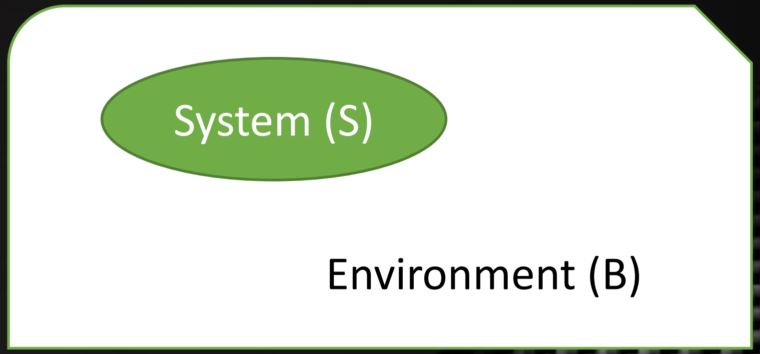

Open Quantum Systems in Quantum Computing

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Why Open Quantum Systems?

- Quantum systems in reality are interacting with an environment (bath) $\Rightarrow$ open quantum systems
- These interactions have a deep impact on the system dynamics.
  - Quantum decoherence (Echo dynamics, Girin et al. Phys. Rep. 2006)
  - Gate error and error mitigation (Temme et al. PRL 2017)
- The study of open quantum systems starts with the combined system.
- The combined system usually has large dimension and is difficult to prepare and simulate directly.
- The theory of open quantum system attempts to identify models that implicitly incorporates the effect of the bath (Breuer & Petruccione).

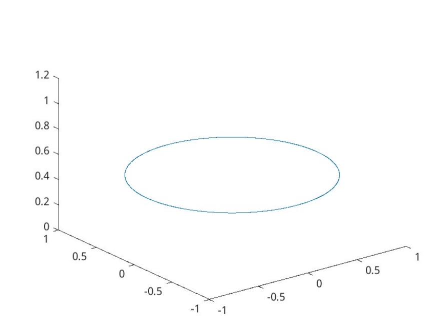
Example: A single-qubit dynamics

Close quantum dynamics

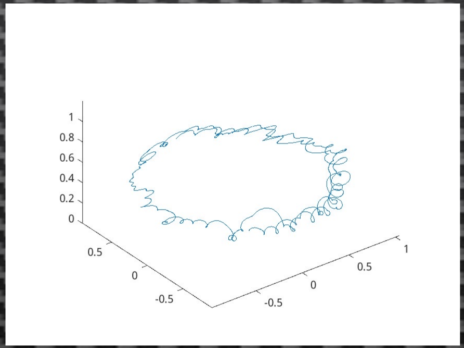
- $H_S = -\frac{1}{20}\sigma_z$
- $|\psi(0)\rangle = \frac{\sqrt{3}}{2}e^{-\frac{i\pi}{4}}|0\rangle + \frac{1}{2}e^{\frac{i\pi}{4}}|1\rangle$
- $x(t) = \langle\psi(t)|\sigma_x|\psi(t)\rangle, y(t)\cdots$

With environment noise (Gaspard-Nagaoka, JCP 1999)

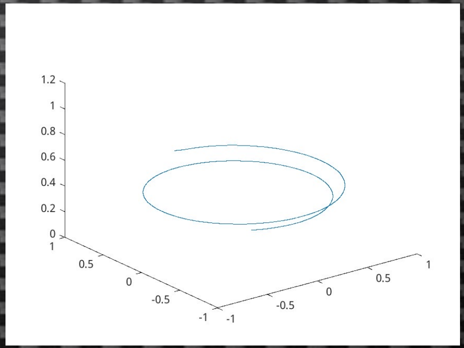
- **Boson bath**
- **Gaussian noise**
- **Coupling constant** $\lambda = 0.1$



