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Modelling realistic open quantum systems with process tensors

Jonathan Keeling
University of St Andrews
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Many-body Open Quantum Systems

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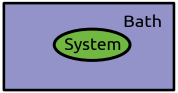
Open quantum systems & Markovian approx.

- Want $\rho_S(t) = \mathrm{Tr}_B(\rho(t))$.



- Standard OQS derivation:

- Time local EOM:
$$\rho^i(t+\Delta) = \left[e^{\Delta\mathcal{L}}\right]^i_j \rho^j(t)$$
- Why non-Markovian/non time-local?

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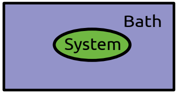

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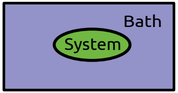

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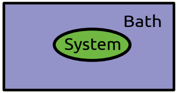

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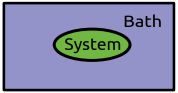

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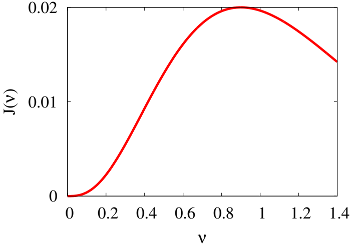

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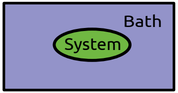

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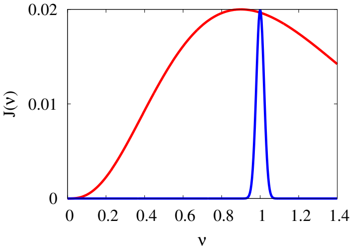

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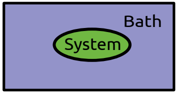

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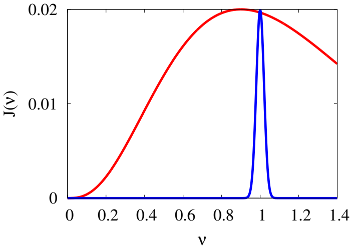

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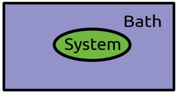

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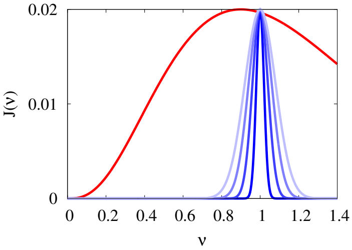

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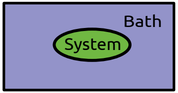

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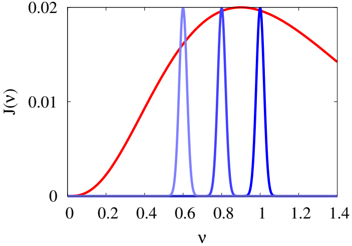

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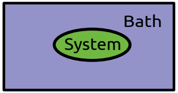

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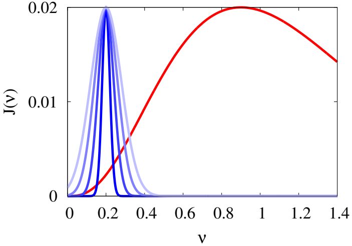

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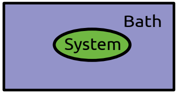

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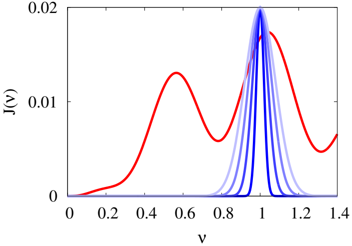

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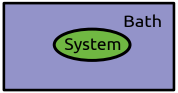

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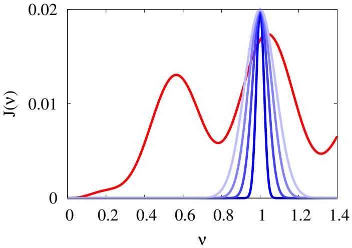

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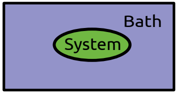

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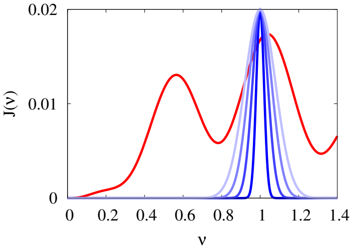

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non-Markovian master equations: How: See [de Vega & Alonso, RMP '17]

- Exactly soluble problems ...
  - e.g. Bosonic: $H = \Psi_i^\dagger M_{ij} \Psi_j + \sum_{i,k} \xi_{i,k}(\psi_i + \psi_i^\dagger)(b_k^\dagger + b_k) + H_{\text{bath}}$
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  $$H \to e^{-V} H e^{V}, \quad V = \sum_k \xi_k (b_k - b_k^\dagger) X_{\text{sys}}$$

  - Renormalize system parameters
  - Perturbative remaining coupling

  [Jang, J. Chem. Phys '09, McCutcheon *et al.* PRB '11, Roy and Hughes PRB '12]
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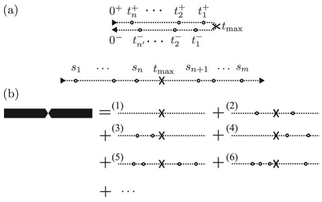

non-Markovian methods: augmentation

- Exponential bath correlations, Hierarchical EOM [Tanimura & Kubo, JPSJ '89]
  Bath $\rightarrow$ sum of Lorenzians modes. n_k describes interaction with mode k.

$$\dot{\rho}_{\mathbf{n},\mathbf{m}} = \mathcal{L}_S \rho_{\mathbf{n},\mathbf{m}} + \sum_{\mathbf{n}',\mathbf{m}'} \mathcal{D}_{\mathbf{n},\mathbf{m},\mathbf{n}',\mathbf{m}'} \rho_{\mathbf{n}',\mathbf{m}'}$$

- Hierarchy of Pure States [Suess, Eisfeld & Strunz, PRL '14; J. Stat. Phys. '15]
  Stochastic unravelling $\rho_{n,m} \rightarrow \sum_l |\psi_n^l\rangle \langle \psi_m^l|$.
- Increase system — include resonant modes

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

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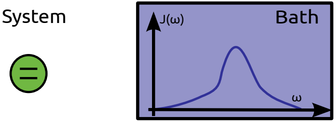
  - 

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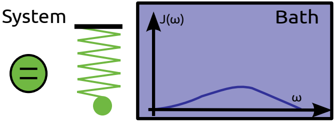
  - 

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  - Include bath $\rightarrow$ chain mapping
    [Chin *et al.* PRL '10; Nat. Phys. '13; Woods *et al.*, J. Math. Phys. '14]
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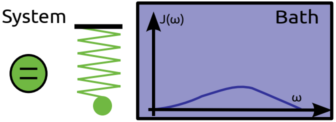
- Exponential bath correlations, Hierarchical EOM [Tanimura & Kubo, JPSJ '89]
  Bath $\to$ sum of Lorenzians modes. n_k describes interaction with mode k.

$$\dot{\rho}_{\mathbf{n},\mathbf{m}} = \mathcal{L}_S \rho_{\mathbf{n},\mathbf{m}} + \sum_{\mathbf{n}',\mathbf{m}'} \mathcal{D}_{\mathbf{n},\mathbf{m},\mathbf{n}',\mathbf{m}'} \rho_{\mathbf{n}',\mathbf{m}'}$$

- Hierarchy of Pure States [Suess, Eisfeld & Strunz, PRL '14; J. Stat. Phys. '15]
  Stochastic unravelling $\rho_{\mathbf{n},\mathbf{m}} \to \sum_t |\psi^t_{\mathbf{n}}\rangle \langle \psi^t_{\mathbf{m}}|$.
- Increase system — include resonant modes
  - 

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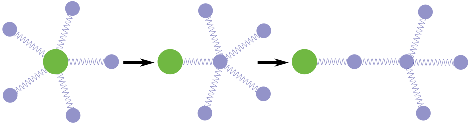
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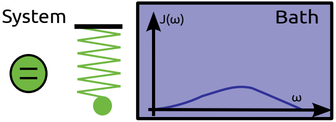
  - 

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    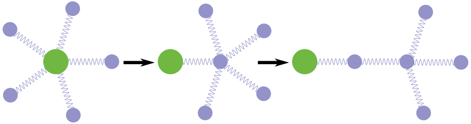
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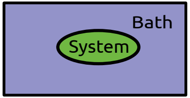
1. Non-Markovian problems & Many-body physics
   - Non-Markovian methods
2. Background: QUAPI & Tensor networks
   - Path integral approach
   - Tensor networks & Matrix product states
   - The TEMPO algorithm
3. Re-interpretation: Process tensors
   - PT-MPO representation
   - Beyond Gaussian environments
4. Applications
   - Optimisation
   - Lattice models
   - Polariton condensation
   - Two-dimensional spectroscopy
5. Future outlook

QUAPI

- System + Harmonic bath



$$H = H_S + \sum_k g_k X_s (b_k + b_k^\dagger) + \omega_k b_k^\dagger b_k$$

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

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

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

- Influence functionals:

$$I_k(j, j') = \begin{cases} e^{\phi_k(j,j')} & k \neq 1 \\ e^{\phi_1(j,j')} \left[e^{\Delta \mathcal{L}_0} \right]_{jj'} & k = 1 \end{cases}$$

[Marki & Makarov J. Chem. Phys. '95]

