Unravelings of the open quantum system dynamics

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Recap:

1. Jump unravelings on the level of density operator

In the pervious lectures GKSL master equation was derived, which described open quantum system dynamics with semi-group property ($\phi(t)\phi(s) = \phi(t+s)$, $\phi(t)[\rho(0)] = \rho(t)$). It has following form

$$\frac{d}{dt}\phi(t) = \mathcal{L}\phi(t) = (\mathcal{L}_R + \underbrace{\sum_k \mathcal{L}_k}_{\mathcal{L}_J})\phi(t), \tag{1}$$

with

$$\begin{aligned}\mathcal{L}_R\rho &= -i(H_{\text{eff}}\rho - \rho H_{\text{eff}}),\\ H_{\text{eff}} &= H - \frac{i}{2}\sum_k \gamma_k L_k^\dagger L_k,\\ \mathcal{L}_k\rho &= \gamma_k L_k \rho L_k^\dagger.\end{aligned}$$

The solution of Eq. (1) reads

$$\phi(t) = \mathrm{e}^{(\mathcal{L}_R+\mathcal{L}_J)t}. \tag{2}$$

As was seen in the previous lectures Eq. (2) can be written as an infinite sum of different "jump trajectories" , which can be easily seen by defining

$$\mathcal{R}_t = \mathrm{e}^{\mathcal{L}_R t} \qquad \Leftrightarrow \qquad \tilde{\mathcal{R}}_u = (u - \mathcal{L}_R)^{-1},$$

where $\tilde{\mathcal{R}}_u$ is the Laplace transform of $\mathcal{R}_t$ and $\widetilde{(\mathrm{e}^{-\alpha t})}_u = \frac{1}{u+\alpha}$.

Write (2) in Laplace representation

$$\tilde{\phi}_u = \tilde{\mathcal{R}}_u(1 - \mathcal{L}_J\tilde{\mathcal{R}}_u)^{-1},$$

which in time domain reads ($\rightarrow$ Neumann series)

$$\rho(t) = \phi(t)\rho(0) = \mathcal{R}_t\rho(0) + \sum_{n=1}^{\infty}\int_0^t dt_n ... \int_0^{t_2} dt_1 \mathcal{R}_{t-t_n}\mathcal{L}_J\mathcal{R}_{t_n - t_{n-1}}...\mathcal{L}_J\mathcal{R}_{t_1}\rho(0) \tag{3}$$

One can consequently "unravel" the reduced state $\rho(t)$ in "jump trajectories"

$$\rho(t) = \underbrace{\mathcal{R}_t\rho(0)}_{\text{no jump}} + \underbrace{\int_0^t dt_1 \overbrace{\mathcal{R}_{t-t_1}\mathcal{L}_J\mathcal{R}_{t_1}\rho(0)}^{\mathcal{K}_1(t,t_1)}}_{\text{all trajectories with one jump}} + \underbrace{\int_0^t dt_2 \int_0^{t_2} dt_1 \overbrace{\mathcal{R}_{t-t_2}\mathcal{L}_J\mathcal{R}_{t_2-t_1}\mathcal{L}_J\mathcal{R}_{t_1}\rho(0)}^{\mathcal{K}_2(t,t_2,t_1)}}_{\text{all trajectories with two jumps}} + ... \tag{4}$$

and a particular n-jump trajectory has a form

$$\mathcal{K}_n(t; t_n, k_n; ...) = \mathcal{R}_{t-t_n}\mathcal{L}_{k_n}...\mathcal{R}_{t_2-t_1}\mathcal{L}_{k_1}\mathcal{R}_{t_1}\rho(0), \tag{5}$$

with $\mathcal{K}_n(t, t_n, ..) = \sum_{k_n,...} \mathcal{K}_n(t; t_n, k_n; ...)$.

Interpretation

- $\mathcal{L}_k$ describes the jumps which occur (due to interaction with the environment) at random times with a rate γ_k
- In-between the jumps the system undergo the relaxing/free evolution generated by $\mathcal{L}_R$.

