

# Efficient Numerical Optimization via Quantum Trajectories

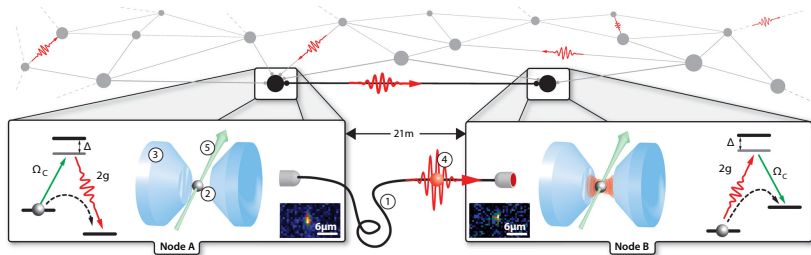
Michael Goerz

Stanford University / Army Research Lab

Gordon Research Conference  
Quantum Control of Light & Matter

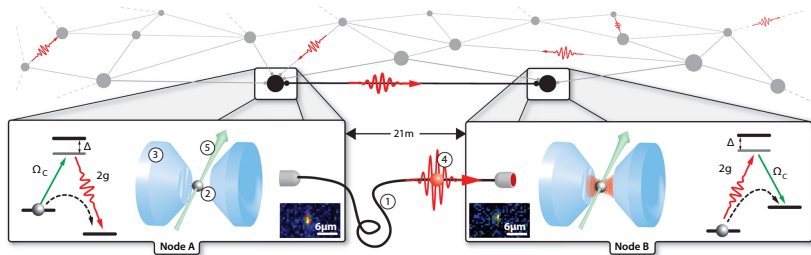
Mount Holyoke College  
August 6, 2017

# quantum networks



from: Reiserer, Rempe. RMP 87, 1379 (2015)

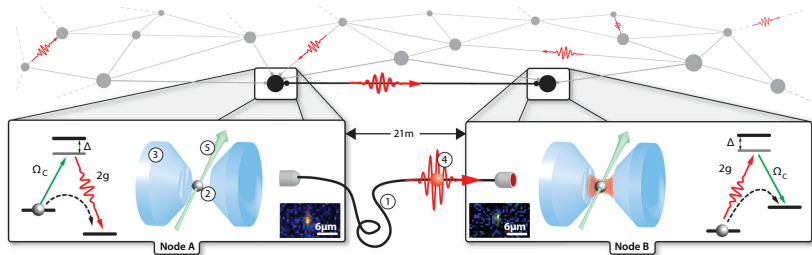
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## applications of networks

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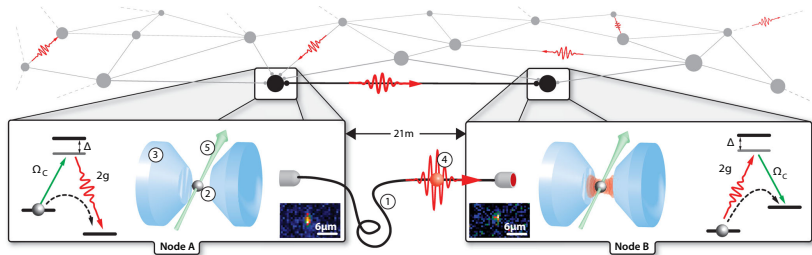


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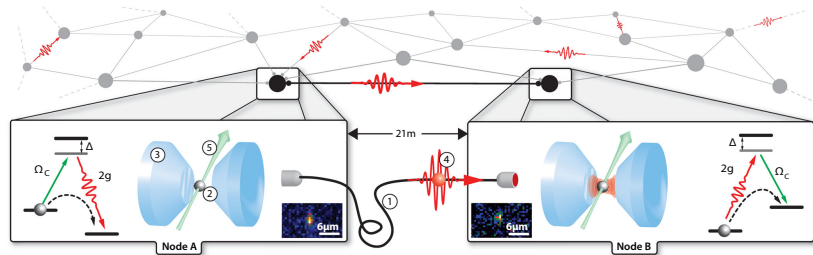