QUAPI

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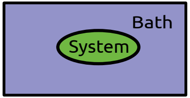

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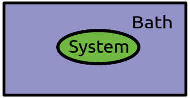

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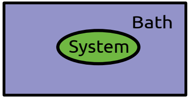

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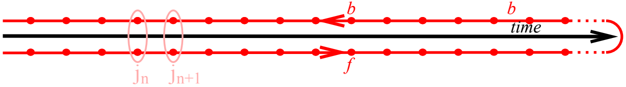

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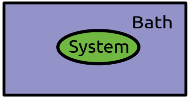

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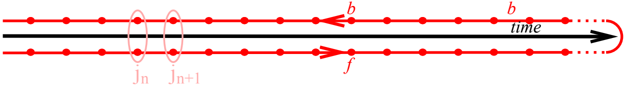

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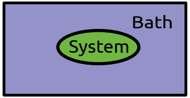

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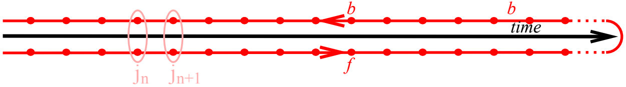

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QUAPI as tensor propagation

- Evaluating path sum:

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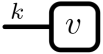
Penrose tensor network notation & contraction

vector v_k 

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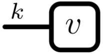
vector	v_k	
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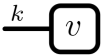
vector	v_k	
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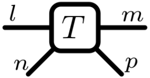
4-rank tensor	$T_{l,m,n,p}$	

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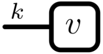

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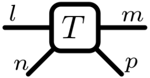

A

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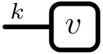

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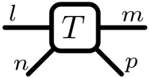
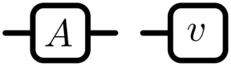


A v



$A_{i,j}$ v_k

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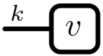
vector	v_k	
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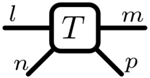
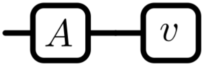
4-rank tensor	$T_{l,m,n,p}$	

A $\qquad v$



$$\sum_k A_{i,k} \quad v_k$$

Penrose tensor network notation & contraction

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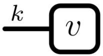

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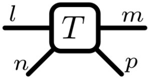

$$A \quad v \quad = \quad w$$

$$\sum_k A_{i,k} \quad v_k \quad = \quad w_i$$

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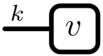
vector v_k 

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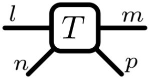
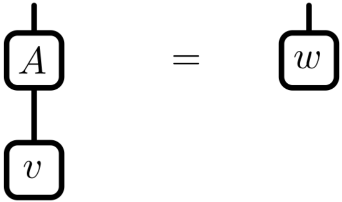
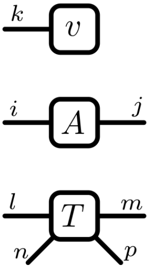
4-rank tensor $T_{l,m,n,p}$ 



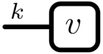
Penrose tensor network notation & contraction

vector	v_k	
matrix	$A_{i,j}$	
4-rank tensor	$T_{l,m,n,p}$	



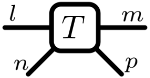
Penrose tensor network notation & contraction

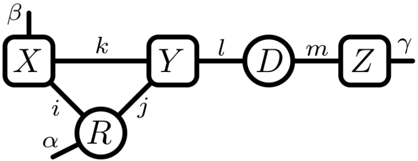
vector v_k



matrix $A_{i,j}$

4-rank tensor $T_{l,m,n,p}$





$$\sum_{ijklm} R_{\alpha ij}\, X_{i\beta k}\, Y_{jkl}\, D_{lm}\, Z_{m\gamma}$$

Penrose tensor network notation & contraction

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matrix $A_{i,j}$

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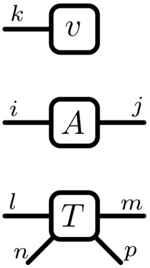
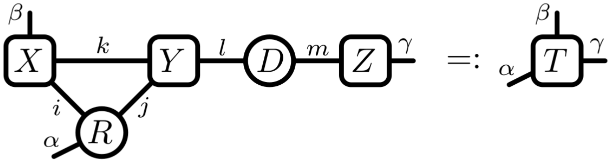




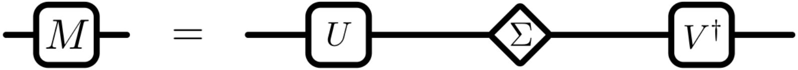
$$\sum_{ijklm} R_{\alpha ij}\, X_{i\beta k}\, Y_{jkl}\, D_{lm}\, Z_{m\gamma} =: T_{\alpha\beta\gamma}$$

Singular value decomposition & compression

$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

- Fixed bond dimension: Keep $\lambda_1 \ldots \lambda_\chi$
- Fixed precision: Keep $\lambda_n > \epsilon_{\mathrm{rel}} \lambda_1$

Singular value decomposition & compression



$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \lambda_3 & \\ & & & \lambda_4 \end{pmatrix} \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

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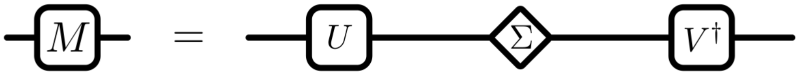

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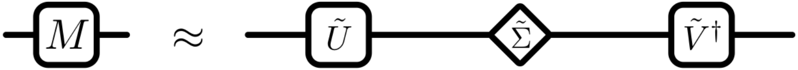

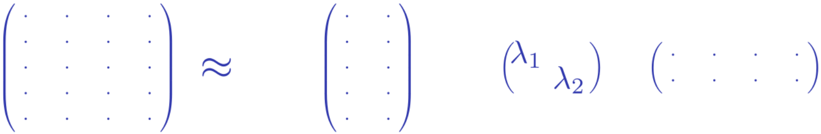

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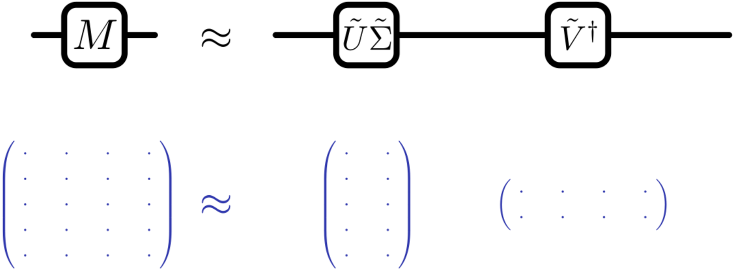

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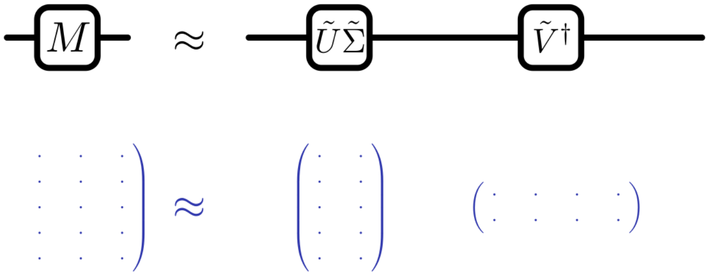

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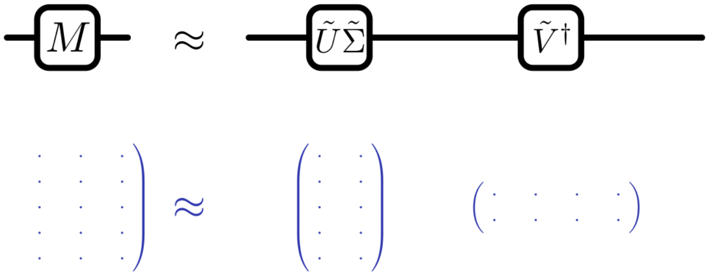

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Matrix product states

$$|\psi\rangle = \sum_{i_1,i_2,\ldots i_N \in \{0,1\}} C_{i_1,i_2,\ldots i_N} |i_1, i_2, \ldots, i_N\rangle$$

e.g. $C_{0,1,1,0,1} = \langle 01101|\psi\rangle$

Reviews: Schollwöck, Ann. Phys. (N.Y.) 326, 96 (2011). Orús, *ibid.* 349, 117 (2014)

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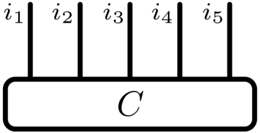

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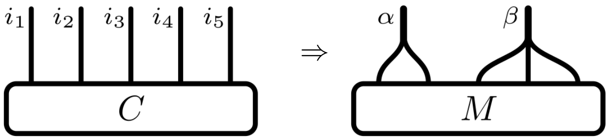

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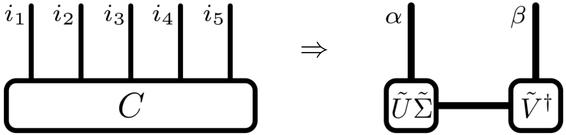

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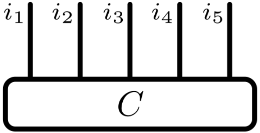
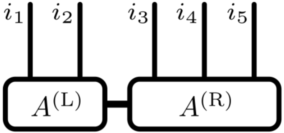


