Non-Markovian Quantum Dynamics of Open Systems: Foundations and Numerical Strategies

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Open Quantum Systems

Total system:

\[ H = H_S + H_E + H_I + H_{\text{field}} \]

\[ \frac{d}{dt} \rho = -i[H, \rho] \]

Open (reduced) system:

\[ \rho_S = \text{tr}_E \{ \rho \} \quad \text{partial trace} \]

\[ \frac{d}{dt} \rho_S = -i \text{tr}_E \{ [H, \rho] \} \]

Applications:

- atomic physics, quantum optics
- condensed matter physics
- quantum chemistry
- nano technologies
- quantum computing, cryptography
- decoherence/quantum error correction
- quantum measurement and control
- entropy production, transport processes
• Quantum Markov Processes

• Non-Markovian Dynamics and Projection Operator Techniques

• Correlated Projection Superoperators

• Conclusions
Quantum Markov Processes

Product initial state: $\rho(0) = \rho_S(0) \otimes \rho_E$

\[\Rightarrow\] Dynamical map $\Phi_t$:

$\rho_S(0) \mapsto \rho_S(t) = \Phi_t \rho_S(0) = \text{tr}_E \left\{ U_t (\rho_S(0) \otimes \rho_E) U_t^\dagger \right\}$

Markov property:

$\Phi_t \Phi_s = \Phi_{t+s}$, $t, s \geq 0$

\[\Rightarrow\] Quantum dynamical semigroup:

$\Phi_t = \exp [\mathcal{L}t]$

Markovian master equation:

$\frac{d}{dt}\rho_S(t) = \mathcal{L}\rho_S(t)$

Generator of time evolution in Lindblad form:

$\mathcal{L}\rho_S = -i[H_S, \rho_S] + \sum_i \gamma_i \left[ A_i \rho_S A_i^\dagger - \frac{1}{2} \left\{ A_i^\dagger A_i, \rho_S \right\} \right]$
Quantum Markov Processes

Structure of Lindblad generator fixed by requirements:

- product initial state
- $\Phi_t$ preserves Hermiticity and trace
- $\Phi_t$ is completely positive:

  reduced state space $\mathcal{H}_S$: $\rho_S \geq 0 \implies \Phi_t \rho_S \geq 0$

  state space $\mathcal{H}_S \otimes \tilde{\mathcal{H}}$: $\rho \geq 0 \implies (\Phi_t \otimes I) \rho \geq 0$

  $\implies$ entanglement theory

- $\Phi_t$ represents a semigroup

$\implies$ microscopic theory:

$\tau_E \ll \tau_S$  separation of time scales
Quantum Markov Processes

Typical applications:

- Interaction of radiation with matter (weak coupling)
- Quantum optics, Cavity-QED (weak damping)
- Decoherence
- Quantum Brownian motion (high temperatures)
- Quantum information: Quantum Error Correction
- Stochastic unravelling (Monte Carlo simulations):
  \[ \rho_S(t) = \text{Mean}[|\psi(t)\rangle\langle\psi(t)|] \]
  \[ |\psi(t)\rangle = \text{stochastic process in Hilbert space} \]
- Laser cooling (Lévy statistics of quantum jumps)
Non-Markovian Dynamics

What is a non-Markovian quantum process?

- Semigroup property violated: slow decay of correlations, strong memory effects
- Initial correlations (classically correlated or entangled initial states)
- Strong couplings and low temperatures (short-time behavior, decoherence)

\[ \frac{d}{dt} \rho(t) = -i\alpha [H_I(t), \rho(t)] \equiv \alpha \mathcal{L}(t) \rho(t) \]
Nakajima-Zwanzig Projection

Projection superoperator (linear map on operators):

\[ \text{total state } \rho(t) \implies \text{relevant part } \mathcal{P} \rho(t) \]

\[
\mathcal{P} \rho = \text{tr}_E \{ \rho \} \otimes \rho_E \\
\mathcal{P}^2 = \mathcal{P}
\]

