UNIVERSITY OF WATERLOO | IQC Institute for Quantum Computing

Open Quantum Systems and Markov Processes II

Theory of Quantum Optics (QIC 895)

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Outline

1. Introduction to open quantum systems and master equations
2. Derivation of an optical master equation
3. Solving the simple Jaynes-Cummings master equation
4. Playing with numerical solutions (Mathematica)

Goal of this lecture

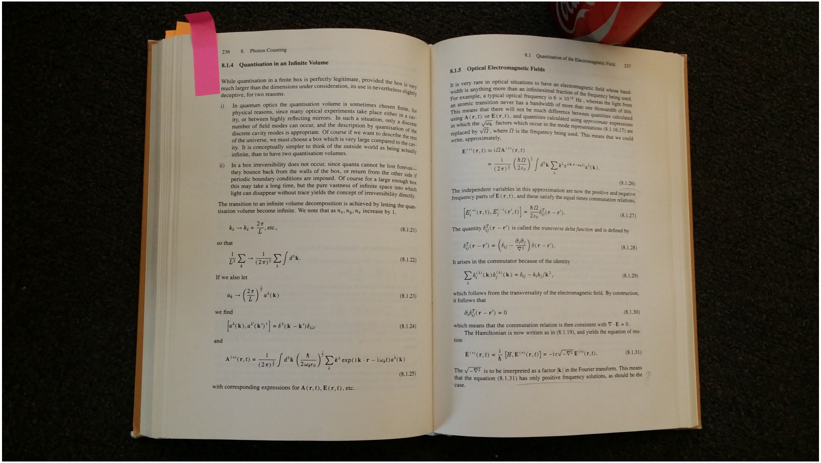
By the end of this lecture you should be able to

1. outline the steps involved in deriving a master equation,
2. explain the Markov approximation, and
3. apply a simple master equation to your own open quantum system problem.

What are open (quantum) systems?

What is irreversibility?

Let us see what Gardiner has to say (*Quantum Noise*, p. 236).



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8.1.4 Quantisation in an Infinite Volume

While quantisation in a finite box is perfectly legitimate, provided the box is very much larger than the dimensions under consideration, its use is nevertheless slightly deceptive, for two reasons.

i) In quantum optics the quantisation volume is sometimes chosen finite, for physical reasons, since many optical experiments take place either in a cavity, or between highly reflecting mirrors. In such a situation, only a discrete number of field modes can occur, and the description by quantisation of the discrete cavity modes is appropriate. Of course if we want to describe the rest of the universe, we must choose a box which is very large compared to the cavity. It is conceptually simpler to think of the outside world as being actually infinite, than to have two quantisation volumes.

ii) In a box irreversibility does not occur, since quanta cannot be lost forever—they bounce back from the walls of the box, or return from the other side if periodic boundary conditions are imposed. Of course for a large enough box this may take a long time, but the pure vastness of infinite space into which light can disappear without trace yields the concept of irreversibility directly.

The transition to an infinite volume decomposition is achieved by letting the quantisation volume become infinite. We note that as n_x, n_y, n_z increase by 1,

$$k_x \to k_x + \frac{2\pi}{L}, \text{etc.,} \tag{8.1.21}$$

so that

$$\frac{1}{L^3}\sum_k \to \frac{1}{(2\pi)^3}\sum_\lambda \int d^3\mathbf{k}. \tag{8.1.22}$$

If we also let

$$a_k \to \left(\frac{2\pi}{L}\right)^{\frac{3}{2}} a^\lambda(\mathbf{k}) \tag{8.1.23}$$

we find

$$\left[a^\lambda(\mathbf{k}), a^{\lambda'}(\mathbf{k}')^\dagger\right] = \delta^3(\mathbf{k}-\mathbf{k}')\delta_{\lambda\lambda'} \tag{8.1.24}$$

and

$$\mathbf{A}^{(+)}(\mathbf{r},t) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int d^3\mathbf{k}\left(\frac{\hbar}{2\omega_k\epsilon_0}\right)^{\frac{1}{2}}\sum_\lambda \hat{\mathbf{e}}^\lambda \exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r} - \mathrm{i}\omega_k t)a^\lambda(\mathbf{k}) \tag{8.1.25}$$

with corresponding expressions for $\mathbf{A}(\mathbf{r},t)$, $\mathbf{E}(\mathbf{r},t)$, etc.