$\Rightarrow$



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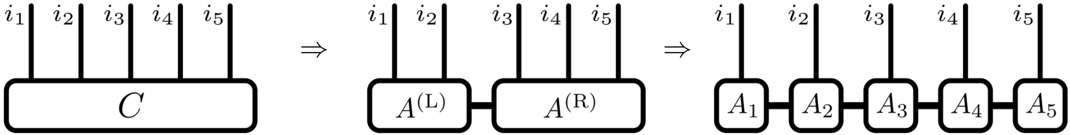

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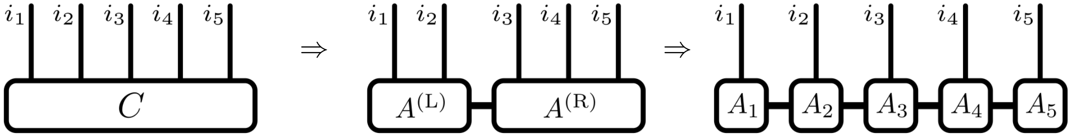

Full state: 2^N numbers

MPS, $2N\chi^2$ numbers

Reviews: Schollwöck, Ann. Phys. (N.Y.) 326, 96 (2011). Orús, *ibid.* 349, 117 (2014)

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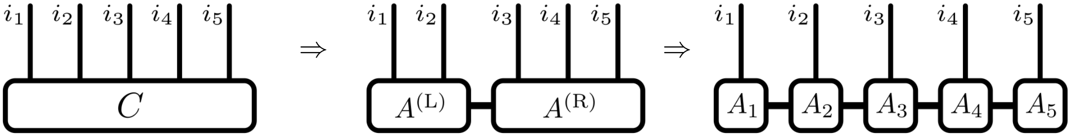

Full state: 2^N numbers

MPS, $2N\chi^2$ numbers

Applies to: Wavefunctions, density matrices, probabilities ....
Also known as “tensor trains”

Reviews: Schollwöck, Ann. Phys. (N.Y.) 326, 96 (2011). Orús, *ibid.* 349, 117 (2014)

From Hilbert space to Liouville space

$$\hat{U}|\psi\rangle$$

From Hilbert space to Liouville space

$\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger$

From Hilbert space to Liouville space

$\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger$ $\qquad$ $\hat{U}\rho\hat{U}^\dagger$

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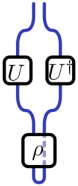
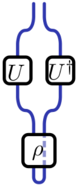
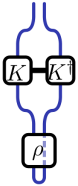


From Hilbert space to Liouville space

$\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger$ $\qquad$ $\hat{U}\rho\hat{U}^\dagger$ $\qquad$ $\hat{U}\rho\hat{U}^\dagger$ $\qquad$ $\sum_\alpha \hat{K}_\alpha \rho \hat{K}_\alpha^\dagger$





From Hilbert space to Liouville space

Hilbert space

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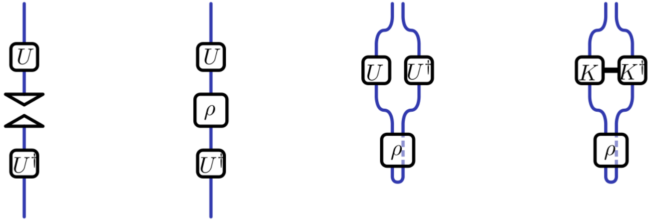
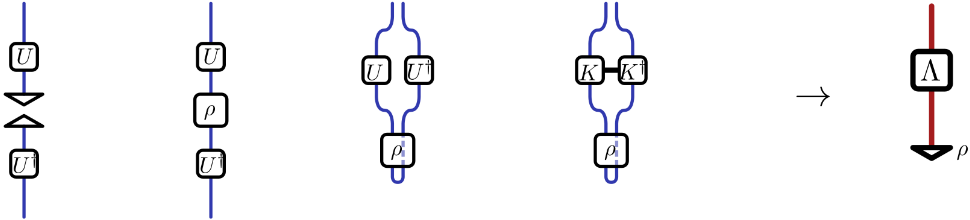


From Hilbert space to Liouville space

Hilbert space | Liouville space

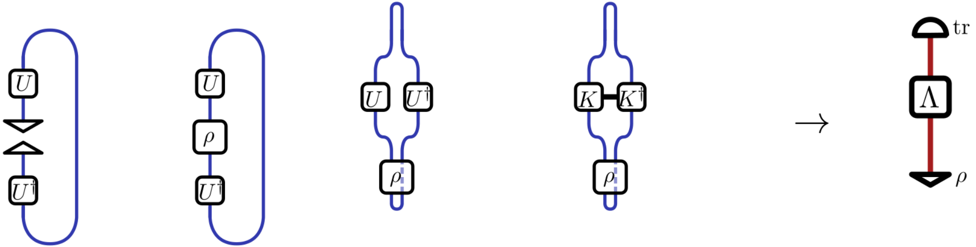
$\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger$ $\quad$ $\hat{U}\rho\hat{U}^\dagger$ $\quad$ $\hat{U}\rho\hat{U}^\dagger$ $\quad$ $\sum_\alpha \hat{K}_\alpha \rho \hat{K}^\dagger_\alpha$ $\quad \rightarrow \quad$ $\Lambda[\rho]$



From Hilbert space to Liouville space

Hilbert space | **Liouville space**

$\mathrm{tr}\left(\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger\right)$ $\quad$ $\mathrm{tr}\left(\hat{U}\rho\hat{U}^\dagger\right)$ $\quad$ $\mathrm{tr}\left(\hat{U}\rho\hat{U}^\dagger\right)$ $\quad$ $\mathrm{tr}\left(\sum_\alpha \hat{K}_\alpha\rho\hat{K}_\alpha^\dagger\right)$ $\quad \rightarrow \quad$ $\mathrm{tr}\left(\Lambda\left[\rho\right]\right)$



QUAPI as tensor network

- 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

[Strathearn *et al.* Nat. Commun. '18]

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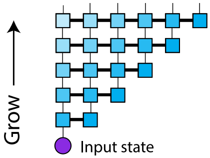

[Strathearn *et al.* Nat. Commun. '18]

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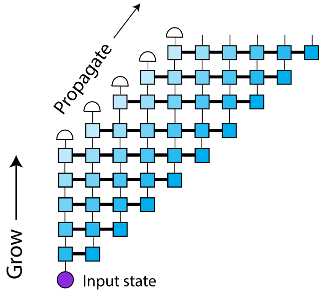

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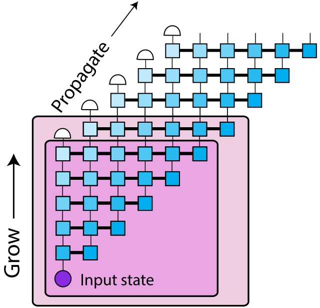

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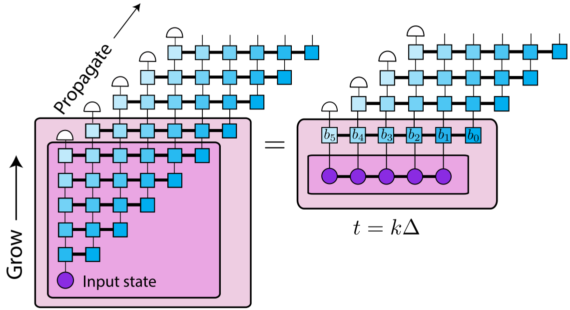

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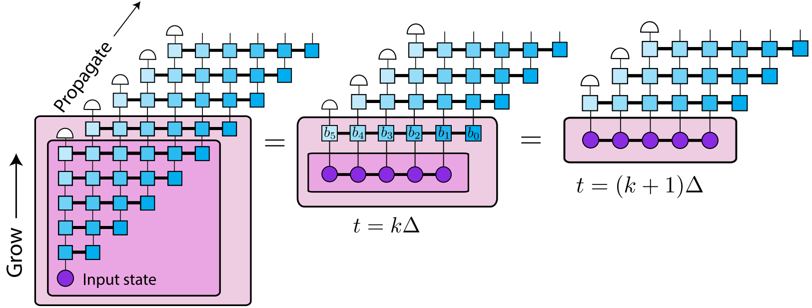
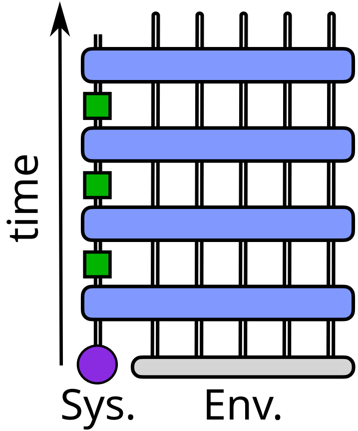


[Strathearn *et al.* Nat. Commun. ’18]

Process tensors



- Gate-based picture of evolution
- Separate out environment—response to sequence of operations
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[Chiribella *et al.* PRL ’08, PRA ’09; Pollock *et al.* PRA ’18, PRL ’18]

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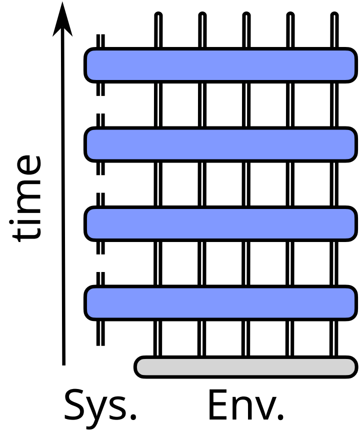