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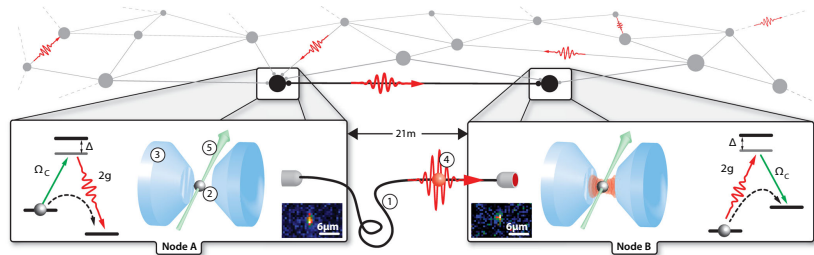


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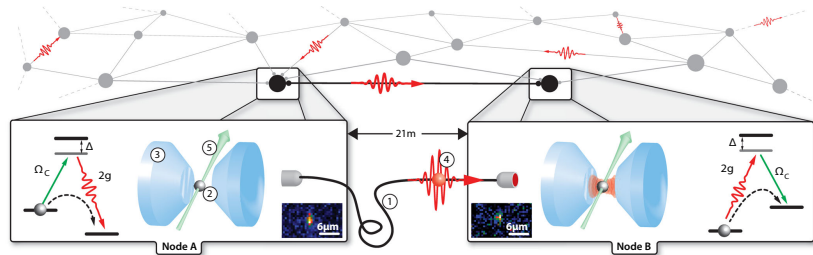
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network advantages:

*scaling, robustness, security*

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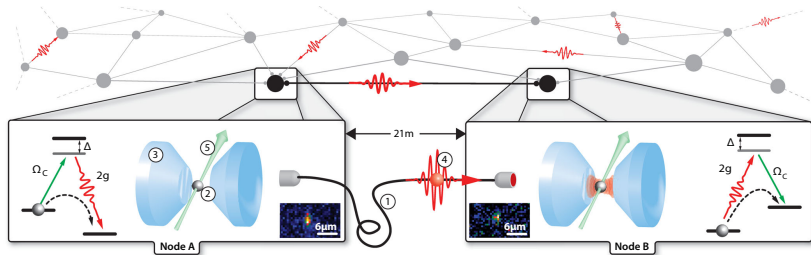
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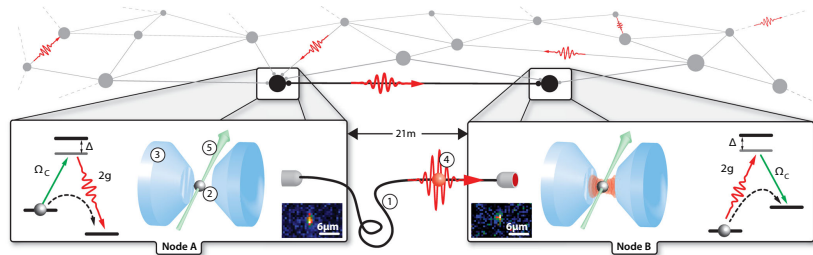
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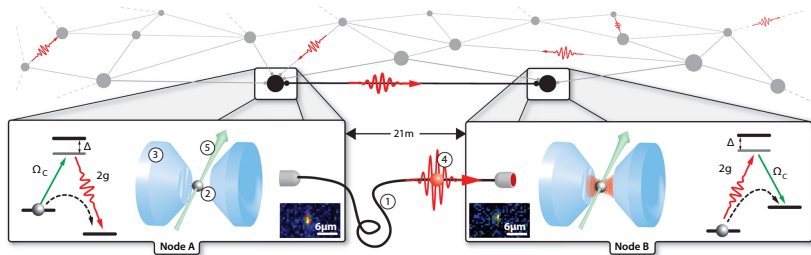
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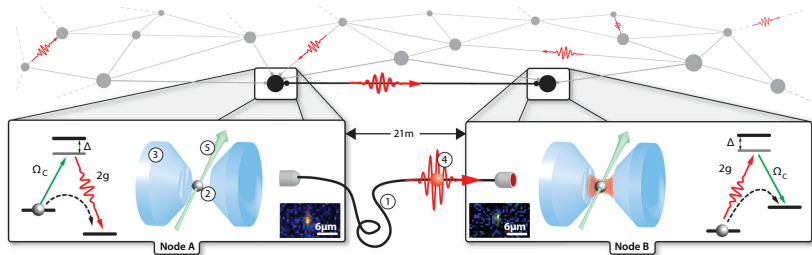
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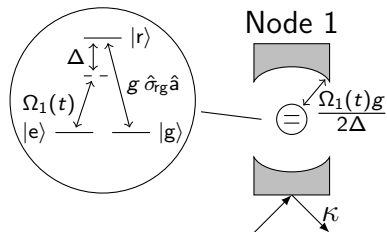
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## control challenges

