# Chemfarm for collective quantum optics
# Tutorial 2: Master equation and Quantum Jumps

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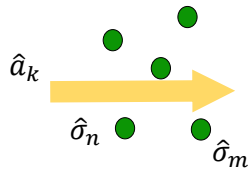
# Outline for today

- Physics: Master equation and Quantum Trajectory methods
  Lecture YouTube Continuos measurement and Quantum Trajectory
- Implementation
- Parallelization using Chemfarm

# Model: atoms + photon modes

$$H = H_A + H_P + H_{AP}$$




"atoms": two-level emitters $n = 1, \dots, N$ at positions $\mathbf{r}_n$

$$H_A = \hbar\omega_a \sum_{n=1}^{N} \hat{\sigma}_n^\dagger \hat{\sigma}_n \qquad \hat{\sigma}_n = |g\rangle_n\langle e| \qquad = \quad \omega_a \;\; \begin{matrix} \text{——} \; |e\rangle \\ \text{——} \; |g\rangle \end{matrix}$$

"photons" = continuum of photon modes $\hat{a}_k$ (modes defined by geometry) $\{k\}$ = mode index

$$H_P = \sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k$$

"atom-photon": dipole interaction (+rotating wave approx.)

$$H_{AP} = -\sum_n \hat{E}(\mathbf{r}_n)\hat{\sigma}_n^\dagger d + h.c. \qquad \hat{E}(\mathbf{r}_n) = -i\sum_k \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0}}\, u_k(\mathbf{r}_n)\hat{a}_k$$

mode profile

# Heisenberg-Langevin approach

[see Lehmberg PRA 2, 883 (1970) for a full derivation]

$$H = \hbar\omega_a \sum_{n=1}^{N} \hat{\sigma}_n^\dagger \hat{\sigma}_n + \sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k - \sum_n \left[\hat{E}(\mathbf{r}_n)\hat{\sigma}_n^\dagger d + h.c.\right]$$

$$\hat{E}(\mathbf{r}_n) = -i \sum_k \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0}} u_k(\mathbf{r}_n)\hat{a}_k$$

$$\hat{\sigma}_n = |g\rangle_n\langle e|$$

Heisenberg Eq. for atom n:

$$\partial_t \hat{\sigma}_n = \frac{i}{\hbar}[H, \hat{\sigma}_n]$$

Use: $[\hat{\sigma}_n^\dagger, \hat{\sigma}_n] = \hat{\sigma}_n^z$ $\quad \hat{\sigma}_n^z = |e\rangle_n\langle e| - |g\rangle_n\langle g|$

$$\partial_t \hat{\sigma}_n = -i\omega_a \hat{\sigma}_n - i\frac{d}{\hbar}\hat{\sigma}_n^z \hat{E}(\mathbf{r}_n)$$

Now wish to find Eq. for field $\hat{E}(\mathbf{r}_n)$ and insert it into the above

# Heisenberg Eq. for field = Maxwell's Eqs. (=Hamilton's Eq. for field...)

$$\nabla \times \hat{E}(r,t) = -\partial_t \hat{B}(r,t) \qquad \nabla \times \hat{B}(r,t) = \frac{1}{c^2}\partial_t \left[\hat{E}(r,t) + \frac{1}{\varepsilon_0}\hat{P}(r,t)\right]$$

Polarization density
= dipoles (of atoms) per volume

$$\hat{P}(\mathbf{r},t) = \sum_n \hat{d}_n(t)\delta(\mathbf{r}-\mathbf{r}_n)$$

$$\hat{d}_n = d\hat{\sigma}_n + \text{h.c.}$$

Freq. domain $\partial_t \to -i\,\omega$

$$\nabla \times \hat{E}(r,\omega) = i\,\omega \hat{B}(r,\omega) \qquad \nabla \times \hat{B}(r,\omega) = -i\frac{\omega}{c^2}\left[\hat{E}(r,\omega) + \frac{1}{\varepsilon_0}\hat{P}(r,\omega)\right]$$