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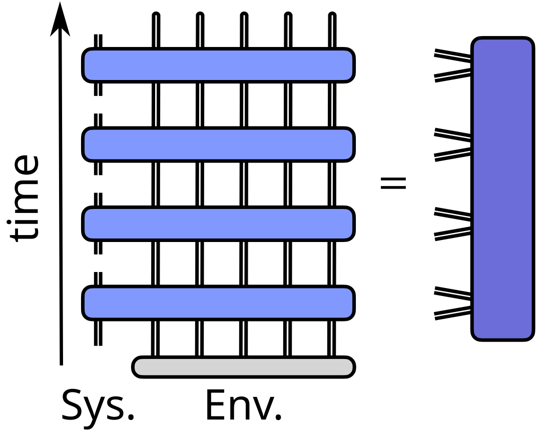

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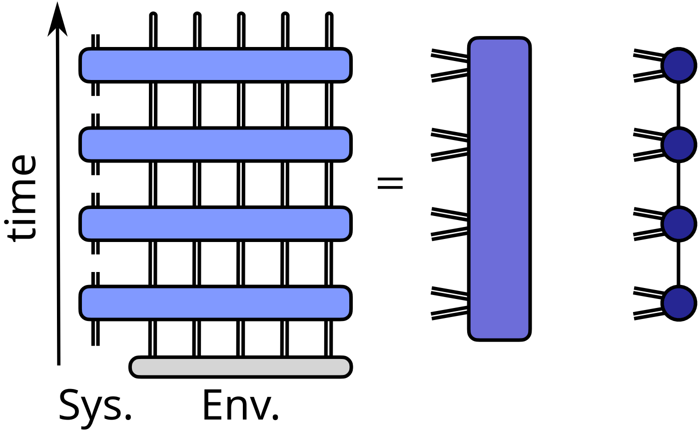

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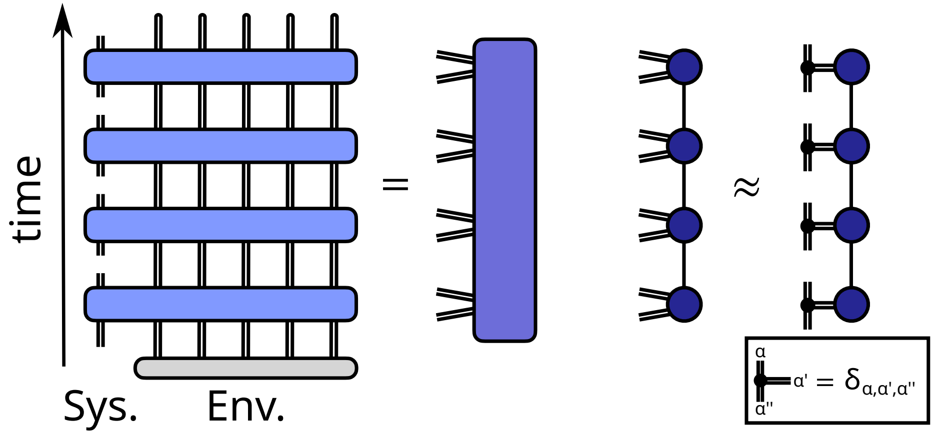

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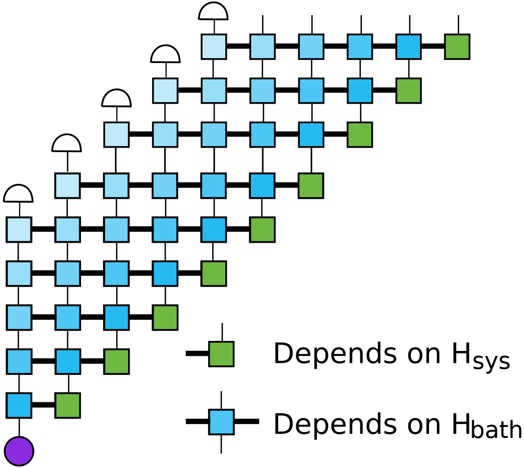
[Chiribella *et al.* PRL ’08, PRA ’09; Pollock *et al.* PRA ’18, PRL ’18]

Re-interpretting TEMPO network → process tensors MPO



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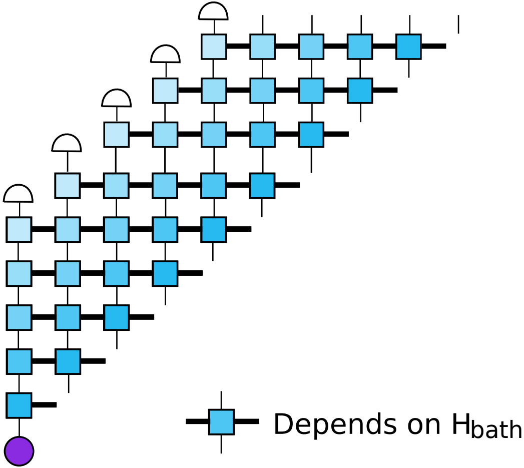

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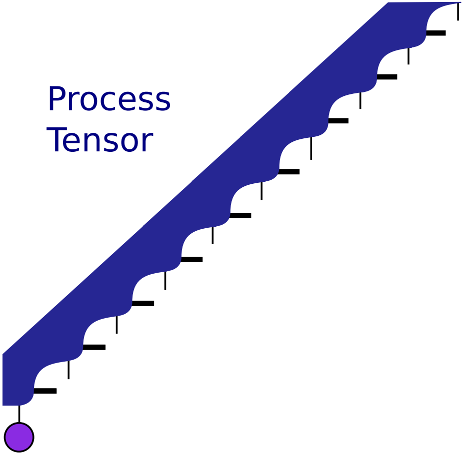

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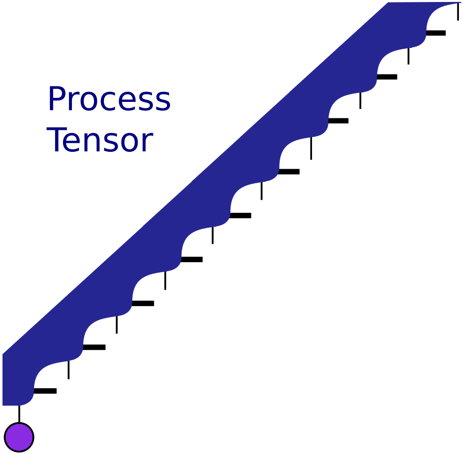

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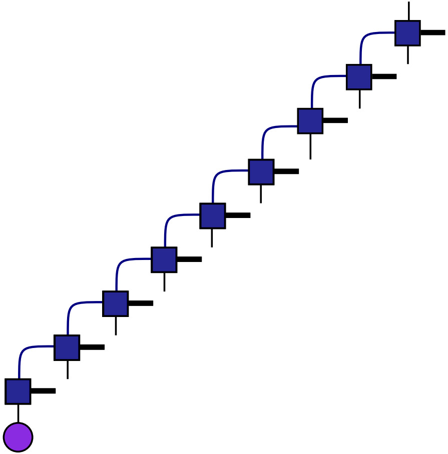

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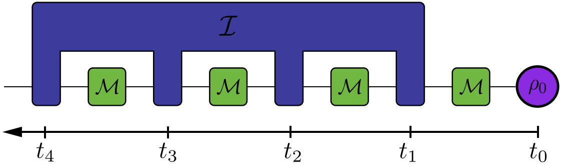
Automatic compression of environments



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[Cygorek *et al.* Nat. Phys. '22]

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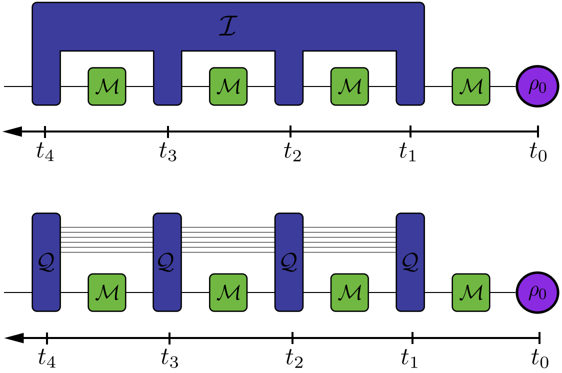

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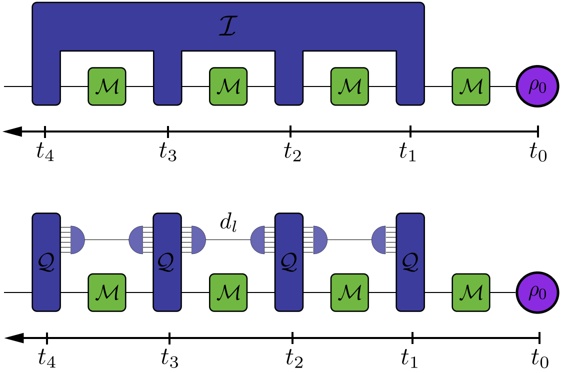

