sum (doubled indices)  $j = (i, j)$ :

$$\rho_N(t_f) = \sum_{j_1, j_2, \dots, j_N} \left( \prod_{n=1}^N \prod_{k=0}^{n-1} h(j_n, j_{n+k}) \right) \rho_j(t_i)$$

- Write  $\rho_j(t)$  as path sum/integral

→ Discrete sum for system

$$1 = \sum_j |\psi_j\rangle\langle\psi_j|$$

$$ghhh = g^{\dagger}ghh^{\dagger}ghhh$$

→ Coordinate path integral for bath

$$1 = \int dx_n |x_n\rangle\langle x_n|$$

$$B^{j_1, j_2, \dots, j_N} = \left( \prod_{n=1}^{N-1} dz_n^{\perp} \right) \prod_{n=1}^N h(j_n, j_{n+1})$$

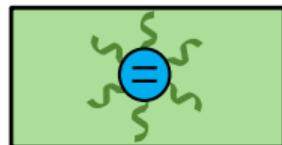
→ Discretize times,  $t_n = N\Delta t$

→ Transfer to path integral form

→ Integrate out bath:

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ADT; products  $\rightarrow$  Growth.

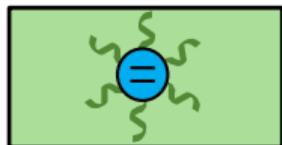
$$g_{ijkl} = g_{ijk} g_{kl}$$

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Product of terms

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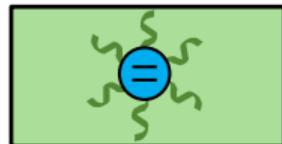
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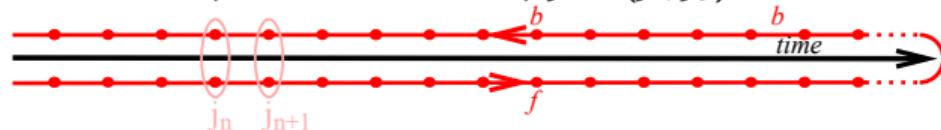
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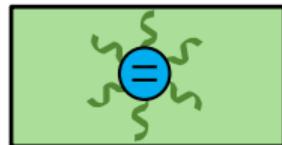
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$$\rho_{j_N}(t_N) = \sum_{j_1 \dots j_{N-1}} \left( \prod_{n=1}^N \prod_{k=0}^{n-1} I_k(j_n, j_{n-k}) \right) \rho_{j_1}(t_1)$$

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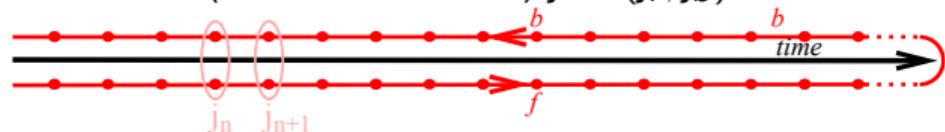
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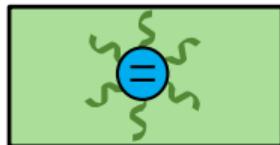
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$$B_{i_{n-1}, \dots, i_1}^{j_n, j_{n-1}, \dots, j_1} = \left( \prod_{k=1}^{n-1} \delta_{i_{n-k}}^{j_{n-k}} \right) \prod_{k=0}^{n-1} I_k(j_n, j_{n-k}).$$

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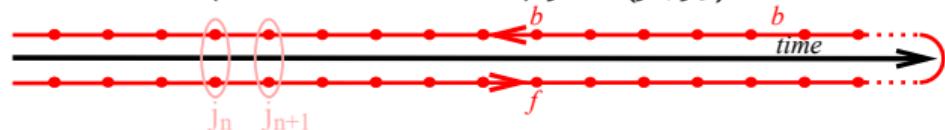
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- Problem:  $n^{\text{th}}$  Tensor size  $\sim d^{2n}$

# QUAPI as tensor network: TEMPO

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

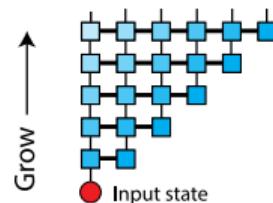
- $B$  is tensor network:  $B^{j_N, j_{N-1}, \dots, j_1} = \{\text{Polar } \left(\frac{1}{\sqrt{2}}(D_{n-1}^{\alpha_n})^{\beta_n}\right) (D_{n-1})^{\gamma_n}\}$ .
- Finite memory approx — neglect correlations  $K$  steps ago