Derive wave equation:

$$\nabla \times \nabla \times \hat{E} = i\,\omega \nabla \times \hat{B} = \frac{\omega^2}{c^2}\left[\hat{E} + \frac{1}{\varepsilon_0}\hat{P}\right]$$

$$\nabla \times \nabla \times \hat{E}(\mathbf{r},\omega) - \frac{\omega^2}{c^2}\hat{E}(\mathbf{r},\omega) = \frac{\omega^2}{c^2}\frac{1}{\varepsilon_0}\hat{P}(\mathbf{r},\omega) = \frac{\omega^2}{c^2}\frac{1}{\varepsilon_0}\sum_n \delta(\mathbf{r}-\mathbf{r}_n)d\hat{\sigma}_n(\omega)$$

# Heisenberg Eq. for field: formal solution (1)

$$\underbrace{\nabla \times \nabla \times \hat{E}(\mathbf{r},\omega) - \frac{\omega^2}{c^2}\hat{E}(\mathbf{r},\omega)}_{\text{Linear operator (\sim "Helmholtz" Eq. for the field)}} = \underbrace{\frac{\omega^2}{c^2}\frac{1}{\varepsilon_0}\sum_n \delta(\mathbf{r}-\mathbf{r}_n)d\hat{\sigma}_n(\omega)}_{\text{point sources ("dipoles") @ atom positions}}$$

→ Solution to point source (=dipole) @ $\mathbf{r}_n$ – Green's function: $G(\mathbf{r}-\mathbf{r}_n)$

$$\hat{E}(\mathbf{r},\omega) = \hat{E}_0(\mathbf{r},\omega) + \underbrace{\frac{\omega^2}{c^2}\frac{d}{\varepsilon_0}\sum_n G(\mathbf{r}-\mathbf{r}_n,\omega)\hat{\sigma}_n(\omega)}_{\text{Field from all "dipole" sources (=radiating atoms)}}$$

Total field

"Source free" solution
= "free" field (in the absence of atoms)
= vacuum fluctuations + incident laser

field propagator = Green's function $G(\mathbf{r}_1,\mathbf{r}_2) = \mathbf{e}_d{}^{\dagger}\cdot\overline{\overline{\boldsymbol{G}}}(\mathbf{r}_1,\mathbf{r}_2)\cdot\mathbf{e}_d$

$$\mathbf{e}_i{}^{\dagger}\cdot\overline{\overline{\boldsymbol{G}}}(\mathbf{r}_1,\mathbf{r}_2)\cdot\mathbf{e}_j = G_{ij}(k,\mathbf{r}_1,\mathbf{r}_2) = \frac{e^{ikr}}{4\pi r}\left[\left(1+\frac{ikr-1}{k^2r^2}\right)\delta_{ij} + \left(-1+\frac{3-3ikr}{k^2r^2}\right)\frac{r^i r^j}{r^2}\right]$$

with $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, $r = |\mathbf{r}|$ and $r^i = \mathbf{e}_i \cdot \mathbf{r}$.

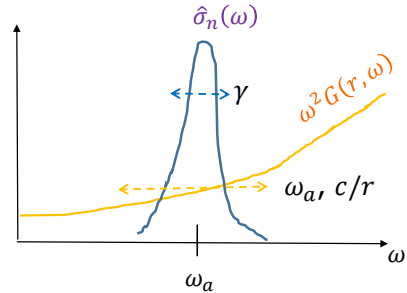
$k = \omega/c$

# Heisenberg Eq. for field: formal solution (2)

$$\hat{E}(\mathbf{r},\omega) = \hat{E}_0(\mathbf{r},\omega) + \frac{\omega^2}{c^2}\frac{d}{\varepsilon_0}\sum_n \hat{\sigma}_n(\omega) G(\mathbf{r}-\mathbf{r}_n,\omega)$$