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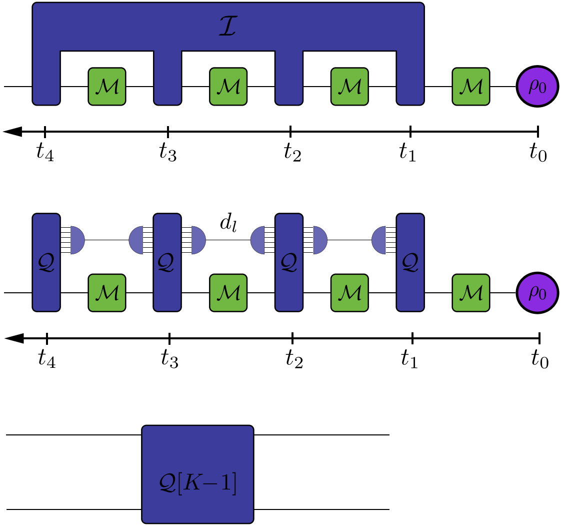

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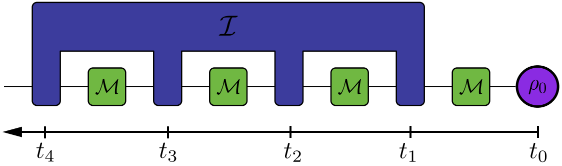

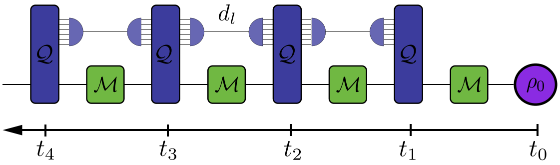

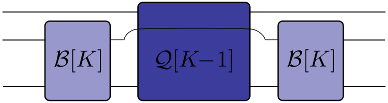

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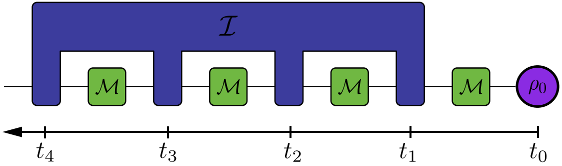

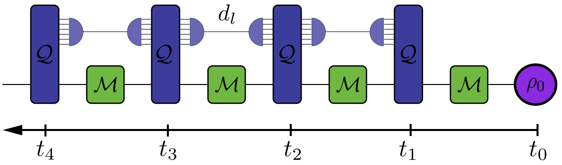

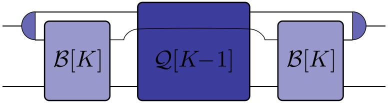

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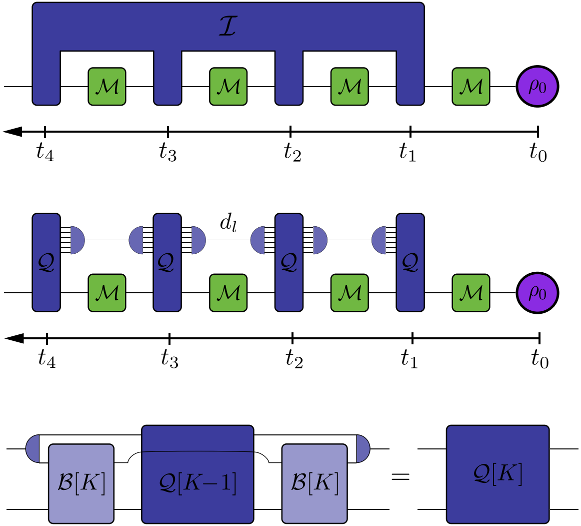

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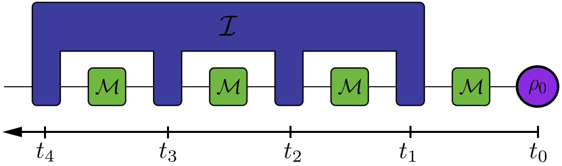

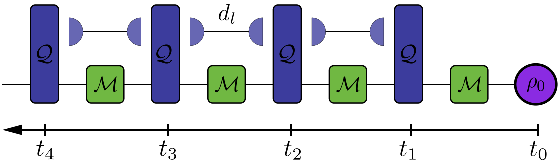

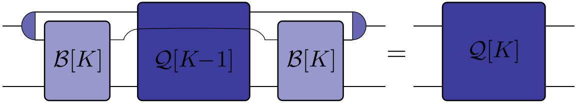

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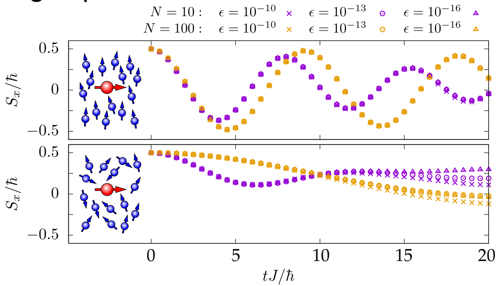
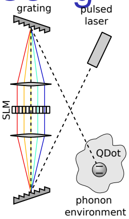


1. Non-Markovian problems & Many-body physics
   - Non-Markovian methods
2. Background: QUAPI & Tensor networks
   - Path integral approach
   - Tensor networks & Matrix product states
   - The TEMPO algorithm
3. Re-interpretation: Process tensors
   - PT-MPO representation
   - Beyond Gaussian environments
4. Applications
   - Optimisation
   - Lattice models
   - Polariton condensation
   - Two-dimensional spectroscopy
5. Future outlook

Using PT-MPO: Optimisation of pulse sequence



- 200s pre-compute, ~ 2 s contract $\times 16000$ points [Fux, Butler *et al.* PRL '21]
- Even faster: derivative w.r.t Hamiltonian via back-propagation

[Butler, Fux *et al.* PRL '24]

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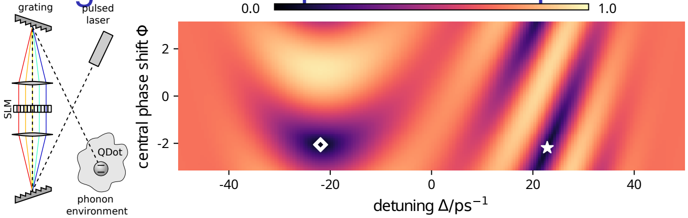

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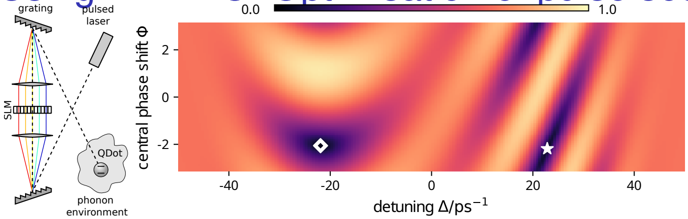

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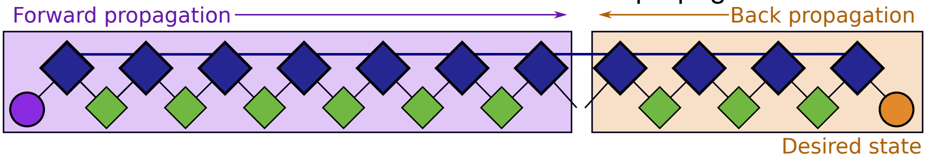

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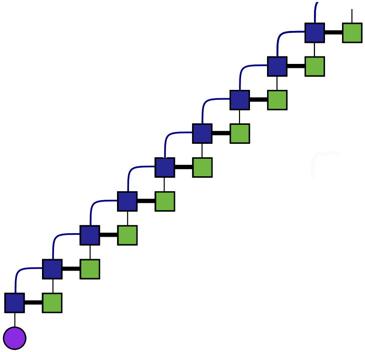
TEMPO and Lattice problems

- One site: PT-MPO



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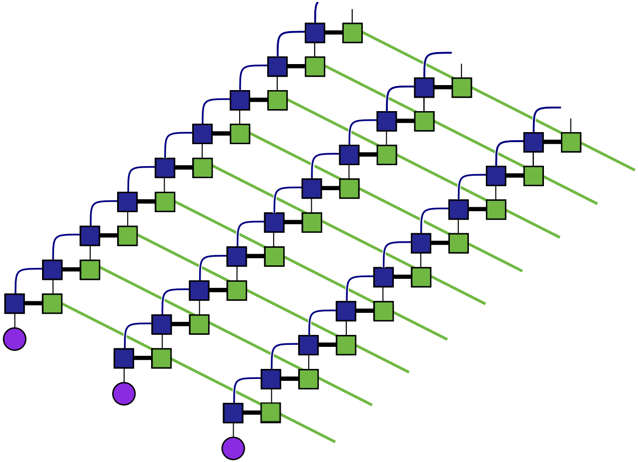
- e.g., thermalisation of 1D chain



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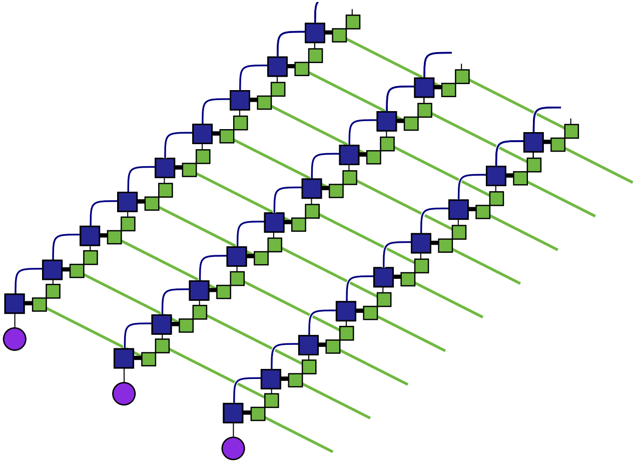