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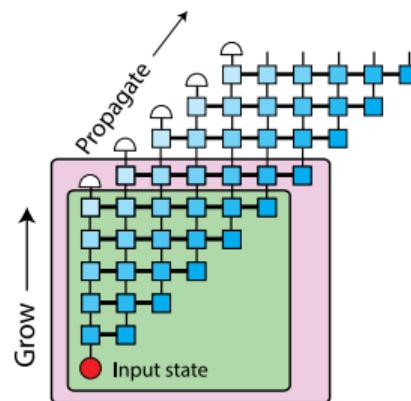
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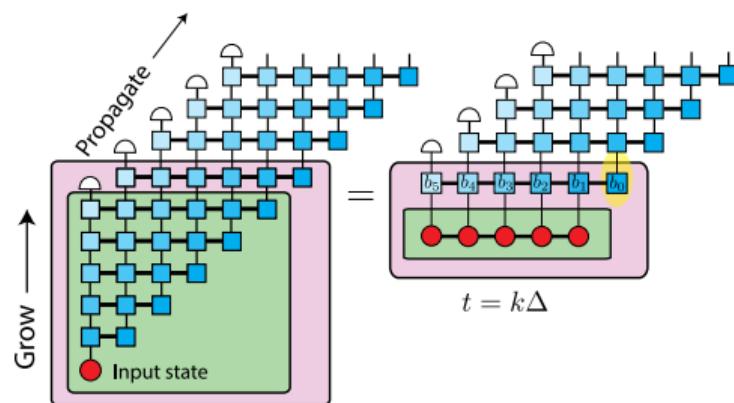
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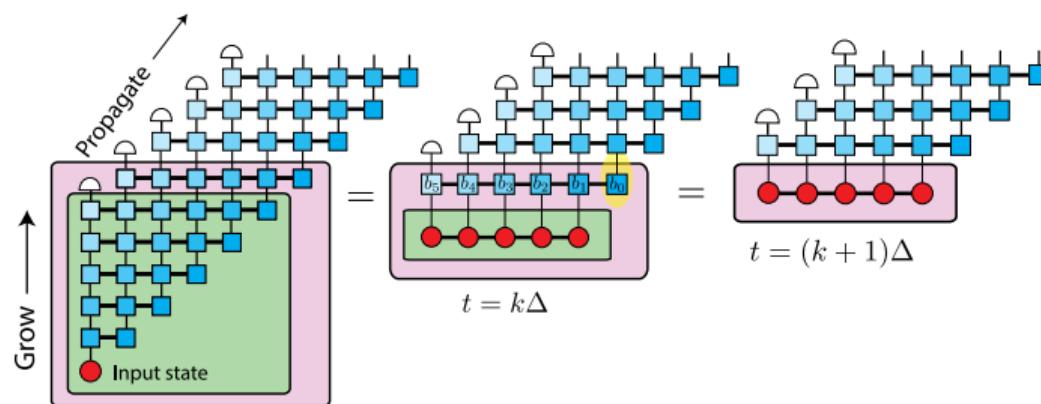
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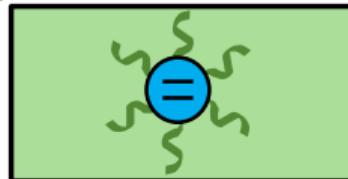
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# spin Boson model

- 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:

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

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

$0 < \alpha < 1/2$  Decaying oscillations,  $\langle S_z \rangle \sim e^{i\omega t - \gamma t}$

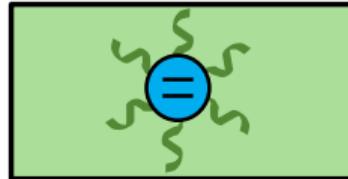
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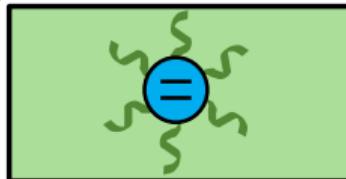
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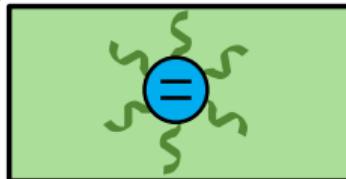
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Challenge in Chapt 1 – find  $K = \tau_0/\Delta$  → non-zero  $\gamma$  for yr

