Open Quantum Systems

Light matter interaction

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Introduction and general description

<u>Motivation</u>:

- Describe a more realistic dynamics of a quantum system in contact with its environment
- Importance: quantum technologies, quantum optics, condensed matter physics, quantum information, quantum biology, among others.
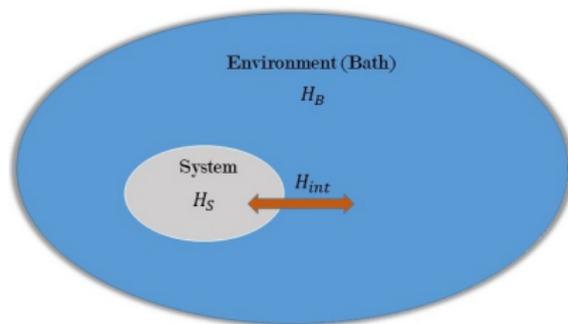

Figure: Schematic representation of an open quantum system

General formalism

Total System Dynamics

$$\hat{\rho}_{\mathcal{S}}\left(t\right) = Tr_{\mathcal{E}}\left\{\hat{U}\left(t\right)\hat{\rho}_{\mathcal{SE}}\left(0\right)\hat{U}^{\dagger}\left(t\right)\right\}$$

$\hat{\rho}_{\mathcal{S}}\left(t\right)$ represents the reduced density matrix of the system of interest

$\hat{U}\left(t\right)$ denotes the time–evolution operator for the composite system

$\hat{\rho}_{\mathcal{SE}}\left(t\right)$ denotes the composite system density operator

Note: this task is very difficult, if not impossible, to carry out in practice for most reasonably complex model systems

Alternative: master equation formalism

General master equation formalism

General master equation of open quantum systems ($\hbar = 1$)

$$\partial_t \hat{\rho}_{\mathcal{S}}(t) = \hat{\mathcal{L}}[\hat{\rho}_{\mathcal{S}}(t)] = \underbrace{-i[H_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)]}_{\text{unitary evolution}} + \underbrace{\hat{\mathcal{D}}[\hat{\rho}_{\mathcal{S}}(t)]}_{\text{decoherence}}$$

$\hat{\mathcal{L}}$ has been decomposed into two parts:

- a unitary part
- nonunitary part that represents decoherence (and possibly also dissipation)

The Born-Markov master equation

It is based in on two core approximations:

- The Born approximation. The system–environment coupling is sufficiently weak and the environment is reasonably large

$$\hat{\rho}(t) \approx \hat{\rho}_{\mathcal{S}}(t) \otimes \hat{\rho}_{\mathcal{E}}$$

- The Markov approximation. Memory effects of the environment are negligible

- The coupling to the environment is described by the interaction Hamiltonian H_{int}

$$H_{int} = \sum_{\alpha} \hat{S}_{\alpha} \otimes \hat{E}_{\alpha}$$

The Born-Markov master equation

The evolution of the reduced density operator $\hat{\rho}_{\mathcal{S}}(t)$ is given by

General Born-Markov master equation

$$\partial_t \hat{\rho}_{\mathcal{S}}(t) = -\imath \left[H_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t) \right] - \sum_\alpha \left[\hat{S}_\alpha, \hat{B}_\alpha \hat{\rho}_{\mathcal{S}}(t) \right] - \sum_\alpha \left[\hat{\rho}_{\mathcal{S}}(t) \hat{C}_\alpha, \hat{S}_\alpha \right]$$

System operators

$$\hat{B}_\alpha = \int_0^\infty d\tau \, \sum_\beta \mathcal{C}_{\alpha\beta}(\tau) \, \hat{S}_\beta(-\tau)$$

$$\hat{C}_\alpha = \int_0^\infty d\tau \, \sum_\beta \mathcal{C}_{\beta\alpha}(-\tau) \, \hat{S}_\beta(-\tau)$$

$\mathcal{C}_{\alpha\beta}(\tau)$ are the environment self–correlation functions $\Rightarrow \mathcal{C}_{\alpha\beta}(\tau) = \left\langle \hat{E}_\alpha(\tau) \hat{E}_\beta \right\rangle_{\hat{\rho}_{\mathcal{E}}}$

Derivation of the master equation for a harmonic oscillator

The system of interest will be a harmonic oscillator (Caldeira-Leggett model)