Time-dependent Schrödinger



Stochastic Schrödinger



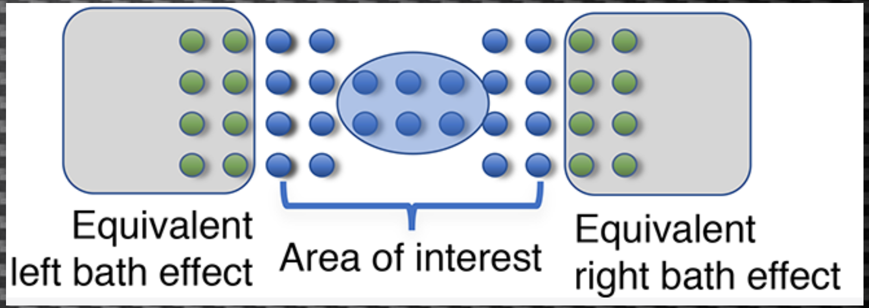
Quantum Master Eq., or Expectation from SSE

Applications outside quantum computing

- Quantum optimal systems
  - Quantum electron dynamics (QED)
  - Photodection
- Echo dynamics in NMR
- Cosmological system
  - Shandera et al 2018 Phys. Rev. D

Electron transport

- The quantum device is connected to leads with different potential



- NEGF from Lindblad (Arrigoni et al PRL 2013).
- Stochastic TDDFT (Di Ventra-D'Agosta, PRL 2007)

Outline

- **Markovian dynamics from the combined quantum system**
- **Quantum algorithms**
  - Time-marching schemes
  - First-order scheme
  - Higher order approximation in the Kraus form
- **Non-Markovian dynamics**
  - Stochastic unravelling of non-Markovian dynamics
  - Markovian embedding of the memory
  - Generalized quantum master equation
  - Quantum algorithms

System-bath dynamics

- Total Hamiltonian: $H = H_S \otimes I_B + I_S \otimes H_B + \lambda H_I$
- Liouville van Neumann equation

$$\frac{d}{dt}\rho_{tot} = -i[H_{tot}, \rho_{tot}] \Rightarrow \rho_{tot}(t) = U_{tot}(t)\rho_{tot}(0)U_{tot}(t)^\dagger$$

- Unitary evolution: $U_{tot}(t) = \exp(-itH_{tot})$.
- $\rho_{tot}(0) = \rho_S(0) \otimes \rho_B(0), \rho_B(0) \propto \exp(-\beta H_B)$
- System density-operator: $\rho_S(t) = tr_B\left(\rho_{tot}(t)\right)$.
- The Kraus form (Lidar et al 2001 Chem Phys.)

$$\rho_S(t) = \sum_j A_j(t)\rho_S(0)A_j(t)^\dagger$$

$$\langle m|A_j(t)|n\rangle = \langle m|\langle\mu|U_{tot}(t)|\nu\rangle|n\rangle, i = (\mu, \nu).$$

Markovian dynamics

- Interaction picture: $\rho_I(t) = U(t)^\dagger \rho(t) U(t)$
  $U(t) = \exp -it(H_S \otimes I_B + I_S \otimes H_B)$
- LvN in the interaction picture
$$\frac{d}{dt}\rho_I = -i\lambda[H_I(t), \rho_I(t)].$$
- For example, $H_I(t) = S(\mathrm{t}) \otimes B(t)$.
- $\rho_I(t)$= $\rho_I(0) - i\lambda \int_0^t [H_I(t'), \rho_I(t')] dt'$
- $\frac{d}{dt}\rho_I = -\lambda^2 \int_0^t [H_I(t), H_I(t'), \rho_I(t')] dt'$
- Assume weak coupling $\lambda \ll 1$
$$\rho_I(t) = \rho_{S,I}(t) \otimes \rho_B + O(\lambda)$$
- In addition, assume that $\langle B(t), B(t') \rangle \approx \delta(t - t')$.
- Then $\frac{d}{dt}\rho_{S,I} = -\lambda^2 c[S, S, \rho_{S,I}(t)]$
- This is a Lindblad equation in the interaction picture. (Cao-Lu J. Math Phys)

From Lindblad ⟷ Kraus?