- node-link interfaces
- entanglement creation & distribution
- signal routing
- local processing



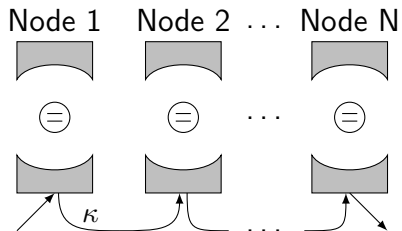
single node:

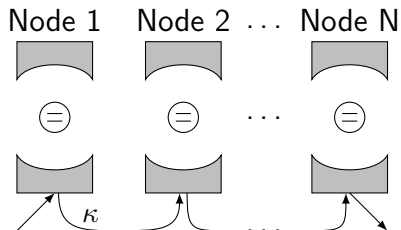
$$\hat{H}^{(1)} = \hat{H}_0 + u_1(t) \left( \hat{\sigma}_{eg} \otimes \hat{\mathbf{a}}_1^\dagger + \text{c.c.} \right)$$

$$\hat{L}^{(1)} = \sqrt{2\kappa} \hat{\mathbf{a}}_1$$

cf. Cirac et al, PRL 78, 3221 (1997)

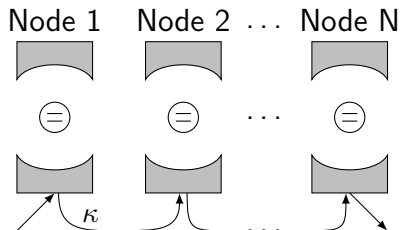
# network model





**SLH formalism** (Gough, James):

$$\{(\hat{\mathbf{H}}^{(i)}, \{\hat{\mathbf{L}}^{(i)}\})\} \text{ of nodes} \rightarrow (\hat{\mathbf{H}}, \{\hat{\mathbf{L}}\}) \text{ of network}$$



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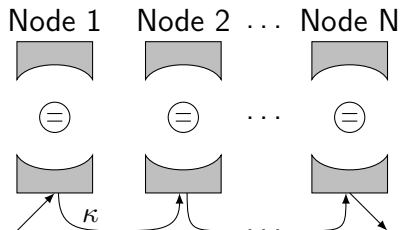


