Structure-preserving Low Rank Scheme for the Lindblad Master Equation

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Outline

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Mater equation

- Master equations are differential equations used to model the dynamics of systems that can be described as a probabilistic combination of some states.

  When the probabilities of the elementary processes are known, one can write down a continuity equation for W, from which all other equations can be derived and which we will call therefore the master equation - Nordsieck, Lam, Uhlenbeck, 1940

- Example: $\frac{d}{dt}p = F(p, t) = Ap$, where p is a vector denoting the probability of the state.
- Quantum master equation deviates from the classical case because we have to take into account superpositions of states.[1]

[1] Campaioli, Cole, Hapuarchchi, 2023.

Quantum mechanics

- Consider a d-dimensional quantum system with Hilbert space $\mathcal{H}$. Let $\mathcal{B} := \{|\phi_1\rangle, |\phi_2\rangle, \dots, |\phi_d\rangle\}$ be an orthonormal basis for $\mathcal{H}$, so that $\langle\phi_i|\phi_j\rangle = \delta_{ij}$. Any pure state of the system can be expressed as

$$|\psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle + \dots + c_d|\phi_d\rangle = \sum_{j=1}^{d} c_j|\phi_j\rangle, \tag{1}$$

  where the coefficient c_j are such that $\langle\psi|\psi\rangle = \sum_{j=1}^{d} |c_j|^2 = 1$. $p_i = |c_i|^2$ denotes the probability in state i.

Quantum mechanics

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where the coefficient c_j are such that $\langle\psi|\psi\rangle = \sum_{j=1}^{d} |c_j|^2 = 1$. $p_i = |c_i|^2$ denotes the probability in state i.

- Schrödinger equation

$$\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar}H|\psi(t)\rangle, \quad (2)$$

where H is the Hamiltonian.

Density matrix

General mixed state can be represented by $\{|\psi_j\rangle, p_j\}$. We can then by the density operator (matrix)

$$\rho = \sum_{j=1}^{d} p_j |\psi_j\rangle\langle\psi_j|, \tag{3}$$

where $|\psi_j\rangle\langle\psi_j|$ is the outer product of $|\psi_j\rangle$ with itself.

1. **Hermitian:** $\rho = \rho^\dagger$. This implies that ρ has only real eigenvalues.
2. **Positive**[2]**:** $\rho > 0$. That is, ρ eigenvalues $p_j \in [0, 1]$ are not negative.
3. $\mathrm{Tr}\rho = 1$, which can also be stated as $\sum_j p_j = 1$, i.e., the sum of its eigenvalues (probabilities) must add up to 1.

The diagonal entries ρ_{ii} (real) are called population, the off-diagonal (complex) entries ρ_{ij} are called coherence. However, ρ_{ii} is not sufficient to describe the state unlike the classical case.

[2] Or, more specifically, *positive semi-definite*.

Example:qubit

We can define a basis of it by the orthonormal vectors: $\{|0\rangle, \ |1\rangle\}$. A pure state of the system would be any unit vector of $\mathcal{H}_2$. It can always be expressed as a $|\psi\rangle = a|0\rangle + b|1\rangle$ with $a, b \in \mathbb{C}$ s. t. $|a|^2 + |b|^2 = 1$.

A mixed state is therefore represented by a positive unit trace operator.

$$\rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} = \rho_{00}|0\rangle\langle 0| + \rho_{01}|0\rangle\langle 1| + \rho_{10}|1\rangle\langle 0| + \rho_{11}|1\rangle\langle 1|, \tag{4}$$

von Neumann equation

- Closed system can be modeled by Schrödinger equation

$$\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar}H|\psi(t)\rangle,$$

where H is the Hamiltonian.

- If H is time independent, we have

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle. \tag{5}$$

As H is a Hermitian operator, the operator $U = e^{-iHt}$ is unitary.

- The von-Neumann equation can be derived

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H, \rho(t)], \tag{6}$$

where we have used the commutator $[A, B] = AB - BA$.

