These notes include: a) an elementary introduction to formalism describing the evolution of density matrix coupled to a thermal bath of harmonic oscillators under conditions typical for quantum optics (i.e. assuming negligible correlation time for the bath); b) an introduction to stochastic wavefunction description of the open systems. These notes are from the Atomic Physics class taught at Harvard in the fall of 2003. The notes were taken by Lily Childress. (The rest of the notes can be found at http://www.courses.fas.harvard.edu/ phys285b/lectures/. Note that some of those have not been carefully proofed and may contain misprints.We would welcome your comments or corrections. Email them to lukin@physics.harvard.edu or to childres@fas.harvard.edu)

Chapter 3

Mathematical methods for open systems in quantum optics

Our primary goal thus far has been to describe the interactions between light and matter. In previous lectures we have developed two different formalisms for atoms interacting with classical and quantum mechanical radiation fields. Even though the latter allowed us to solve the problem of spontaneous emission, the full quantum mechanical treatment is cumbersome at best, and in many cases unnecessary. We would like to describe both coherent phenomena (such as classical field Rabi oscillations) and incoherent processes (such as spontaneous emission) in a more efficient manner. By truncating our description to include only the few modes or atomic levels of interest, we can treat much more complicated systems.

In more formal language, we seek a quantum mechanical treatment of open systems. The ”system” interacts not only with controllable classical signals, but also with a large number of degrees of freedom we call the ”environment” or ”reservoir”, and over which we have no control. If we do not care about the reservoir state, we would like to be able to describe the system without also calculating the reservoir dynamics. For instance, the system might be an atom interacting with both a controllable laser field and an environment composed of the vacuum modes of the electromagnetic field; by properly eliminating the radiation field degrees of freedom while retaining their effect on the atom, we can obtain a simpler but equally accurate picture of the atomic evolution.

3.1 The density operator

Although the state of a quantum mechanical system is represented by $|\psi\rangle$, a vector in Hilbert space, this description does not provide a useful picture for many practical situations, and certainly cannot treat macroscopic objects. Any quantum mechanical state can also be represented as a density operator; moreover, the density operator can describe classical ensembles as well.

Suppose our system can be in one of a number of quantum states $|\psi_\alpha\rangle$ and it occupies each state with some probability p_α. The density operator for the system is

$$\hat{\rho} = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|. \tag{3.1}$$

If there exists a basis in which $\hat{\rho} = |\phi\rangle\langle\phi|$ for some state $|\phi\rangle$, the system is said to be in a "pure state". If such a basis cannot be found, the system is in a "mixed state", and has lost some of its purely quantum mechanical character. Finally, if a basis can be found in which the off-diagonal elements of the density operator vanish, the system can be described by a classical ensemble, and is called a "statistical mixture".

From this definition, one can immediately derive several important properties which any density operator must satisfy:

(1) $\hat{\rho} = \hat{\rho}^\dagger$
(2) $\mathrm{Tr}[\hat{\rho}] = \sum_n \langle n|\hat{\rho}|n\rangle = 1$ where $\{|n\rangle\}$ form an orthonormal basis
(3) $\langle n|\hat{\rho}^2|m\rangle \leq \langle n|\hat{\rho}|m\rangle$ where $|m\rangle$ and $|n\rangle$ are any pure states

The first is self evident, the second follows from conservation of probability, and the third is an equality only when the density operator describes a pure state.

Operator expectation values may be calculated directly from the density operator. If $\hat{S}$ is a system observable, its expectation value should be calculated in all possible quantum states weighted by their probability of occupation:

$$\begin{aligned}
\langle\hat{S}\rangle &= \sum_\alpha p_\alpha \langle\psi_\alpha|\hat{S}|\psi_\alpha\rangle && (3.2)\\
&= \sum_{\alpha,n} p_\alpha \langle\psi_\alpha|\hat{S}|n\rangle\langle n|\psi_\alpha\rangle && (3.3)\\
&= \sum_n \langle n| \underbrace{\left(\sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|\right)}_{\hat{\rho}} \hat{S}|n\rangle && (3.4)\\
&= \mathrm{Tr}[\hat{\rho}\hat{S}]. && (3.5)
\end{aligned}$$

By inserting a completeness relation $\sum_n |n\rangle\langle n| = 1$ and rearranging terms, a considerable simplification is obtained.

In this context, the mathematical meaning of the trace may be unclear. However, given a basis $\{|n\rangle\}$, we may write the operators $\hat{S}$ and $\hat{\rho}$ as matrices, whereby their trace is the usual sum of diagonal elements. The so-called density matrix has elements $\rho_{n,n'}$ such that

$$\hat{\rho} = \sum_{n,n'} |n\rangle \underbrace{\langle n|\hat{\rho}|n'\rangle}_{\rho_{n,n'}} \langle n'|. \tag{3.6}$$

These elements have a physical meaning, and there are two cases worth distinguishing:

(1) Diagonal elements $\rho_{nn} = \langle (|n\rangle\langle n|) \rangle$ correspond to the probability of occupying state $|n\rangle$.