QNET: computer (quantum) algebra software

<https://github.com/mabuchilab/QNET>

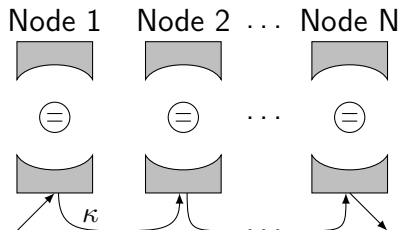


# network model



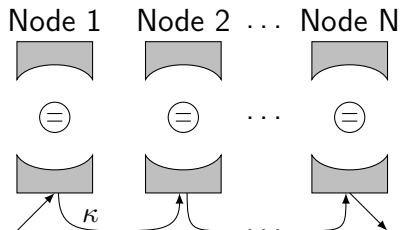
$$\hat{\mathbf{H}} = \sum_{i=1}^N \hat{\mathbf{H}}^{(i)} + \sum_{i \neq j} i\kappa \hat{\mathbf{a}}_i^\dagger \hat{\mathbf{a}}_j + \text{c.c.}; \quad \hat{\mathbf{L}} = \sqrt{2\kappa} \sum_{i=1}^N \hat{\mathbf{a}}_i$$

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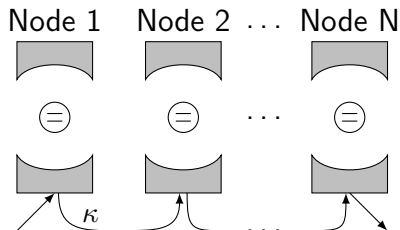
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- Hilbert space dimension exponential with  $N$

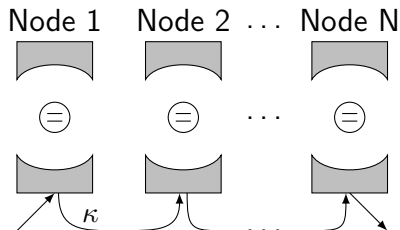
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- Hilbert space dimension exponential with  $N$
  - node-node interaction and decay both  $\propto \kappa$
- $\Rightarrow$  dark state  $\langle \Psi | \hat{\mathbf{L}}^\dagger \hat{\mathbf{L}} | \Psi \rangle = 0$

# quantum jump method (MCWF)

see Dum et al. PRA 4879 (1992); Mølmer et al. JOSAB 10, 524 (1993)

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propagate until  $|\Psi_k(t)|^2 = r$ .



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instantaneous jump  $|\Psi_k(t)\rangle \rightarrow \hat{\mathbf{L}}_l |\Psi_k(t)\rangle$  (normalized)

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- 4 new random number  $r \in [0, 1)$  and continue the propagation.

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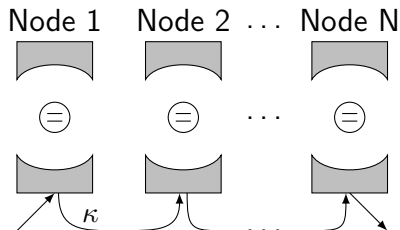
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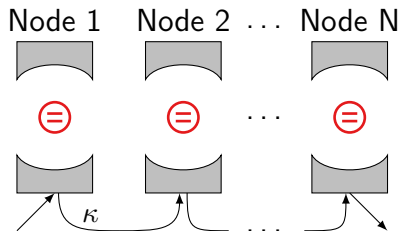
## trajectory averaging:

$$\hat{\rho} = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{k=1}^M |\Psi_k\rangle \langle \Psi_k|$$

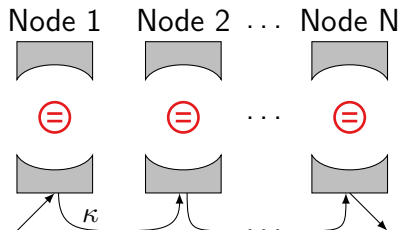
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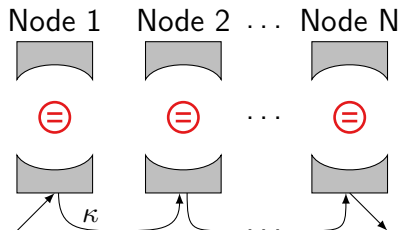


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**Dicke state:** distribute a fixed excitation number over all nodes

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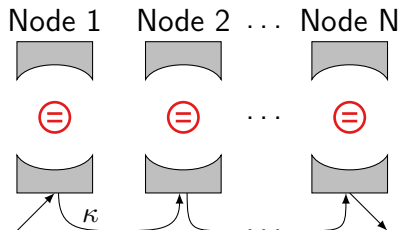