- Markovian + CPTP ⇒ Lindblad-Gorini-Kossakowski-Sudarshan equation

$$\frac{d}{dt}\rho = -i[H_S,\rho] + \sum_j L_j \rho L_j^\dagger - \frac{1}{2}\{L_j^\dagger L_j, \rho\}$$

- Lindblad equation ⇒ Channel representations?
- Let's try the Euler's method
- Time steps: $t_0, t_1, \cdots, t_N = T; t_n = n\Delta t.$
- Euler: $\rho_{n+1} = \rho_n + \Delta t G \rho_n + \Delta t \rho_n G^\dagger + \Delta t \sum_j L_j \rho L_j^\dagger$

$$G = -iH - \frac{1}{2}\sum_j L_j^\dagger L_j$$

- Kraus form:

$$\rho_{n+1} = (I + \Delta t G)\rho_n (I + \Delta G)^\dagger + \Delta t \sum_j L_j \rho L_j^\dagger + O(\Delta t^2)$$

- $A_0 = I + \Delta t(-iH + G)$
- $A_j = \sqrt{\Delta t} L_j$

Why quantum algorithms

- Classical computation for Lindblad has a complexity that is polynomial in the dimension N.
- For example, it involves matrix vector multiplication.
- Quantum algorithms may have complexity $\log N \Rightarrow$ exponential speed
- Existing methods
  - Natural representation (Schlimgen et al PRR 2022)
  - Stinespring form (Wang et al, using Ham-generated unitary, PRL 2013)
  - Kraus form
- We will consider algorithms with high accuracy and complexity estimates.

Time-marching schemes

- Lindblad equation: $\frac{d}{dt}\rho = \mathcal{L}\rho$
- One-step approximation: $\mathrm{e}^{\Delta t\mathcal{L}}\rho \approx \mathcal{E}_{\Delta t}\rho$
- Global approximation: $\mathrm{e}^{T\mathcal{L}}\rho \approx \mathcal{E}_{\Delta t}^{\frac{T}{\Delta t}}\rho$
- Stinespring form.

$$\rho(\mathrm{t}+\Delta\mathrm{t}) = \mathrm{e}^{\Delta t\mathcal{L}}\rho \approx tr_A(U|0\rangle\langle 0| \otimes \rho(t)U^\dagger)$$

- Only need to specify the first col of U.
- For example. $U = \exp -i\sqrt{\Delta t}J$. (Cleve-Wang 2017)
- Global error $\mathrm{O}(\mathrm{T}\Delta t)$.
- Complexity $\mathrm{O}\left(\frac{\mathrm{T}^2}{\epsilon}\right)$.
- Improved method (T. Li and Childs 2017): $\mathrm{O}\left(\frac{\mathrm{T}^{\frac{3}{2}}}{\epsilon^{\frac{1}{2}}}\right)$.
- Nearly optimal complexity $O(m^2q^2T\log\frac{1}{\epsilon})$ (Cleve-Wang 2017 $\mathcal{L}$ expressed as Paulis)

$$J = \begin{bmatrix} \sqrt{\Delta t}H_S & L_1^\dagger & L_2^\dagger & \cdots & L_m^\dagger \\ L_1 & & & & \\ L_2 & & & & \\ \vdots & & & & \\ L_m & & & & \end{bmatrix}$$

Structure-Preserving Methods

- How to find a higher-order Kraus form?
- A direct time discretization $\nRightarrow$ CPTP map
- A structure-preserving method (Cao-Lu 2021)
- Decompose a Lindbladian: $\mathcal{L} = \mathcal{L}_D + \mathcal{L}_J$
- $\mathcal{L}_D = \left[-iH - \frac{1}{2}\sum_{j=1}^{m} L_j^\dagger L_j\,,\ \cdot\ \right]; \mathcal{L}_J\rho = \sum_{j=1}^{m} L_j \rho L_j^\dagger$