Back to time-domain – perform IFT:

$$\hat{E}(\mathbf{r},t) = \hat{E}_0(\mathbf{r},t) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_n \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t}\hat{\sigma}_n(\omega)\ \omega^2 G(\mathbf{r}-\mathbf{r}_n,\omega)$$




- Dominant "free" dynamics: oscillations at $\omega_a$
- Slow dynamics due to radiation ~ decay/shift $\gamma$

Wide function around $\omega_a$
Width ~ $\omega_a,\ c/r$

Markov approximation: $\omega_a,\ c/r \gg \gamma$

$$\hat{E}(\mathbf{r},t) \approx \hat{E}_0(\mathbf{r},t) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_n {\omega_a}^2 G(\mathbf{r}-\mathbf{r}_n,\omega_a)\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t}\hat{\sigma}_n(\omega)$$

$$= \hat{E}_0(\mathbf{r},t) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_n {\omega_a}^2 G(\mathbf{r}-\mathbf{r}_n,\omega_a)\hat{\sigma}_n(t)$$

# Heisenberg-Langevin Eq. for atoms (1)

$$\partial_t \hat{\sigma}_n = -i\omega_a \hat{\sigma}_n - i\frac{d}{\hbar}\hat{\sigma}_n^z \hat{E}(\mathbf{r}_n)$$

We got for field: $\hat{E}(\mathbf{r}) = \hat{E}_0(\mathbf{r}) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_n {\omega_a}^2 G(\mathbf{r}-\mathbf{r}_n,\omega_a)\hat{\sigma}_n$

→ Field "felt" by **atom** $n$, $\mathbf{r} = \mathbf{r}_n$ :

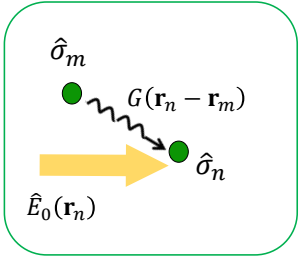
$$\hat{E}(\mathbf{r}_n) = \hat{E}_0(\mathbf{r}_n) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_m {\omega_a}^2 G(\mathbf{r}_n-\mathbf{r}_m)\hat{\sigma}_m$$

= "free" field (in the absence of atoms)
= vacuum fluctuations + incident laser

$$\hat{E}_0(\mathbf{r}_n) = -i\sum_k \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0}} u_k(\mathbf{r}_n)\hat{a}_k(0)e^{-i\omega_k t}$$

Field from all "dipole" sources (=radiating atoms)

field propagator = $G(\mathbf{r}_n - \mathbf{r}_m)$



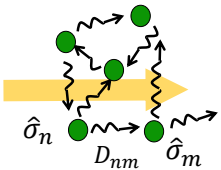
# Heisenberg-Langevin Eq. for atoms (2)

$$\partial_t \hat{\sigma}_n = -i\omega_a \hat{\sigma}_n - i\hat{\sigma}_n^z \frac{d}{\hbar}\left[\hat{E}_0(\mathbf{r}_n) + \frac{{\omega_a}^2}{c^2}\frac{d}{\varepsilon_0}\sum_m G(\mathbf{r}_n - \mathbf{r}_m)\hat{\sigma}_m\right]$$

$$D_{nm} = -i\frac{3}{2}\gamma\lambda G(\mathbf{r}_n - \mathbf{r}_m) \qquad \gamma = \frac{{d^2\omega_a}^3}{3\pi\varepsilon_0\hbar c^3}$$

$$\lambda = 2\pi c/\omega_a$$

$$\partial_t \hat{\sigma}_n = -i\omega_a \hat{\sigma}_n + \hat{\sigma}_n^z\left[\hat{F}_n + \sum_m D_{nm}\,\hat{\sigma}_m\right]$$




**→ Collective response**

(= multiple scattering
= dipole-dipole)

quantum noise (vacuum) + incident laser

$$\hat{F}_n = -i\frac{d}{\hbar}\hat{E}_0(\mathbf{r}_n) = -d\sum_k \sqrt{\frac{\omega_k}{2\varepsilon_0\hbar}}u_k(\mathbf{r}_n)\hat{a}_k(0)e^{-i\omega_k t}$$