However, $\mathcal{R}_t\rho(0)$ is not normalized, $\mathcal{R}_t$ is trace decreasing:

$$\mathrm{e}^{\mathcal{L}_R t}\rho = \mathrm{e}^{-itH_{\text{eff}}}\rho\mathrm{e}^{itH_{\text{eff}}} > 0$$

$$\frac{d}{dt}\mathrm{Tr}(\mathrm{e}^{\mathcal{L}_R t}\rho) = \mathrm{Tr}(\mathcal{L}_R\mathrm{e}^{\mathcal{L}_R t}\rho) = -\mathrm{Tr}(\mathcal{L}_J\mathrm{e}^{\mathcal{L}_R t}\rho) < 0.$$

Interpretation

- $\mathrm{Tr}(\mathcal{R}_t\rho(0)) = P_0(t)$ - the probability that no jump occurs till time t
- $\mathrm{Tr}(\mathcal{K}_n(t; t_n, k_n; ...)\rho(0)) = P_n(t; t_n, k_n; ...)$ - the probability density that (solely) n jumps k_n in the vicinity of times $t_n, ...$ occur till time t
- As the events corresponding to different trajectories are mutually exclusive, the

probability density that some n jumps in the vicinity of times $t_n, ...$ occur till time t equals $\mathrm{Tr}(\mathcal{K}_n(t, t_n, ..)\rho(0)) = P_n(t, t_n, ...) = \sum\limits_{k_n, ...} P_n(t; t_n, k_n; ...)$

Indeed the interpretation makes sense, as

$$1 = \mathrm{Tr}(\rho(t)) = P_0(t) + \sum_{n=1}^{\infty} \int_0^t dt_n ... \int_0^{t_2} dt_1 P_n(t, t_n, ...) \tag{6}$$

So by defying normalised states

$$\rho_n(t; t_n, k_n; ...) = \frac{\mathcal{K}_n(t; t_n, k_n; ..)}{\mathrm{Tr}(\mathcal{K}_n(t; t_n, k_n; ...))}$$

one obtains

$$\rho(t) = \sum\!\!\!\!\!\!\int P_n(t; t_n, k_n; ...)\rho_n(t; t_n, k_n; ...) = \mathcal{M}(\rho_n(t; t_n, k_n; ...)).$$

- To find $\rho(t)$ one can find individual trajectories and then build a weighted average.
- The state transformation for single trajectory has a form of POVM measurement, accordingly measurement interpretation of the trajectories is given (Ozawa theorem). Interpretation: The open system is continously monitored by the environment.
- Each trajectory corresponds to some measurement record - clicking of an apparatus at some fixed times; no clicking is also an event - H_{eff} driving the free evolution is not Hermitian.
- By the absence of information which record was detected one builds unconditional state: $\rho(t)$.
- We gain a physical interpretation: Discontinuous/jump trajectories

For more reading see "Introduction to Decoherence Theory" by Hornberger in "Entanglement and Decoherence, Foundations and Modern Trends" edited by Buchleitner, Viviescas and Tiersch.

2. Jump unravelings on the level of pure states

In the above examined situation trajectory at fixed time is a N^2-dimensional object (for N-dimensional system) - for large N difficult to handle. However, each density operator can be decompose in pure states - N-dimensional objects, $\rho(0) = \sum p^m |\phi^m(0)\rangle\langle\phi^m(0)|$. Constructing the jump trajectories on the level of these pure states can be computationally advantageous!

The construction of these jump trajectories is analogous to the above case. One firstly draw an initial pure state $|\phi^m(0)\rangle$ with probability p^m. Then one can construct with this initial state a trajectory. The unnormalized trajectory with n-jumps k_n till time t at fixed times $(t_n, ..., t_1)$ and a fixed initial state m is

$$|\phi_n^m(t; t_n, k_n; ...)\rangle = \mathrm{e}^{-iH_{\mathrm{eff}}(t-t_n)}\sqrt{\gamma_{k_n}}L_{k_n}...\mathrm{e}^{-iH_{\mathrm{eff}}(t_2-t_1)}\sqrt{\gamma_{k_1}}L_{k_1}\mathrm{e}^{-iH_{\mathrm{eff}}t_1}|\phi^m(0)\rangle,$$

so one gets the connection $\mathcal{K}_n(t; t_n, k_n; ...) = \sum_m p^m |\phi_n^m(t; t_n, k_n; ...)\rangle\langle\phi_n^m(t; t_n, k_n; ...)|$. The corresponding probabilities and the normalised state can be obtained analogously to above consideration.