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8.1.5 Optical Electromagnetic Fields

It is very rare in optical situations to have an electromagnetic field whose bandwidth is anything more than an infinitesimal fraction of the frequency being used. For example, a typical optical frequency is 6×10^{14} Hz, whereas the light from an atomic transition never has a bandwidth of more than one thousandth of this. This means that there will not be much difference between quantities calculated using $\mathbf{A}(\mathbf{r},t)$ or $\mathbf{E}(\mathbf{r},t)$, and quantities calculated using *approximate* expressions in which the $\sqrt{\omega_\mathbf{k}}$ factors which occur in the mode representations (8.1.16,17) are replaced by $\sqrt{\Omega}$, where Ω is the frequency being used. This means that we could write, approximately,

$$\begin{aligned}\mathbf{E}^{(+)}(\mathbf{r},t) &\approx \mathrm{i}\Omega\mathbf{A}^{(+)}(\mathbf{r},t)\\ &= \frac{\mathrm{i}}{(2\pi)^{\frac{3}{2}}}\left(\frac{\hbar\Omega}{2\epsilon_0}\right)^{\frac{1}{2}}\int d^3\mathbf{k}\sum_\lambda \hat{\mathbf{e}}^\lambda e^{\mathrm{i}(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}a^\lambda(\mathbf{k}).\end{aligned} \tag{8.1.26}$$

The independent variables in this approximation are now the positive and negative frequency parts of $\mathbf{E}(\mathbf{r},t)$, and these satisfy the equal times commutation relations,

$$\left[E_i^{(+)}(\mathbf{r},t), E_j^{(-)}(\mathbf{r}',t)\right] = \frac{\hbar\Omega}{2\epsilon_0}\delta_{ij}^T(\mathbf{r}-\mathbf{r}'). \tag{8.1.27}$$

The quantity $\delta_{ij}^T(\mathbf{r}-\mathbf{r}')$ is called the *transverse delta function* and is defined by

$$\delta_{ij}^T(\mathbf{r}-\mathbf{r}') = \left(\delta_{ij} - \frac{\partial_i\partial_j}{\nabla^2}\right)\delta(\mathbf{r}-\mathbf{r}'). \tag{8.1.28}$$

It arises in the commutator because of the identity

$$\sum_\lambda \hat{\mathbf{e}}_i^{(\lambda)}(\mathbf{k})\hat{\mathbf{e}}_j^{(\lambda)}(\mathbf{k}) = \delta_{ij} - k_i k_j/\mathbf{k}^2, \tag{8.1.29}$$

which follows from the transversality of the electromagnetic field. By construction, it follows that

$$\partial_i\delta_{ij}^T(\mathbf{r}-\mathbf{r}') = 0 \tag{8.1.30}$$

which means that the commutation relation is then consistent with $\nabla\cdot\mathbf{E} = 0$.

The Hamiltonian is now written as in (8.1.19), and yields the equation of motion

$$\dot{\mathbf{E}}^{(+)}(\mathbf{r},t) = \frac{\mathrm{i}}{\hbar}\left[H, \mathbf{E}^{(+)}(\mathbf{r},t)\right] = -\mathrm{i}c\sqrt{-\nabla^2}\,\mathbf{E}^{(+)}(\mathbf{r},t). \tag{8.1.31}$$

The $\sqrt{-\nabla^2}$ is to be interpreted as a factor $|\mathbf{k}|$ in the Fourier transform. This means that the equation (8.1.31) has only positive frequency solutions, as should be the case.

What are open (quantum) systems?

Theory of Markov processes

Great simplification: we only need to know the probability distribution at the current point in time in order to predict the future distributions: the reservoir does not act as a system memory.

There are two main analytic tools for *classical* Markov processes:

1. Stochastic differential equations
2. Fokker-Planck equations

Extension to quantum regime not easy, as the following shows.

What are open (quantum) systems?
A simple approach to introduce losses

How would you introduce losses, characterized by a relaxation rate $\gamma/2$, to the operators of the Hamiltonian $\mathcal{H} = \hbar\omega_c a^\dagger a$?
In the Heisenberg picture we could try:

$$a(t) = a e^{-\left(i\omega_c + \frac{\gamma}{2}\right)t} \quad (1)$$

$$a^\dagger(t) = a^\dagger e^{\left(i\omega_c - \frac{\gamma}{2}\right)t} \quad (2)$$

But this would violate the fundamental commutation relation:

$$\left[a(t), a^{\dagger}(t)\right] = \mathbb{1} e^{-\gamma t} \quad (3)$$

We need a **noise generator**, which has sufficient output even at absolute zero temperature: vacuum noise preserves commutation relation.