Complementary projection onto irrelevant part:

\[ Q = I - \mathcal{P} \]

\[ \implies \text{Nakajima-Zwanzig equation:} \]

\[ \frac{d}{dt} \mathcal{P} \rho(t) = \int_0^t ds \ K(t, s) \mathcal{P} \rho(s) + \mathcal{I}(t) Q \rho(0) \]

\[ K(t, s) = \text{memory kernel} \]
Eliminating the memory kernel:

\[ \rho_S(t) = \Phi_t \rho_S(0) \quad \text{and} \quad \frac{d}{dt} \rho_S(t) = \dot{\Phi}_t \rho_S(0) \]

\[ \Rightarrow \text{time-local master equation (TCL):} \]

\[ \frac{d}{dt} \rho_S(t) = \left( \Phi_t \Phi_t^{-1} \right) \rho_S(t) \equiv \mathcal{K}(t) \rho_S(t) \]

Important properties:

- No time-convolution involved, equation \text{local in time}
- Interpretation of \( \Phi_t^{-1} \): The inverse of \( \Phi_t \), but not completely positive (not even positive)
- Inhomogeneous term in case of initial correlations
General form of master equation:
\[
\frac{d}{dt} \mathcal{P} \rho(t) = \mathcal{K}(t) \mathcal{P} \rho(t) + \mathcal{I}(t) \mathcal{Q} \rho(0)
\]

General form of TCL generator:
\[
\mathcal{K}(t) \rho_S = -i [H_S(t), \rho_S] + \sum_i \left[ C_i(t) \rho_S D_i^\dagger(t) + D_i(t) \rho_S C_i^\dagger(t) \right]
- \frac{1}{2} \sum_i \left\{ D_i^\dagger(t) C_i(t) + C_i^\dagger(t) D_i(t), \rho_S \right\}
\]

\[
\implies \text{Not in Lindblad form: } C_i(t) \neq D_i(t)
\]
Time Convolutionless Master Equation

Perturbation expansion:

\[ \mathcal{K}(t) = \sum_{n=1}^{\infty} \alpha^n \mathcal{K}_n(t) \]

The \( n \)-th-order contribution:

\[ \mathcal{K}_n(t) = \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-2}} dt_{n-1} \times \langle \mathcal{L}(t) \mathcal{L}(t_1) \mathcal{L}(t_2) \ldots \mathcal{L}(t_{n-1}) \rangle_{oc} \]

Ordered cumulants (partially time-ordered):

\[ \langle \mathcal{L}(t) \mathcal{L}(t_1) \mathcal{L}(t_2) \ldots \mathcal{L}(t_{n-1}) \rangle_{oc} \equiv \sum (-1)^q \mathcal{P} \mathcal{L}(t) \ldots \mathcal{L}(t_i) \mathcal{P} \mathcal{L}(t_j) \ldots \mathcal{L}(t_k) \mathcal{P} \ldots \mathcal{P} \]

Example:

\[ \mathcal{K}_2(t) = \int_0^t dt_1 \mathcal{P} \mathcal{L}(t) \mathcal{L}(t_1) \mathcal{P} \]
Damped Jaynes-Cummings Model

\[ H_S + H_E = \omega_0 \sigma_+ \sigma_- + \sum_k \omega_k b\dagger_k b_k \]

\[ H_I = \sum_k g_k \sigma_+ b_k + g_k^* \sigma_- b\dagger_k \]

Spectral density: \[ J(\omega) = \frac{1}{2\pi} \frac{\gamma_0 \lambda^2}{(\omega_0 - \Delta - \omega)^2 + \lambda^2} \]

Expansion: \[ \alpha = \frac{\tau_E}{\tau_S} = \frac{\gamma_0}{\lambda} \]
Exact TCL master equation:

$$\frac{d}{dt}\rho_S(t) = -\frac{i}{2}S(t)[\sigma_+\sigma_-, \rho_S(t)]$$

$$+ \gamma(t) \left[ \sigma_-\rho_S(t)\sigma_+ - \frac{1}{2} \{\sigma_+\sigma_-, \rho_S(t)\} \right]$$

⇒ Generator not in Lindblad form:

- Coefficients are time-dependent
- $\Phi_t = \text{completely positive map, but no semigroup}$!
- Decay rate $\gamma(t)$ takes negative values
Applications

