Open quantum systems – lecture 6

lecture
winter semester 2022/2023
Technische Universität Dresden

Dr. Gernot Schaller

November 24, 2022

1.6.2 Dual master equation

Analogous to the Heisenberg picture, instead of solving the master equation for the density matrix, we can equally aim to solve for expectation values of operators $\langle A\rangle = \mathrm{Tr}\{A\rho\}$. This yields

$$\frac{d\langle A_i\rangle}{dt} = +\mathrm{i}\langle[H,A_i]\rangle + \sum_\alpha \left\langle L_\alpha^\dagger A_i L_\alpha - \frac{1}{2}\left\{L_\alpha^\dagger L_\alpha, A_i\right\}\right\rangle . \tag{1.1}$$

For a d-dimensional system described by a $d\times d$ density matrix, one has at most d^2-1 operators A_i that can ge generated on the r.h.s.

However, sometimes one is lucky and the equations close with fewer operators – e.g. if the Lindblad operators are linear in annihilation and creation operators and the Hamiltonian is at most quadratic. For example, consider the previously discussed harmonic oscillator coupled to a thermal bath, for which one gets independent equations

$$\begin{aligned}
&\frac{d}{dt}\langle a^\dagger a\rangle = \Gamma\left(n_B - \langle a^\dagger a\rangle\right), \qquad \frac{d}{dt}\langle a\rangle = \left(-\mathrm{i}\Omega - \frac{\Gamma}{2}\right)\langle a\rangle , \qquad \frac{d}{dt}\langle a^\dagger\rangle = \left(+\mathrm{i}\Omega - \frac{\Gamma}{2}\right)\langle a^\dagger\rangle ,\\
&\frac{d}{dt}\langle a^2\rangle = (-2\mathrm{i}\Omega - \Gamma)\langle a^2\rangle , \qquad \frac{d}{dt}\langle a^{2\dagger}\rangle = (+2\mathrm{i}\Omega - \Gamma)\langle a^{2\dagger}\rangle
\end{aligned} \tag{1.2}$$

From the first we learn that the average occupation converges to a thermal equilibrium value, whereas $\langle a\rangle$ and $\langle a^\dagger\rangle$ decay, such that the related position and momentum $\langle x\rangle = \sqrt{\frac{\hbar}{2m\Omega}}\langle a^\dagger + a\rangle$ and $\langle p\rangle = \sqrt{\frac{\hbar m\Omega}{2}}\mathrm{i}\langle a^\dagger - a\rangle$ spiral to the origin. For example, starting in a coherent state $|\Psi_0\rangle = |\alpha\rangle$ described by complex parameter α, this means that the initial spread of the coherent state $\langle x^2\rangle_0 - \langle x\rangle_0^2 = \frac{\hbar}{2m\Omega}$ and $\langle p^2\rangle_0 - \langle p\rangle_0^2 = \frac{\hbar m\Omega}{2}$ will increase to the spread of the thermal state $\langle x^2\rangle_\infty - \langle x\rangle_\infty^2 = \frac{\hbar}{2m\Omega}(1+2n_B)$ and $\langle p^2\rangle_\infty - \langle p\rangle_\infty^2 = \frac{\hbar m\Omega}{2}(1+2n_B)$.

1.6.3 Quantum trajectories

Solving the Lindblad equation can be quite memory consuming – it squares the effort compared to a closed quantum system described by the Schrödinger equation. A method commonly used to describe open quantum systems, are **quantum trajectories**, also known as **quantum jumps** or **Monte-Carlo wave functions**. The main idea is not to solve the master equation, but to stochastically evolve wavefunctions, such that the average of these wavefunctions reproduces the dynamics of the Lindblad master equation.

To gain some intuition, split the Lindblad equation as

$$\frac{d\rho}{dt} = -\mathrm{i}(H_{\mathrm{eff}}\rho - \rho H_{\mathrm{eff}}^\dagger) + \sum_\alpha L_\alpha \rho L_\alpha^\dagger , \tag{1.3}$$

where H_{eff} is an effective non-Hermitian Hamiltonian given by

$$H_{\mathrm{eff}} = H_S - \frac{\mathrm{i}}{2}\sum_\alpha L_\alpha^\dagger L_\alpha . \tag{1.4}$$

The last term in (1.3) represents discrete jumps, while the first represents a no-jump evolution. In terms of superoperators, we can write

