Low rank approximation for the numerical simulation of high dimensional Lindblad equations

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Outline

High dimensional Lindblad equations

- The Lindblad master equation governing open-quantum systems:

$$\frac{d}{dt}\rho = -i[H,\rho] - \tfrac{1}{2}(L^\dagger L\rho + \rho L^\dagger L) + L\rho L^\dagger,$$

  where ρ is the density operator ($\rho^\dagger = \rho$, $\mathrm{Tr}\,(\rho) = 1$, $\rho \geq 0$), H is an Hermitian operator and L is any operator on the Hilbert space $\mathcal{H}$ of dimension $n = \dim \mathcal{H}$.
- Usually, $n = \prod_{j=1}^{c} n_j$ large comes from $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_c$ where each $\mathcal{H}_j$ is of small or intermediate dimension $n_j \ll n$. Moreover, the operators H and L are usually defined as sums with few terms of simple tensor products of operators acting only on some $\mathcal{H}_j$.
- Typical situations of composite systems: coherent feedback scheme, circuit/cavity QED, ...

Quantum Monte-Carlo (QMC) simulations[1]

The Lindbald equation $\frac{d}{dt}\rho = -i[H,\rho] - \frac{1}{2}(L^\dagger L\rho + \rho L^\dagger L) + L\rho L^\dagger$, is the master equation of the stochastic system

$$d|\psi_t\rangle = \left(-iH - \frac{1}{2}L^\dagger L + \langle\psi_t|L^\dagger L|\psi_t\rangle\right)|\psi_t\rangle\, dt + \left(\frac{L|\psi_t\rangle}{\sqrt{\langle\psi_t|L^\dagger L|\psi_t\rangle}} - |\psi_t\rangle\right)\, dN_t$$

with $dN_t \in \{0,1\}$, $\mathbb{E}(dN_t) = \langle\psi_t|L^\dagger L|\psi_t\rangle\, dt$ (Poisson process).

Monte-Carlo simulations: simulate N realizations of such stochastic Schrödinger equation $[0,T] \ni t \mapsto |\psi_t^k\rangle$, $k = 1,\ldots N$: for N large (typically $N \sim 1000$)

$$\rho_t \approx \frac{1}{N}\sum_{k=1}^{N} |\psi_t^k\rangle\langle\psi_t^k|.$$

[1] J. Dalibard, Y. Castion, and K. Mølmer. Wave-function approach to dissipative processes in quantum optics. *Phys. Rev. Lett.*, 68(5):580–583, 1992.

Approximation by projection methods[2] [3]

Based on physical intuition, select an adapted sub-set of density matrices, i.e. a sub-manifold $\mathcal{D}$ of the vector space of Hermitian matrices equipped with Frobenius Euclidian metric. The approximate evolution is given by the orthogonal projection $\Pi^\rho(d\rho/dt)$ of $d\rho/dt$ onto the tangent space at ρ to $\mathcal{D}$:

$$\text{for } \rho \in \mathcal{D}, \quad \frac{d}{dt}\rho = \overbrace{\Pi^\rho\Big(- i[H,\rho] - \tfrac{1}{2}(L^\dagger L\rho + \rho L^\dagger L) + L\rho L^\dagger \Big)}^{\text{vector field on } \mathcal{D}}.$$

In [3], Mabuchi considers a reduced order model for a spin-spring system. The sub-manifold $\mathcal{D}$ was the (real) 5-dimensional manifold constructed with the tensor products of arbitrary two-level states and pure coherent states.

Computation of $\Pi^\rho(d\rho/dt)$ in local coordinates is not trivial and yields usually to nonlinear ODEs.

[2] R. van Handel and H. Mabuchi. Quantum projection filter for a highly nonlinear model in cavity qed. *Journal of Optics B: Quantum and Semiclassical Optics*, 7(10):S226, 2005.

[3] H. Mabuchi. Derivation of Maxwell-Bloch-type equations by projection of quantum models. *Phys. Rev. A*, 78:015801, Jul 2008.