(2) Off-diagonal elements $\rho_{nm} = \langle (|n\rangle\langle m|) \rangle$ correspond to the expectation value of the coherence between level $|n\rangle$ and $|m\rangle$, e.g. the atomic dipole operator.

For example, the density operator for a two-level atom may be written as a 2x2 matrix,

$$\hat{\rho} = \rho_{11}|1\rangle\langle 1| + \rho_{12}|1\rangle\langle 2| + \rho_{21}|2\rangle\langle 1| + \rho_{22}|2\rangle\langle 2|. \tag{3.7}$$

A pure state $|\psi\rangle = c_1|\psi\rangle + c_2|\psi\rangle$ then has a density matrix with $\rho_{ij} = c_i c_j^*$. One example of a mixed state is the two-level atom with transition frequency ω in thermal equilibrium. In the basis $\{|1\rangle, |2\rangle\}$ its density operator takes the form

$$\begin{aligned} \hat{\rho} &= \frac{e^{-\hat{H}/k_BT}}{\mathrm{Tr}[e^{-\hat{H}/k_BT}]} && (3.8) \\ &= \frac{1}{1+e^{-\hbar\omega/k_BT}} \begin{pmatrix} 1 & 0 \\ 0 & e^{-\hbar\omega/k_BT} \end{pmatrix} && (3.9) \\ &= \frac{1}{2\cosh \hbar\omega/2k_BT} \begin{pmatrix} e^{\hbar\omega/2k_BT} & 0 \\ 0 & e^{-\hbar\omega/2k_BT} \end{pmatrix}. && (3.10) \end{aligned}$$

Clearly, the equilibrium population depends on the relative scale of the atomic transition frequency and the temperature. For instance, at room temperature $T = 300K$, $k_BT/(2\pi\hbar) \approx 6 \cdot 10^{12}$ Hz, which corresponds to a frequency between microwave and near-infrared. If the atomic transition frequency is well above this scale, the atom will be in its ground state in equilibrium; otherwise, it will be in a statistical mixture of ground and excited states.

The density matrix for a thermal radiation field illustrates how the density operator formalism connects up with statistical mechanics. A single mode with frequency ν_j has a density operator

$$\hat{\rho}^{(j)} = \frac{e^{-\hbar\nu_j \hat{a}_j^\dagger \hat{a}_j/k_B T}}{\mathrm{Tr}[e^{-\hbar\nu_j \hat{a}_j^\dagger \hat{a}_j/k_B T)}} \tag{3.11}$$

with matrix elements between Fock states $|n\rangle, |m\rangle$

$$\hat{\rho}^{(j)}_{nm} = \delta_{nm} e^{-\hbar\nu_j n/k_B T}\left(1 - e^{-\hbar\nu_j/k_B T)}\right). \tag{3.12}$$

Note that only the diagonal elements are nonzero since the field is a statistical mixture of photon number states. Consequently, the expectation value for the annihilation operator vanishes,

$$\langle \hat{a}_j \rangle = \sum_n \langle n|\hat{a}_j \hat{\rho}|n\rangle = \sum_n \rho_{n,n-1}\sqrt{n} = 0, \tag{3.13}$$

but the average photon number obeys the Bose-Einstein distribution,

$$\bar{n}_j = \langle \hat{a}_j^\dagger \hat{a}_j \rangle = \sum_n \rho_{nn} = \frac{1}{e^{-(\hbar\nu_j/k_B T)} - 1}. \tag{3.14}$$

3.2 System and environment

The density operator formalism is well suited for treating a system composed of two parts when only one subsystem is relevant. For clarity, we will call the total system the universe, and its component parts are the system and the environment. The universe can be described by a quantum state $|\psi\rangle$, with the corresponding density operator $\hat{\rho} = |\psi\rangle\langle\psi|$, and in principle we can solve for the dynamics of the system by first finding how the universe evolves. Since we are really only interested in the system, we would like to find a more efficient description which does not require us to calculate precisely what happens to the environment degrees of freedom.

We proceed by first expanding the total state vector in terms of a basis $\{|n\rangle|e\rangle\}$ where $|n\rangle$ is a state of the system and $|e\rangle$ is a state of the environment, so that

$$|\psi\rangle = \sum_{\{n,e\}} |n\rangle|e\rangle\langle n,e|\psi\rangle. \tag{3.15}$$

Consider the expectation value in this state of an operator $\hat{S}$ which acts only on the system degrees of freedom,

$$\begin{aligned}
\langle\hat{S}\rangle &= \sum_{n,e,n',e'} \langle n,e|\hat{S}|n',e'\rangle\langle n',e'|\psi\rangle\langle\psi|n,e\rangle && (3.16)\\
&= \sum_{n}\langle n|\hat{S}\,\underbrace{(\sum_{e}\langle e|\psi\rangle\langle\psi|e\rangle)}_{\hat{\rho}_S}\,|n\rangle && (3.17)\\
&= \mathrm{Tr}_S[\hat{S}\hat{\rho}_S]. && (3.18)
\end{aligned}$$

The subscript S (R) on the trace indicates that only the system (reservoir) states are included in the sum. The expectation value of a system operator can always be found in terms of a reduced density operator

$$\hat{\rho}_S = \mathrm{Tr}_R[\hat{\rho}]. \qquad (3.19)$$

Note that $\hat{\rho}_S$ has all the properties of a density operator, and can be expressed as a probabilistic mixture of system states, $\hat{\rho}_S = \sum_\alpha p\alpha|\psi^S_\alpha\rangle\langle\psi^S_\alpha|$. In general, however, $\hat{\rho}_S$ does not have to describe a pure state, and this reflects the fact that the system under consideration interacts with the environment, i.e. it is an open system.