**Dipole-dipole coupling** (with all atomic dipoles)

$$D_{nm} = \gamma_{nm}/2 + i\Delta_{nm}$$

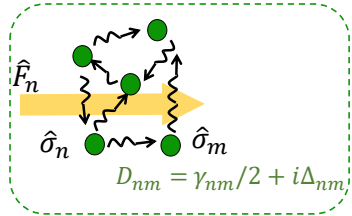
dipole-dipole kernel
(photon Green's function)

$$\partial_t \hat{\sigma}_n = -\left(i\omega_a + \frac{\gamma}{2}\right)\hat{\sigma}_n + \hat{\sigma}_n^z\left[\hat{F}_n + \sum_{m\neq n} D_{nm}\,\hat{\sigma}_m\right]$$

$$\mathrm{Re}\; D_{nn} = \gamma/2$$

$$\mathrm{Im}\; D_{nn} + \omega_a \rightarrow \omega_a$$

# Many-body physics of quantum emitters (atoms)




Heisenberg-Langevin Eq. for atoms:

$$\partial_t \hat{\sigma}_n = \frac{i}{\hbar}[H_{\text{eff}}, \hat{\sigma}_n] + \hat{\sigma}_n^z \hat{F}_n$$

Effective Hamiltonian (non-Hermitian): **collectivity**

$$H_{\text{eff}} = \hbar\left(\omega_a - i\frac{\gamma}{2}\right)\sum_{n=1}^{N}\hat{\sigma}_n^\dagger\hat{\sigma}_n + \hbar\sum_{n=1}^{N}\sum_{m\neq n}\left(\Delta_{nm} - i\frac{\gamma_{nm}}{2}\right)\hat{\sigma}_n^\dagger\hat{\sigma}_m$$

Quantum noise
(has to exist due to dissipation)

$$\hat{F}_n = -d\sum_k \sqrt{\frac{\omega_k}{2\varepsilon_0\hbar}}\, u_k(\mathbf{r}_n)\hat{a}_k(0)e^{-i\omega_k t}$$

**Dipole-dipole interaction**
(reversible excitation exchange)

**Collective radiation**
(dissipation)

Equivalent description: quantum master equation $\partial_t\hat{\rho} = -\frac{i}{\hbar}\left(H_{\text{eff}}\hat{\rho} - \hat{\rho}H_{\text{eff}}^\dagger\right) + \sum_{n,m}\gamma_{nm}\hat{\sigma}_n\hat{\rho}\hat{\sigma}_m^\dagger$

Output light $\hat{E}(\mathbf{r}) = \hat{E}_0(\mathbf{r}) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_n \omega_a{}^2 G(\mathbf{r}-\mathbf{r}_n,\omega_a)\hat{\sigma}_n$

Quantum noise: "jump term"

# Zoo of Quantum Master equations for superradiance

$$\frac{\partial \rho}{\partial t} = -i(H_{\text{eff}}\rho - \rho H_{\text{eff}}^{\dagger}) + \sum_{n,m=1}^{N} \gamma_{nm}\sigma_n \rho \sigma_m^{\dagger} \tag{1a}$$

$$H_{\text{eff}} = \sum_{n} (\Omega_n^{*}\sigma_n + \Omega_n \sigma_n^{\dagger}) + \sum_{n,m=1}^{N} \left(\Delta_{nm} - i\frac{\gamma_{nm}}{2}\right)\sigma_n^{\dagger}\sigma_m \tag{1b}$$

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Cases:

- Driven Dicke model: $\Omega_n = \Omega$, $\Delta_{nm} = \Delta$, $\gamma_{nm} = \gamma$
- Waveguide QED: $\Omega_n = \Omega e^{ikx_n}$, $\Delta_{nm} = \frac{\gamma_{1D}}{2}\sin(k|z_n - z_m|)$, $\gamma_{nm} = \gamma_{1D}\cos(k|z_n - z_m|)$
- Waveguide QED with individual decay: $\Omega_n = \Omega e^{ikx_n}$, $\Delta_{nm} = \frac{\gamma_{1D}}{2}\sin(k|z_n - z_m|)$, $\gamma_{nm} = \gamma_{1D}\cos(k|z_n - z_m|) + \gamma_s \delta_{nm}$
- Cavity $z_n = n\lambda$
- Free space; 2D array; 3D array, etc.