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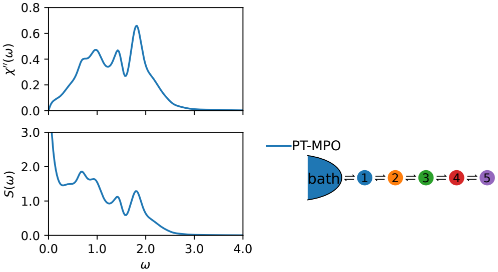

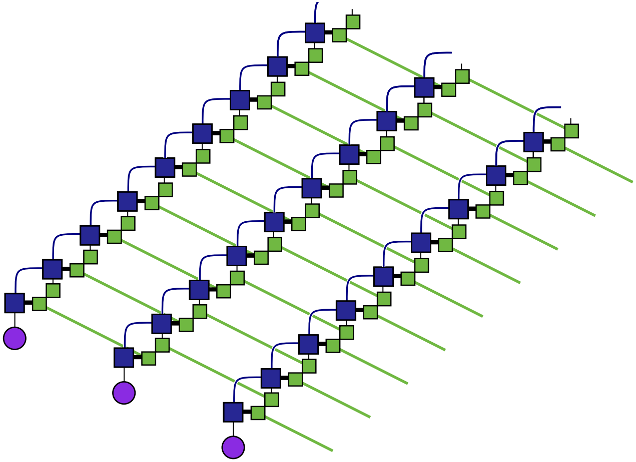

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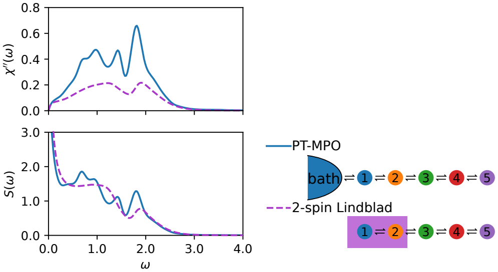

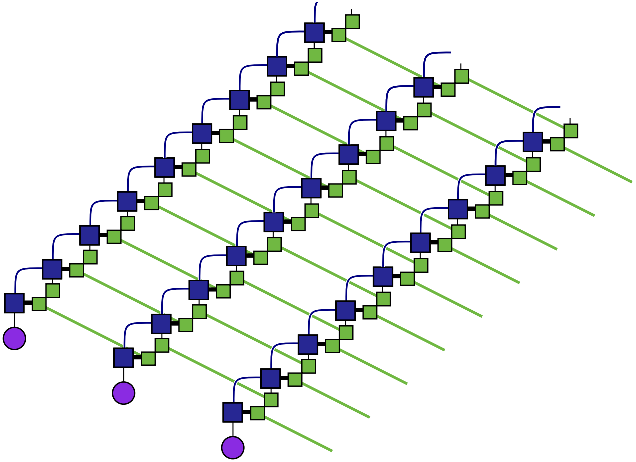

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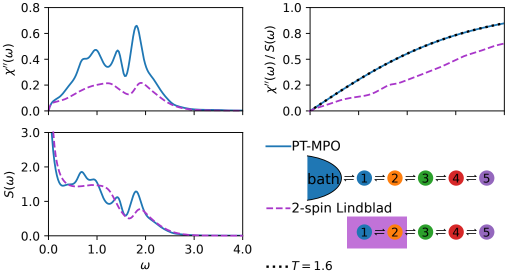

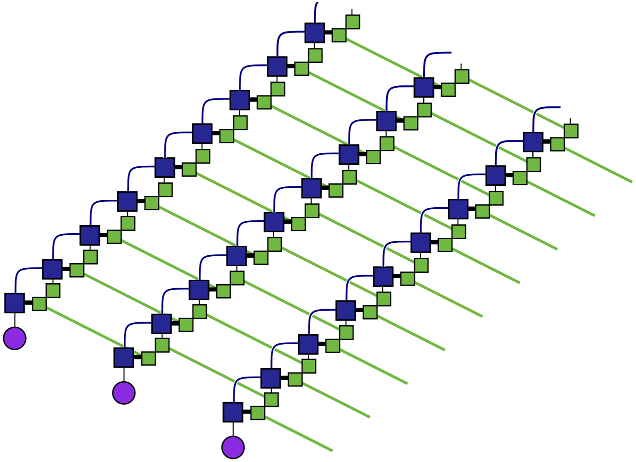

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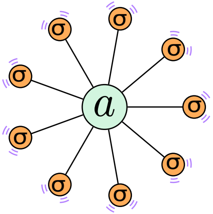
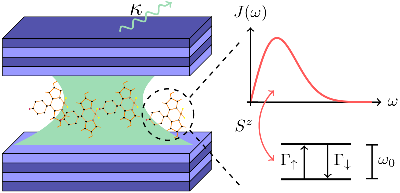
Mean-field TEMPO: Polariton condensation

- Tavis-Cummings model + bath



$$H = \omega a^\dagger a + \sum_{i=1}^{\mathcal{N}_m} \Big[g(a\sigma_i^+ + \text{H.c.}) + \omega_0 \sigma_i^+ \sigma_i^- + \sum_k \xi_{i,k}(b_{i,k} + b_{i,k}^\dagger)\sigma_i^z + \omega_{k,v} b_{i,k}^\dagger b_{i,k} \Big]$$

- $J(\omega)$, match BODIPY-Br



- Process tensor → fast evaluation
- Phase diagram vs $\omega_c, g, T_{\text{bath}}$
- Large $\mathcal{N}_m$, mean-field decoupling

[Fowler-Wright *et al.* PRL '22] see also [Mu *et al.* PRL '26] beyond MF

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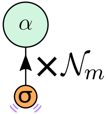

$$H_i = g(\langle a\rangle \sigma_i^x + \text{H.c.}) + \omega_0 \sigma_i^+ \sigma_i^-$$

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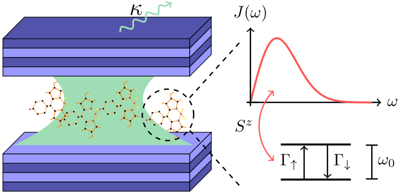

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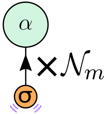

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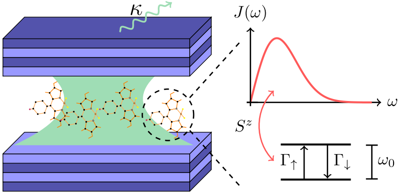

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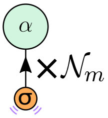

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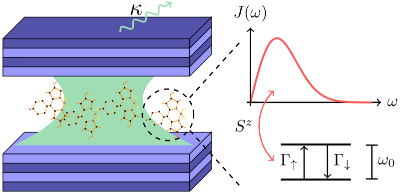

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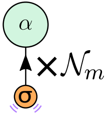

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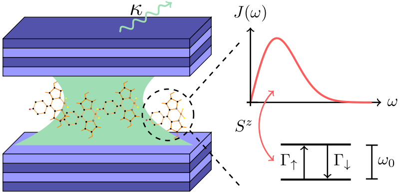
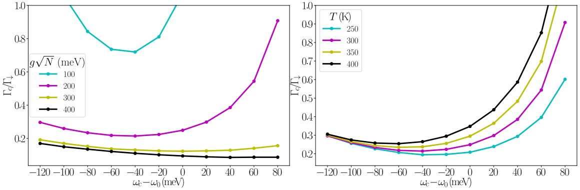


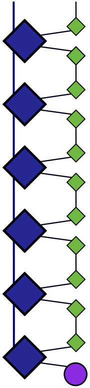
- Process tensor → fast evaluation
- Phase diagram vs ω_c, g, T_bath



[Fowler-Wright *et al.* PRL '22] see also [Mu *et al.* PRL '26] beyond MF

Multi-time correlations → 2D spectroscopy

Process tensor:



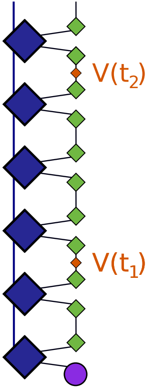
- 2D spectroscopy:

- 2D Spectra:
  Fourier transform w.r.t $t_2 - t_1$

[De Wit *et al.* PRR ’25]

Multi-time correlations → 2D spectroscopy

Process tensor: → natural tool for multi-time correlations



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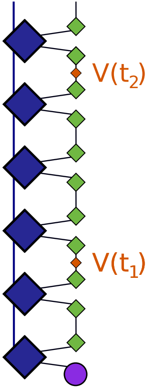

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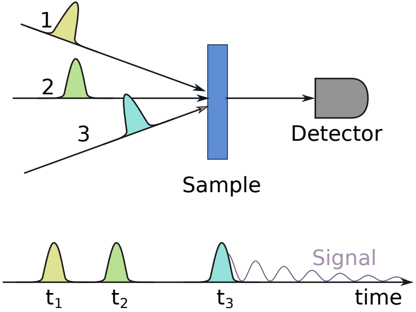

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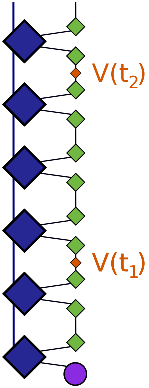

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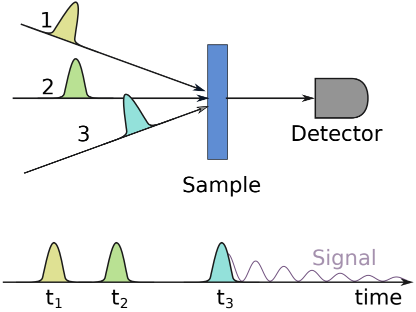