3.3 The dynamics of an open system

We will use the density operator as a tool to aid derivation of an efficient description for an open system interacting with its environment. To understand how the reduced density operator evolves in time, consider first its evolution with a Hamiltonian $\hat{H}_S$ acting only on the system:

$$\begin{aligned}
i\hbar\dot{\hat{\rho}}_S &= \sum_\alpha p_\alpha(\underbrace{i\hbar|\dot{\psi}^S_\alpha\rangle}_{\hat{H}_S|\psi^S_\alpha\rangle}\langle\psi^S_\alpha| + |\psi^S_\alpha\rangle\ \underbrace{i\hbar\langle\dot{\psi}^S_\alpha|}_{-\langle\psi^S_\alpha|\hat{H}_S}\ ) && (3.20)\\
&= \frac{1}{i\hbar}[\hat{H}_S,\hat{\rho}_S]. && (3.21)
\end{aligned}$$

Suppose now that there is some coupling between the system and the environment described by an interaction Hamiltonian $\hat{H}_{SR}$. The dynamics will become quite a bit more involved, since even if the system and environment start out independent of one another, the initial product state $|\psi_S\rangle\otimes|\psi_R\rangle$ will evolve under the influence of $\hat{H}_{SR}$ into a state which cannot in general be factored into independent system and environment states. The system and environment are then said to be entangled.

As an illustration we return to the example of an atom spontaneously emitting a photon into the vacuum. If the atom starts out in a superposition state, $|\psi_0\rangle = (c_1|1\rangle + c_2|2\rangle) \otimes |0\rangle$, at time t it will be in a state $|\psi(t)\rangle = c_1|1\rangle \otimes |0\rangle + c_2(t)|2\rangle \otimes |0\rangle + \sum_k c_k(t)|1\rangle \otimes |1_l\rangle$ which can no longer be written as a direct product of atomic and electromagnetic states. The elements of the atomic reduced density matrix can then be calculated n terms of the decay rate γ:

$$\hat{\rho} = \mathrm{Tr}[|\psi(t)\rangle\langle\psi(t)|] = \begin{pmatrix} 1 - \rho_{22}(0)e^{-\gamma t} & \rho_{12}(0)e^{-\gamma t/2} \\ \rho_{21}(0)e^{-\gamma t/2} & \rho_{22}(0)e^{-\gamma t} \end{pmatrix} \tag{3.22}$$

Note that the off-diagonal elements decay at half the rate of the excited state population. This is characteristic of interactions which conserve energy.

3.3.1 General formalism

The total Hamiltonian may be represented as a sum of three terms,

$$\hat{H} = \hat{H}_S + \hat{H}_R + \hat{H}_{SR}. \tag{3.23}$$

The first term only affects system degrees of freedom and the second only affects the reservoir while the third contains cross products of system operators with reservoir operators. The total density matrix obeys the equation of motion

$$\begin{aligned} \dot{\hat{\rho}} &= \frac{1}{i\hbar}[\hat{H}, \hat{\rho}] && (3.24) \\ &= \frac{1}{i\hbar}[\hat{H}_S + \hat{H}_R + \hat{H}_{SR}, \hat{\rho}], && (3.25) \end{aligned}$$

and we may trace over the reservoir degrees of freedom on both sides of the equation to obtain the evolution for the system reduced density operator:

$$\begin{aligned} \dot{\hat{\rho}}_S &= \mathrm{Tr}[\dot{\hat{\rho}}] && (3.26) \\ &= \frac{1}{i\hbar}[\hat{H}_S, \hat{\rho}_S] + \frac{1}{i\hbar}\underbrace{\mathrm{Tr}[[\hat{H}_R, \hat{\rho}]]}_{=0} + \frac{1}{i\hbar}\mathrm{Tr}[[\hat{H}_{SR}, \hat{\rho}]]. && (3.27) \end{aligned}$$

Each of the three terms contributes differently. The system Hamiltonian has the same effect it would have in the absence of the reservoir. The reservoir Hamiltonian has no net effect on $\hat{\rho}_S$ because the trace is invariant under cyclic permutations of the reservoir operators, so the commutator must vanish. The interaction Hamiltonian, however, involves both system and reservoir operators and requires special treatment. Although we have obtained the equation of motion as a general result, no further progress can be made without specifying at least some of the properties of the interaction Hamiltonian and the reservoir itself.

3.3.2 Density operator method for a Markovian reservoir

By limiting the system and reservoir to certain kinds of interactions relevant to atomic physics and quantum optics, we can develop a framework for analyzing open systems. In particular, we will consider environments which have a very short correlation time, so that the system is only influenced by the instantaneous state of the reservoir.