Open quantum system

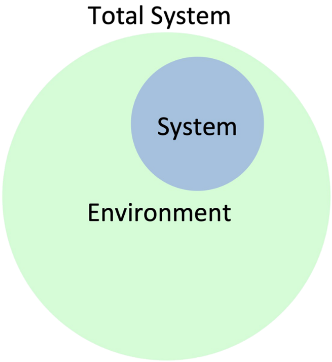

FIG. 1. A total system divided into the system of interest, "system" and the environment.

Figure: From: D. Manzano, A short introduction to the Lindblad master equation, 2020

The Lindblad master equation

The Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) master equation, often known as the *Lindblad* master equation,

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H, \rho(t)] + \sum_k \gamma_k \left(L_k \rho(t) L_k^\dagger - \frac{1}{2}\left\{ L_k^\dagger L_k, \rho(t) \right\} \right), \tag{7}$$

where $\{L_k\}$ are the *Lindblad*/jump/collapse operators representing some non-unitary processes like relaxation or decoherence that occur at some rates $\{\gamma_k\}$. $\{A, B\} = AB + BA$.

Example: $L_\downarrow = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, non-Hermitian.

CPTP map

$B(\mathcal{H})$: space of all density matrices in the Hilbert space $\mathcal{H}$. A map $\mathcal{V} : B(\mathcal{H}) \to B(\mathcal{H})$ is called a *completely positive and trace-preserving map (CPTP-map)* if it is

- Trace preserving. $\mathrm{Tr}[\mathcal{V}A] = \mathrm{Tr}[A], \forall A \in B(\mathcal{H})$.
- Completely positive (see next page).

Completely positive

Definition

A map $\mathcal{V}$ is positive iff $\forall A \in B(\mathcal{H})$ s.t. $A \geq 0 \Rightarrow \mathcal{V}A \geq 0$.

Maps a positive matrix to a positive matrix.

Completely positive

Definition

A map $\mathcal{V}$ is positive iff $\forall A \in B(\mathcal{H})$ s.t. $A \geq 0 \Rightarrow \mathcal{V}A \geq 0$.

Maps a positive matrix to a positive matrix. However, this is not enough.

Definition

A map $\mathcal{V}$ is completely positive iff $\forall n \in \mathbb{N}$, $\mathcal{V} \otimes \mathbb{1}_n$ is positive.

Meaning: there exist composite systems, and our density matrix could be the partial trace of a more complicated state.

Completely positive

Complete positive $\Rightarrow$ Positive, but not vice versa.
Example: matrix transpose operator is positive, but not complete positive.

Theorem (Choi's Theorem)

A linear map $\mathcal{V} : B(\mathcal{H}) \rightarrow B(\mathcal{H})$ is completely positive iff it can be expressed as

$$\mathcal{V}\rho = \sum_i V_i^\dagger \rho V_i \tag{8}$$

with $V_i \in B(\mathcal{H})$.

Choi-Kraus

Theorem (Choi-Kraus' Theorem)

A linear map $\mathcal{V} : B(\mathcal{H}) \to B(\mathcal{H})$ *is completely positive and trace-preserving iff it can be expressed as*

$$\mathcal{V}\rho = \sum_l V_l^\dagger \rho V_l \tag{9}$$

with $V_l \in B(\mathcal{H})$ *fulfilling*

$$\sum_l V_l V_l^\dagger = \mathbb{1}_{\mathcal{H}}. \tag{10}$$

A beautiful result

If the solution to

$$\frac{d}{dt}\rho = \mathcal{L}\rho \tag{11}$$

induces a CPTP map from $\rho(0)$ to $\rho(t)$, then (11) can be written in the form of Lindblad master equation.

Markovian CPTP generator $\Longleftrightarrow$ Lindblad master equation

Outline

Numerical schemes

We would like to design numerical methods with the following properties

- CPTP, i.e. the map from ρ^n to ρ^{n+1} is CPTP map.
- High order accurate.
- Low rank. For quantum systems with low entropy or that are weakly coupled to the environment or for the early stage of the dynamics of systems initialized in a pure state, ρ can be approximated by low rank matrix.