Total system Hamiltonian

$$H = H_{\mathcal{S}} + H_{\mathcal{E}} + H_{int}$$

$$H_{\mathcal{S}} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\Omega^2\hat{x}^2$$

$$H_{\mathcal{E}} = \sum_i \left(\frac{\hat{p}_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2\hat{q}_i^2 \right)$$

$$H_{int} = \hat{x} \otimes \sum_i c_i\,\hat{q}_i = \hat{x} \otimes \hat{E}$$

$H_{\mathcal{S}}$ is the self–Hamiltonian of the system

$H_{\mathcal{E}}$ is the self–Hamiltonian of the environment

H_{int} is the interaction Hamiltonian
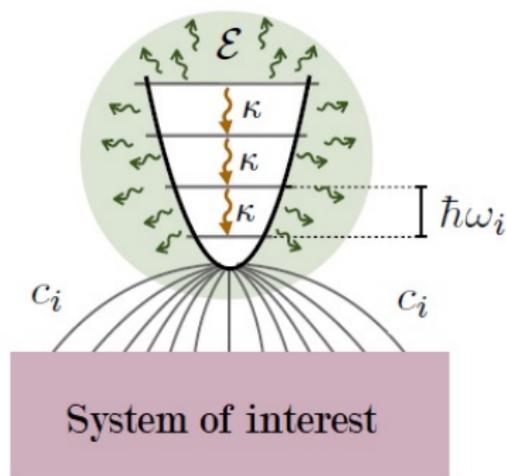
Illustrative representation

Figure: Caldeira-Leggett model. The system of interest interacting with a set of quantum oscillators.

Environment self–correlation functions

Since H_{int} contains a single term, only one such function will need to be computed

Evaluation

$$\mathcal{C}(\tau) = \left\langle \hat{E}(\tau)\hat{E} \right\rangle_{\hat{\rho}_{\mathcal{E}}} = \sum_{i,j} c_i c_j \left\langle \hat{q}_i(\tau)\hat{q}_j \right\rangle_{\hat{\rho}_{\mathcal{E}}}$$

For $i \neq j$ (oscillators do not interact with each other)

$$\left\langle \hat{q}_i(\tau)\hat{q}_j \right\rangle_{\hat{\rho}_{\mathcal{E}}} = \left\langle \hat{q}_i(\tau) \right\rangle_{\hat{\rho}_{\mathcal{E}}} \left\langle \hat{q}_j \right\rangle_{\hat{\rho}_{\mathcal{E}}} = 0$$

For $i = j$

$$\mathcal{C}(\tau) = \sum_i c_i^2 \left\langle \hat{q}_i(\tau)\hat{q}_i \right\rangle_{\hat{\rho}_{\mathcal{E}}}$$

Environment self–correlation functions

Time evolution of the operator $\hat{q}_i$ in the interaction picture ($\hbar = 1$)

$$\hat{q}_i\left(\tau\right) = \sqrt{\frac{1}{2m_i\omega_i}}\left(\hat{a}_i e^{-\imath\omega_i\tau} + \hat{a}_i^\dagger e^{\imath\omega_i\tau}\right)$$

which leads to

$$\langle\hat{q}_i\left(\tau\right)\hat{q}_i\rangle_{\hat{\rho}_\varepsilon} = \frac{1}{2m_i\omega_i}\left\{\left\langle\hat{a}_i\hat{a}_i^\dagger\right\rangle e^{-\imath\omega_i\tau} + \left\langle\hat{a}_i^\dagger\hat{a}_i\right\rangle e^{\imath\omega_i\tau}\right\}, \ N_i = \left\langle\hat{a}_i^\dagger\hat{a}_i\right\rangle$$

Environment in thermal equilibrium

$$N_i \equiv N_i\left(T\right) = \frac{1}{e^{\omega_i/k_B T} - 1}$$

Environment self–correlation functions

Using $\left[\hat{a}_i, \hat{a}_i^\dagger\right] = 1$

$$\langle \hat{q}_i (\tau) \hat{q}_i \rangle_{\hat{\rho}_\varepsilon} = \frac{1}{2m_i\omega_i} \left\{ coth\left(\frac{\omega_i}{2k_B T}\right) cos(\omega_i\tau) - \imath\, sin(\omega_i\tau) \right\}$$