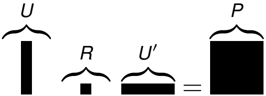
Low rank Kalman filters[4]

For $dx = Ax\,dt + G\,d\omega$, $dy = C\,dx + H\,d\eta$, computation of the best estimate of x at t knowing the past values of the output y relies on the computation of the conditional error covariance matrix P solution of the Riccati matrix equation

$$\frac{d}{dt}P = AP + PA' + GG' - PC'(HH')^{-1}CP.$$

When $G = 0$, the Riccati equation is rank preserving. It defines then a vector field on the sub-manifold of rank $m < n$ covariance matrices ($n = \dim x$ here). This sub-manifold admits the over-parameterization

$$(U, R) \mapsto URU' = P \leftrightsquigarrow$$



where U belongs to the set of $n \times m$ orthogonal matrices ($U'U = \mathbb{I}_m$) and R is $m \times m$, positive definite and symmetric.

Lift of dP/dt ($P = URU'$ solution the above Riccati equation):

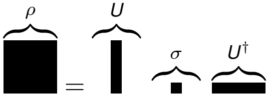
$$\frac{d}{dt}U = (\mathbb{I}_n - UU')AU, \quad \frac{d}{dt}R = U'AUR + RU'AU - RU'C(HH')^{-1}CUR$$

[4] S. Bonnabel and R. Sepulchre. The geometry of low-rank Kalman filters. *preprint arXiv:1203.4049v1*, March 2012.

Projection and lift for rank-m density operators of $\mathbb{C}^{n\times n}$

The sub-manifold $\mathcal{D}_m$ of density matrices ρ of rank $m < n$ is over-parameterized via

$$\rho = U\sigma U^\dagger \leftrightsquigarrow$$



where σ is a $m \times m$ strictly positive Hermitian matrix, U a $n \times m$ matrix with $U^\dagger U = \mathbb{I}_m$.
The family of lifts for $d\rho/dt = -i[H,\rho] - \frac{1}{2}(L^\dagger L\rho + \rho L^\dagger L) + L\rho L^\dagger$

$$\frac{d}{dt}U = -iAU + (\mathbb{I}_n - UU^\dagger)\left(-i(H-A) - \tfrac{1}{2}L^\dagger L + LU\sigma U^\dagger L^\dagger U\sigma^{-1}U^\dagger\right)U,$$

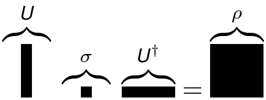
$$\frac{d}{dt}\sigma = -i[U^\dagger(H-A)U,\sigma] - \tfrac{1}{2}(U^\dagger L^\dagger LU\sigma + \sigma U^\dagger L^\dagger LU) + U^\dagger LU\sigma U^\dagger L^\dagger U$$
$$+ \tfrac{1}{m}\mathrm{Tr}\left((L^\dagger(\mathbb{I}_n - UU^\dagger)L\; U\sigma U^\dagger\right)\mathbb{I}_m.$$

where the gage degree of freedom A is any time varying $n \times n$ Hermitian matrix.

The computation of the lifted dynamics

Tangent map of the submersion:

$$(U,\sigma) \mapsto U\sigma U^\dagger = \rho \leftrightsquigarrow$$



with the infinitesimal variations $\delta U = \imath\eta U$ and $\delta\sigma = \varsigma$:

$$(\eta,\varsigma) \mapsto i[\eta,\rho] + U\varsigma U^\dagger$$

where η is any $n \times n$ Hermitian matrix, ς is any $m \times m$ Hermitian matrix with zero trace.

A $n \times n$ Hermitian matrix ξ in the tangent space at $\rho = U\sigma U^\dagger$ to $\mathcal{D}_m$ admits the parameterization $\xi = i[\eta,\rho] + U\varsigma U^\dagger$.

The projection $\Pi_m^\rho(\frac{d}{dt}\rho)$ corresponds to the tangent vector ξ associated to η and ς minimizing

$$\mathrm{Tr}\left(\left(-i[H,\rho] - (L^\dagger L\rho + \rho L^\dagger L)/2 + L\rho L^\dagger - i[\eta,\rho] - U\varsigma U^\dagger\right)^2\right),$$

First order stationary conditions give η and ς as function of $\rho = U\sigma U^\dagger$: the lifted evolution is given by $\frac{d}{dt}U = i\eta U$ and $\frac{d}{dt}\sigma = \varsigma$ where the arbitrary matrix A appears.