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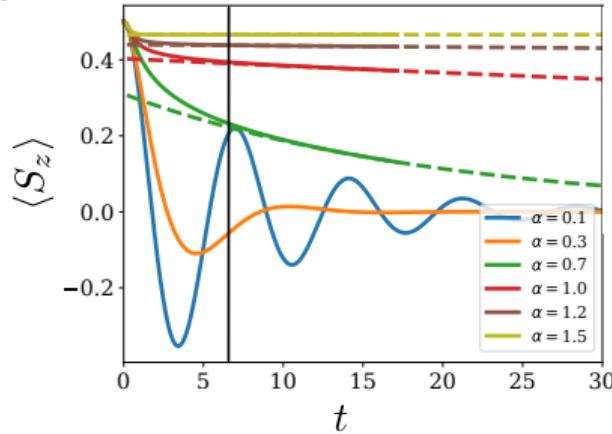
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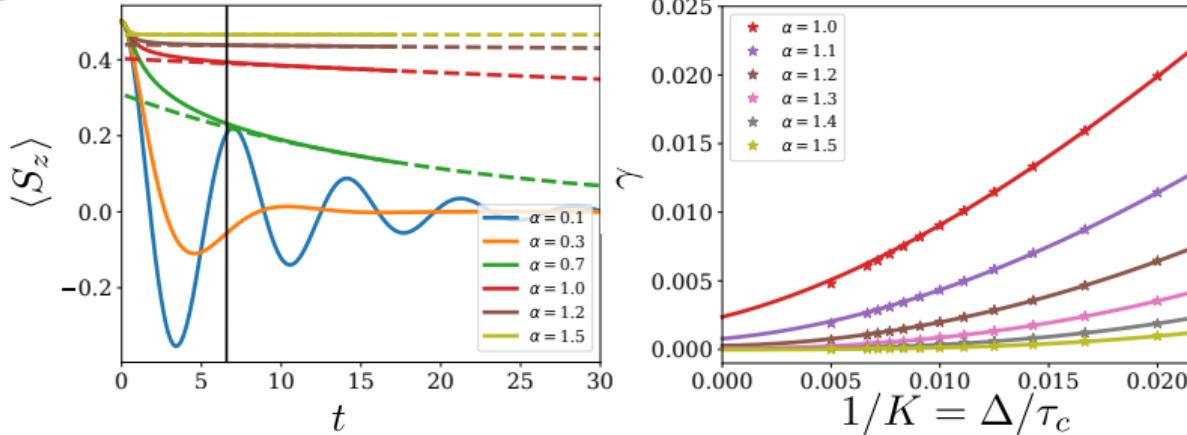
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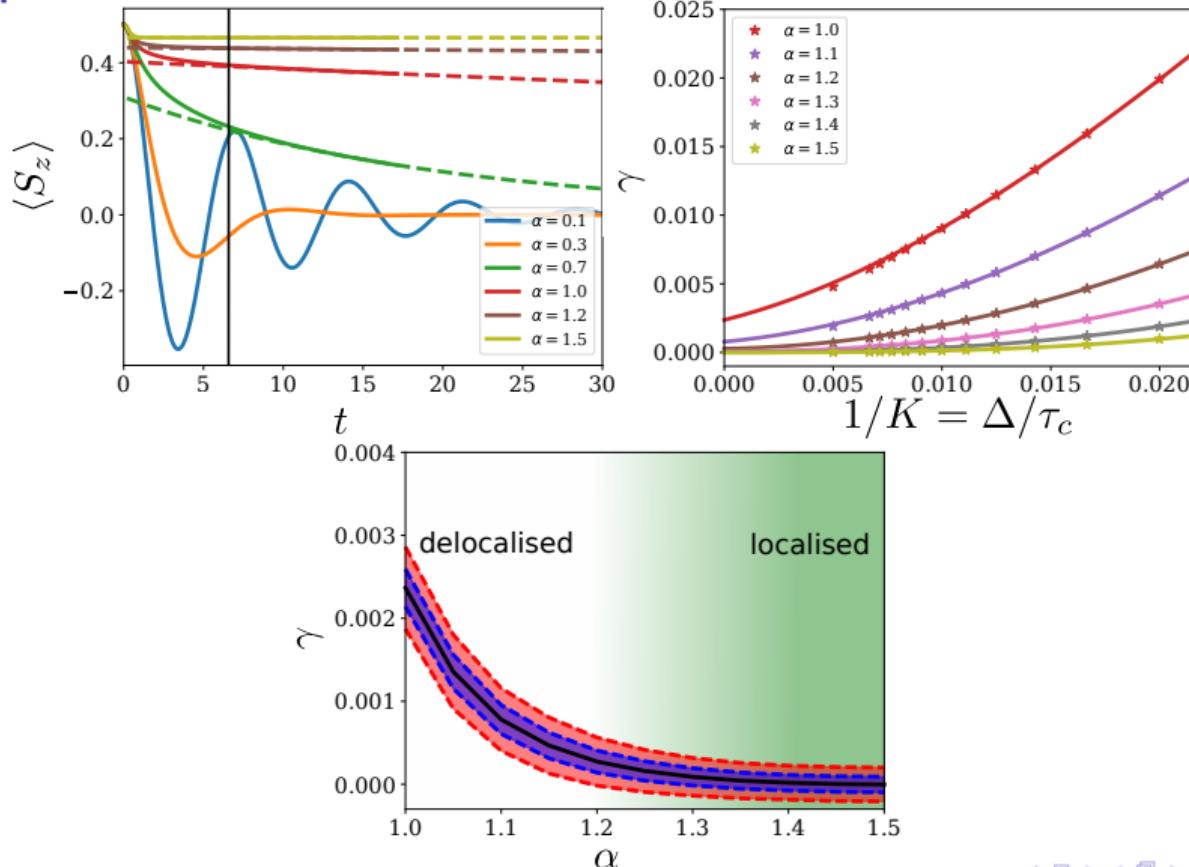
# TEMPO spin Boson results



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# Environment induced revivals

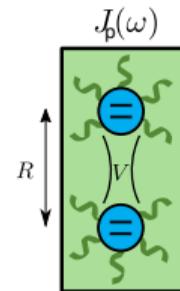
- Two spins in common environment

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

• Phase factors,  $g_{i,\nu} = g_i e^{-i k_\nu R}$ ,  $\omega_i = |k_i|$

• Propagation: revivals at  $t = R, 2R, \dots$

• Spin Boson,  $J(\omega) = J_p(\omega)(1 - \cos(\omega R))$



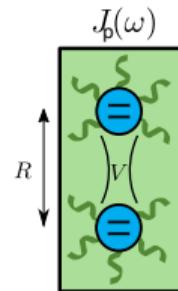
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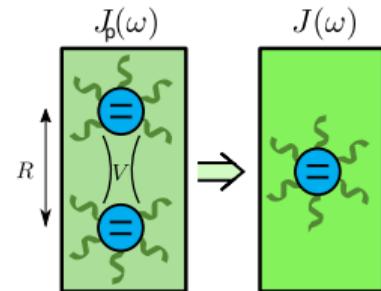