- Quantum Brownian motion, spin-boson systems
- Atom laser (slow algebraic decay of correlations)
- QED: Non-Ohmic spectral densities, strong memory effects
- Spin star
Highly Non-Markovian Behavior

Interaction with finite reservoir:

\[
\begin{align*}
H &= H_S + H_E + V \\
V &= \lambda \sum_{n_1, n_2} c(n_1, n_2) \sigma_+ |n_1\rangle\langle n_2| + \text{h.c.} \\
\langle c(n_1, n_2)c^*(n_1', n_2') \rangle &= \delta_{n_1, n_1'} \delta_{n_2, n_2'}
\end{align*}
\]

Highly Non-Markovian Behavior

Standard master equation in Born-Markov approximation:

$$\frac{d}{dt} \rho_S(t) = \gamma_2 \left[ \sigma - \rho_S(t) \sigma + - \frac{1}{2} \{ \sigma + \sigma -, \rho_S(t) \} \right]$$

Markovian relaxation rate:

$$\gamma_2 = \frac{2\pi \chi^2 N_2}{\delta \varepsilon} \quad \Rightarrow \quad \frac{\gamma_2}{\delta \varepsilon} \sim 10^{-3}$$
Failure of the Born-Markov Approximation

2-point correlation:

\[ f_2(t, t_1) = \text{tr}_E\{B(t)B^\dagger(t_1)\rho_E\} \approx \gamma_2 h(t - t_1) \]

\[ B(t) = \lambda \sum_{n_1, n_2} c(n_1, n_2)e^{-i\omega(n_1, n_2)t}|n_1\rangle\langle n_2| \]

band width = \(\delta\varepsilon\) \(\Rightarrow\) \(\tau_E = \delta\varepsilon^{-1}\)

\(\Rightarrow\) Markov property seems to be satisfied if:

\[ \gamma_2 \ll \delta\varepsilon \]

Conclusion: Highly non-Markovian behavior although standard Markov condition is fulfilled

\(\Rightarrow\) Investigate higher order correlations!
Failure of the Born-Markov Approximation

4-point correlation:

\[ f_4(t, t_1, t_2, t_3) = \text{tr}_E\{B(t)B^\dagger(t_1)B(t_2)B^\dagger(t_3)\rho_E\} \]
\[ \approx \gamma_2^2 h(t - t_1)h(t_2 - t_3) + \gamma_1 \gamma_2 h(t - t_3)h(t_1 - t_2) \]

TCL master equation to fourth order:

\[ \frac{d}{dt}\rho_S(t) = \Gamma(t) \left[ \sigma - \rho_S\sigma + \frac{1}{2}\{\sigma+\sigma-, \rho_S\} \right] \]
\[ + \tilde{\Gamma}(t) \left[ \sigma+\sigma - \rho_S\sigma+\sigma - \frac{1}{2}\{\sigma+\sigma-, \rho_S\} \right] \]

Time-dependent relaxation rates:

\[ \Gamma(t) = \gamma_2(1 - \gamma_1 t) \]
\[ \tilde{\Gamma}(t) = \gamma_1 \gamma_2 t \]
\[ \gamma_{1,2} = \frac{2\pi \lambda^2 N_{1,2}}{\delta\varepsilon} \]

\[ \implies \text{4th order small if: } \gamma_1 t \ll 1 \]
Failure of the Born-Markov Approximation

Coherences:
\[
\rho_{01}(t) = \rho_{01}(0) \exp[-\gamma_2 t / 2]
\]

Populations:
\[
\rho_{11}(t) = \rho_{11}(0) \exp[-\gamma_2 t + \gamma_1 \gamma_2 t^2 / 2]
\]

- Short-time behavior correctly reproduced
- Breakdown of description for long times
- TCL expansion cannot be truncated at any finite order
- No uniform convergence
- Non-perturbative approach necessary
Correlated Projection Superoperators

How do we treat such highly non-Markovian behavior?

\[ \text{total state } \rho(t) \implies \text{relevant part } \mathcal{P}\rho(t) \]

General requirements:

\[ \mathcal{P}^2 = \mathcal{P} \]
\[ \rho_S \equiv \text{tr}_E \rho = \text{tr}_E \{ \mathcal{P} \rho \} \]