Gage $A = H$ adapted to weak dissipation

In

$$\frac{d}{dt}U = -iAU + (\mathbb{I}_n - UU^\dagger)\left(-i(H - A) - \tfrac{1}{2}L^\dagger L + LU\sigma U^\dagger L^\dagger U\sigma^{-1}U^\dagger\right)U,$$

$$\frac{d}{dt}\sigma = -i[U^\dagger(H - A)U, \sigma] - \tfrac{1}{2}(U^\dagger L^\dagger LU\sigma + \sigma U^\dagger L^\dagger LU) + U^\dagger LU\sigma U^\dagger L^\dagger U + \tfrac{1}{m}\mathrm{Tr}\left((L^\dagger(\mathbb{I}_n - UU^\dagger)L\, U\sigma U^\dagger\right)\mathbb{I}_m.$$

set $A = H$:

$$\frac{d}{dt}U = -iHU + (\mathbb{I}_n - UU^\dagger)\left(-\tfrac{1}{2}L^\dagger L + LU\sigma U^\dagger L^\dagger U\sigma^{-1}U^\dagger\right)U,$$

$$\frac{d}{dt}\sigma = -\tfrac{1}{2}(U^\dagger L^\dagger LU\sigma + \sigma U^\dagger L^\dagger LU) + U^\dagger LU\sigma U^\dagger L^\dagger U + \tfrac{1}{m}\mathrm{Tr}\left((L^\dagger(\mathbb{I}_n - UU^\dagger)L\, U\sigma U^\dagger\right)\mathbb{I}_m,$$

H only appears in the dynamics of U and not in the dynamics of σ.
Appropriate when H dominates L: a slow evolution of σ as compared to a fast evolution of U (important for the numerical procedure)

A numerical integration scheme adapted to weak dissipation

U_k and σ_k the numerical approximations of $U(k\delta t)$ and $\sigma(k\delta t)$.
The update from time $k\delta t$ to time $(k+1)\delta t$ is split into 3 steps for U and 2 steps for σ

$$U_{k+\frac{1}{3}} = \left(\mathbb{I}_n - \tfrac{i\delta t}{2} H - \tfrac{\delta t^2}{8} H^2 + i \tfrac{\delta t^3}{48} H^3\right) U_k$$

$$U_{k+\frac{2}{3}} = U_{k+\frac{1}{3}} + \delta t (\mathbb{I}_n - U_{k+\frac{1}{3}} U^\dagger_{k+\frac{1}{3}}) \left(-\tfrac{1}{2} L^\dagger L U_{k+\frac{1}{3}} + L U_{k+\frac{1}{3}} \sigma_k U^\dagger_{k+\frac{1}{3}} L^\dagger U_{k+\frac{1}{3}} \sigma_k^{-1}\right)$$

$$U_{k+1} = \Upsilon\left(\left(\mathbb{I}_n - \tfrac{i\delta t}{2} H - \tfrac{\delta t^2}{8} H^2 + i \tfrac{\delta t^3}{48} H^3\right) U_{k+\frac{2}{3}}\right) \quad (\Upsilon \text{ ortho-normalization})$$

$$\sigma_{k+\frac{1}{2}} = \sigma_k + \delta t \; U^\dagger_{k+\frac{1}{3}} L U_{k+\frac{1}{3}} \sigma_k U^\dagger_{k+\frac{1}{3}} L^\dagger U_{k+\frac{1}{3}} + \delta t \, \frac{\mathrm{Tr}\left((U^\dagger_{k+\frac{1}{3}} L^\dagger L U_{k+\frac{1}{3}} - U^\dagger_{k+\frac{1}{3}} L^\dagger U_{k+\frac{1}{3}} U^\dagger_{k+\frac{1}{3}} L U_{k+\frac{1}{3}}) \sigma_k \right) \; \mathbb{I}_m}{m}$$

$$\sigma_{k+1} = \frac{(\mathbb{I}_m - \frac{\delta t}{2} U^\dagger_{k+\frac{1}{3}} L^\dagger L U_{k+\frac{1}{3}}) \sigma_{k+\frac{1}{2}} (\mathbb{I}_m - \frac{\delta t}{2} U^\dagger_{k+\frac{1}{3}} L^\dagger L U_{k+\frac{1}{3}})}{\mathrm{Tr}\left((\mathbb{I}_m - \frac{\delta t}{2} U^\dagger_{k+\frac{1}{3}} L^\dagger L U_{k+\frac{1}{3}}) \sigma_{k+\frac{1}{2}} (\mathbb{I}_m - \frac{\delta t}{2} U^\dagger_{k+\frac{1}{3}} L^\dagger L U_{k+\frac{1}{3}}) \right)}.$$

This scheme preserves $U^\dagger U = \mathbb{I}_m$, $\sigma^\dagger = \sigma$, $\sigma > 0$ and $\mathrm{Tr}(\sigma) = 1$.