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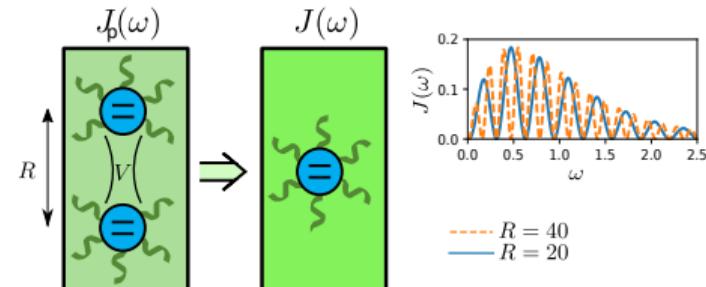


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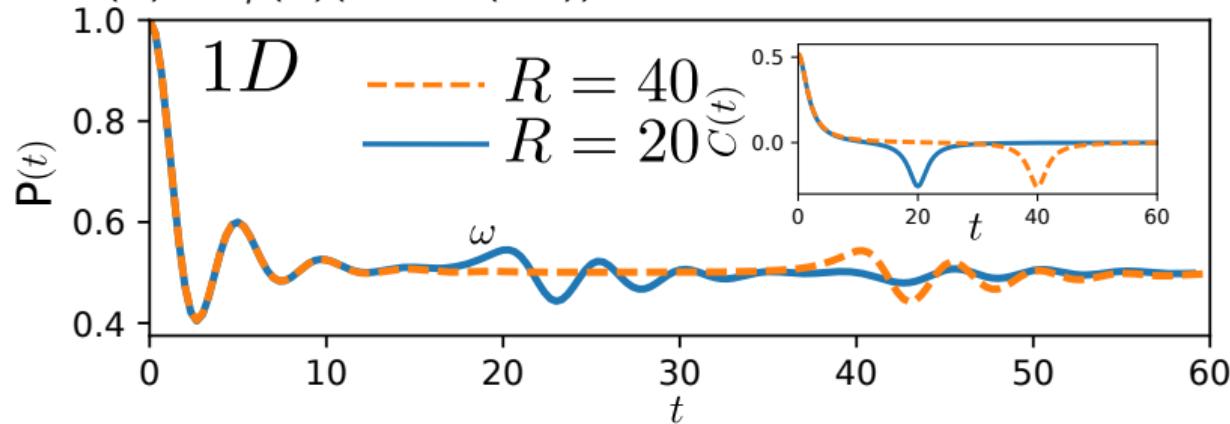
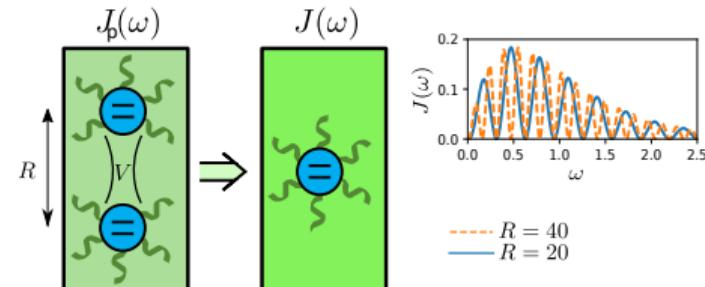


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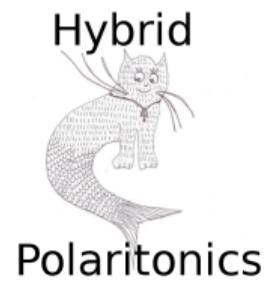
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# Acknowledgements

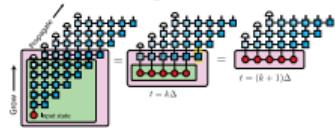


## FUNDING:

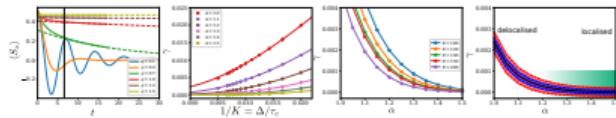


# Summary

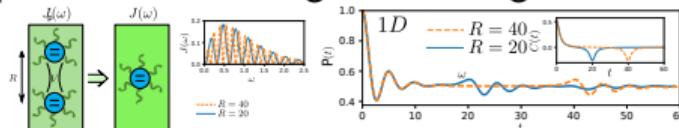
- TEMPO Algorithm for general non-Markovian problems



- Captures localisation transition of spin Boson model



- Capable to handling oscillating DoS.



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

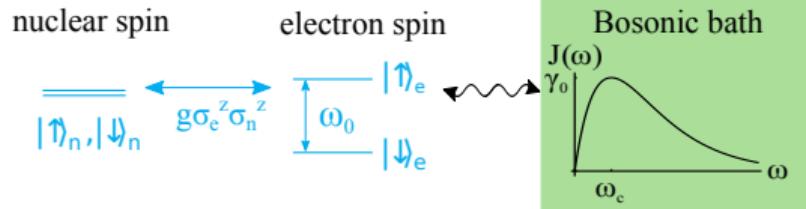
[Strathearn, Kirton, Kilda, Keeling & Lovett, Nat. Comm. (2018)]

5

## Protected coherence

# Protected coherence: Two coupled spins

- Coupled electron + nucleus



$\Leftarrow T = 0$  — single emission, final coherence.