What are open (quantum) systems?
Markov processes for quantum systems: master equation

The quantum analog of the Fokker-Planck equation is the **master equation**, which we will now derive. We follow the exposition in Louisell's book *Quantum Statistical Properties of Radiation*.

Derivation of an optical master equation
Milestones

Our goal is to find **an explicit** equation of motion for the reduced density operator for the system in the Schrödinger picture.

1. Write down general equation of motion for the reduced density operator for the system in the Schrödinger picture $S(t)$.
2. Write down the equation of motion for the density operator in the interaction picture $\chi(t)$.
3. Use 2$^{\text{nd}}$-order perturbation theory to simplify the time evolution of $\chi(t)$.
4. Use and justify Markov approximation, which collapses the integrals.
5. Insert the resulting equation of motion for the reduced system density operator in the interaction picture into the one in the Schrödinger picture.

The total Hamiltonian (system plus reservoir plus interaction) is

$$H_T = H + R + V = H_0 + V \tag{4}$$

with the interaction typically of the form

$$V = \hbar \sum_j \left(\kappa_j b_j a^\dagger + \kappa_j^* b_j^\dagger a \right) \quad . \tag{5}$$

The total density operator in the Schrödinger picture is $\rho(t)$, which is related to the one interaction picture:

$$\rho(t) = e^{-\frac{i}{\hbar}H_0(t-t_0)}\chi(t)e^{\frac{i}{\hbar}H_0(t-t_0)} \tag{6}$$

In the Schrödinger picture the reduced density operator for the system is

$$S(t) = \mathrm{Tr}_R(\rho(t)) \tag{7}$$

and is related to the one in the interaction picture:

$$S(t) = e^{-\frac{i}{\hbar}H(t-t_0)}s(t)e^{\frac{i}{\hbar}H(t-t_0)} \tag{8}$$

with $s(t) = \mathrm{Tr}_R\chi(t)$.

Derivation of an optical master equation

Relevant equations of motion for density operators

The general equation of motion for $S(t)$:

$$\frac{\partial S(t)}{\partial t} = e^{-\frac{i}{\hbar}H(t-t_0)} \left\{ \frac{1}{i\hbar}[H, s(t)] + \frac{\partial s}{\partial t} \right\} e^{\frac{i}{\hbar}H(t-t_0)} \tag{9}$$

However, it is much easier to work out the explicit form in the interaction picture:

$$\frac{\partial \chi(t)}{\partial t} = \frac{1}{i\hbar}[V(t-t_0), \chi(t)] \tag{10}$$

with

$$V(t-t_0) = e^{\frac{i}{\hbar}H_0(t-t_0)} V e^{-\frac{i}{\hbar}H_0(t-t_0)} \tag{11}$$

Derivation of an optical master equation

2^{nd}-order perturbation theory for $\chi(t)$

Expand

$$\frac{\partial \chi(t)}{\partial t} = \frac{1}{i\hbar}[V(t-t_0), \chi(t)] \tag{12}$$

to second order:

$$\begin{aligned} \chi(t) &= \chi(t_0) + \frac{1}{i\hbar}\int_{t_0}^{t} dt' [V(t'-t_0), \chi(t_0)] \\ &+ \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' [V(t-t'), [V(t''-t_0), \chi(t_0)]] \\ &+ \ldots \end{aligned} \tag{13}$$

Derivation of an optical master equation

2^{nd}-order perturbation theory for $s(t)$

Now take trace over reservoir and use the fact

$$\rho(t_0) = \chi(t_0) = f_0(R)s(t_0) \tag{14}$$

$$\begin{aligned} s(t) - s(t_0) &= \frac{1}{i\hbar}\int_{t_0}^{t} dt' \mathrm{Tr}_R([V(t'-t_0), f_0(R)s(t_0)]) \\ &+ \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \mathrm{Tr}_R([V(t-t'), [V(t''-t_0), f_0(R)s(t_0)]]) \\ &+ \ldots \end{aligned} \tag{15}$$