General ansatz:

\[ \mathcal{P} \rho = \sum_i \text{tr}_E \{ A_i \rho \} \otimes B_i \]

With arbitrary environmental operators \( A_i, B_i \) satisfying:

\[ \text{tr}_E \{ A_j B_i \} = \delta_{ij} \]
\[ \sum_i A_i \text{tr}_E B_i = I_E \]
Correlated Projection Superoperators

Example 1:

\[ A = I_E \quad B = \rho_E \]

\[ \implies P\rho = \text{tr}_E \{\rho\} \otimes \rho_E \quad \text{standard projection} \]

Example 2:

\[ A_i = B_i = \frac{1}{\sqrt{N_i}} \Pi_i \quad \{\Pi_i\} = \text{orthogonal projections} \]

\[ \implies P\rho = \sum_i \text{tr}_E \{\Pi_i \rho\} \otimes \frac{1}{N_i} \Pi_i \quad \text{new projection} \]

- Description of initial correlations
- Projections onto separable (classically correlated) or nonseparable (entangled) quantum states
- Non-perturbative
Correlated Projection Superoperators

Example: Interaction with finite reservoir

Use new TCL projection:

$$\mathcal{P} \rho = \text{tr}_E \{ \Pi_1 \rho \} \otimes \frac{1}{N_1} \Pi_1 + \text{tr}_E \{ \Pi_2 \rho \} \otimes \frac{1}{N_2} \Pi_2$$

Two density matrices:

$$\rho_S^{(1)} = \text{tr}_E \{ \Pi_1 \rho \} \quad \rho_S^{(2)} = \text{tr}_E \{ \Pi_2 \rho \}$$

$$\implies \rho_S = \rho_S^{(1)} + \rho_S^{(2)}$$

Coupled system of equations of motion:

$$\frac{d}{dt} \rho_S^{(1)} = \gamma_1 \sigma + \rho_S^{(2)} \sigma - \frac{\gamma_2}{2} \{ \sigma + \sigma, \rho_S^{(1)} \}$$

$$\frac{d}{dt} \rho_S^{(2)} = \gamma_2 \sigma - \rho_S^{(1)} \sigma + \frac{\gamma_1}{2} \{ \sigma - \sigma, \rho_S^{(2)} \}$$
Correlated Projection Superoperators

\[ \frac{\gamma_{1,2}}{\delta \varepsilon} \sim 1 \]

Dynamics of populations:

\[ \frac{d}{dt} \rho_{11}(t) = - (\gamma_1 + \gamma_2) \rho_{11}(t) + \gamma_1 \rho_{11}(0) \]

- No semigroup, but positive dynamical map!
- Highly non-Markovian: System never forgets its initial data!
Correlated Projection Superoperators

Non-perturbative aspect: Different projection operators generate solutions that differ in all orders of the coupling:

- Standard projection, 4th order:

\[ \rho_{11}(t) = \rho_{11}(0) \exp[-\gamma_2 t + \gamma_1 \gamma_2 t^2 / 2] \]

- New projection, 4th order:

\[ \rho_{11}(t) = \rho_{11}(0) \left[ \frac{\gamma_1}{\gamma_1 + \gamma_2} + \frac{\gamma_2}{\gamma_1 + \gamma_2} e^{-\Gamma t} \right] \]

\[ \Gamma = (\gamma_1 + \gamma_2) \left[ 1 + \frac{\gamma_1 + \gamma_2}{2 \delta \varepsilon} \right] \]
Conclusions

- Non-Markovian dynamics and projection superoperators
- Standard approach can fail although usual Markov condition is satisfied $\implies$ Higher-order correlations
- Correlated projection superoperators:
  \[
P \rho = \sum_i \text{tr}_E \{A_i \rho\} \otimes B_i
  \]
  - Choose an appropriate set $\{A_i, B_i\}$
  - Carry out expansion and investigate higher orders
  - Different $P$’s lead to solutions that differ in all orders
- Theory of entanglement and non-Markovian dynamics:
  Dynamical significance of classically correlated and nonseparable states
References

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Exact Monte-Carlo Technique:


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