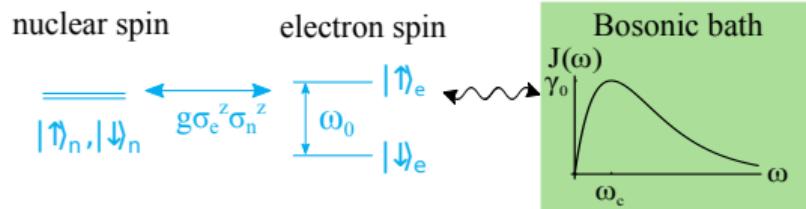
$$H = \frac{\omega_0}{2} \sigma_e^z + g \sigma_e^z \sigma_n^z + \sum_k \xi_k (\sigma_e^+ b_k + \text{H.c.}) + H_B$$

- Electron spin flip – effect on nuclear coherence

[Cammack *et al.* PRA '18]

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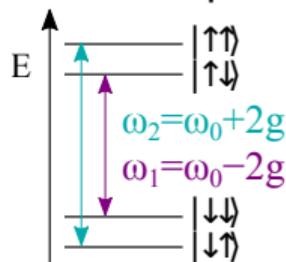
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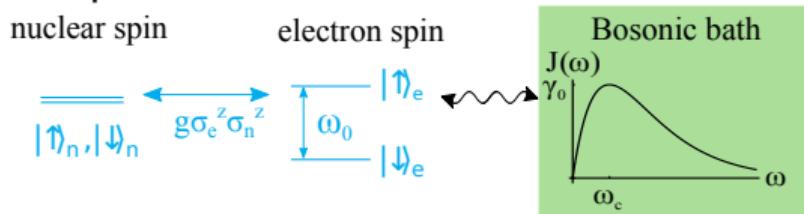
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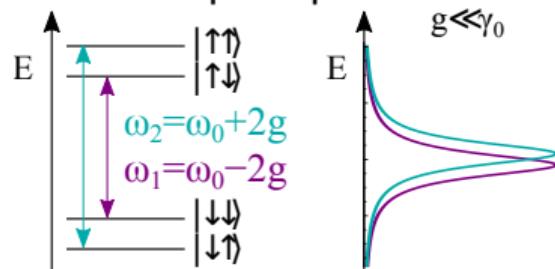
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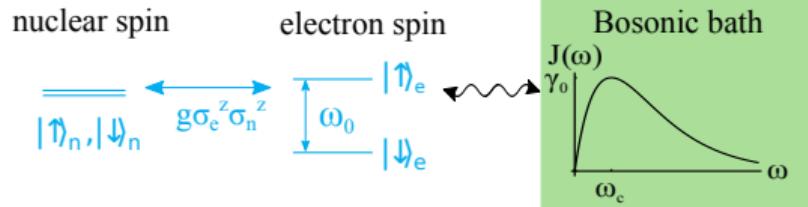
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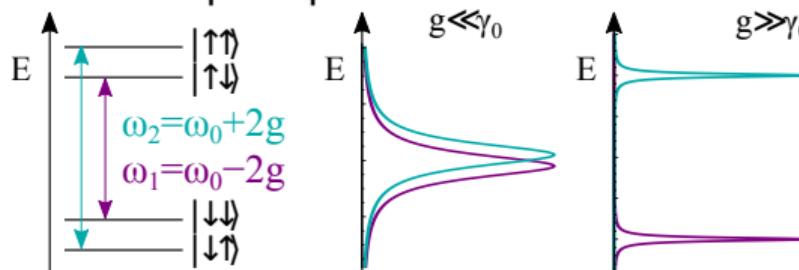
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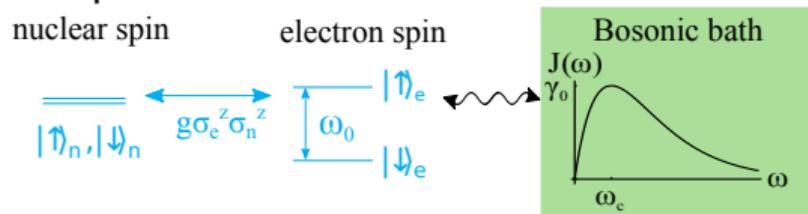
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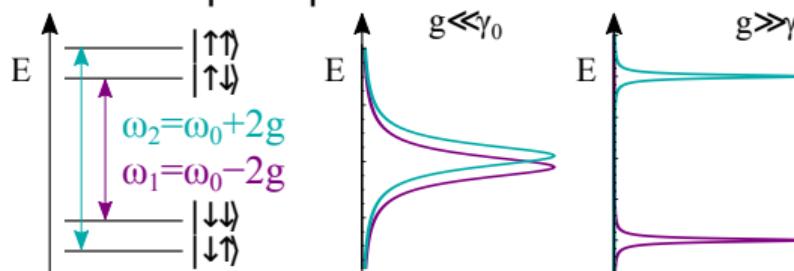
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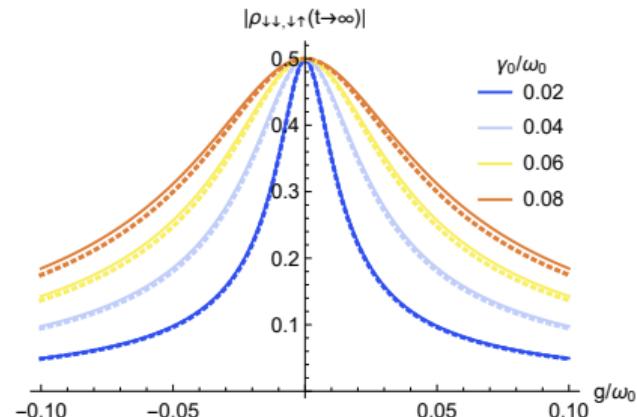
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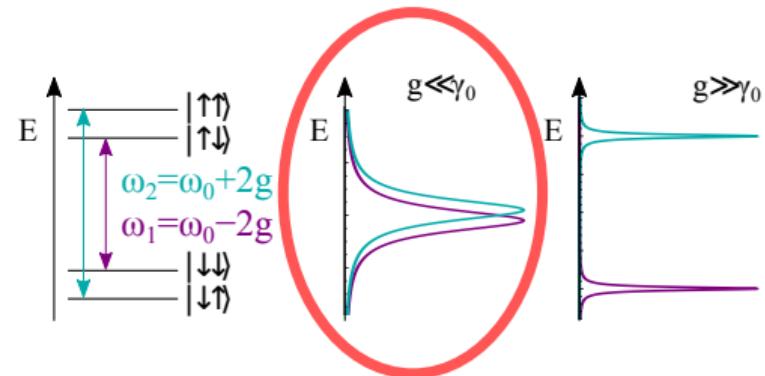
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# Protected coherence: Finite temperature