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1 \qquad : \mathcal{L}_0\rho \hat{=} -\mathrm{i}(H_{\mathrm{eff}}\rho - \rho H_{\mathrm{eff}}^\dagger), \qquad \mathcal{L}_1\rho \hat{=} \sum_\alpha L_\alpha\rho L_\alpha^\dagger , \tag{1.5}$$

such that $\mathcal{L}_1$ contains the quantum jumps, whereas the no-jump evolution is in $\mathcal{L}_0$. We can expand the propagator into a Dyson series

$$e^{\mathcal{L}t} = e^{\mathcal{L}_0 t} + \int_0^t dt_1 e^{\mathcal{L}_0(t-t_1)}\mathcal{L}_1 e^{\mathcal{L}_0 t_1} + \int_0^t dt_2 \int_0^{t_2} dt_1 e^{\mathcal{L}_0(t-t_2)}\mathcal{L}_1 e^{\mathcal{L}_0(t_2-t_1)}\mathcal{L}_1 e^{\mathcal{L}_0 t_1} + \dots \tag{1.6}$$

This has the interpretation of periods of free evolutions, interupted by 0 (first term), 1 (second term), 2 (third term), and more (not shown) quantum jumps. Numerically, we observe that the calculation of the free propagator requires the complexity of the Schrödinger equation only $e^{\mathcal{L}_0 t}\rho \hat{=} e^{-\mathrm{i}H_{\mathrm{eff}}t}\rho e^{+\mathrm{i}H_{\mathrm{eff}}^\dagger t}$, albeit at the expense of introducing a non-Hermitian Hamiltonian. Evaluating the probability of a no-jump evolution, we obtain for small timesteps Δt and assuming that initially we are in a pure state

$$P_{\mathrm{stay}}(\Delta t) = \mathrm{Tr}\left\{(e^{\mathcal{L}_0 \Delta t}\left|\Psi\right\rangle\!\left\langle\Psi\right|)\right\} = 1 - \sum_\alpha \left\langle\psi\right| L_\alpha^\dagger L_\alpha \left|\psi\right\rangle \Delta t + \mathcal{O}\{\Delta t^2\}\,. \tag{1.7}$$

Accordingly, we can identify $P_{\mathrm{jump}}(\Delta t) = \sum_\alpha \left\langle\psi\right| L_\alpha^\dagger L_\alpha \left|\psi\right\rangle \Delta t$ as the probability of a quantum jump to occurr in interval Δt, and more specific, $P_\alpha(\Delta t) = \left\langle\psi\right| L_\alpha^\dagger L_\alpha \left|\psi\right\rangle \Delta t$ as the probability of jump α. Note that depending on the L_α operators, the requirement that these probabilities are small $\sum_\alpha P_\alpha(\Delta t) \ll 1$ may pose strong constraints on the maximum timestep Δt.

Thus, we already obtain a naive algorithm for solving the Lindblad equation stochastically. It requires to update the state $\left|\psi(t)\right\rangle$ during timestep Δt according to simple rules:

- with probability $P_\alpha = \left\langle\psi\right| L_\alpha^\dagger L_\alpha \left|\psi\right\rangle \Delta t$,

$$\left|\psi(t+\Delta t)\right\rangle = \left|\psi_{\mathrm{jump}}^\alpha\right\rangle = \frac{L_\alpha \left|\psi(t)\right\rangle}{\sqrt{\left\langle\psi(t)\right| L_\alpha^\dagger L_\alpha \left|\psi(t)\right\rangle}}\,, \tag{1.8}$$

  i.e., we act with the corresponding jump operator and normalize.

- with probability $P_{\mathrm{stay}} = 1 - \sum_\alpha P_\alpha$,

$$\left|\psi(t+\Delta t)\right\rangle \to \left|\psi_{\mathrm{stay}}\right\rangle = \frac{e^{-\mathrm{i}H_{\mathrm{eff}}\Delta t}\left|\psi(t)\right\rangle}{\sqrt{\left\langle\psi(t)\right| e^{+\mathrm{i}H_{\mathrm{eff}}^\dagger \Delta t} e^{-\mathrm{i}H_{\mathrm{eff}}\Delta t}\left|\psi(t)\right\rangle}}\,, \tag{1.9}$$

  i.e., we propagate with the effective non-Hermitian Hamiltonian by Δt and normalize.