Decomposition $\mathcal{C}(\tau) = \nu(\tau) - \imath\,\eta(\tau)$

$$\nu(\tau) = \sum_i \frac{c_i^2}{2m_i\omega_i} coth\left(\frac{\omega_i}{2k_B T}\right) cos(\omega_i\tau) \equiv \int_0^\infty d\omega\, J(\omega) coth\left(\frac{\omega}{2k_B T}\right) cos(\omega\tau)$$

and

$$\eta(\tau) = \sum_i \frac{c_i^2}{2m_i\omega_i} sin(\omega_i\tau) \equiv \int_0^\infty d\omega\, J(\omega) sin(\omega\tau)$$

Environment self–correlation functions

with

$$J(\omega) = \sum_i \frac{c_i^2}{2m_i\omega_i} \delta(\omega - \omega_i)$$

It is called the spectral density of the environment

Spectral densities encapsulate the physical properties of the environment

In modeling the environment, we often goes to a continuum limit

Master equation

The general expression for the Born–Markov master equation

$$\partial_t \hat{\rho}_{\mathcal{S}}(t) = -\imath \left[H_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t) \right] - \int_0^\infty d\tau \left\{ \nu(\tau) \left[\hat{x}, \left[\hat{x}(-\tau), \hat{\rho}_{\mathcal{S}}(t) \right] \right] \right.$$
$$\left. -\imath \eta(\tau) \left[\hat{x}, \left\{ \hat{x}(-\tau), \hat{\rho}_{\mathcal{S}}(t) \right\} \right] \right\}$$

The explicit form of the interaction-picture position operator

$$\hat{x}(\tau) = \hat{x} \cos(\Omega \tau) + \frac{\hat{p}}{m\Omega} \sin(\Omega \tau)$$

Final form

$$\partial_t \hat{\rho}_{\mathcal{S}}(t) = -\imath \left[H_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t) \right] - \imath \gamma \left[\hat{x}, \left\{ \hat{p}, \hat{\rho}_{\mathcal{S}}(t) \right\} \right] - D \left[\hat{x}, \left[\hat{x}, \hat{\rho}_{\mathcal{S}}(t) \right] \right]$$

Master equation

Coefficients

$$\gamma \equiv \frac{1}{M\Omega} \int_0^\infty d\tau \, \eta(\tau) \, sin(\Omega\tau)$$

$$D \equiv \int_0^\infty d\tau \, \nu(\tau) \, cos(\Omega\tau)$$

<u>Note</u>: to evaluate the coefficients we must choose a specific functional form for the spectral density appearing in the expressions for $\nu(\tau)$ and $\eta(\tau)$

Spectral density

- Usually, the frequency dependence of $J(\omega)$ is taken to follow a power-law dependence of the form $J(\omega) \propto \omega^{\alpha}$
- We usually choose a high-frequency cutoff Λ to include a term that damps $J(\omega)$ for frequencies $\omega > \Lambda$

Lorentz–Drude form for $J(\omega)$

$$J(\omega) = \frac{2m\gamma_0}{\pi} \omega \frac{\Lambda^2}{\Lambda^2 + \omega^2}$$

Coefficients of the master equation

$$\gamma = \gamma_0 \text{ and } D = 2m\gamma_0 k_B T, \text{ for } \Omega \ll k_B T$$

Physical interpretation

Master equation

$$\partial_t \hat{\rho}_{\mathcal{S}}(t) = -\imath \left[H_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t) \right] - \imath \gamma \left[\hat{x}, \{ \hat{p}, \hat{\rho}_{\mathcal{S}}(t) \} \right] - D \left[\hat{x}, \left[\hat{x}, \hat{\rho}_{\mathcal{S}}(t) \right] \right]$$

First commutator

$$-\imath \left[H_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t) \right]$$

It describes the reversible unitary dynamics of the harmonic oscillator

Second commutator

$$-\imath \gamma \left[\hat{x}, \{ \hat{p}, \hat{\rho}_{\mathcal{S}}(t) \} \right]$$

It describes momentum damping due to the interaction with the environment since

$$\langle \hat{p} \rangle_t \propto e^{-2\gamma t} \langle \hat{p} \rangle_0$$

Physical interpretation

Third commutator

$$-D\left[\hat{x},\left[\hat{x},\hat{\rho}_{\mathcal{S}}\left(t\right)\right]\right]$$