**Dicke state:** distribute a fixed excitation number over all nodes  
for single excitation:

$$|10\dots 0\rangle \rightarrow \frac{1}{\sqrt{N}} (|10\dots 0\rangle + |01\dots 0\rangle + \dots + |00\dots 1\rangle)$$



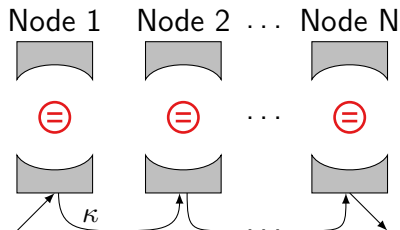
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## optimal control problem

find control fields  $u_1(t) \dots u_N(t)$   
that drive  $|\Psi(0)\rangle \rightarrow |\Psi(T)\rangle = |\Psi\rangle_{\text{tgt}}$

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minimize  $J_T = 1 - \langle\langle \hat{\rho}(T) | \hat{\mathbf{P}}_{\text{tgt}} \rangle\rangle$

# gradient optimization

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Khaneja et al, JMR 172, 296 (2005)

on time grid:  $u_{ij} = u_i(t_j)$ ;  $\mathcal{E}_j = \mathcal{E}(t_j, t_{j-1})$

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aux. functional  $J = J_T + \sum_i \frac{\lambda_i}{S_i(t)} \int_0^T [u_i^{(1)}(t) - u_i^{(0)}(t)]^2 dt$

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$$\text{minimize} \quad J_T = 1 - \langle\langle \hat{\rho}(T) | \hat{\mathbf{P}}_{\text{tgt}} \rangle\rangle$$

## GRAPE/LBFGS

Khaneja et al, JMR 172, 296 (2005)

on time grid:  $u_{ij} = u_i(t_j)$ ;  $\mathcal{E}_j = \mathcal{E}(t_j, t_{j-1})$

$$\Delta u_{ij} \propto \frac{\partial J_T}{\partial u_{ij}} = - \langle\langle \hat{\mathbf{P}}^{(0)}(t_j) \left| \frac{\partial \mathcal{E}_j}{\partial u_{ij}} \right| \hat{\rho}^{(0)}(t_{j-1}) \rangle\rangle,$$

## Krotov's method

Reich et al, JCP 136, 104103 (2012)

aux. functional  $J = J_T + \sum_i \frac{\lambda_i}{S_i(t)} \int_0^T [u_i^{(1)}(t) - u_i^{(0)}(t)]^2 dt$

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**optimize using quantum trajectories?**

# optimal control of trajectories

$$J_T = 1 - \langle\langle \hat{\rho}(T) | \hat{\mathbf{P}}_{\text{tgt}} \rangle\rangle \quad \longleftarrow \quad \hat{\rho} = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{k=1}^M |\Psi_k\rangle \langle \Psi_k|$$

# optimal control of trajectories

$$J_T = 1 - \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{k=1}^M \left| \underbrace{\langle \Psi_k(T) | \Psi_{\text{tgt}} \rangle}_{\equiv \tau_k} \right|^2$$

# optimal control of trajectories

$$J_T = 1 - \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{k=1}^M \underbrace{|\langle \Psi_k(T) | \Psi_{\text{tgt}} \rangle|}_{\equiv \tau_k}^2$$

## GRAPE/LBFGS

$$\frac{\partial J_T}{\partial u_{ij}} = - \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{k=1}^M \left[ \frac{\partial \tau_k}{\partial u_{ij}} \tau_k^* + \tau_k \left( \frac{\partial \tau_k}{\partial u_{ij}} \right)^* \right]$$

$$\frac{\partial \tau_k}{\partial u_{ij}} = \left\langle \Psi_{\text{tgt}}^{(0)}(t_j) \left| \frac{\partial \hat{U}_{jk}}{\partial u_{ij}} \right| \Psi_k^{(0)}(t)_{j-1} \right\rangle$$