Duhamel's principle

- $\rho(t) = e^{t\mathcal{L}_D}\rho(0) + \int_0^t e^{(t-t_1)\mathcal{L}_D}\mathcal{L}_J\rho(t_1)dt_1$
- $\rho(t) = e^{t\mathcal{L}_D}\rho(0) + \int_0^t e^{(t-t_1)\mathcal{L}_D}\mathcal{L}_J e^{t_1\mathcal{L}_D}\rho(0)dt_1 + O(t^2)$

Higher-order methods in Kraus form

- Repeat for the formula K times

$$\rho(t) = e^{t\mathcal{L}_D}\rho(0) + \sum_{k=1}^{K} \int e^{(t-t_k)\mathcal{L}_D}\mathcal{L}_J e^{(t_k-t_{k-1})\mathcal{L}_D} \cdots \rho(0) dt_1 \cdots dt_k$$
$$+O(\frac{(2\|L\|t)^{K+1}}{(K+1)!}$$

Observations

- $e^{t\mathcal{L}_D}\rho(0) = D\rho(0)D^\dagger, D = \exp -t(iH + \frac{1}{2}\sum_{j=1}^{m} L_j^\dagger L_j)$
- It is a CP map in the Kraus form.
- $\mathcal{L}_J\rho = \sum_{j=1}^{m} L_j \rho L_j^\dagger$ is also CP in the Kraus form
- A composition of CP maps is CP
- Overall the solution is expressed in a Kraus form.

Approximating the integrals

- The integrals are treated with Gaussian quadrature
- Gaussian quadrature $(s_1, s_2, \cdots, s_q), (w_1, w_2, \cdots, w_q)$
- $\int_0^1 f(t)dt = \sum_{j=1}^{q} w_j f(s_j) + O\left(\frac{q||f^{2q}||}{(2q)!2^{4q-1}}\right).$
- $\int e^{(t-t_k)\mathcal{L}_D} \mathcal{L}_J e^{(t_k-t_{k-1})\mathcal{L}_D} \cdots \rho(0) dt_1 \cdots dt_k$

$$\approx \sum_{j_1=1}^{q} \sum_{j_2=1}^{q} \cdots \sum_{j_k=1}^{q} w_{j_k}, w_{(j_k,j_{k-1})}, \cdots w_{(j_k,\cdots j_1)} F_k\left(s_{j_k}, s_{(j_k,j_{k-1})}, \cdots s_{(j_k,\cdots j_1)}\right) + O\left(\frac{||G||^{2q} 2^{2k} t^{2q+k}}{(k-1)!\,(2q)!}\right)$$

- The sum of the coefficients $\Sigma_{j_1}\Sigma_{j_2} \cdots \Sigma_{j_k} w_{j_k}, w_{(j_k,j_{k-1})}, \cdots w_{(j_k,\cdots j_1)} = \frac{\mathrm{t}^{\mathrm{k}}}{(\mathrm{k}+1)!}$
- Truncation: $K, q = \frac{\log 1/\epsilon}{\log\ \log 1/\epsilon}.$

Implementing the Kraus forms

- A general CPTP map in a Kraus form

$$\mathcal{E}\rho = A_0\rho A_0^\dagger + \sum_{j=1}^{M} A_j\rho A_j^\dagger .$$

- Block-encode A_j: $A_j \approx s_j\big(\langle 0| \otimes I)U_j(|0\rangle \otimes I\big)$
- $|\mu\rangle \propto \sum_j s_j|j\rangle$.
- $W = \sum_j |j\rangle\langle j| \otimes U_j|\mu\rangle|0\rangle \otimes I$.
- $\sum_j |j\rangle A_j|\psi\rangle \approx I \otimes \langle 0| \otimes I) \sum_j |j\rangle\langle j| \otimes U_j|\mu\rangle|0\rangle\,|\psi\rangle$
- $|\rho_{new}\rangle = \big(A_0|\psi\rangle, \cdots, A_j|\psi\rangle, \cdots\big)$
- $\mathcal{E}\rho = \mathrm{tr}_\mathrm{A}(|\rho_{new}\rangle\langle\rho_{new}|)$