Computational cost versus QMC procedure

$$d|\psi_t\rangle = \left(-iH - \tfrac{1}{2}L^\dagger L + \langle\psi_t|L^\dagger L|\psi_t\rangle\right)|\psi_t\rangle\ dt + \left(\frac{L|\psi_t\rangle}{\sqrt{\langle\psi_t|L^\dagger L|\psi_t\rangle}} - |\psi_t\rangle\right)\ dN_t$$

$$U_{k+\frac{1}{3}} = \left(\mathbb{I}_n - \tfrac{i\delta t}{2}H - \tfrac{\delta t^2}{8}H^2 + i\tfrac{\delta t^3}{48}H^3\right)U_k$$

$$U_{k+\frac{2}{3}} = U_{k+\frac{1}{3}} + \delta t(\mathbb{I}_n - U_{k+\frac{1}{3}}U^\dagger_{k+\frac{1}{3}})\left(-\tfrac{1}{2}L^\dagger L U_{k+\frac{1}{3}} + LU_{k+\frac{1}{3}}\sigma_k U^\dagger_{k+\frac{1}{3}}L^\dagger U_{k+\frac{1}{3}}\sigma_k^{-1}\right)$$

$$U_{k+1} = \Upsilon\Big(\left(\mathbb{I}_n - \tfrac{i\delta t}{2}H - \tfrac{\delta t^2}{8}H^2 + i\tfrac{\delta t^3}{48}H^3\right)U_{k+\frac{2}{3}}\Big)$$

Both methods use essentially right multiplications of H, L, $L^\dagger$ by $n\times 1$ or $n\times m$ matrices, as, for example, the products $H|\psi\rangle$, $L|\psi\rangle$ or HU, LU, $L^\dagger(LU)$. No string $n\times n$ matrices since H and L are defined as tensor products of operators of small dimensions. When n is very large and m is small, this point is crucial for an efficient numerical implementation: evaluations of products like HU or LU can be parallelized.

Empirical estimation[5] of truncation error

- Based on Frobenius norms of $\dot\rho = \frac{d}{dt}\rho$ and $\dot\rho_\perp = \dot\rho - \Pi_m^\rho(\dot\rho)$ for $\rho = U\sigma U^\dagger$ using:

$$\dot\rho = -i[H,\rho] - \tfrac{1}{2}\big(L^\dagger L\rho + \rho L^\dagger L\big) + L\rho L^\dagger\Big)$$

$$\dot\rho_\perp = (\mathbb{I}_n - P_\rho)L\rho L^\dagger(\mathbb{I}_n - P_\rho) - \frac{\mathrm{Tr}\big(L\rho L^\dagger(\mathbb{I}_n - P_\rho)\big)}{m}P_\rho$$

  where $P_\rho = UU^\dagger$.
- Good approximation when $\mathrm{Tr}\left(\dot\rho_\perp^2\right) \ll \mathrm{Tr}\left(\dot\rho^2\right)$.
- At each time step, $\mathrm{Tr}\left(\dot\rho^2\right)$ and $\mathrm{Tr}\left(\dot\rho_\perp^2\right)$ may be numerically evaluated with a complexity similar to the complexity of the numerical scheme (no need to explicitly compute $\dot\rho$ and $\dot\rho_\perp$ as $n \times n$ matrices before taking their Frobenius norms).

[5] Inspired from R. van Handel and H. Mabuchi. Quantum projection filter for a highly nonlinear model in cavity qed. *Journal of Optics B: Quantum and Semiclassical Optics*

Initialization procedure

σ_0 and U_0 need to be deduced from a given initial condition ρ_0:

- When the rank of $\rho_0 \geq m$: σ_0 diagonal matrix made of the largest m eigenvalues of ρ_0 with sum normalized to one; U_0 the associated normalized eigenvectors.
- When the rank of $\rho_0 = 1$ and $m > 1$: $\rho_0 = |\psi_0\rangle\langle\psi_0|$. It is then natural to take for σ_0 a diagonal matrix where the first diagonal element is $1 - (m-1)\epsilon$ and the over ones are equal to $\epsilon \ll 1$. Then U_0 is constructed, up to an ortho-normalization preserving the first column, with $|\psi_0\rangle$ as the first column, $H|\psi_0\rangle$ as the second column, ..., $H^{m-1}|\psi_0\rangle$ as the last column.
- When the rank of ρ_0 in $]1, m[$: combine the above initialization scheme ...