# optimal control of trajectories

$$J_T = 1 - \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{k=1}^M \left| \underbrace{\langle \Psi_k(T) | \Psi_{\text{tgt}} \rangle}_{\equiv \tau_k} \right|^2$$

## GRAPE/LBFGS

$$\frac{\partial \tau_k}{\partial u_{ij}} = \left\langle \Psi_{\text{tgt}}^{(0)}(t_j) \left| \frac{\partial \hat{U}_{jk}}{\partial u_{ij}} \right| \Psi_k^{(0)}(t_{j-1}) \right\rangle$$

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$$J_T = 1 - \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{k=1}^M \underbrace{|\langle \Psi_k(T) | \Psi_{\text{tgt}} \rangle|}_{\equiv \tau_k}^2$$

## GRAPE/LBFGS

$$\frac{\partial \tau_k}{u_{ij}} = \left\langle \Psi_{\text{tgt}}^{(0)}(t_j) \left| \frac{\partial \hat{U}_{jk}}{\partial u_{ij}} \right| \Psi_k^{(0)}(t_{j-1}) \right\rangle$$

## Krotov's method

Palao, Kosloff, PRA 68, 062308 (2003).

$$\Delta u_i(t) = \frac{S_i(t)}{M\lambda_i} \sum_{k=1}^M \underbrace{\Im \langle \chi_k^{(0)}(t) | \hat{H}_i | \Psi_k^{(1)}(t) \rangle}_{\equiv \Delta u_{ik}(t)},$$

with  $\chi_k^{(0)}(T) = -\frac{\partial J_T}{\partial \langle \Psi_k |} = \tau_k^{(0)} |\Psi_{\text{tgt}}\rangle$

# optimal control of trajectories

$$J_T = 1 - \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{k=1}^M \underbrace{|\langle \Psi_k(T) | \Psi_{\text{tgt}} \rangle|^2}_{\equiv \tau_k}$$

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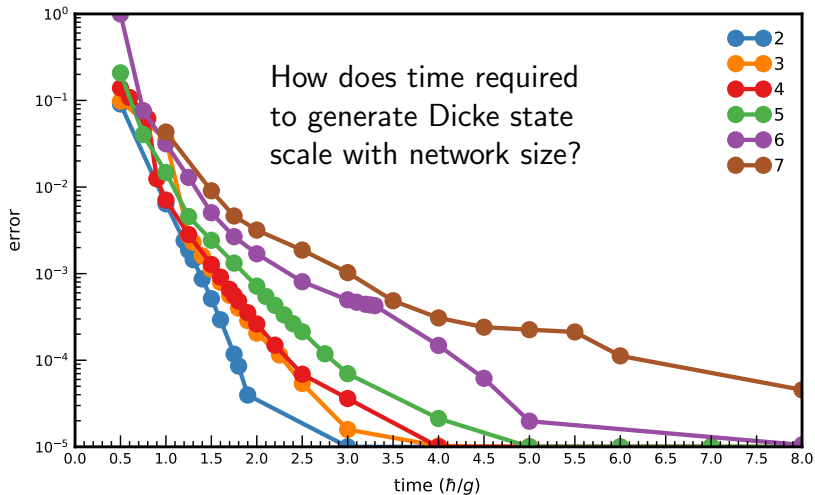
## Krotov's method

Palao, Kosloff, PRA 68, 062308 (2003).