Main theorems

- Norm of the Linbladian: $||\mathcal{L}||_{be} = \alpha_0 + \sum_{j=1}^{m} \alpha_j^2$.
- Theorem (Li and Wang 2023). Suppose that we have the block encodings of H_S and $L_j, j = 1,2 \cdots, m$. For all $t, \epsilon > 0$, there is a quantum algorithm that yields an approximate density operator $\rho(t) = e^{t\mathcal{L}}\rho(0)$, with error within ϵ using $O(t||\mathcal{L}||_{be}\text{polylog}\frac{t}{\epsilon})$ queries and $O(tm||\mathcal{L}||_{be}\text{polylog}\frac{t}{\epsilon})$ additional 1- and 2-qubit gates.

Non-Markovian dynamics

- Why non-Markvoian?
- When there is no scale separation, non-Markovian properties emerge.
    - Divergence from standard properties [Gröblacher, non-Ohmic spectral density, 2015].
    - Measuring non-Markovianity [Breuer 2009].
    - Modeling a non-Markovian quantum dynamics
    - Controlling a non-Markovian dynamics
- There is a backflow of information.
- There is no universal form for the QME.
- It is difficult to preserve the CP property.
- The form of the equations depends heavily on the bath properties
- Our approach: Stochastic unravelling.

The connection with SSE

- A stochastic Schrödinger equation is a more intuitive description
- Stochastic Schrödinger

$$id\psi = (H_S - \frac{i\lambda^2}{2}\sum_{j=1}^{M} L_j^\dagger L_j)\psi dt + \lambda \sum_{j=1}^{M} L_j \psi dW_j$$

- The equation is written in the Ito form.
- dW_j: complex-valued white noise (multiplicative)
- SDE: $dz_t = a(z_t)dt + b(z_t) \circ dW_t$ (Stratonovich)
- Then $z_t = e^{D_t} z_0$, (Stochastic flow Kunita 1994)

$$D_t = tX_0 + W_t X_1 + \frac{1}{2}\left(\int_0^t s dW_s - \int_0^t W_s ds\right)[X_0, X_1] + \cdots$$

$$X_0 = a \cdot \nabla_{z_0}, X_1 = b \cdot \nabla_{z_0}.$$

- Application to SSE (Li and Li PRE 2020).

$$|\psi(t)\rangle = \exp\left(-itH - \frac{t}{2}(L^\dagger + L)L + LW_t + K_{(0,1)}\left(\frac{1}{2}[L^\dagger, L])L + i[H, L]\right) + \cdots\right)|\psi(0)\rangle$$

- The covariance $\rho(t) = E[|\psi(t)\rangle\langle\psi(t)|]$ satisfies Lindblad Eq.
- Can we use SSE to derive non-Markovian dynamics?

Stochastic Schrödinger Equation

- Schrödinger equation $i\partial_t\Psi = H\Psi$.
- A complete basis in $\mathcal{H}_B$. $H_B|n\rangle = \varepsilon_n|n\rangle, |n\rangle = \chi_n(r_B)$.
- Expand $\Psi = \sum_n \varphi_n(r_S, t)\chi_n(r_B)$.
- An infinite set of equations for $\varphi_n(\cdot, t)$ with
- Assume that $H = H_S \otimes I_B + I_S \otimes H_B + \lambda S \otimes B, 0 < \lambda \ll 1$.
- Using perturbations: (ϕ as a realization of φ_n) [Gaspard-Nagaoka 1999]

$$i\partial_t\phi = H_S\phi - i\lambda^2 S^\dagger \int_0^t C(\tau)e^{-iH_S\tau}S\phi(t-\tau)d\tau - i\lambda S\eta\,(t)$$

$$C(t) = tr\left(\rho_B^{eq}B(t)B(0)\right).$$

- The correlation is related to the spectral density
- This NM SSE does not have an exact QME.