Derivation of an optical master equation

Insert system-reservoir interaction

The system and reservoir interact via

$$V = \hbar \sum_i Q_i F_i \tag{16}$$

for example

$$Q_1 = a^\dagger \qquad F_1 = \sum_j \kappa_j b_j \tag{17}$$

$$Q_2 = a \qquad F_2 = \sum_j \kappa_j^* b_j^\dagger \tag{18}$$

The relation between interaction and Schrödinger picture is:

$$V(t - t_0) = \hbar \sum_i Q_i(t - t_0) F_i(t - t_0) \tag{19}$$

$$Q_i(t - t_0) = e^{\frac{i}{\hbar} H(t-t_0)} Q_i e^{-\frac{i}{\hbar} H(t-t_0)} \tag{20}$$

$$F_i(t - t_0) = e^{\frac{i}{\hbar} R(t-t_0)} Q_i e^{-\frac{i}{\hbar} R(t-t_0)} \tag{21}$$

Derivation of an optical master equation
First separation of system and reservoir

$$
\begin{aligned}
s(t) - s(t_0) &= -i \sum_i \int_{t_0}^{t} dt' [Q_i', s(t_0)] \langle F_i' \rangle_R \\
&- \sum_{i,j} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \Big\{ [Q_i' Q_j'' s(t_0) - Q_j'' s(t_0) Q_i'] \langle F_i' F_j'' \rangle_R \\
&\qquad - [Q_i' s(t_0) Q_j'' - s(t_0) Q_j'' Q_i'] \langle F_j'' F_i' \rangle_R \Big\} \\
&+ \ldots
\end{aligned} \tag{22}
$$

where prime and double prime indicate $t' - t_0$ and $t'' - t_0$ time dependence, respectively. The $\langle F_i' F_j'' \rangle_R$ and $\langle F_j'' F_i' \rangle_R$ are the reservoir correlation functions.

Now use system operators in Schrödinger picture:

$$Q_i(t) = e^{\frac{i}{\hbar}Ht} Q_i e^{-\frac{i}{\hbar}Ht} = e^{i\omega_i t} Q_i \tag{23}$$

e.g. $a \to a e^{-i\omega_c t}$ and change integration variables

$$\begin{aligned}
& s(t) - s(t_0) \\
= \quad & -i \sum_i \langle F_i \rangle_R \, [Q_i, s(t_0)] \int_0^{t-t_0} d\xi \, e^{i\omega_i \xi} \\
- \quad & \sum_{i,j} \int_0^{t-t_0} d\xi \Big\{ [Q_i Q_j s(t_0) - Q_j s(t_0) Q_i] \int_0^{t-t_0-\xi} d\tau \, e^{i\omega_i \tau} \langle F_j(\tau) F_i \rangle_R \\
& \quad -[Q_i s(t_0) Q_j - s(t_0) Q_j Q_i] \int_0^{t-t_0-\xi} d\tau \, e^{i\omega_i \tau} \langle F_i F_j(\tau) \rangle_R \Big\} e^{i(\omega_i + \omega_j)\xi} \\
+ \quad & \ldots
\end{aligned} \tag{24}$$

Observe: for sufficiently short time scales, excitation is not coming back to the system, which is what we want. In other words, the system loses all its past memories, which happens when

$$\tau_c \ll t - t_0 \ll \gamma^{-1} \tag{25}$$

which means the fluctuations of the system are

1. smoothed out during reservoir correlation time τ_c but not
2. on a time scale where system is damped.

Derivation of an optical master equation

2nd-order perturbation theory for $s(t)$ with Markov approximation

$$
\begin{aligned}
s(t) - s(t_0) &= -i \sum_i \langle F_i \rangle_R [Q_i, s(t_0)] I(\omega_i) \\
&- \sum_{i,j} \Big\{ [Q_i Q_j s(t_0) - Q_j s(t_0) Q_i] w_{ij}^+ \\
&\qquad - [Q_i s(t_0) Q_j - s(t_0) Q_j Q_i] w_{ji}^- \Big\} I(\omega_i + \omega_j) \\
&+ \ldots
\end{aligned} \tag{26}
$$

with

$$
I(\omega_i) = \int_0^{t-t_0} d\xi e^{i\omega_i \xi} \quad \text{and} \quad I(\omega_i + \omega_j) = \int_0^{t-t_0} d\xi e^{i(\omega_i+\omega_j)\xi} \tag{27}
$$

and the reservoir spectral densities

$$
w_{ij}^+ = \int_0^\infty d\tau e^{i\omega_i \tau} \langle F_i(\tau) F_j \rangle_R \quad \text{and} \quad w_{ji}^- = \int_0^\infty d\tau e^{i\omega_i \tau} \langle F_j F_i(\tau) \rangle_R \tag{28}
$$