3. Time-continuous unravelings on the level of pure states

Now we will get to know an example of time-continuous trajectories on the level of the pure states. The description is of course highly non-unique. Here, we consider the unraveling where the single trajectories are driven by stochastic Schrödinger equations (Diósi and Strunz, Phys. Lett. A, 235(6):569, 1997), see, e.g., "Stochastic Processes in Physics and Chemistry" by Van Kampen for what the stochastic processes are. We start with microscopic derivation of the description, so considering both the reduced state and the environment.

We model the environment with harmonic oscillators:

$$H = H_S + H_I + H_E = H_S + \sum_\lambda (g_\lambda^* L a_\lambda^\dagger + g_\lambda L^\dagger a_\lambda) + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda$$

We go to interaction picture with respect to the environment

$$H_{\mathrm{tot}}(t) = \mathrm{e}^{iH_E} H \mathrm{e}^{-iH_E} - H_E = H_S + \sum_\lambda (g_\lambda^* L a_\lambda^\dagger \mathrm{e}^{i\omega_\lambda t} + g_\lambda L^\dagger a_\lambda \mathrm{e}^{-i\omega_\lambda t}) = H_S + LB^\dagger(t) + L^\dagger B(t),$$

and assume that initially the system is a pure state and the environment is in the ground state: $|\Psi(0)\rangle = |\phi_0\rangle|0_1\rangle..|0_\lambda\rangle... =: |\phi_0\rangle|0\rangle$.

The Schrödinger equation describing the evolution of the total system reads

$$i\partial_t|\Psi(t)\rangle = H_{\mathrm{tot}}(t)|\Psi(t)\rangle. \tag{7}$$

The key point is to expand the environmental degrees of freedom in terms of Bargmann coherent states. They are defined in a following way

$$||z\rangle = \mathrm{e}^{za^\dagger}|0\rangle = \mathrm{e}^{|z|^2/2}|z\rangle,$$

where $|z\rangle$ is a "standard" coherent state.

- The Bargmann coherent states are not normalized $\langle z'||z\rangle = \mathrm{e}^{z'z^*}$.
- They form an overcomplete basis

$$1 = \int \frac{d^2z}{\pi}\mathrm{e}^{-|z|^2}||z\rangle\langle z||.$$

- $||z\rangle$ is analytic in z (no z^* dependency).
- $\langle z||a^\dagger = z^*\langle z||$
- $\langle z||a = \frac{\partial}{\partial z^*}\langle z||$.

The total state can be consequently written as

$$\begin{aligned}|\Psi(t)\rangle = \int \frac{d^2z_1}{\pi}..\int \frac{d^2z_\lambda}{\pi}..\mathrm{e}^{-(|z_1|^2+...+|z_\lambda|^2+...)}||z_1\rangle...||z_\lambda\rangle...\langle z_\lambda||...\langle z_1||\Psi(t)\rangle \\ =: \int \frac{d^2z}{\pi}\mathrm{e}^{-|z|^2}||z\rangle\langle z||\Psi(t)\rangle =: \int \frac{d^2z}{\pi}\mathrm{e}^{-|z|^2}|\phi(t,z^*)\rangle||z\rangle.\end{aligned}$$

- $|\phi(t,z^*)\rangle$ - the state "relative" to $||z\rangle$ - is analytic in z^*_λ.
- By having $|\phi(t,z^*)\rangle$ one can obtain the whole state! - statements about common properties like correlations/entanglement between open system and its environment possible.

Project Schrödinger equation (7) on the Bargmann coherent states

$$\langle z||\partial_t|\Psi(t)\rangle = \partial_t|\phi(t,z^*)\rangle = H_S|\phi(t,z^*)\rangle + Lz_t^*|\phi(t,z^*)\rangle - L^\dagger\int_0^t ds\alpha(t-s)\frac{\delta|\phi(t,z^*)\rangle}{\delta z_s^*}. \tag{8}$$

- $z_t^* := -i\sum_\lambda g_\lambda^* z_\lambda^* \mathrm{e}^{i\omega_\lambda t}$
- We used $\frac{\partial}{\partial z_\lambda^*} = \int ds \frac{\partial z_s^*}{\partial z_\lambda^*}\frac{\delta}{\delta z_s^*}$.
- $\alpha(t)$ is a bath correlation function at zero temperature $\alpha(t) = \langle B(t)B^\dagger(s)\rangle$, with $B(t)$ - bath coupling operator.
- No Born-Markov approximation used by derivation of Eq. (8) - in principle arbitrary "memory effects" can be described (arbitrary correlation function $\alpha(t)$). However, one has to know what the functional derivative $\frac{\delta|\phi(t,z^*)\rangle}{\delta z_s^*}$ is.