Again, we will assume $\hat{H} = \hat{H}_S + \hat{H}_R + \hat{H}_{SR}$, and we will work in the interaction picture, where the relevant operators are

$$\begin{aligned} \tilde{\rho} &= e^{i(\hat{H}_R+\hat{H}_S)t/\hbar}\hat{\rho}e^{-i(\hat{H}_R+\hat{H}_S)t/\hbar} && (3.28) \\ \tilde{H}_{SR} &= e^{i(\hat{H}_R+\hat{H}_S)t/\hbar}\hat{H}_{SR}e^{-i(\hat{H}_R+\hat{H}_S)t/\hbar}. && (3.29) \end{aligned}$$

The unitary transformation automatically accounts for the free evolution of the system and reservoir, so that the only remaining dynamics are due to the interactions, i.e.

$$\frac{d}{dt}\tilde{\rho} = \frac{1}{i\hbar}[\tilde{H}_{SR}, \tilde{\rho}]. \tag{3.30}$$

Our analysis requires a specific form for the interaction,

$$\hat{H}_{SR} = \hat{S}\hat{R}^\dagger + \hat{R}\hat{S}^\dagger, \tag{3.31}$$

where $\hat{S}$ ($\hat{R}$) is a general system (reservoir) operator. In practice, the interaction Hamiltonian may have a sum over such terms: the analysis proceeds in exactly the same manner, and the effects may be accounted for by considering each term of the sum separately and summing at the end. In the interaction picture, we will represent the Hamiltonian by

$$\tilde{H}_{SR} = \hat{S}\hat{F}_R(t)^\dagger + \hat{F}_R(t)\hat{S}^\dagger, \tag{3.32}$$

where all the time dependence is explicitly included in the reservoir operator $\hat{F}_R(t)$.

For example, consider the Hamiltonian for a single atom interacting with the radiation field in the Schrodinger picture,

$$\hat{H}_{SR} = \underbrace{-\sum_j \hbar g_j \hat{a}_j}_{\hat{R}} \underbrace{|2\rangle\langle 1|}_{\hat{S}^\dagger} - \sum_j \hbar g_j^* \hat{a}_j^\dagger |1\rangle\langle 2|, \tag{3.33}$$

where we can identify the system and reservoir operators appropriate to our more general form of the interaction. Likewise, in the interaction picture the Hamiltonian includes the phase factors associated with free evolution of the system and reservoir:

$$\tilde{H}_{SR} = \underbrace{-\sum_j \hbar g_j \hat{a}_j e^{-i(\nu_j-\omega)t}}_{\hat{F}_R(t)} \underbrace{|2\rangle\langle 1|}_{\hat{S}^\dagger} - \sum_j \hbar g_j^* \hat{a}_j^\dagger e^{i(\nu_j-\omega)t} |1\rangle\langle 2|, \tag{3.34}$$

and we incorporate these phase factors into the new reservoir operator $\hat{F}_R(t)$.

In addition to the specified form for the interaction given by Eq. (3.32), our analysis requires two assumptions regarding the nature of the reservoir itself, namely

(1) The reservoir is large

(2) The reservoir has a broad bandwidth.

The first assumption indicates that the reservoir state is not significantly affected by its interaction with the system. Consequently for our analysis we may take the reservoir to be in a stationary (time-independent) state, for example a statistical mixture at some temperature T. The second assumption implies that the correlation time $\tau_c$for the reservoir is short; in particular, we require that τ_c be much smaller than the typical timescale τ_S on which the system evolves. These assumptions together constitute the "Born-Markov Approximation", and a reservoir which satisfies them is called Markovian.

The effect of the reservoir on the system can be simplified by averaging over a timescale Δt which is in between the correlation time and characteristic system evolution time, $\tau_c \ll \Delta t \ll \tau_S$. This approach is akin to perturbation theory in τ_c/τ_S, and will provide equations of motion for the system reduced density operator which are valid for times greater than Δt.

Starting from Eq. (3.30), we can formally integrate to obtain the density operator at a later time,

$$\underbrace{\tilde{\rho}(t+\Delta t) - \tilde{\rho}(t)}_{\Delta\tilde{\rho}} = \frac{1}{i\hbar} \int_t^{t+\Delta t} dt' [\tilde{H}_{SR}(t'), \tilde{\rho}(t')]. \tag{3.35}$$

Expanding $\tilde{\rho}(t')$ in the same manner (which is valid since $t' - t < \Delta t$), we obtain

$$\begin{aligned} \Delta\tilde{\rho} \;=\; & \tfrac{1}{i\hbar}\int_t^{t+\Delta t} dt' [\tilde{H}_{SR}(t'), \tilde{\rho}(t')] \\ & + \tfrac{1}{(i\hbar)^2}\int_t^{t+\Delta t} dt' \int_t^{t'} dt'' [\tilde{H}_{SR}(t'), [\tilde{H}_{SR}(t''), \tilde{\rho}(t'')]. \end{aligned} \tag{3.36}$$