- $T > 0$ , Born-Markov approx

- Separation of timescales. Decay rates  $\gamma_1 \gg \gamma_2$
- For  $\gamma_1/\kappa_0 \gg \gamma_2/\kappa_0 \gg 1$ , quasi-steady state  
 $p = \rho$

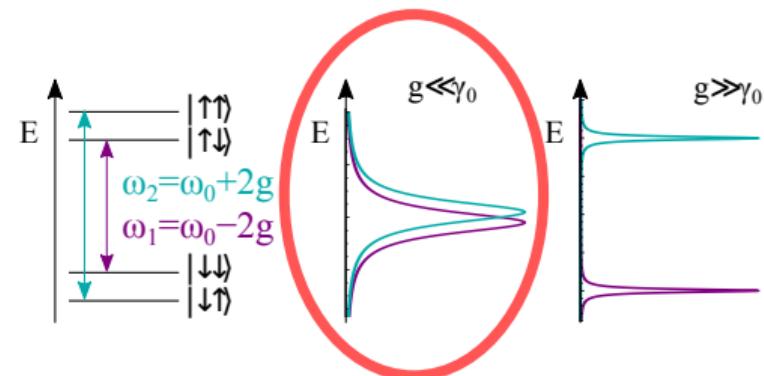


- High T: Large ratio of timescales
- High T protects coherence for longer!
- But: Born-Markov invalid at high T

[Cammack *et al.* PRA '18]