- Assume $\frac{\delta|\phi(t,z^*)\rangle}{\delta z_s^*} = O(t,s,z^*)|\phi(t,z^*)\rangle$, then Eq. (8) is convolutionless/time-local (this is also often the case when "memory effects" occur).

- The states $|\phi(t,z^*)\rangle$ are still not normalized: the equation for normalized state is not linear!

- In general only single-shot measurement interpretation of the trajectories.

With the resolution of the identity in terms of Bargmann coherent states it is easy to see that the $|\phi(t,z^*)\rangle$ indeed build the unraveling of the reduced dynamics

$$\rho(t) = \mathrm{Tr}_E(|\Psi(t)\rangle\langle\Psi(t)|) = \int \frac{d^2z}{\pi} \mathrm{e}^{-|z|^2} \langle z||\Psi(t)\rangle\langle\Psi(t)||z\rangle$$
$$= \int \frac{d^2z}{\pi} \mathrm{e}^{-|z|^2} |\phi(t,z^*)\rangle\langle\phi(t,z^*)| = \mathcal{M}_z(|\phi(t,z^*)\rangle\langle\phi(t,z^*)|)$$

and the function z_t can be interpreted as a Gaussian complex noise (see, e.g., "Stochastic Processes: Theory for Applications" by Robert G. Gallager for Gaussian complex process) with

$$\mathcal{M}_z(z_t) = 0, \qquad \mathcal{M}_z(z_t z_s^*) = \alpha(t-s), \qquad \mathcal{M}_z(z_t z_s) = 0.$$

From the stochastic Schrödinger equation (8) one can derive a master equation for the reduced state.

With $\overline{O}(t,z^*) = \int_0^t ds\alpha(t-s)O(t,s,z^*)$, $\rho(t) = \mathcal{M}_z(|\phi(t,z^*)\rangle\langle\phi(t,z^*)|) = \mathcal{M}_z(P_t)$ and $\mathcal{M}_z(z_t P_t) = \mathcal{M}_z(\int_0^t ds\alpha(t-s)\frac{\delta}{\delta z_s^*}P_t) = \mathcal{M}_z(\overline{O}(t,z^*)P_t)$[1] one gets

$$\partial_t\rho(t) = -i[H_S,\rho(t)] + [L,\mathcal{M}_z(P_t\overline{O}^\dagger(t,z^*))] + [\mathcal{M}_z(\overline{O}(t,z^*)P_t),L^\dagger]. \tag{9}$$

- If $\overline{O}(t,z^*) = \overline{O}(t)$ (no dependence on the noise) the Eq. (9) simplifies

$$\partial_t\rho(t) = -i[H_S,\rho(t)] + [L,\rho(t)\overline{O}^\dagger(t)] + [\overline{O}(t)\rho(t),L^\dagger].$$

- in Markov limit: $\alpha(t-s) = \gamma\delta(t-s)$ and with $O(t,t,z^*) = L$ we obtain again GKSL master equation

$$\partial_t\rho(t) = -i[H_S,\rho(t)] + \frac{\gamma}{2}[L,\rho(t)L^\dagger] + \frac{\gamma}{2}[L\rho(t),L^\dagger].$$

[1] Novikov theorem, using the Gaussianity of the complex noise. Explicitly: $\mathcal{M}_z(z_t P_t) = -i\sum_\lambda g_\lambda \mathrm{e}^{i\omega_\lambda t}\int\frac{d^2z}{\pi}(\frac{\partial}{\partial z_\lambda^*}\mathrm{e}^{-|z_\lambda|^2})P_t = i\sum_\lambda g_\lambda \mathrm{e}^{i\omega_\lambda t}\int\frac{d^2z}{\pi}\mathrm{e}^{-|z_\lambda|^2}\frac{\partial}{\partial z_\lambda^*}P_t$ and then use $\frac{\partial}{\partial z_\lambda^*} = \int ds\frac{\partial z_s^*}{\partial z_\lambda^*}\frac{\delta}{\delta z_s^*}$.