Lindblad equation of oscillation revivals

The collective symmetric behavior of N_a two-level atoms resonantly interacting with a quantized field:

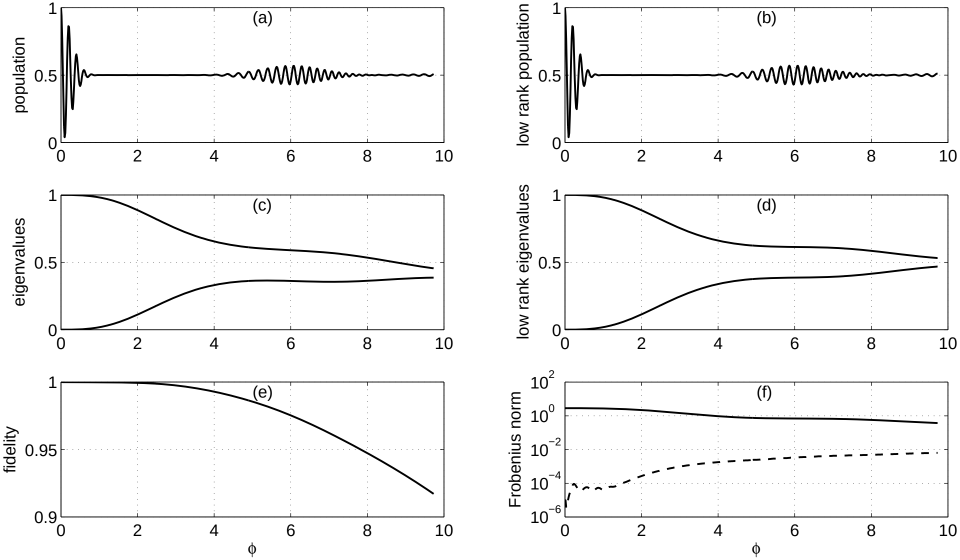
$$\frac{d}{dt}\rho = \frac{\Omega_0}{2}[\mathbf{a}^\dagger J^- - \mathbf{a}J^+, \rho] - \kappa(\mathbf{n}\rho/2 + \rho\mathbf{n}/2 - \mathbf{a}\rho\mathbf{a}^\dagger)$$

Preliminary tests via two different type of simulations including the first complete revival:

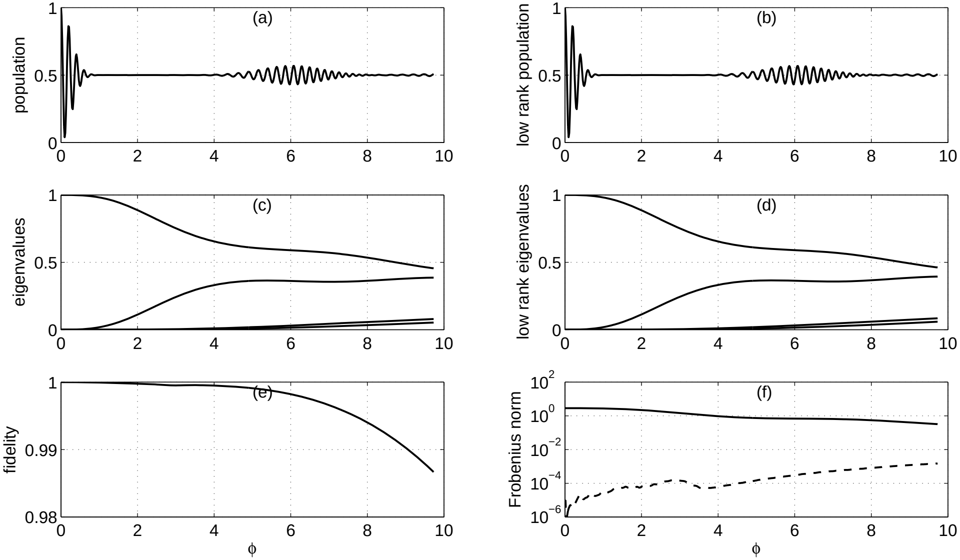
- $N_a = 1$ atom initially in the excited state, a field initially in a coherent state with $\bar{n} = 15$ photons (truncation to 30 photons): comparisons between the full-rank and rank-2-4-6 solutions with $\kappa = \Omega_0/500$:
- $N_a = 50$ atoms all initially in excited states, a field with $\bar{n} = 200$ (truncation to 300 photons): comparison of the analytic approximate weak-damping model proposed in [6] (predicts a reduction of a factor $r = 2$ of the complete first revival between $\kappa = 0$ and $\kappa = \log(r)\Omega_0/(4\pi\bar{n}^{3/2})$) with the rank-8 approximation given by the above integration scheme with $\delta t = 1/(\Omega_0\sqrt{\bar{n}}N_a)$.