One may then verify that the ensemble-averaged evolution can be written as to order Δt^2 as

$$\begin{aligned}\overline{\rho(t+\Delta t)} &= (1 - \sum_\alpha P_\alpha)|\psi_{\mathrm{stay}}\rangle\langle\psi_{\mathrm{stay}}| + \sum_\alpha P_\alpha |\psi_{\mathrm{jump}}^\alpha\rangle\langle\psi_{\mathrm{jump}}^\alpha| \\ &= \rho(t) - \mathrm{i}\Delta t\Big[H_{\mathrm{eff}}\rho(t) - \rho(t)H_{\mathrm{eff}}^\dagger\Big] + \Delta t \sum_\alpha L_\alpha \rho(t) L_\alpha^\dagger + \mathcal{O}\{\Delta t^2\}\,,\end{aligned} \tag{1.10}$$

which is equivalent to the discretized version of Eq. (1.3). This also implies that the expectation value of any observable O can also be evaluated by averaging over the trajectories $\langle O\rangle = \mathrm{Tr}\,\{\rho(t)O\} = \overline{\left\langle\psi(t)\right| O \left|\psi(t)\right\rangle}$.

The above procedure however may not be very efficient: To keep the scheme valid, one is forced to use very small timesteps Δt, which will lead to the outcome that in most timesteps, we will just

propagate by the jump-free evolution (non-Hermitian Hamiltonian and normalization). Instead, one could evolve these trivial (jump-free) periods more efficiently by sampling the waiting time to the next jump.

Therefore, we write the above procedure as a stochastic differential equation.

Def. 1 (Stochastic Schrödinger equation)**.** *A master equation of Lindblad form*

$$\dot{\rho} = -\mathrm{i}\left[H,\rho\right] + \sum_\alpha \left[L_\alpha \rho L_\alpha^\dagger - \frac{1}{2}\left\{L_\alpha^\dagger L_\alpha, \rho\right\}\right] \tag{1.11}$$

can be effectively modeled by solving the stochastic differential equation

$$|d\psi\rangle = \left[-\mathrm{i}H - \frac{1}{2}\sum_\alpha L_\alpha^\dagger L_\alpha + \frac{1}{2}\sum_\alpha \langle\psi| L_\alpha^\dagger L_\alpha |\psi\rangle\right]|\Psi\rangle dt + \sum_\alpha \left(\frac{L_\alpha|\psi\rangle}{\sqrt{\langle\psi| L_\alpha^\dagger L_\alpha |\psi\rangle}} - |\psi\rangle\right) dN_\alpha\,, \tag{1.12}$$

with Poisson increments dN_α satisfying

$$dN_\alpha dN_\beta = \delta_{\alpha\beta} dN_\alpha \qquad : \qquad \overline{dN_\alpha} = \langle\psi| L_\alpha^\dagger L_\alpha |\psi\rangle dt\,. \tag{1.13}$$

- Being intended to be read as $|\psi\rangle \to |\psi\rangle + |d\psi\rangle$, the above just implements the previous recipe. To see that note that $dN_\alpha \in \{0,1\}$ and that no two quantum jumps can occur at the same time. Then, if $dN_\alpha = 1$ for a particular jump, the state is just updated like in (1.8) and the change due to $dt \ll dN_\alpha$ is neglected. When $dN_\alpha = 0$ for all jumps, we have to solve $\frac{|d\psi\rangle}{dt} = \left(-\mathrm{i}H_\mathrm{eff} + \frac{1}{2}\sum_\alpha \langle\psi| L_\alpha^\dagger L_\alpha |\psi\rangle\right)|\psi\rangle$. The solution to this nonlinear differential equation is given by $|\psi(t)\rangle = \frac{e^{-\mathrm{i}H_\mathrm{eff}t}|\psi_0\rangle}{\sqrt{\langle\psi_0|e^{+\mathrm{i}H_\mathrm{eff}^\dagger t}e^{-\mathrm{i}H_\mathrm{eff}t}|\psi_0\rangle}}$, in analogy to Eq. (1.9).

- It is actually neither necessary nor efficient to discretize time for the propagation: For the no-jump evolution, we just need to propagate according to the effective non-Hermitian Hamiltonian. Numerically, it is therefore much more efficient to stochastically determine the time when the next jump occurs according to the waiting-time distribution between any two jumps

$$\omega(\tau) = -\frac{d}{d\tau}\langle\psi| e^{+\mathrm{i}H_\mathrm{eff}^\dagger \tau} e^{-\mathrm{i}H_\mathrm{eff}\tau} |\psi\rangle\,. \tag{1.14}$$

  Technically, such a distribution of waiting times is obtained via the cumulative distribution $W(\tau) = \int_0^\tau \omega(\tau')d\tau' = 1 - \langle\psi| e^{+\mathrm{i}H_\mathrm{eff}^\dagger \tau} e^{-\mathrm{i}H_\mathrm{eff}\tau} |\psi\rangle$: For random random numbers that are uniformly distributed $r_i \in [0,1]$, one can find the associated waiting times $\tau_i \in [0,\infty]$ that are distributed according to the waiting time distribution $\omega(\tau)$ by solving $r_i = W(\tau_i)$. Thus, the waiting-time sampled stochastic solution scheme could be summarized as follows:

  – generate a random number $r_i \in [0,1]$ and for state $|\psi(t)\rangle$ solve the equation

$$r_i = 1 - \langle\psi(t)| e^{+\mathrm{i}H_\mathrm{eff}^\dagger \tau_i} e^{-\mathrm{i}H_\mathrm{eff}\tau_i} |\psi(t)\rangle \tag{1.15}$$

  numerically (or, if possible, analytically) for τ_i,

– propagate by the waiting time τ_i to the next jump time and normalize the solution

$$|\psi(t+\tau_i)\rangle = \frac{e^{-\mathrm{i}H_{\mathrm{eff}}\tau_i}\,|\psi(t)\rangle}{\sqrt{\langle\psi(t)|\,e^{+\mathrm{i}H_{\mathrm{eff}}^\dagger\tau_i}e^{-\mathrm{i}H_{\mathrm{eff}}\tau_i}\,|\psi(t)\rangle}}\,. \tag{1.16}$$

– perform a quantum jump of type α with conditional probability

$$P_{\alpha,\mathrm{jump}} = \frac{\langle\psi(t+\tau_i)|\,L_\alpha^\dagger L_\alpha\,|\psi(t+\tau_i)\rangle}{\sum_\beta\langle\psi(t+\tau_i)|\,L_\beta^\dagger L_\beta\,|\psi(t+\tau_i)\rangle}\,. \tag{1.17}$$

For such trajectories, we do not even need to specify a timestep.

- Computing a single trajectory this way may require significantly less storage effort than solving the original Lindblad equation in superoperator notation. Typically, this numerical advantage is not scotched by the required sampling (a process which is easily parallelizable).

- As the Lindblad equation is invariant under unitary transformations of the Lindblad operators and also under the simultaneous transformations

$$L_\alpha \to L_\alpha + a_\alpha\mathbf{1}\,, \qquad H \to H + \frac{1}{2\mathrm{i}}\sum_\alpha\left(a_\alpha^* L_\alpha - a_\alpha L_\alpha^\dagger\right) + b\mathbf{1}\,, \tag{1.18}$$

where $a_\alpha \in \mathbb{C}$ and $b \in \mathbb{R}$, the numerical solution scheme is not unique. One talks of different unravellings of the master equation [1].

- In case the jump operators describe transition between different energy eigenstates, i.e., $H = \sum_a E_a\,|a\rangle\langle a|$ and $L_\alpha \to L_{ab} = \sqrt{R_{ab}}\,|a\rangle\langle b|$ with transition rate from $|b\rangle$ to $|a\rangle$ given by $R_{ab} > 0$, and when the initial state is just a specific energy eigenstate $|n\rangle$, the above stochastic differential equation reduces to Gillespie algorithm for propagating rate equations.

As example, consider the harmonic oscillator, for which we have $L_\downarrow = \sqrt{\Gamma(1+n_B)}a$ and $L_\uparrow = \sqrt{\Gamma n_B}a^\dagger$, which leads to the non-Hermitian Hamiltonian

$$H_{\mathrm{eff}} = \Omega a^\dagger a - \frac{\mathrm{i}}{2}\Gamma\left((1+n_B)a^\dagger a + n_B a a^\dagger\right)\,, \tag{1.19}$$

and the probabilities for excitation and de-excitation during a timestep Δt become

$$P_\uparrow(t) = \Gamma\Delta t n_B\langle\psi(t)|\,aa^\dagger\,|\psi(t)\rangle\,, \qquad P_\downarrow(t) = \Gamma\Delta t(1+n_B)\langle\psi(t)|\,a^\dagger a\,|\psi(t)\rangle\,. \tag{1.20}$$

To obtain a non-trivial example, let us consider a coherent initial state

$$|\psi_0\rangle = |\alpha\rangle = e^{\alpha a^\dagger - \alpha^* a}\,|0\rangle = e^{-|\alpha|^2/2}\sum_{n=0}^\infty\frac{\alpha^n}{\sqrt{n!}}\,|n\rangle\,. \tag{1.21}$$

From that, one can calculate a trajectory, and upon averaging many trajectories, one can recover the evolution by the master equation, see Fig. 1.1.