An Embedding Approach

- It is typically expensive to solve the non-Markovian SSE directly
- We start with the SSE:

$$i\partial_t\phi = H_S\phi - i\lambda^2 S^\dagger \int_0^t C(\tau)e^{-i\tau H_S}S\phi(t-\tau)d\tau - i\lambda S\eta(t)$$

- Approximating $\eta(t)$ by a complex OU process (Risken)
  - $i\dot{\zeta} = -\alpha\zeta + \gamma\dot{W}(t)$.
  - If $\gamma^2 = 2Im[\alpha], c(t,t') = \langle\zeta(t)^*\zeta(t')\rangle = e^{-i\alpha^*(t-t')}, t \geq t'$.
  - Idea: Use $c(t,t')$ and $\zeta(t)$ as building blocks to approximate $C(t)$ and $\eta(t)$
- Approximation by exponentials:
  - Set $C(t) = \theta^2 e^{-i\alpha^* t}, \eta(t) = \theta\zeta(t)$.
    $\Rightarrow \langle\eta(t)^*\eta(s)\rangle = C(t-s)$.
  - Define $\chi = \frac{\lambda}{\theta}\int_0^t C(\tau)e^{-i\tau H_S}S\phi(t-\tau)d\tau$. An auxiliary orbital.
  - Equation for χ: $i\partial_t\chi = (H_S + \alpha^*)\chi + i\lambda\theta S\phi$.

Approximating the BCF

- An extended stochastic system

$$i\partial_t \phi = H_S \phi - i\lambda\theta S^\dagger \chi + \lambda\theta S \phi \zeta(t)$$
$$i\partial_t \chi = (H_S + \alpha^*)\chi + i\lambda\theta S \phi.$$
$$i\dot{\zeta} = -\alpha\zeta + \gamma \dot{W}(t).$$

- Multiple exponential functions:

$$C(t) \approx \sum_k \theta_k^2 e^{i\alpha_k^* t}.$$

- The power spectrum

$$|G(\omega)|^2 \approx \sum_k \frac{2\theta_k^2 \nu_k}{(\omega + \mu_k)^2 + \nu_k^2}$$

- This is a sum of Lorentzians.

Ritschel-Eisfeld 2014 JCP

$$\alpha(t) = \frac{1}{\pi}\int_0^\infty d\omega J(\omega)\left(\coth\left(\frac{\omega}{2T}\right)\cos(\omega t) - i\sin(\omega t)\right),$$
$$J_k(\omega) = \frac{1}{(\omega - \Omega_k)^2 + \gamma_k^2}.$$
$$J_{DL}(\omega) = 2\pi\lambda\omega\frac{\gamma}{\omega^2 + \gamma^2},$$
$$J_{ohm}(\omega) = \eta\omega e^{-\omega/\Lambda},$$
$$J_{vib}(\omega) = \frac{X\ \omega^2 J_{ohm}(\omega)}{(\omega - \tilde{g}(\omega))^2 + J_{ohm}^2(\omega))}$$
$$J_{bg}(\omega) = \frac{\pi S\omega}{\sqrt{2\pi}\sigma} e^{-[\ln(\omega/\omega_c]^2/2\sigma^2}.$$

The non-Markovian dynamics is now embedded in an extended, but Markovian dynamics.

The computation is much more efficient.