[6] T. Meunier, A. Le Diffon, C. Ruef, P. Degiovanni, and J.-M. Raimond. Entanglement and decoherence of N atoms and a mesoscopic field in a cavity. *Phys. Rev. A*, 74:033802, 2006.

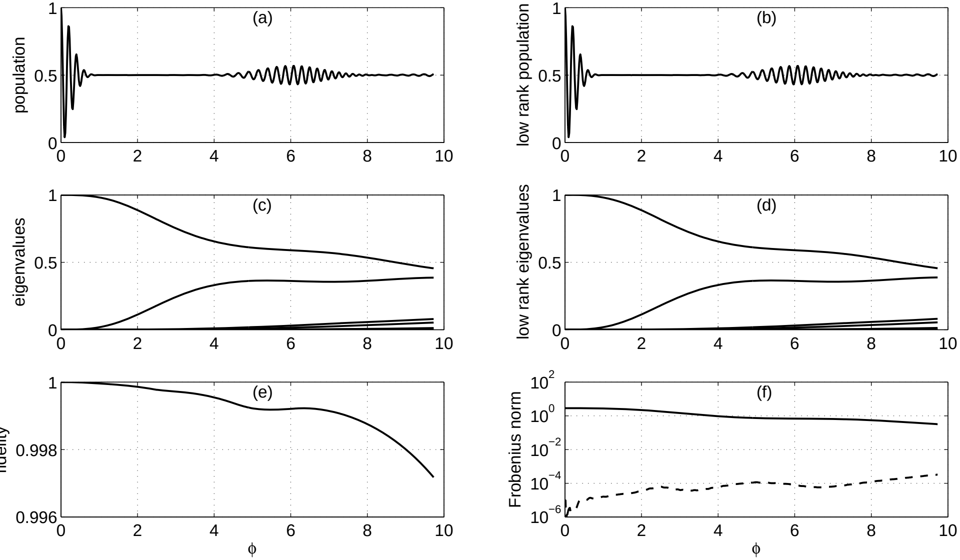
Full rank (left) versus rank 2 (right) ($N_a = 1$, $\bar{n} = 15$, $\phi = \Omega_0 t / 2\sqrt{\bar{n}}$)



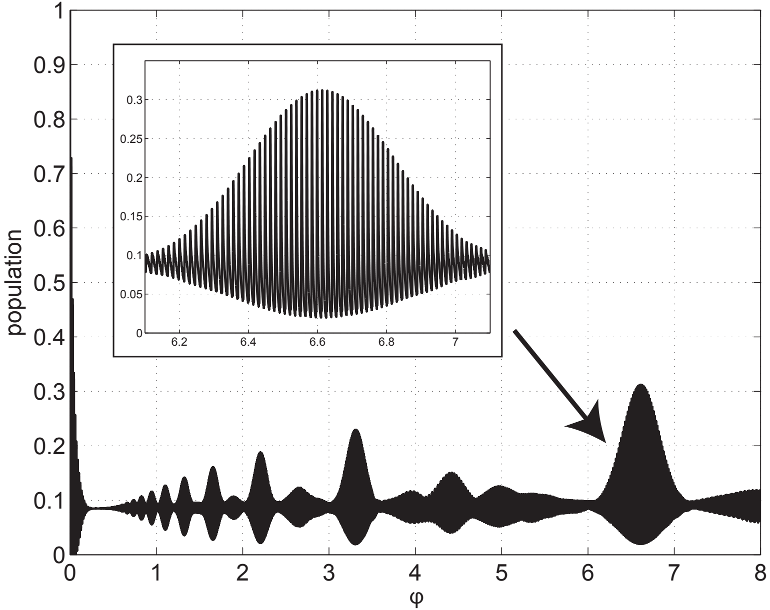
Full rank (left) versus rank 4 (right) ($N_a = 1$, $\bar{n} = 15$, $\phi = \Omega_0 t/2\sqrt{\bar{n}}$)