It describes diffusion in momentum

$$\left\langle\hat{p}^2\right\rangle_t \propto Dt$$

Such influences in the central system brings loss of coherence

Purity

Change in purity $\varsigma = Tr \, \hat{\rho}_{\mathcal{S}}^2$

$$\partial_t \varsigma \left(t \right) = -4D \left[\left\langle \hat{x}^2 \right\rangle_t - \left\langle \hat{x} \right\rangle_t^2 \right] = -4D\Delta x^2 \left(t \right)$$

$\Delta x^2 \left(t \right)$ is the dispersion in position space

The instantaneous decrease in purity, and thus the amount of decoherence, is minimized if this spatial dispersion is minimized

Coherent states are selected by the interaction with the environment and represent the pointer states

Dynamics of Gaussian packets: decoherence

Alternative form of the master equation (Wigner representation)

$$\partial_t W(x, p, t) = \left[-\frac{p}{m}\partial_x + \gamma\partial_p p + D\partial_p^2 \right] W(x, p, t)$$

which is recognized as the Fokker-Planck equation

Initial wave function of the system (coherent superposition)

$$\Psi(x, 0) = \Psi_1(x) + \Psi_2(x)$$

$$\Psi(x, 0) = N \exp\left[-\frac{(x - x_0)^2}{2\delta^2} \right] \exp(\imath p_0 x) + N \exp\left[-\frac{(x + x_0)^2}{2\delta^2} \right] \exp(-\imath p_0 x)$$

Dynamics of Gaussian packets: decoherence

The Wigner function corresponding to the initial state $\Psi(x, 0)$

$$W_{1,2}(x, p, 0) = N^2 \delta^2 exp\left[-\frac{(x \mp x_0)^2}{\delta^2} - \delta^2 (p \mp p_0)^2\right]$$

$$W_{int}(x, p, 0) = 2N^2 \delta^2 exp\left[-\frac{x^2}{\delta^2} - \delta^2 p^2\right] cos[2x_0 p + 2p_0 x]$$
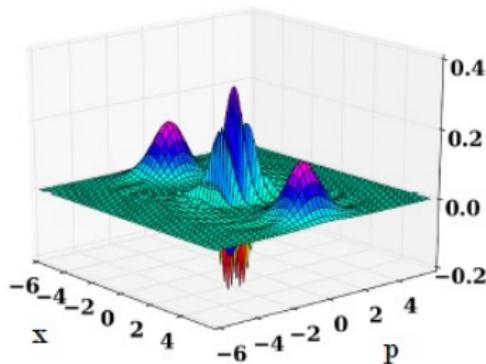

Figure: Superposition of two Gaussian wave packets in the Wigner picture at time $t = 0$

Dynamics of Gaussian packets: decoherence

The resulting time-evolved Wigner function

$$W_{1,2}(x, p, t) = N^2 \delta^2 \frac{\delta_2}{\delta_1} exp\left[-\frac{(x \mp x_c)^2}{\delta_1^2} \right] exp\left[-\delta_2^2 (p \mp p_c - \beta(x \mp x_c))^2 \right]$$

$$W_{int}(x, p, t) = 2N^2 \delta^2 \frac{\delta_2}{\delta_1} exp(-A_{int}) exp\left[-\frac{x^2}{\delta_1^2} - \delta_2^2 (p - \beta x)^2 \right] \times$$

$$\times cos\left[2\kappa_p p + 2(\kappa_x - \beta\kappa_p) x \right]$$

The coefficients δ_1, δ_2, x_c, p_c, β, A_{int}, κ_x and κ_p are in general time-dependent

The term $exp(-A_{int})$ describes the damping of the oscillations

Dynamics of Gaussian packets: decoherence

Dynamics associated with the loss of coherence:

Equation of motion for A_{int}

$$\partial_t A_{int} = 4D\kappa_p^2$$

The diffusion coefficient D is connected with the suppression of the interference terms

Conclusion

- Open quantum systems allow the description of a more realistic quantum dynamics

- The environment influence on the dynamics of a quantum system can be computed through a master equation

- The interplay between dissipation x decoherence may perturb the intrinsic dynamics of your central system

- The interaction with the environment selects pointer states

- Superposition states experiences decoherence through the diffusion process, which tends to suppress the interference terms