Now we trace over the reservoir degrees of freedom to find the change in the system reduced density operator over time Δt,

$$\begin{aligned} \Delta\tilde{\rho}_S \;=\; & \tfrac{1}{i\hbar}\int_t^{t+\Delta t} dt' \ \mathrm{Tr}_R[\tilde{H}_{SR}(t'), \tilde{\rho}(t')] \\ & + \tfrac{1}{(i\hbar)^2}\int_t^{t+\Delta t} dt' \int_t^{t'} dt'' \ \mathrm{Tr}_R[\tilde{H}_{SR}(t'), [\tilde{H}_{SR}(t''), \tilde{\rho}(t'')]. \end{aligned} \tag{3.37}$$

To proceed we must now make yet another assumption: the initial state is factorizable,

$$\tilde{\rho}(t) = \tilde{\rho}_S(t) \otimes \tilde{\rho}_R(t). \tag{3.38}$$

For times shortly thereafter, $t < t' < t + \Delta t$, the total density operator is approximately factorizable with some small correction,

$$\tilde{\rho}(t') \approx \tilde{\rho}_S(t') \otimes \tilde{\rho}_R(t') + \tilde{\rho}_{corr}(t'). \tag{3.39}$$

Provided that $\Delta t \ll \tau_S$, we can neglect $\tilde{\rho}_{corr}$ in the RHS of Eq. (3.37) to leading order, replacing the total density operator by the product of a system and reservoir density operator.

Using the explicit forms for $\tilde{H}_{SR}(t)$ and $\tilde{\rho}(t)$, we will now examine the two terms in Eq. (3.37). The first term, $\Delta\tilde{\rho}_S^{(1)}$, has a straightforward effect on the system,

$$\Delta\tilde{\rho}_S^{(1)} = \frac{1}{i\hbar}\int_t^{t+\Delta t} dt' \ \mathrm{Tr}_R[\hat{S}\hat{F}_R(t')^\dagger + \hat{F}_R(t')\hat{S}^\dagger, \tilde{\rho}_S(t') \otimes \tilde{\rho}_R(t')] \tag{3.40}$$

$$= \frac{1}{i\hbar}\int_t^{t+\Delta t} dt' \ [\hat{S}, \tilde{\rho}_S(t')] \otimes \mathrm{Tr}_R\{\hat{F}_R(t')^\dagger, \tilde{\rho}_R(t')\} + h.c. \tag{3.41}$$

$$= \frac{1}{i\hbar}\int_t^{t+\Delta t} dt' \ [\hat{S}, \tilde{\rho}_S(t')] \otimes 2\langle\hat{F}_R(t')^\dagger\rangle + h.c. \tag{3.42}$$

$$= \frac{1}{i\hbar}\int_t^{t+\Delta t} dt' \ [\underbrace{2\hat{S}\langle\hat{F}_R(t')^\dagger\rangle + 2\hat{S}^\dagger\langle\hat{F}_R(t')\rangle}_{\hat{H}'_S}, \tilde{\rho}_S(t')]. \tag{3.43}$$

Since the reservoir is large and does not change much under the influence of the system, $\langle\hat{F}_R(t')^\dagger\rangle$ is essentially a constant. The effect of the first term may thereby be interpreted an addition to the system Hamiltonian, $\hat{H}_S + \hat{H}'_S$. In many cases including the atom-field interaction, $\langle \hat{F}_R(t')^\dagger \rangle = 0$, and the first term vanishes altogether.

The second term, $\Delta\tilde{\rho}_S^{(2)}$, is responsible for the nontrivial effects of the reservoir. We will evaluate it in terms of two-time correlation functions of the reservoir operators, defined by

$$\begin{aligned}
g^{--}(t',t'') &= \mathrm{Tr}[\hat{F}_R(t')\hat{F}_R(t'')\tilde{\rho}_R] && (3.44)\\
g^{+-}(t',t'') &= \mathrm{Tr}[\hat{F}_R(t')^\dagger\hat{F}_R(t'')\tilde{\rho}_R] && (3.45)\\
g^{-+}(t',t'') &= \mathrm{Tr}[\hat{F}_R(t')\hat{F}_R(t'')^\dagger\tilde{\rho}_R] && (3.46)\\
g^{++}(t',t'') &= \mathrm{Tr}[\hat{F}_R(t')^\dagger\hat{F}_R(t'')^\dagger\tilde{\rho}_R]. && (3.47)
\end{aligned}$$

For example, we can explicitly evaluate one of these correlators for an environment formed by the radiation field, where

$$g^{+-}(t',t'') = \hbar^2 \sum_{j,k} g_j^* g_k \langle \hat{a}_j^\dagger \hat{a}_k \rangle e^{i(\nu_j-\omega)t' - i(\nu_k-\omega)t''}. \tag{3.48}$$

If the radiation field is in a thermal state,$\langle \hat{a}_j^\dagger \hat{a}_k \rangle = \delta_{jk}\bar{n}_j$, so the correlator becomes

$$g^{+-}(t',t'') = \hbar^2 \sum_j |g_j|^2 \bar{n}_j e^{i(\nu_j-\omega)(t'-t'')}. \tag{3.49}$$