# Methods for solving the master equation

$$\dot{\rho} = \mathcal{L}\rho, \qquad \mathcal{L} \in \mathrm{Mat}(d^2, d^2), \qquad \text{Non-Hermitian symmetric matrix} \tag{2}$$

Differential equation solvers: Runge–Kutta, adaptive step size, etc. (Qutip `mesolve`, SciPy `solve_ivp`)

**Boring but straightforward**

For steady state: solve $\mathcal{L}\rho_{\mathrm{ss}} = 0$ (Qutip `steadystate`, SciPy `null_space`)

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Diagonalization: $\rho(t) = e^{\mathcal{L}t}\rho(0)$, eigenvalues of $\mathcal{L}$ give decay rates and oscillation frequencies (Qutip `eigenstates`, SciPy `eig`)

**Today or Next time**

Only a few eigenvalues are relevant for long-time dynamics, so we can use sparse diagonalization (SciPy `eigs`)

**Very intresing: next time**

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Quantum Trajectories: Monte Carlo wavefunction method, unraveling the master equation into stochastic trajectories of pure states (Qutip `mcsolve`)

**Today**

MPS + MPO methods (Tensor)

**Very advanced...**

# Runge–Kutta time stepping

Goal: solve $\dot{y} = f(t, y)$ by stepping forward in time.

$$k_1 = f(t, y), \quad k_2 = f\left(t + \tfrac{h}{2},\, y + \tfrac{h}{2}k_1\right), \quad k_3 = f\left(t + \tfrac{h}{2},\, y + \tfrac{h}{2}k_2\right), \quad k_4 = f(t + h,\, y + hk_3) \tag{3}$$

$$y(t + h) = y(t) + \tfrac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{4}$$

- RK4 is 4th order: local error $\sim h^5$, global error $\sim h^4$
- Adaptive RK uses error estimates to adjust $h$ automatically
- In master equations, set $y = \mathrm{vec}(\rho)$ and solve $\dot{y} = \mathcal{L}y$

Python direct implementation: Qutip `mesolve`; SciPy `solve_ivp` with method='RK45' or 'RK23'

# Driven Dicke model

$\Omega_n = \Omega$, $\Delta_{nm} = \Delta$, $\gamma_{nm} = \gamma$
Master equation:

$$\frac{\partial \rho}{\partial t} = -i\Omega \sum_n [\sigma_n + \sigma_n^\dagger, \rho] - i\Delta \sum_{n,m} [\sigma_n^\dagger \sigma_m, \rho] + \gamma \sum_{n,m} \left( \sigma_n \rho \sigma_m^\dagger - \frac{1}{2} \{\sigma_n^\dagger \sigma_m, \rho\} \right) \tag{5}$$

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Collective spin operators: $S^\alpha = \sum_n \sigma_n^\alpha$; $S^+ = \sum_n \sigma_n^+$; $S^- = \sum_n \sigma_n^-$

$$\frac{\partial \rho}{\partial t} = -i\Omega [S^x, \rho] - i\Delta [S^+ S^-, \rho] + \gamma \left( S^- \rho S^+ - \frac{1}{2} \{S^+ S^-, \rho\} \right) \tag{6}$$

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Non-Hermitian Hamiltonian: $H_{\text{eff}} = \Omega S^x + \Delta S^+ S^- - i\frac{\gamma}{2} S^+ S^-$
Master equation:

$$\frac{\partial \rho}{\partial t} = -i(H_{\text{eff}} \rho - \rho H_{\text{eff}}^\dagger) + \gamma S^- \rho S^+$$