CPTP scheme

CPTP scheme: trace preserving, and

$$\rho^{n+1} \equiv \mathcal{G}\rho^n = \sum_l G_l^\dagger \rho^n G_l$$

with G_l to be determined.

- TP is relatively easy (can be done by renormalization).
- Key is to have a scheme that is in Kraus form.
- A negative result: no explicit Runge-Kutta method is CP [3].

[3] Riesch, Jirasuchek, 2019

CPTP scheme

- Steinbach, Garraway, Knight, 1995 construct a first high order CPTP scheme using Taylor expansion.
- Other techniques include Picard iteration, and stochastic unraveling Cao, Lu, 2021, Wang, Li, 2024, Ding, Li, Lin, 2024.
- We reformulate the equation [4] (for simplicity, we write only one jump operator)

$$\frac{d}{dt}\rho(t) = \left(J\rho(t) + \rho(t)J^\dagger\right) + L\rho(t)L^\dagger \equiv \mathcal{L}_J\rho(t) + \mathcal{L}_L\rho(t), \quad (12)$$

where $J = -iH_{\text{eff}},\ H_{\text{eff}} = H + \frac{1}{2i}L^\dagger L$. We treat $\mathcal{L}_J\rho(t)$ implicitly, and $\mathcal{L}_L\rho(t)$ explicitly.
Note: connection with differential Lyapunov equation.

[4] Steinbach, Garraway, Knight, 1995

Lawson integrator (Integrating factor)

$$\frac{d}{dt}q(t) = Jq(t) + q(t)J^\dagger \Longleftrightarrow \frac{d}{dt}V(t) = JV(t), q = VV^\dagger \qquad (13)$$

With $V(t+\Delta t) = U(\Delta t)V(t)$, we have $q(t+\Delta t) = U(\Delta t)q(t)U(\Delta t)^\dagger$, which is on Kraus form.

Therefore, we apply the Lawson integrator and get

$$\rho^{(i)} = U(c_i\Delta t)\rho_0 U(c_i\Delta t)^\dagger + \Delta t \sum_{j=1}^{i-1} a_{ij} U((c_i - c_j)\Delta t)\mathcal{L}_L \rho^{(j)} U((c_i - c_j)\Delta t)^\dagger, \quad i = 1, \dots, s,$$

$$\rho_1 = U(\Delta t)\rho_0 U(\Delta t)^\dagger + \sum_{i=1}^{s} b_i \Delta t U((1 - c_i)\Delta t)\mathcal{L}_L \rho^{(i)} U((1 - c_i)\Delta t)^\dagger, \qquad (14)$$

As long as a_{ij}, b_i are non-negative, this is CP. In practice, the operator $U(\Delta t)$ can be taken as explicit/implicit scheme that matches with the order of accuracy of the lawson/RK method.

Low rank method

- Idea: we solve for $V(t)$ (the Cholesky factor), and perform low rank truncation according to error threshold. Chen, Farquhar, Parrish 21, Donatella, Denis, Le Boite, C. Ciuti, 21, McCaul, Jacobs, Bondar, 21
- This is done by rounding.
  $\mathbf{R} = R_1 R_1^\dagger + \dots R_k R_k^\dagger$, with $R_j \in \mathbb{C}^{N\times r_j}$. Suppose $W = [R_1, \dots, R_k]$, then $\mathbf{R} = WW^\dagger$ and the low rank truncation $\mathcal{T}_{\epsilon, r_{\max}}[\mathbf{R}]$ is defined as the truncated SVD of $\mathbf{R}$ according to the rank threshold $r_{\max}$ and energy cutoff ϵ.

Low rank method

Question: will this truncation destroy CP?

Low rank method

Question: will this truncation destroy CP? No.

Theorem

The truncated SVD operator $\mathcal{T}_{\epsilon,r_{\max}}[A]$, where A is SPSD, is on Kraus form, and thus is a CP map.

Proof.