The two time correlation function now depends only on the difference in time, $t'' - t' = \tau$, and it is a sharply peaked function of τ whose width corresponds to the reservoir correlation time τ_c. In the limit that the radiation field volume $V \to \infty$, $\tau_c \to 0$, we recover the Wigner-Weisskopf approximation for which the correlator is a delta function in time. Note that for the radiation field, $g^{--} = g^{++} = 0$, and g^{-+} is the same as g^{+-} with $\langle \hat{a}_j^\dagger \hat{a}_j \rangle$ replaced by $\langle \hat{a}_j \hat{a}_j^\dagger \rangle = \langle \hat{a}_j^\dagger \hat{a}_j \rangle + 1$. Expressed in terms of correlation functions, the second term becomes

$$\begin{aligned}
\Delta\tilde{\rho}_S^{(2)} \;=\; & \tfrac{1}{(i\hbar)^2}\int_t^{t+\Delta t} dt' \int_t^{t'} dt'' \Big\{ g^{+-}(t',t'') \left(\hat{S}\hat{S}^\dagger\tilde{\rho}_S - \hat{S}^\dagger\tilde{\rho}_S\hat{S} \right) \\
& + g^{-+}(t',t'') \left(\hat{S}^\dagger\hat{S}\tilde{\rho}_S - \hat{S}\tilde{\rho}_S\hat{S}^\dagger \right) \Big\} + h.c.,
\end{aligned} \tag{3.50}$$

where we have neglected contributions from g^{--} and g^{++}. The only significant time dependence enters through the sharply-peaked correlation functions. In the case of the radiation field we may evaluate the inner integral using the same procedure performed in the Wigner Weisskopf approximation, obtaining

$$
\begin{aligned}
-\frac{1}{\hbar^2}\int_t^{t'} dt'' g^{+-}(t',t'') &= \sum_j \int_t^{t'} |g_j|^2 \bar{n}_j e^{i(\omega-\nu_j)(t''-t')} && (3.51)\\
&= -\pi \sum_j |g_j|^2 \bar{n}_j \delta(\nu_j - \omega) && (3.52)\\
&= -\gamma/2\bar{n}(\omega). && (3.53)
\end{aligned}
$$

Here we have neglected the energy shift arising from the principal part of the integral, because that can be incorporated into the bare system Hamiltonian. As mentioned above, the calculation for g^{-+} proceeds in the same manner, yielding

$$
-\frac{1}{\hbar^2}\int_t^{t'} dt'' g^{-+}(t',t'') = -\gamma/2(\bar{n}(\omega)+1). \qquad (3.54)
$$

The remaining integral may be approximated by $\Delta t\cdot$ integrand because Δt is now small compared to the time variation of the integrand. Dividing through by Δt, we obtain a time-averaged differential equation for $\tilde{\rho}_S$:

$$
\frac{\Delta\tilde{\rho}_S}{\Delta t} = -\frac{\gamma}{2}\bar{n}(\omega)\left(\hat{S}\hat{S}^\dagger\tilde{\rho}_S - \hat{S}^\dagger\tilde{\rho}_S\hat{S}\right) - \frac{\gamma}{2}\left(\bar{n}(\omega)+1\right)\left(\hat{S}^\dagger\hat{S}\tilde{\rho}_S - \hat{S}\tilde{\rho}_S\hat{S}^\dagger\right) + h.c. \qquad (3.55)
$$

This result is known as the "master equation", and it provides an essential tool for studying the evolution of open systems coupled to Markovian reservoirs.

3.3.3 Remarks on the generalized master equation

In the previous lecture we derived the equation governing the evolution of an open system coupled to a Markovian reservoir. In the Schrodinger picture, this so-called master equation takes the form

$$
\begin{aligned}
\frac{\Delta\hat{\rho}_S}{\Delta t} = & -\textstyle\sum_p \frac{\gamma_p}{2}\bar{n}\left(\hat{S}_p\hat{S}_p{}^\dagger\hat{\rho}_S - \hat{S}_p{}^\dagger\hat{\rho}_S\hat{S}_p\right) + h.c.\\
& -\textstyle\sum_p \frac{\gamma_p}{2}\left(\bar{n}+1\right)\left(\hat{S}_p{}^\dagger\hat{S}_p\hat{\rho}_S - \hat{S}_p\hat{\rho}_S\hat{S}_p{}^\dagger\right) + h.c. \qquad (3.56)\\
& +\tfrac{1}{i\hbar}[\hat{H}_S, \hat{\rho}_S].
\end{aligned}
$$

The system time dependence is built into the last term, and we have included a sum over different interactions with the reservoir. Explicitly, the system-reservoir interaction takes the form $\hat{H}_{SR} = \sum_p \hat{S}_p\hat{R}_p^\dagger + h.c.$, and each term has its associated rate γ_p. In order to incorporate multiple system-reservoir interaction terms, we implicitly make an assumption that the different terms are incoherent, so that the interference between them vanishes. While this requirement is satisfied most of the time, one should bear in mind that there exist cases where such interference is important.

Although Eq. (3.56) allows us to efficiently account for the effects of the reservoir, this added information has a price. When only an isolated n-level system need be considered, its evolution is governed by n differential equations for the amplitude of each basis vector. When the effect of the environment is included, the system must be described by $\mathcal{O}(n^2)$ differential equations. The large number of equations can complicate the mathematics, and we will frequently need more sophisticated tools to extract a solution.