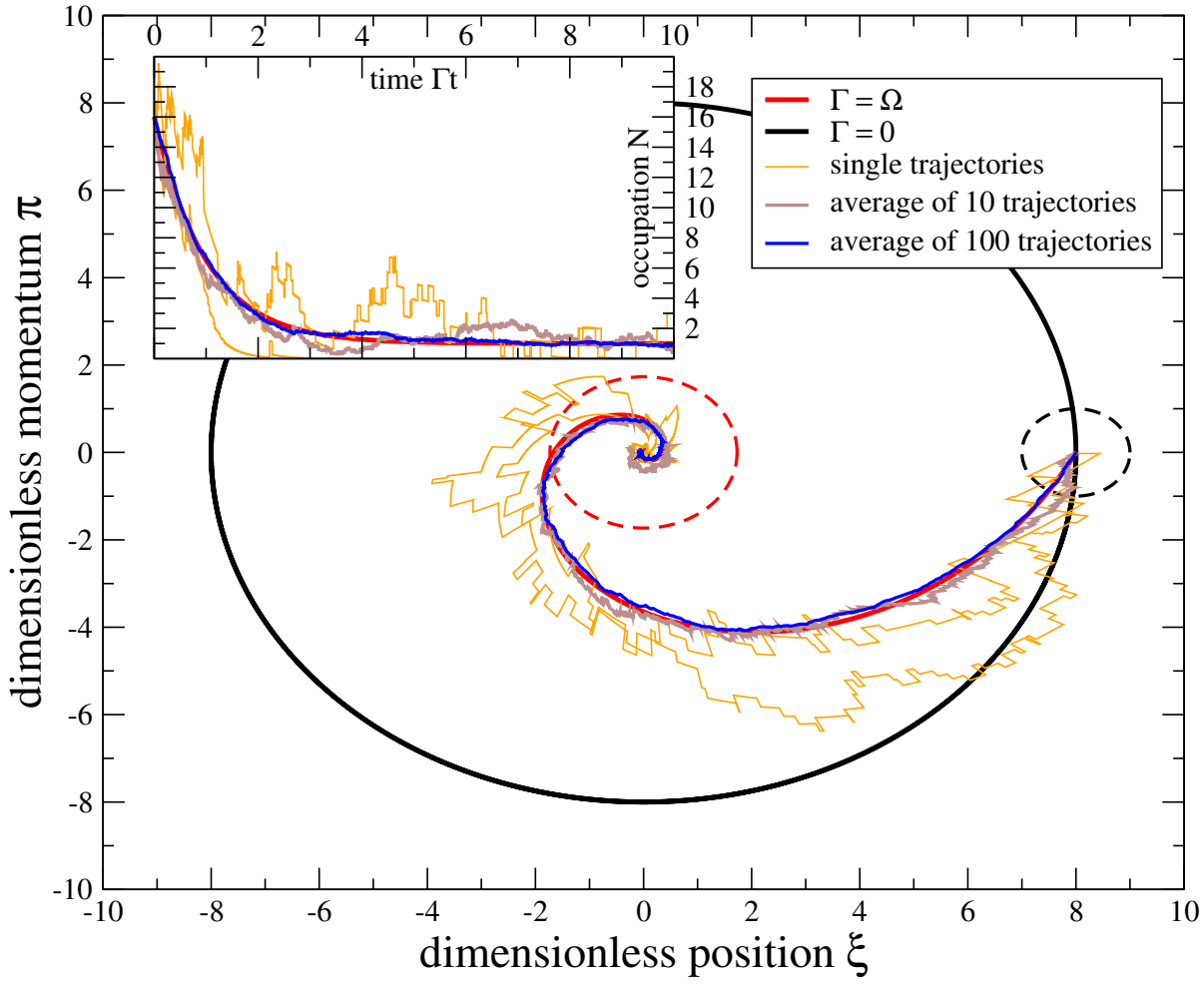

Figure 1.1: Plot of the master equation average values (continuous black and red curves) in terms of dimensionless position $\xi = x\sqrt{\frac{2m\Omega}{\hbar}}$ and $\pi = p\sqrt{\frac{2}{\hbar m\Omega}}$ starting from an initial coherent state with $\alpha = 4$ and for a bath with Bose occupation number $n_B = 1$. Individual trajectories (orange) may divert significantly from the average master equation solution, but the average of sufficiently many trajectories (brown and blue) will reproduce it. Dashed circles denote expected standard deviations for the initial (black) and final (red) states. Inset: Analog for $\langle a^\dagger a \rangle$ versus time. With the chosen cutoff of $N_{\text{cut}} = 100$, the brute-force vectorization recipe would have produced a Liouillian of dimension 10000×10000.

Bibliography

[1] H. M. Wiseman and G. J. Milburn. *Quantum Measurement and Control*. Cambridge University Press, Cambridge, 2010.