Embedding into *Linear* SSEs

- Define an auxiliary orbital: $\chi^{II} = i\phi(t)\zeta(t)$
- Keep up to $\mathcal{O}(\lambda^2)$ terms,

$$i\partial_t\phi = H_S\phi - i\lambda\theta S^\dagger\chi^I - i\lambda\theta S\chi^{II}$$
$$i\partial_t\chi^I = (H_S + \alpha^*)\chi^I + i\lambda\theta S\phi.$$
$$i\partial_t\chi^{II} = (H_S - \alpha)\chi^{II} + i\gamma\phi\dot{W}(t).$$

- We obtain linear SDEs.
- $\mathcal{O}(\lambda^3)$ approximations,

$$i\partial_t\chi^I = (H_S + \alpha^*)\chi^I + i\lambda\theta S\phi.$$
$$i\partial_t\chi^{II} = (H_S - \alpha)\chi^{II} - i\lambda\theta S^\dagger\chi^{III} - i\lambda\theta S\chi^{IV} + i\gamma\phi\dot{W}(t).$$
$$i\partial_t\chi^{III} = i\lambda\theta S\chi^{II} + (H_S + \alpha^* - \alpha)\chi^{III} + i\gamma\chi^I\dot{W}(t).$$
$$i\partial_t\chi^{IV} = i\lambda\theta S^\dagger\chi^{II} + (H_S - 2\alpha)\chi^{IV} + 2i\gamma\chi^{II}\dot{W}(t).$$

Multiple Jump Operators

- Non-Markovian SSE

$$i\frac{d}{dt}\psi = H\psi - i\lambda^2 \sum_{\alpha,\beta=1}^{M} \int_0^t C_{\alpha,\beta}(\tau) S_\alpha^\dagger e^{-i\tau H} S_\beta \psi(t-\tau) d\tau$$

$$+\lambda \sum_{\alpha=1}^{M} \eta_\alpha(t) S_\alpha \psi(t).$$

- Time correlation: $\mathrm{E}\left[\eta_\alpha(t)\eta_\beta(t')^\dagger\right] = C_{\alpha,\beta}(t-t')$.
- Approx. BCF: $C(t) \approx \sum_{j=1}^{J} \theta_j^2 |R_j\rangle\langle R_j| e^{-id_j t}. Imd_j \geq 0.$
- Auxiliary wave function, $\{\chi_{j,\beta}^{I}, \chi_{j,\beta}^{II}, \chi_{j,\beta}^{III}, \chi_{j,\beta}^{IV}\}$

The generalized quantum master eqn (GQME)

- Linearity $\Rightarrow$ closed form of the density-matrix equation.
- $\Gamma = \mathrm{E}[|\Phi\rangle\langle\Phi|]$. $\Phi = [\phi\ \chi^{I}\ \chi^{II}]$. $\rho_S = \mathrm{E}[|\phi\rangle\langle\phi|]$.
- Extended system: $i\partial_t \Phi = H\Phi + \sum_k V_k \phi \dot{W}(t)$. Unravelling of NM dynamics
- QME: $i\partial_t \Gamma = H\Gamma - \Gamma H^{\dagger} + \sum_k V_k \rho V_k^{\dagger}$.
  - It is not exactly Lindblad.
  - It preserves the positivity.
- The initial condition: $\Gamma(0) = \begin{bmatrix} \rho_S(0) & & & & \\ & 0 & & & \\ & & \rho_S(0) & & \\ & & & 0 & \\ & & & & \rho_S(0) \end{bmatrix}$.
- Density: $\rho_S(t) = Q\Gamma(t)Q^T, (Q = |0\rangle \otimes I)$ is the first diagonal block. $tr(\rho_S) = 1 + O(\lambda^3)$

The GQME (contd)

- The Hamiltonian
- $H_0 = \begin{bmatrix} H_S & -i\lambda\theta_1 S^\dagger & \lambda c_1 S & -i\lambda\theta_2 S^\dagger & \lambda c_2 S & \cdots \\ i\lambda\theta_1 S & H_s + \alpha_1^* & 0 & 0 & 0 & \cdots \\ \lambda c_1 S^\dagger & 0 & H_s - \alpha_1 & 0 & 0 & \cdots \\ i\lambda\theta_2 S & 0 & 0 & H_s + \alpha_2^* & 0 & \cdots \\ \lambda c_2 S^\dagger & 0 & 0 & 0 & H_s - \alpha_2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$
- $H = I_A \otimes H_S + H_A \otimes I_S + i\lambda \sum_k D_k \otimes T_k + i\lambda \sum_k E_k \otimes T_k^\dagger$
- The space is enlarged to mimic the influence of the environment.