Derivation of an optical master equation

2^{nd}-order perturbation theory for $s(t)$ with Markov approximation

For integration times much longer than a period of the free motion of the system

$$I(\omega_i) = 0 \quad \text{and} \quad I(\omega_i + \omega_j) = (t - t_0)\delta(\omega_i, -\omega_j) \tag{29}$$

$$\begin{aligned} \frac{s(t) - s(t_0)}{t - t_0} &= -\sum_{i,j} \delta(\omega_i, -\omega_j) \Big\{ [Q_i Q_j s(t_0) - Q_j s(t_0) Q_i] w_{ij}^{+} \\ &\quad - [Q_i s(t_0) Q_j - s(t_0) Q_j Q_i] w_{ji}^{-} \Big\} + \dots \end{aligned} \tag{30}$$

Derivation of an optical master equation

2^{nd}-order perturbation theory for $s(t)$ with Markov approximation

Now we can go back to our general equation of motion for the reduced density operator for the system

$$\frac{\partial S(t)}{\partial t} = e^{-\frac{i}{\hbar}H(t-t_0)} \left\{ \frac{1}{i\hbar}[H, s(t)] + \frac{\partial s}{\partial t} \right\} e^{\frac{i}{\hbar}H(t-t_0)} \tag{31}$$

and

$$\frac{\partial S(t)}{\partial t} \approx e^{-\frac{i}{\hbar}H(t-t_0)} \left[\lim_{t_0 \to t} \left\{ \frac{1}{i\hbar}[H, s(t)] + \frac{s(t) - s(t_0)}{t - t_0} \right\} \right] e^{\frac{i}{\hbar}H(t-t_0)} \tag{32}$$

(33)

Now we are very close... and it is now easy to obtain...

$$\begin{aligned} \frac{\partial S(t)}{\partial t} &\approx \frac{1}{i\hbar}[H, S(t)] \\ &- \sum_{i,j} \delta(\omega_i, -\omega_j) \left\{ [Q_i Q_j S(t_0) - Q_j S(t_0) Q_i] w_{ij}^{+} \right. \\ &\left. -[Q_i S(t_0) Q_j - S(t_0) Q_j Q_i] w_{ji}^{-} \right\} \end{aligned} \tag{34}$$

The simple Jaynes-Cummings Hamiltonian describes a single atom coupled to a single field mode (inside a cavity:

$$H_{JC} = \hbar\Delta a^{\dagger} a + \hbar\Theta\sigma^{+}\sigma^{-} + \hbar g \left(a^{\dagger}\sigma^{-} + a\sigma^{+}\right) \tag{35}$$

This Hamiltonian is in the interaction picture with RWA applied. One can add a laser driving term $\hbar\epsilon \left(a + a^{\dagger}\right)$, which replenishes lost cavity photons. The following solution is without this term (for simplicity and space reasons). The simulations later include it, however.

There are two important loss mechanisms we consider:

1. Cavity mirrors are partially reflective: cavity field can decay!
2. The cavity is not fully closed: atom can radiate out the side of the cavity.

These two couplings to the field outside the cavity (environment) is encapsulated by the following master equation:

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= -\frac{i}{\hbar}[H_{JC},\rho] \\ &+ \kappa\left(2a\rho a^\dagger - a^\dagger a\rho - \rho a^\dagger a\right) + \frac{\gamma}{2}\left(2\sigma^-\rho\sigma^+ - \sigma^+\sigma^-\rho - \rho\sigma^+\sigma^-\right)\end{aligned} \tag{36}$$

The simple Jaynes-Cummings master equation
Operator expectation values

In many situations we are not interested in density operators but expectation values of certain operators

$$\langle A \rangle = \mathrm{Tr}(A\rho) \tag{37}$$

for which we have to solve the so-called **rate equations**

$$\frac{d}{dt}\langle A \rangle = \mathrm{Tr}\left(A\frac{d}{dt}\rho\right) \tag{38}$$