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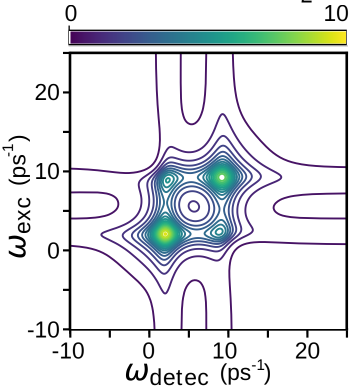

Outlook—future directions

- Complex systems: organic molecules, biological chromophores
  Large Hilbert space, see [Cochin *et al.* 2603.06840]
- Many-body problems
- Process tensor representations beyond MPO
  - Tree tensor network, e.g.[Dowling *et al.* PRX '24]

See [Keeling, Stoudenmire, Bañuls, Reichman: 2509.07661]

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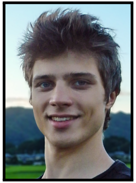
Acknowledgements







FUNDING:

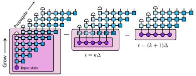
EPSRC
Engineering and Physical Sciences
Research Council

CM-CDT

QOpen
Many-body Open Quantum Systems

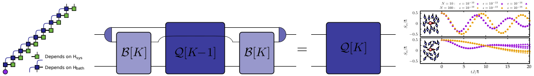
Summary

- TEMPO Algorithm for general non-Markovian problems



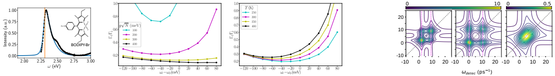
[Strathearn, Kirton, Kilda, Keeling & Lovett, Nat. Comm. '18]

- Reformulation as process tensor, Automatic Compression of Environments



[Fux *et al.* PRL '21] [Cygorek *et al.* Nat. Phys. '22]

- Can combine with Lattices, Mean-Field theory, 2D spectroscopy



[Fux, Kilda *et al.* PRR '23] [Fowler-Wright *et al.* PRL '22] [de Wit *et al.* PRR '25]

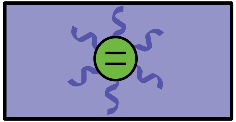
- Perspective: [Keeling *et al.* arXiv:2509.07661]
- **Open source code available:**
  `https://github.com/tempoCollaboration/OQuPy` [Fux *et al.* JCP '24]

6 Application: Spin-Boson problem

- Tensor networks & Matrix product states

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 $\omega_c \gg \Omega$:

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 $t \rightarrow \infty$.

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

spin Boson model

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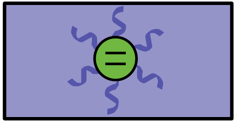

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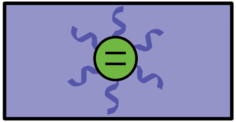

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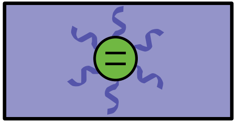

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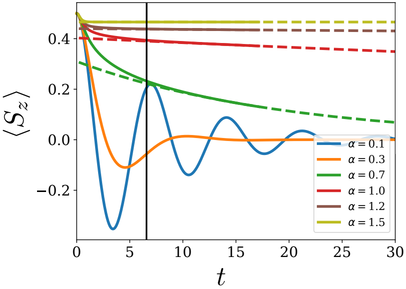
TEMPO spin Boson results



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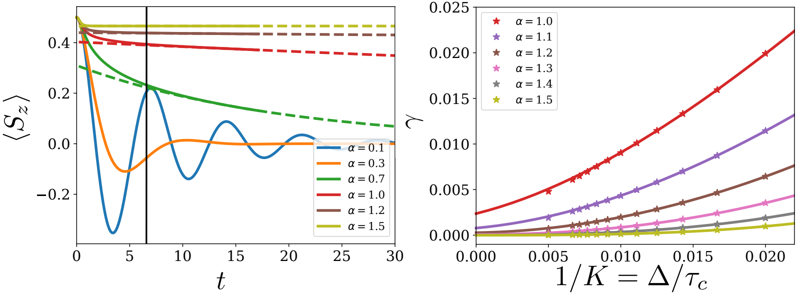

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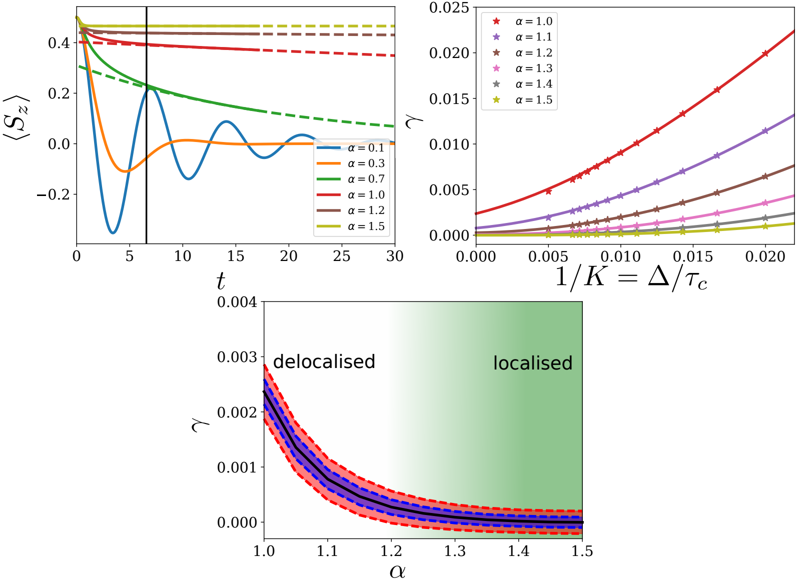
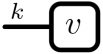


Penrose tensor network notation & contraction

vector v_k 

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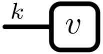
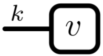
vector	v_k	
matrix	$A_{i,j}$	

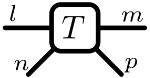
Penrose tensor network notation & contraction

vector v_k



matrix $A_{i,j}$

4-rank tensor $T_{l,m,n,p}$



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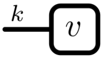

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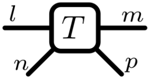

A

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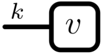

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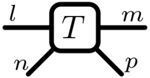
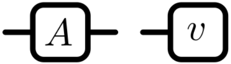


A v



$A_{i,j}$ v_k

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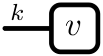

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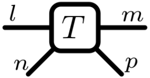
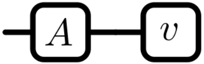


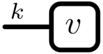
$A \qquad v$



$$\sum_k A_{i,k} \quad v_k$$

Penrose tensor network notation & contraction

vector v_k



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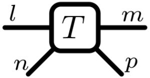

$$A \qquad v \qquad = \qquad w$$

$$\sum_k A_{i,k} \quad v_k \quad = \quad w_i$$

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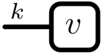
vector v_k 

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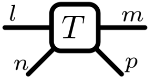
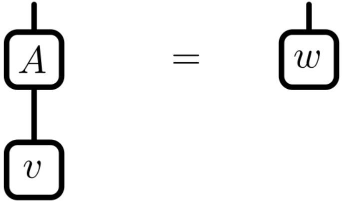
4-rank tensor $T_{l,m,n,p}$ 



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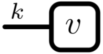

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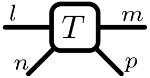

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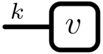
vector	v_k	
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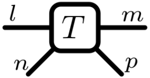
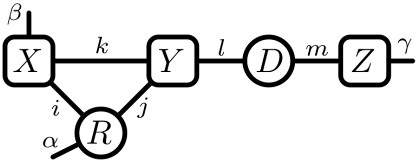
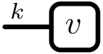
4-rank tensor	$T_{l,m,n,p}$	

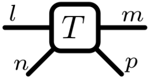


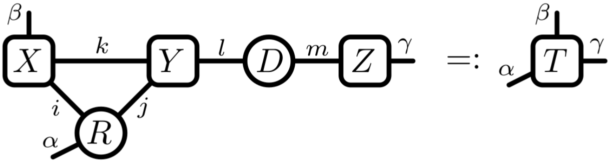
$$\sum_{ijklm} R_{\alpha ij}\, X_{i\beta k}\, Y_{jkl}\, D_{lm}\, Z_{m\gamma}$$

Penrose tensor network notation & contraction

vector	v_k	
matrix	$A_{i,j}$	
4-rank tensor	$T_{l,m,n,p}$	







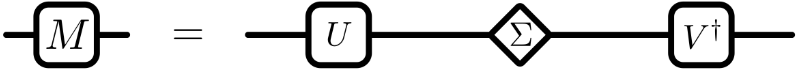
$$\sum_{ijklm} R_{\alpha ij}\, X_{i\beta k}\, Y_{jkl}\, D_{lm}\, Z_{m\gamma} =: T_{\alpha\beta\gamma}$$

Singular value decomposition & compression

$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

- Fixed bond dimension: Keep $\lambda_1 \ldots \lambda_\chi$
- Fixed precision: Keep $\lambda_n > \epsilon_{\mathrm{rel}} \lambda_1$

Singular value decomposition & compression



$$
\begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \lambda_3 & \\ & & & \lambda_4 \end{pmatrix} \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}
$$