Full rank (left) versus rank 6 (right) ($N_a = 1$, $\bar{n} = 15$, $\phi = \Omega_0 t / 2\sqrt{\bar{n}}$)

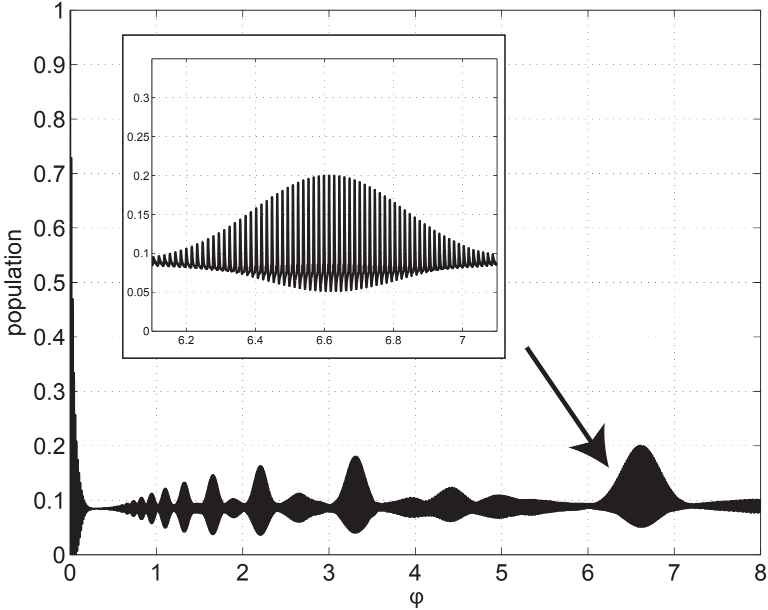


Oscillation revival with $\kappa = 0$ ($N_a = 50$, $\bar{n} = 200$, $\phi = \Omega_0 t/2\sqrt{\bar{n}}$)



Schrödinger simulation time 1h15 (Dell precision M4440 with Matlab)

Rank-8 solution with $\kappa = \log(2)\Omega_0/(4\pi\bar{n}^{3/2})$ ($N_a = 50$, $\bar{n} = 200$)



Rank-8 simulation time 17h00 (Dell precision M4440 with Matlab)

Concluding remarks

A single tuning parameter: the rank $m \ll n$.
Extension to an arbitrary number of Lindblad operators:

$$\frac{d}{dt}\rho = -i[H,\rho] + \sum_\nu L_\nu \rho L_\nu^\dagger - \tfrac{1}{2}(L_\nu^\dagger L_\nu \rho + \rho L_\nu^\dagger L_\nu)$$

$$\frac{d}{dt}U = -iHU + (\mathbb{I}_n - UU^\dagger)\left(\sum_\nu -\tfrac{1}{2} L_\nu^\dagger L_\nu + L_\nu U\sigma U^\dagger L_\nu^\dagger U\sigma^{-1}U^\dagger\right)U$$

$$\frac{d}{dt}\sigma = \sum_\nu \tfrac{-1}{2}(U^\dagger L_\nu^\dagger L_\nu U\sigma + \sigma U^\dagger L_\nu^\dagger L_\nu U) + U^\dagger L_\nu U\sigma U^\dagger L_\nu^\dagger U$$

$$+ \tfrac{1}{m}\mathrm{Tr}\left(\sum_\nu (L_\nu^\dagger(\mathbb{I}_n - UU^\dagger)L_\nu \; U\sigma U^\dagger\right)\mathbb{I}_m.$$

Similar low-rank approximations could be done for continuous-time quantum filters . . .
Implemented in simulation packages such as QuTip[7]?
Adaptation when n is huge[8] ? Low-rank quantum tomography ?

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[7] J.R Johansson, P.D. Nation, F.Nori: QuTiP an open-source Python framework for dynamics of open quantum systems. Computers Physics Communications 183 (2012) 1760–1772.

[8] Ilya Kuprov: Spinach - software library for spin dynamics simulation of large spin systems. PRACQSYS 2010.