# Revealing the master equation with Quantum Trajectories

$$\rho(t+\mathrm{d}t) = \rho(t) - i(H_{\mathrm{eff}}\rho - \rho H_{\mathrm{eff}}^{\dagger})\mathrm{d}t + \gamma S^{-}\rho S^{+}\mathrm{d}t \tag{7}$$

Krauss operators: $K_0 = 1 - iH_{\mathrm{eff}}\mathrm{d}t$, $K_1 = \sqrt{\gamma \mathrm{d}t}S^{-}$

$$\rho(t+\mathrm{d}t) = K_0\rho K_0^{\dagger} + K_1\rho K_1^{\dagger} \tag{8}$$

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Assume the system is in a pure state $|\psi\rangle$ at time $t$. Then we can write the state at time $t+\mathrm{d}t$ as:

$$|\psi(t+\mathrm{d}t)\rangle = \begin{cases} \frac{K_0|\psi\rangle}{\|K_0|\psi\rangle\|} & \text{with probability } p_0 = \|K_0\,|\psi\rangle\|^2 \\ \frac{K_1|\psi\rangle}{\|K_1|\psi\rangle\|} & \text{with probability } p_1 = \|K_1\,|\psi\rangle\|^2 \end{cases} \tag{9}$$

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Dynamics: $\rho(t+\mathrm{d}t) = p_0|\psi_0\rangle\langle\psi_0| + p_1|\psi_1\rangle\langle\psi_1|$, where $|\psi_0\rangle = \frac{K_0|\psi\rangle}{\|K_0|\psi\rangle\|}$ and $|\psi_1\rangle = \frac{K_1|\psi\rangle}{\|K_1|\psi\rangle\|}$

# Algorithm for Quantum Trajectories: Monte Carlo wavefunction method

Realization in Python: Qutip `mcsolve`

1. Initialize the system in a pure state $|\psi_0\rangle$
2. Evolve the state under the non-Hermitian Hamiltonian $H_{\text{eff}}$ for a time step $\mathrm{d}t$: $|\psi'\rangle = e^{-iH_{\text{eff}}\mathrm{d}t}\,|\psi\rangle$
3. Calculate the norm of the evolved state: $p_0 = \||\psi'\rangle\|^2$
4. Generate a random number $r$ uniformly distributed in the interval $[0, 1]$
5. If $r < p_0$, the system evolves to $|\psi_0\rangle = \frac{|\psi'\rangle}{\||\psi'\rangle\|}$ (no jump occurs)
6. If $r \geq p_0$, a quantum jump occurs, and the system evolves to $|\psi_1\rangle = \frac{K_1|\psi\rangle}{\|K_1|\psi\rangle\|}$ (jump occurs)
7. Repeat steps 2-6 for the desired number of time steps. Average over many trajectories to obtain the density matrix $\rho(t) = \frac{1}{N_{\text{traj}}} \sum_{i=1}^{N_{\text{traj}}} |\psi_i(t)\rangle \langle\psi_i(t)|$

# Advantages of the method

- Computational efficiency: The method allows for efficient simulation of open quantum systems by reducing the computational complexity associated with the density matrix formalism. Instead of evolving a density matrix, which has a size that scales as the square of the Hilbert space dimension, we evolve pure states, which scale linearly with the Hilbert space dimension.
- Physical insight: The method provides a clear physical picture of the dynamics of open quantum systems. The quantum jumps correspond to discrete events that can be interpreted as measurements or interactions with the environment, allowing for a more intuitive understanding of the system's behavior.
- Flexibility: The method can be applied to a wide range of open quantum systems, including those with time-dependent Hamiltonians, multiple decay channels, and non-Markovian dynamics.

# Implementation

1. JupyterHub on ChemFarm: Notebook with example on Dicke model (Qutip `mcsolve`)
2. Python script for cavity model + PBS submission script for running on ChemFarm