- Fixed bond dimension: Keep $\lambda_1 \ldots \lambda_\chi$
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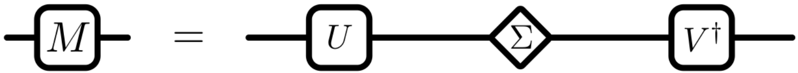

$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \cancel{\lambda_3} & \\ & & & \cancel{\lambda_4} \end{pmatrix} \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

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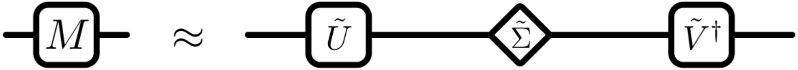

$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} \approx \begin{pmatrix} \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \end{pmatrix} \begin{pmatrix} \lambda_1 & \\ & \lambda_2 \end{pmatrix} \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

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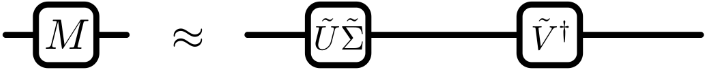

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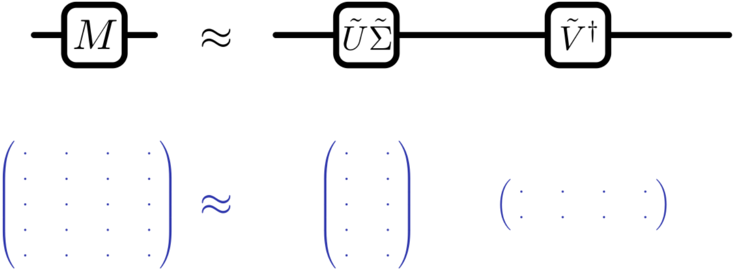

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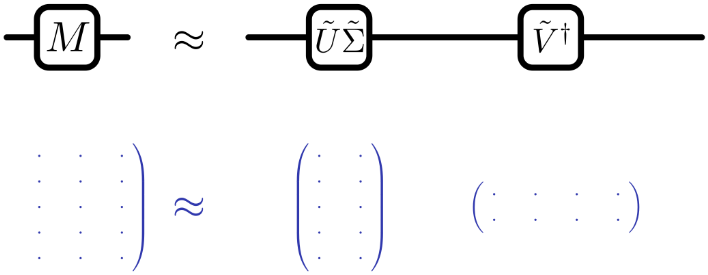

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Matrix product states

$$|\psi\rangle = \sum_{i_1,i_2,\ldots i_N \in \{0,1\}} C_{i_1,i_2,\ldots i_N} |i_1, i_2, \ldots, i_N\rangle$$

e.g. $C_{0,1,1,0,1} = \langle 01101|\psi\rangle$

Reviews: Schollwöck, Ann. Phys. (N.Y.) 326, 96 (2011). Orús, *ibid.* 349, 117 (2014)

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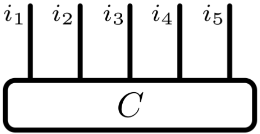

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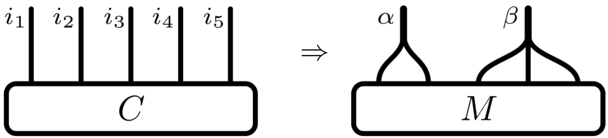

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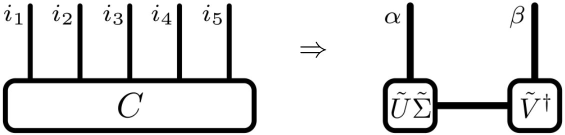

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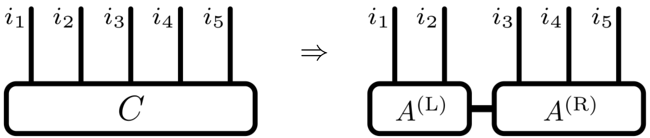

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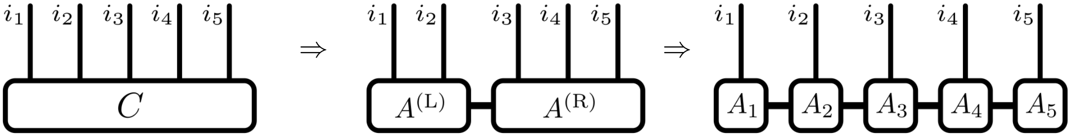

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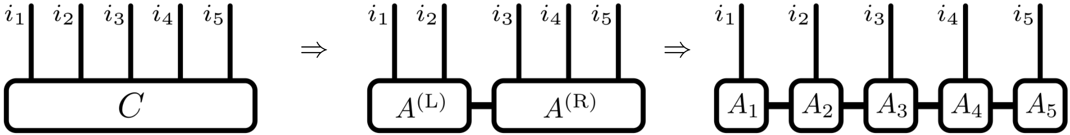

Full state: 2^N numbers

MPS, $2N\chi^2$ numbers

Reviews: Schollwöck, Ann. Phys. (N.Y.) 326, 96 (2011). Orús, *ibid.* 349, 117 (2014)

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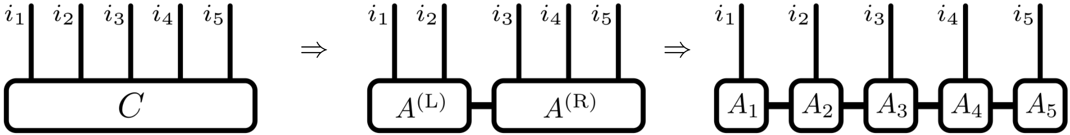


Full state: 2^N numbers

MPS, $2N\chi^2$ numbers

Applies to: Wavefunctions, density matrices, probabilities ....
Also known as “tensor trains”

Reviews: Schollwöck, Ann. Phys. (N.Y.) 326, 96 (2011). Orús, *ibid.* 349, 117 (2014)

From Hilbert space to Liouville space

$\hat{U}|\psi\rangle$

From Hilbert space to Liouville space

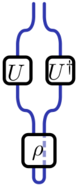
$$\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger$$

From Hilbert space to Liouville space

$$\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger \qquad \hat{U}\rho\hat{U}^\dagger$$

From Hilbert space to Liouville space

$\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger$ $\quad$ $\hat{U}\rho\hat{U}^\dagger$ $\quad$ $\hat{U}\rho\hat{U}^\dagger$



From Hilbert space to Liouville space

$\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger$

$\hat{U}\rho\hat{U}^\dagger$

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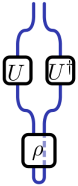
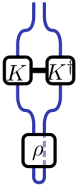


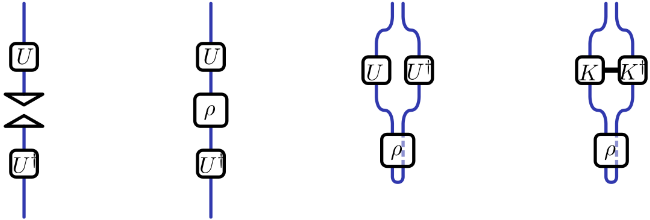
$\sum_\alpha \hat{K}_\alpha \rho \hat{K}_\alpha^\dagger$



From Hilbert space to Liouville space

Hilbert space

$\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger$ $\quad$ $\hat{U}\rho\hat{U}^\dagger$ $\quad$ $\hat{U}\rho\hat{U}^\dagger$ $\quad$ $\sum_\alpha \hat{K}_\alpha\rho\hat{K}_\alpha^\dagger$

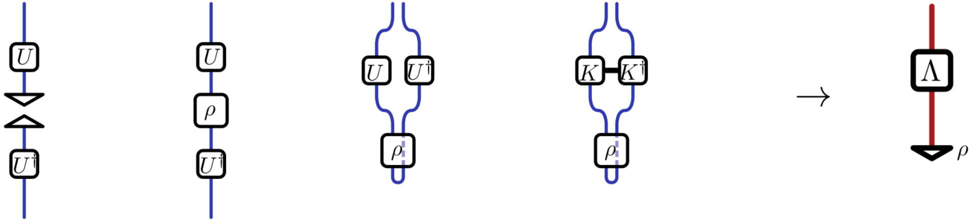


From Hilbert space to Liouville space

Hilbert space

Liouville space

$\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger$ $\quad$ $\hat{U}\rho\hat{U}^\dagger$ $\quad$ $\hat{U}\rho\hat{U}^\dagger$ $\quad$ $\sum_\alpha \hat{K}_\alpha \rho \hat{K}_\alpha^\dagger$ $\quad \rightarrow \quad$ $\Lambda[\rho]$

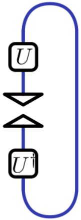


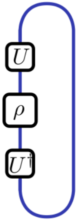
From Hilbert space to Liouville space

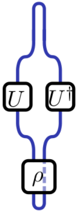
Hilbert space

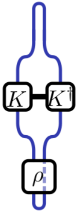
Liouville space

$\mathrm{tr}\left(\hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger\right)$ $\mathrm{tr}\left(\hat{U}\rho\hat{U}^\dagger\right)$ $\mathrm{tr}\left(\hat{U}\rho\hat{U}^\dagger\right)$ $\mathrm{tr}\left(\sum_\alpha \hat{K}_\alpha\rho\hat{K}_\alpha^\dagger\right)$ $\rightarrow$ $\mathrm{tr}\left(\Lambda\left[\rho\right]\right)$









$\rightarrow$