Since A is SPSD, its SVD has the form $A = U\Lambda U^\dagger$, and $\mathcal{T}_{\epsilon,r_{\max}}[A] = UD\Lambda D^\dagger U^\dagger$ where $D = \mathrm{diag}(\underbrace{1,\ldots 1,}_{r} 0\ldots,0)$. Therefore,

$\mathcal{T}_{\epsilon,r_{\max}}[A] = UDU^\dagger A(UDU^\dagger)^\dagger$ is on Kraus form. □

In contrast, TDVP on Lindblad will destroy the structure.

Numerical results: CP

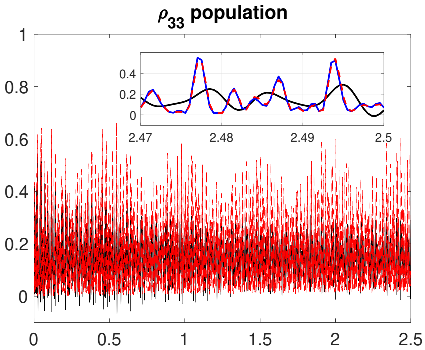

Figure: Evolution of the population ρ_{33}. RK4 method (black) , IF-exp (red, dashed), IF-Taylor 6 (blue) using a timestep of 0.1 femto-seconds.

Numerical results: Jaynes-Cumming Model

$$H = \lambda(b\sigma^+ + b^\dagger\sigma^-), L = \sqrt{\kappa} b$$

Here

$$b = I_{2\times 2} \otimes \hat{b}, \quad \sigma^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \otimes I_{m\times m}, \quad \sigma^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes I_{m\times m}$$

and $\hat{b}$ is the $m \times m$ lowering matrix with elements $\hat{b}_{l,l+1} = \sqrt{l}, l = 1, \ldots, m-1$. Initial condition $\rho = VV^\dagger$, with

$$V = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \frac{\mathbf{v}}{\|\mathbf{v}\|}.$$

$$\mathbf{v} \sim \sum_{n=0}^{m-1} \frac{|v|^n}{\sqrt{n!}} \mathbf{e}_n,$$

Here we choose $v = \sqrt{m/3}$ so that the last terms in the sum for $\mathbf{v}$ are small also for moderate m.

Numerical results

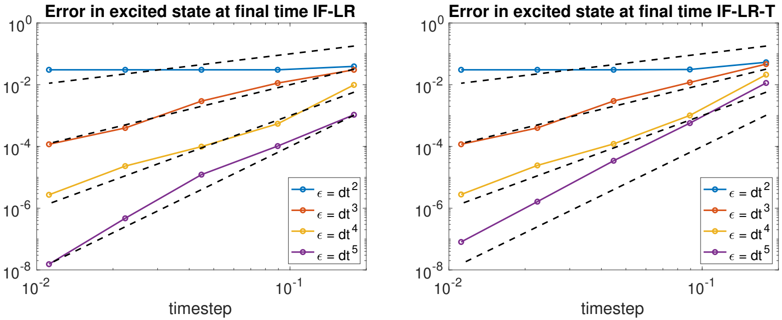

Figure: Errors at the final time for the two low-rank methods (matrix exponentiation (left) and Taylor series (right)) as a function of the timestep. The dashed lines are orders, one to four.

Numerical results

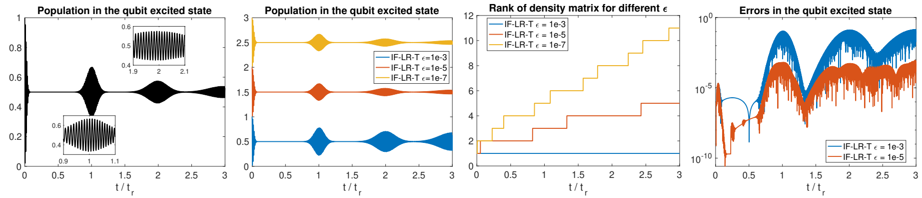

Figure: Low-rank computation of revival for $m = 150$.

Conclusions and outlook

- We propose a simple framework for constructing low rank CPTP scheme.
- Future work: generalize to time-dependent Hamiltonian and jump operators.
- Future work: tensor network.

The END! Thank You!