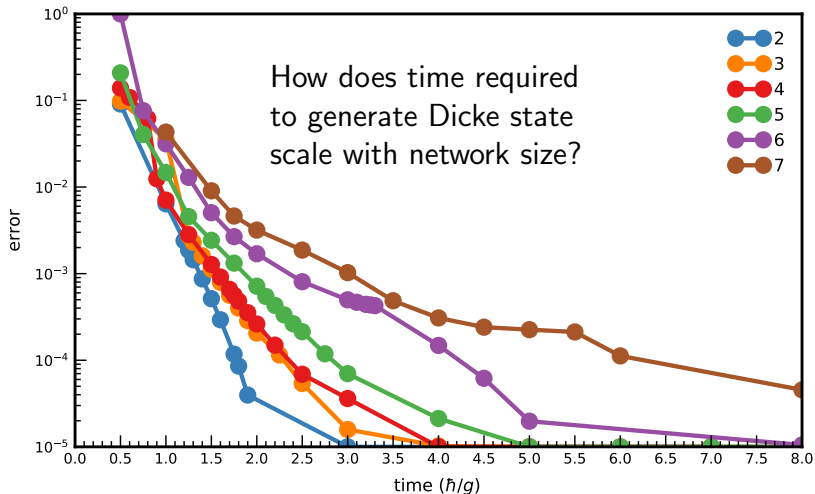
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# quantum speed limit for Dicke state generation



# quantum speed limit for Dicke state generation



⇒ single trajectory allows to determine speed limit

## Krotov's method

Palao, Kosloff, PRA 68, 062308 (2003).

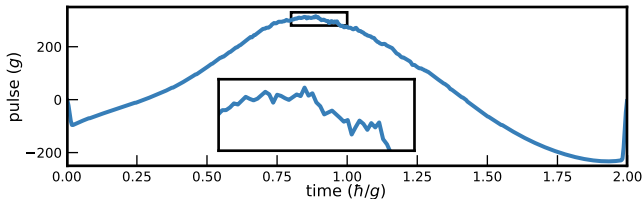
$$\Delta u_i(t) = \frac{S_i(t)}{M\lambda_i} \sum_{k=1}^M \underbrace{\Im \langle \chi_k^{(0)}(t) | \hat{\mathbf{H}}_i | \psi_k^{(1)}(t) \rangle}_{\equiv \Delta u_{ik}(t)},$$

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## ■ noisy pulses



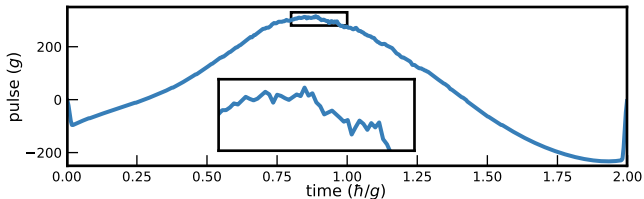
⇒ smooth pulses every few iterations

## Krotov's method

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### ■ noisy pulses



⇒ smooth pulses every few iterations

### ■ no monotonic convergence



## Krotov's method (in Liouville space)

$$\Delta u_i(t) = \frac{S_i(t)}{\lambda_i} \left\langle\left\langle \hat{\mathbf{P}}^{(0)}(t) \left| \frac{\partial \mathcal{L}}{\partial u_i(t)} \right| \hat{\rho}^{(1)}(t) \right\rangle\right\rangle$$

$$\hat{\rho} = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{k=1}^M |\psi_k\rangle \langle \psi_k| \quad \uparrow$$

## Krotov's method (in Liouville space)

$$\Delta u_i(t) = \frac{S_i(t)}{M^2 \lambda_i} \sum_{k,k'=1}^M \Im \left[ \left\langle \xi_k^{(0)}(t) \left| \hat{\mathbf{H}}_i \right| \psi_{k'}^{(1)}(t) \right\rangle \right. \\ \left. \times \left\langle \psi_{k'}^{(1)}(t) \left| \xi_k^{(0)}(t) \right\rangle \right]$$

$$\text{with } \hat{\mathbf{P}}^{(0)}(t) = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{k=1}^M |\xi_k\rangle \langle \xi_k|$$