The properties of the GQME

- Perturbation form: $\partial_t \Gamma = \mathcal{L}_0 \Gamma + \lambda \mathcal{L}_1 \Gamma$

Theorem: The solution of the unperturbed GQME is bounded for all time:

$$||\Gamma_0(t)|| \leq C||\Gamma_0(0)||, \forall t \geq 0.$$

The block of $\Gamma(t)$, $\tilde{\rho}(t)$ follows unitary evolution.

The trace is given by: $\mathrm{tr}\big(\Gamma_0(t)\big) = 2K + 1 + \sum_{1\leq k\leq K} e^{-4\nu_k t}$.

The trace of $\Gamma(t)$ has the bound

$$\mathrm{tr}\big(\Gamma(t)\big) = 2K + 1 + \sum_{1\leq k\leq K} e^{-4\nu_k t} + O(\lambda^2).$$

The block of $\Gamma(t)$, $\tilde{\rho}(t)$: $tr\big(\tilde{\rho}(t)\big) = 1 + O(\lambda^3)$.

Modeling Error in terms of λ

- Model Error: From the system dynamics, one can apply an asymptotic analysis.
- $\rho_S(t) = \rho_S^{(0)}(t) + \cancel{\lambda\rho_S^{(1)}(t)} + \lambda^2\rho_S^{(2)}(t) + O(\lambda^3).$
- The first order term disappears after the partial trace
- The second order term involves the BCF.

Theorem (Li-Wang 2023). Let $\hat{\rho}_S(t)$ be the first diagonal block of Γ: $\hat{\rho}_S = \langle 0|\Gamma|0\rangle$. Then

- $\left\| \hat{\rho}_S(t) - \left(\rho_S^{(0)}(t) + \lambda^2\rho_S^{(2)}(t) \right) \right\| \le C\lambda^3.$
- The GQME is consistent with the second order expansion.

Simulating the non-Markovian dynamics

- Kraus form from an infinitesimal approximation:

$$M_{\Delta t}\rho = A_0 \rho A_0^\dagger + \sum_m A_m \rho A_m^\dagger$$

- $A_0 = I - i\Delta t H$
- $A_m = \sqrt{\Delta t} V_m$
- $\left|M_{\Delta t}\rho - e^{\Delta t L}\right|_\diamond \leq 5\left|\left|L\right|\right|^2 \Delta t^2$. But it can be improved to higher order.

Theorem (Li-Wang, CMP, 2023). Suppose that we are given the access to block encodings of H_S and S_m, m $\in [M]$, $\lambda > 0$, $d_k, k \in [K]$, and $\rho_S(0)$ that exists a quantum algorithm that produces $\rho_S(t)$ s.t. $\left|\left|\rho_S(t) - \langle 0| \otimes I\Gamma(t)|0\rangle \otimes I\right|\right| < \epsilon$. The algorithm uses $O\left(\text{tpolylog}\left(\frac{t}{\epsilon}\right)\text{poly}(M, K, \lambda)\right)$ queries to H_S and S_m and additional 1 and 2-qubit gates.

Open issues

Extensions of Lindblad simulations

- Multiple time scales
- Time-dependent Lindbladians

Non-Markovian QME

- Time local Lindbladians
- Hierarchical equations of motions (HEOM)

What can we use these simulators for?

- Reaching thermal state?
- Control of open quantum systems.
- Quantum error mitigation?
- Electron transport. (how to deal with the nonlinear potential?)

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