One more caveat deserves attention: In our previous derivation, we assumed that the state of the universe was factorizable, i.e.

$$\tilde{\rho}(t') \approx \tilde{\rho}_S(t) \otimes \tilde{\rho}_R(t), \tag{3.57}$$

where $t' - t \leq \Delta t$. We made this statement with little justification, but we will now show that our assumption is valid for a reservoir with no memory, $\tau_c = 0$.

Suppose that the system and reservoir do not interact until a time $t = t_i$, so that for all times prior to t_i the universe density operator is factorizable. At some time $t > t_i$, we may certainly write

$$\tilde{\rho}(t) = \tilde{\rho}_S(t_i) \otimes \tilde{\rho}_R(t_i) + \tilde{\rho}_{corr}(t_i, t) \tag{3.58}$$

where $\tilde{\rho}_{corr}(t_i, t)$ depends on the correlations built up between the system and the reservoir *prior* to the time interval $t \rightarrow t + \Delta t$ for which we calculated the correlations. We will use perturbation theory to estimate the contributions to $\Delta\tilde{\rho}_S = \tilde{\rho}_S(t + \Delta t) - \tilde{\rho}_S(t)$ which we neglected by setting $\tilde{\rho}_{corr}(t_i, t) = 0$. To leading order,

$$\tilde{\rho}_{corr}(t_i, t) \approx \frac{1}{i\hbar} \int_{t_i}^{t} [\tilde{H}_{SR}(t'), \tilde{\rho}_S(t_i) \otimes \tilde{\rho}_R(t_i)], \tag{3.59}$$

so that the neglected change in the system density operator is

$$\Delta\tilde{\rho}_S \propto \int_{t_i}^{t} dt' \int_{t}^{t+\Delta t} dt'' \underbrace{\langle \tilde{H}_{SR}(t'') \tilde{H}_{SR}(t') \rangle}_{\propto\ \delta(t''-t')}. \tag{3.60}$$

Recall that the time correlation function for a reservoir with no memory is a delta function; since the time intervals for integration do not overlap, the delta function is zero everywhere within the region of integration. The contributions to $\Delta\hat{\rho}_S$ due to $\tilde{\rho}_{corr}(t_i, t)$ thus vanish to leading order (and all higher orders) for $\tau_c = 0$. In fact, a more rigorous analysis shows that the corrections scale as τ_c^2.

We have now shown that a reservoir with no memory has a local interaction with the system; that is, it immediately forgets about all previous correlations and depends only on the current state. This amnesia implies irreversibility since information is lost (so entropy must increase). For practical purposes, irreversible vs reversible dynamics will provide our boundary between system and environment. Any part of the environment which exhibits time reversibility we will include in the system even if we are not explicitly interested in its evolution.

We have highlighted two situations where the master equation may not suffice: (1) when there is interference between different interaction terms and (2) when the reservoir interaction is reversible. A more thorough discussion of the assumptions and approximations implicit in the master equation may be found in e.g. Cohen-Tannoudji *et al.*, "Atom-Photon Interactions".

3.3.4 Example: The two-level atom

The master equation is frequently used to describe the evolution of a driven two-level system coupled to a dissipative environment. The coherent interaction with the driving field takes the form

$$\hat{H}_S = -\hbar\delta|2\rangle\langle 2| - \hbar\Omega|1\rangle\langle 2| - \hbar\Omega^*|2\rangle\langle 1|, \tag{3.61}$$

while the reservoir effects enter the density matrix equation:

$$\begin{aligned}\frac{\Delta\hat{\rho}_S}{\Delta t} \;=\; & -\tfrac{\gamma}{2}(\bar{n}+1)\left(\sigma_{22}\hat{\rho}_S - \sigma_{12}\hat{\rho}_S\sigma_{21}\right) + h.c. \\ & -\tfrac{\gamma}{2}\bar{n}\left(\sigma_{11}\hat{\rho}_S - \sigma_{21}\hat{\rho}_S\sigma_{12}\right) + h.c. \\ & +\tfrac{1}{i\hbar}[\hat{H}_S, \hat{\rho}_S],\end{aligned} \tag{3.62}$$

where $\hat{S} = |1\rangle\langle 2| = \sigma_{12}$. Taking the matrix elements yields four differential equations for the components of the density matrix,

$$\dot{\rho}_{22} = -\gamma(\bar{n}+1)\rho_{22} + \gamma\bar{n}\rho_{11} + i\Omega\rho_{21} - i\Omega^*\rho_{12} \tag{3.63}$$

$$\dot{\rho}_{11} = \gamma(\bar{n}+1)\rho_{22} - \gamma\bar{n}\rho_{11} - i\Omega\rho_{21} + i\Omega^*\rho_{12} \tag{3.64}$$

$$\dot{\rho}_{12} = -\frac{\gamma}{2}(2\bar{n}+1)\rho_{12} + i\delta\rho_{12} - i\Omega(\rho_{22} - \rho_{11}) \tag{3.65}$$

$$\dot{\rho}_{21} = -\frac{\gamma}{2}(2\bar{n}+1)\rho_{21} - i\delta\rho_{21} + i\Omega^*(\rho_{22} - \rho_{11}). \tag{3.66}$$

Note that only two of these equations are independent, since the evolution equations must preserve probability, $\rho_{11} + \rho_{22} = \mathrm{Tr}[\hat{\rho}_S] = 1$, and hermiticity, $\rho_{12} = \rho_{21}^*$.