Inserting master equation and simplifying yields:

$$\begin{aligned} \frac{d}{dt}\langle A \rangle &= -\frac{i}{\hbar}\langle [H_{JC}, A] \rangle \qquad (39) \\ &+ \kappa \langle 2aAa^\dagger - a^\dagger a A - A a^\dagger a \rangle + \frac{\gamma}{2}\langle 2\sigma^- A \sigma^+ - \sigma^+\sigma^- A - A\sigma^+\sigma^- \rangle \end{aligned}$$

$$\frac{d}{dt}\langle a^\dagger a\rangle = ig\langle a\sigma_+ - a^\dagger\sigma_-\rangle - 2\kappa\langle a^\dagger a\rangle \quad (40)$$

$$\frac{d}{dt}\langle \sigma_+\sigma_-\rangle = -ig\langle a\sigma_+ - a^\dagger\sigma_-\rangle - \gamma\langle \sigma_+\sigma_-\rangle \quad (41)$$

$$\begin{aligned}\frac{d}{dt}\langle a\sigma_+ + a^\dagger\sigma_-\rangle &= i(\Theta-\Delta)\langle a\sigma_+ - a^\dagger\sigma_-\rangle \\ &- \left(\kappa+\frac{\gamma}{2}\right)\langle a\sigma_+ + a^\dagger\sigma_-\rangle \end{aligned}\quad (42)$$

$$\begin{aligned}\frac{d}{dt}\langle a\sigma_+ - a^\dagger\sigma_-\rangle &= i(\Theta-\Delta)\langle a\sigma_+ + a^\dagger\sigma_-\rangle \\ &+ 2ig\langle a^\dagger a\rangle - 2ig\langle \sigma_+\sigma_-\rangle - 4ig\langle a^\dagger a\sigma_+\sigma_-\rangle \\ &- \left(\kappa+\frac{\gamma}{2}\right)\langle a\sigma_+ - a^\dagger\sigma_-\rangle \end{aligned}\quad (43)$$

$$\frac{d}{dt}\langle a^\dagger a\rangle = ig\langle a\sigma_+ - a^\dagger\sigma_-\rangle - 2\kappa\langle a^\dagger a\rangle \tag{44}$$

$$\frac{d}{dt}\langle \sigma_+\sigma_-\rangle = -ig\langle a\sigma_+ - a^\dagger\sigma_-\rangle - \gamma\langle \sigma_+\sigma_-\rangle \tag{45}$$

$$\begin{aligned}\frac{d}{dt}\langle a\sigma_+ + a^\dagger\sigma_-\rangle &= i(\Theta-\Delta)\langle a\sigma_+ - a^\dagger\sigma_-\rangle \\ &- \left(\kappa + \frac{\gamma}{2}\right)\langle a\sigma_+ + a^\dagger\sigma_-\rangle \end{aligned} \tag{46}$$

$$\begin{aligned}\frac{d}{dt}\langle a\sigma_+ - a^\dagger\sigma_-\rangle &= i(\Theta-\Delta)\langle a\sigma_+ + a^\dagger\sigma_-\rangle \\ &+ 2ig\langle a^\dagger a\rangle - 2ig\langle \sigma_+\sigma_-\rangle - 4ig\langle a^\dagger a\sigma_+\sigma_-\rangle \\ &- \left(\kappa + \frac{\gamma}{2}\right)\langle a\sigma_+ - a^\dagger\sigma_-\rangle \end{aligned} \tag{47}$$

Semi-classical approximation:

$$\langle a^\dagger a \sigma_+ \sigma_- \rangle \approx \langle a^\dagger a \rangle \langle \sigma_+ \sigma_- \rangle \tag{48}$$

Effectively neglecting atom-field correlation fluctuations.

The simple Jaynes-Cummings master equation
Analytic Solution

Mathematica's DSOLVE does not find an analytic solution.

Mathematica's NDSOLVE finds numerical solutions. Let's have a look at them and play!

Summary

Let's face it: stochastic *and* coupled *and* quantum systems are ugly. However:

1. You saw what is involved in deriving a master equation that describes a quantum optical system interacting with it's environment.
2. Playing with parameters actually yields quantitative predictions for regimes where experiments can work.
3. Now go, and fight decay!