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



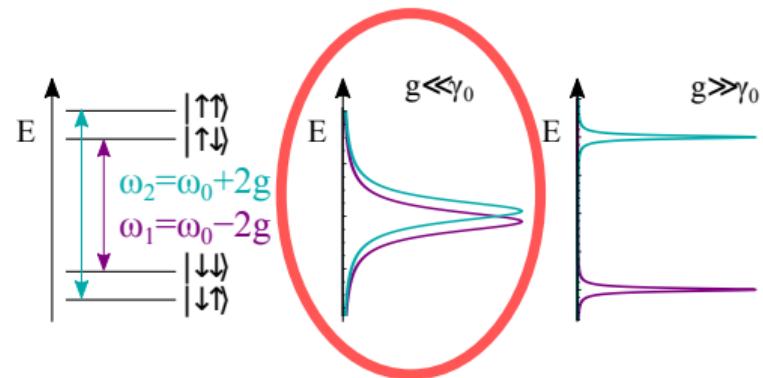
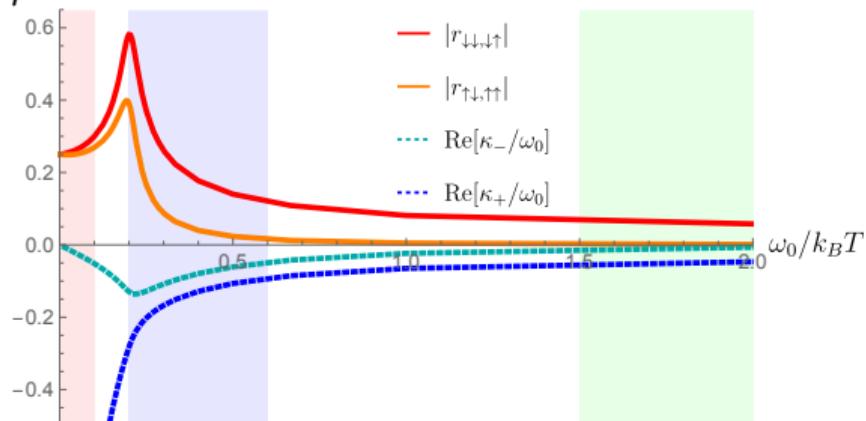
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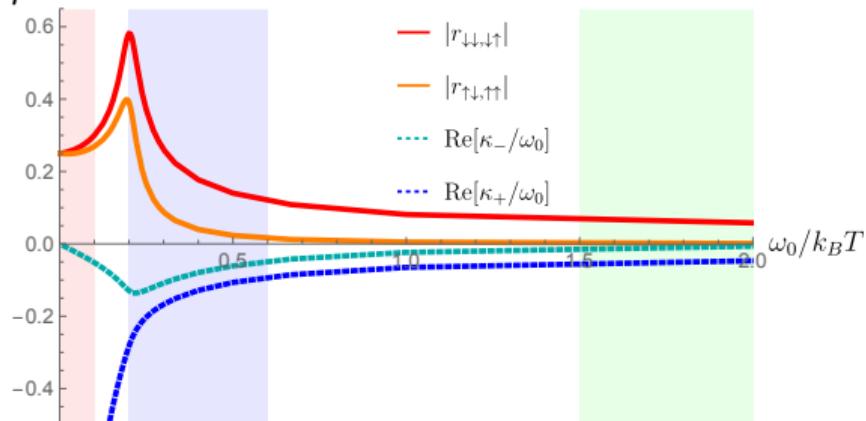
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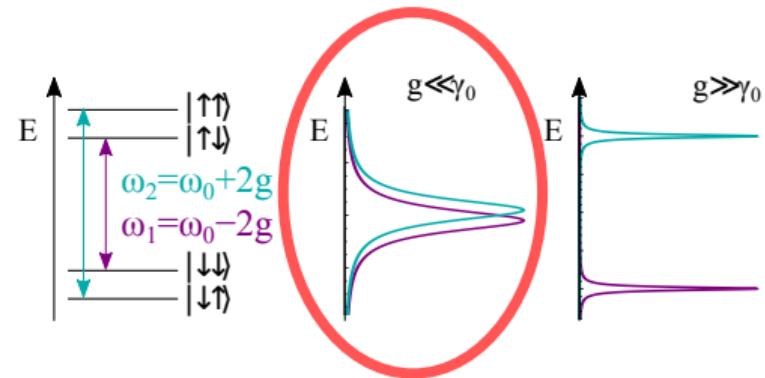
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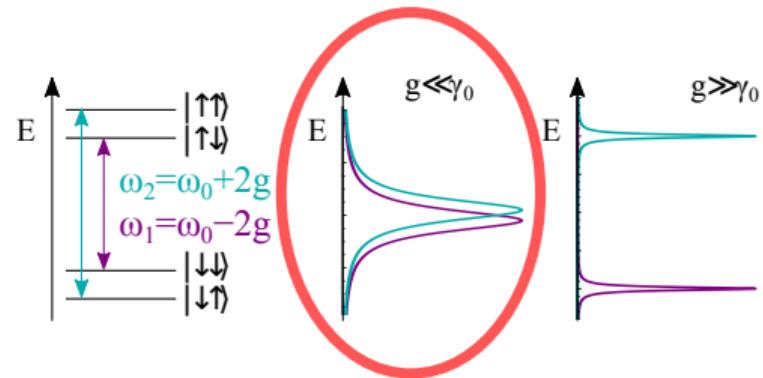
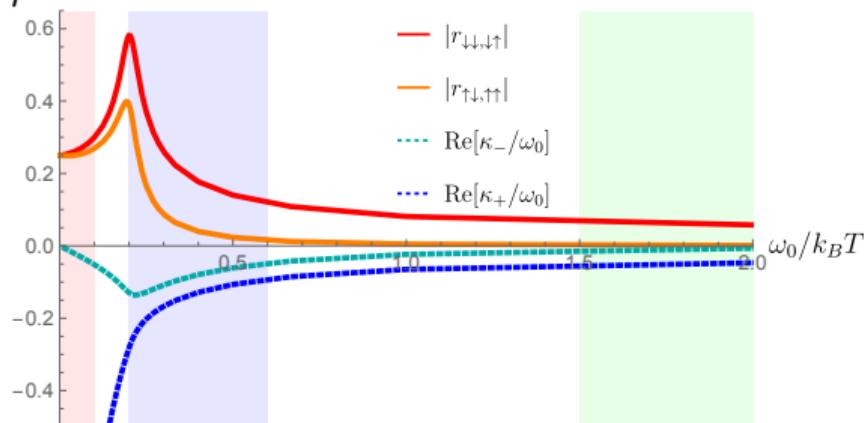