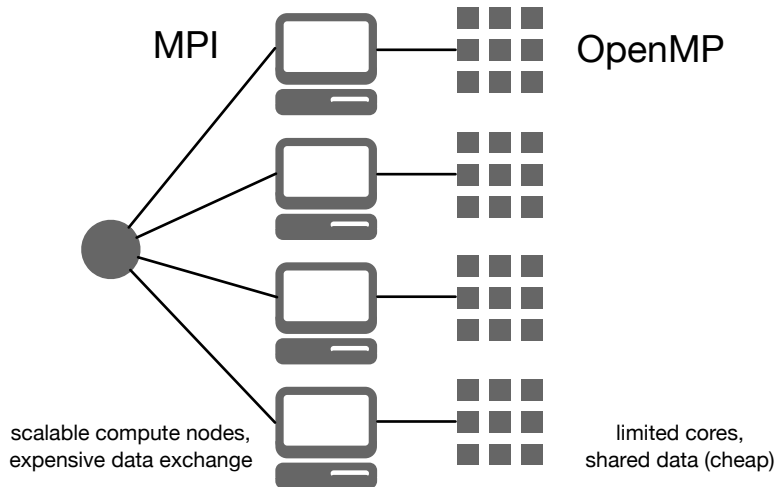
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$$\text{with } \hat{\mathbf{P}}^{(0)}(t) = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{k=1}^M |\xi_k\rangle \langle \xi_k|$$

cross-trajectory terms!

# parallelization approaches



## Krotov's method

$$\Delta u_i(t) = \frac{S_i(t)}{M^2 \lambda_i} \sum_{k,k'=1}^M \Im \left[ \left\langle \xi_k^{(0)}(t) \left| \hat{H}_i \right| \psi_{k'}^{(1)}(t) \right\rangle \right. \\ \left. \times \left\langle \psi_{k'}^{(1)}(t) \left| \xi_k^{(0)}(t) \right\rangle \right]$$

## Krotov's method

$$\Delta u_i(t) = \frac{S_i(t)}{M^2 \lambda_i} \sum_{k,k'=1}^M \Im \left[ \left\langle \xi_k^{(0)}(t) \left| \hat{H}_i \right| \psi_{k'}^{(1)}(t) \right\rangle \right. \\ \left. \times \left\langle \psi_{k'}^{(1)}(t) \left| \xi_k^{(0)}(t) \right\rangle \right]$$

- sending update  $\Delta u_i(t)$  is cheap

## Krotov's method

$$\Delta u_i(t) = \frac{S_i(t)}{M^2 \lambda_i} \sum_{k,k'=1}^M \Im \left[ \langle \xi_k^{(0)}(t) | \hat{H}_i | \Psi_{k'}^{(1)}(t) \rangle \right. \\ \left. \times \langle \Psi_{k'}^{(1)}(t) | \xi_k^{(0)}(t) \rangle \right]$$

- sending update  $\Delta u_i(t)$  is cheap
- sending states  $|\xi_k\rangle, |\Psi_{k'}\rangle$  is expensive

## Krotov's method

$$\Delta u_i(t) = \frac{S_i(t)}{M^2 \lambda_i} \sum_{k, k'=1}^M \Im \left[ \left\langle \xi_k^{(0)}(t) \left| \hat{H}_i \right| \psi_{k'}^{(1)}(t) \right\rangle \right. \\ \left. \times \left\langle \psi_{k'}^{(1)}(t) \left| \xi_k^{(0)}(t) \right\rangle \right]$$

- sending update  $\Delta u_i(t)$  is cheap
- sending states  $|\xi_k\rangle, |\psi_{k'}\rangle$  is expensive

⇒ proposal:

only cross-reference trajectories  $k, k'$  that are local



# acknowledgments

## conclusion

large Hilbert space & dissipative dynamics

→ optimal control of MCWF trajectories with Krotov's method

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<https://github.com/mabuchilab/QNET>

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<https://github.com/mabuchilab/QNET>



Christiane Koch  
Kassel (Germany)



quantum dynamics and control

<https://www.qdyn-library.net>