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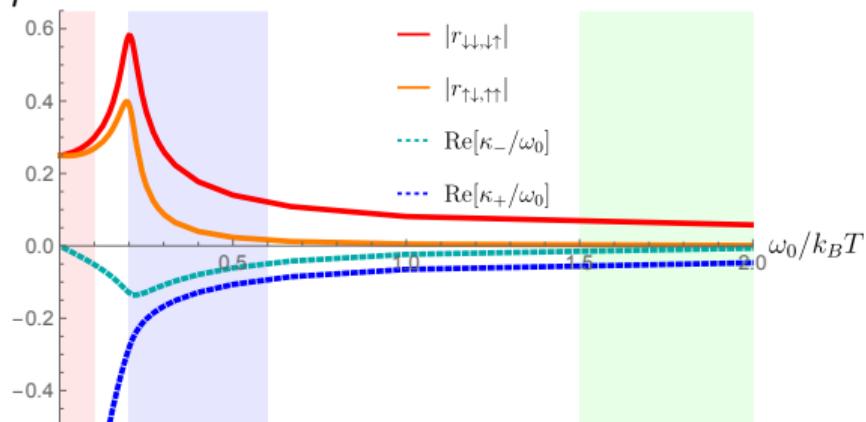
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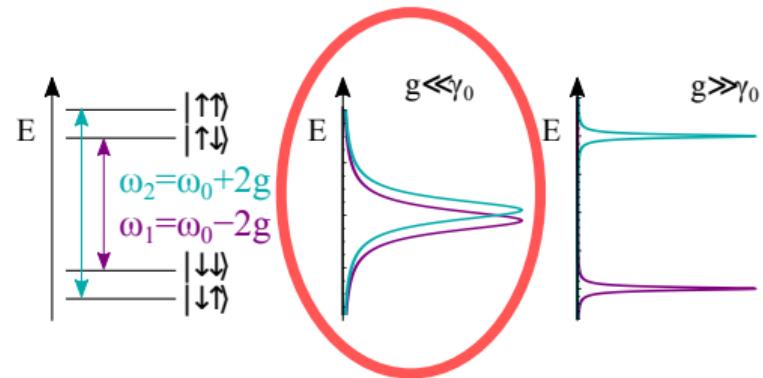
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# Protected coherence: High temperature TEMPO

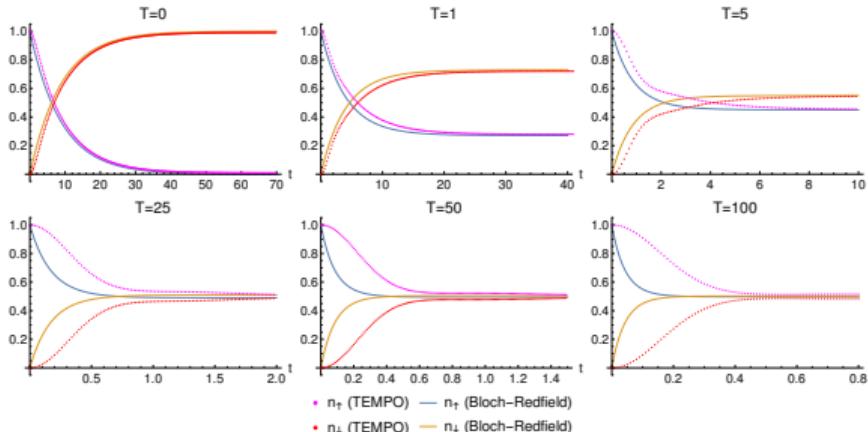
- Modify coupling for TEMPO form:  $H = \frac{\omega_0}{2}\sigma_e^z + g\sigma_e^z\sigma_n^z + \sum_k \xi_k \sigma_e^x(b_k + b_k^\dagger) + H_B$
- Populations — see Markov breakdown  $\rightarrow$  Longer coherence at high  $T$

[Work by A. Dunnett]

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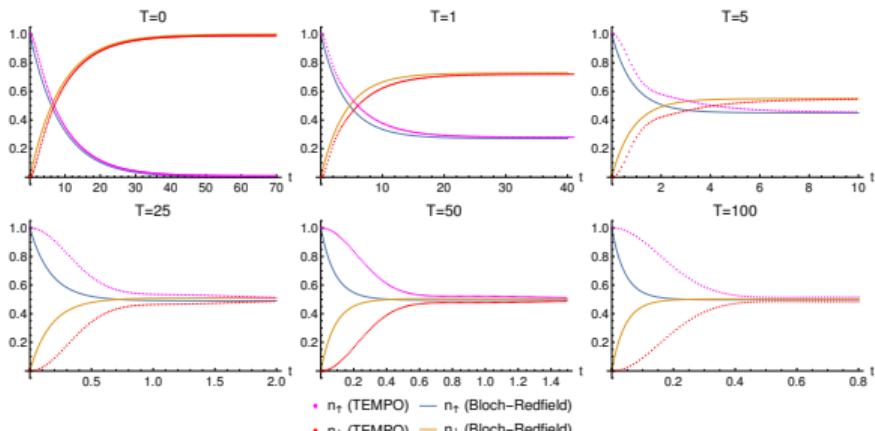


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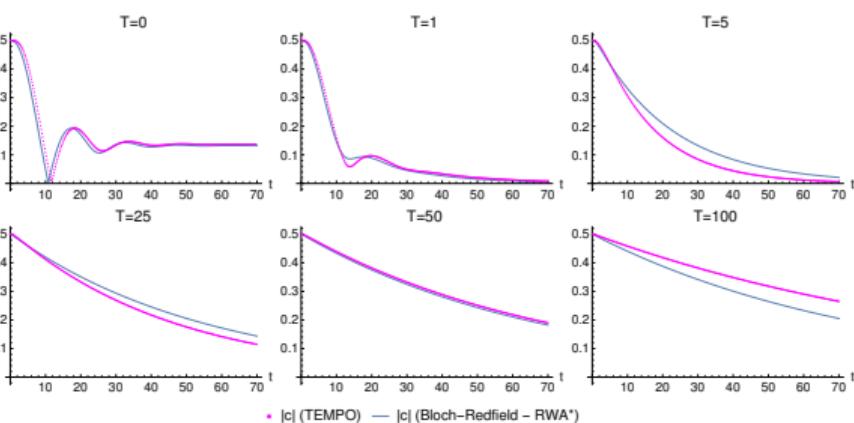
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