Three types of processes contribute to the system evolution described by Eq. (3.66):

(1) coherent driving $\propto \Omega$,

(2) thermal photons $\propto \gamma\bar{n}$, and

(3) spontaneous emission $\propto \gamma$.

Coherent interactions are characteristic of the ideal two-level system introduced in previous lectures, and come from the system Hamiltonian terms. Thermal photons lead to incoherent transitions in *both* directions, whereas spontaneous emission only allows population in ρ_{22} to leak into ρ_{11}:

$$\begin{aligned} \dot{\rho}_{22} &= \gamma\bar{n}(\rho_{11} - \rho_{22}) - \gamma\rho_{22} + \dots \qquad (3.67) \\ \dot{\rho}_{11} &= \gamma\bar{n}(\rho_{22} - \rho_{11}) + \gamma\rho_{22} + \dots \qquad (3.68) \end{aligned}$$

Although incoherent processes can increase and decrease the populations ρ_{11} and ρ_{22}, they only decrease the off-diagonal terms. The decay rate of the coherences, γ_{12} is related to the rate of population decay out of state $|1\rangle$, $\gamma_1 = \gamma\bar{n}$, and $|2\rangle$, $\gamma_2 = \gamma(\bar{n} + 1)$, with

$$\gamma_{12} = \frac{\gamma_1 + \gamma_2}{2}. \qquad (3.69)$$

This relation holds for any two states and their associated coherence, and only depends on the rates out of the states, not into them.

In general, however, there exist processes which decrease the coherences without affecting the populations. These are typically incorporated phenomenologically into the master equation by setting

$$\gamma_{12} = \frac{\gamma_1 + \gamma_2}{2} + \gamma_d. \qquad (3.70)$$

where γ_d is the so-called decoherence rate. Such decoherence can result from a variety of sources including, for example, finite linewidth of an applied laser field or atom-atom interactions.

3.3.5 Atomic response to a resonant field

We will consider two special cases to gain physical insight into the dynamics of an atom as it undergoes simultaneousmaster coherent and incoherent pumping.

Weak applied field

For sufficiently small applied fields Ω, the master equation can be treated perturbatively. Since the populations change by terms $\propto \Omega^2$, to lowest order we may set $\rho_{11} \approx \rho_{11}^{(0)}, \rho_{22} \approx \rho_{22}^{(0)}$, and consider only the evolution of the coherences,

$$\dot{\rho}_{12} \approx -(\gamma_{12} - i\delta)\rho_{12} + i\Omega(\rho_{11}^{(0)} - \rho_{22}^{(0)}). \tag{3.71}$$

Since this equation is now linear in Ω, we may solve it by taking the Fourier transform of ρ_{12} and Ω,

$$\begin{aligned} \rho_{12}(t) &= \int d(\delta\nu) e^{-i\delta\nu t} \rho_{12}(\delta\nu) && (3.72) \\ \Omega(t) &= \int d(\delta\nu) e^{-i\delta\nu t} \Omega(\delta\nu). && (3.73) \end{aligned}$$

With this substitution, we find that in the weak field limit the coherence at frequency $\delta\nu$ is a Lorentzian with effective detuning $\delta + \delta\nu$:

$$\rho_{12}(\delta\nu) = \Omega(\delta\nu) \frac{i(\rho_{11}^{(0)} - \rho_{22}^{(0)})}{\gamma_{12} + i(\delta + \delta\nu)}. \tag{3.74}$$

This approach may be generalized to multilevel atoms, so that

$$\rho_{ij}(\delta\nu) = \Omega_{ij}(\delta\nu) \frac{i(\rho_{ii}^{(0)} - \rho_{jj}^{(0)})}{\gamma_{ij} + i(\delta_{ij} + \delta\nu)}. \tag{3.75}$$

whenever the populations ρ_{ii} and ρ_{jj} are essentially frozen in time.

Continuous-wave fields of arbitrary strength

When the applied field is constant in time, we expect that the system will undergo Rabi oscillations which are damped by the reservoir interaction. The decay terms drive the system into an equilibrium state after a time $\propto 1/\gamma_{12}$, and a steady-state description of the system is easily found by setting the time derivative of its density matrix elements to zero. Solving for the coherence,

$$\dot{\rho}_{12} = 0 \Rightarrow \rho_{12} = \frac{i\Omega(\rho_{11} - \rho_{22})}{\gamma_{12} - i\delta} \tag{3.76}$$

we then find the steady state population

$$\rho_{22} = \frac{R_{opt}}{\gamma + 2R_{opt}} \tag{3.77}$$

where $R_{opt} = 2|\Omega/\Gamma_{12}|^2$ and $\Gamma_{12} = \gamma_{12} - i\delta$. R_{opt} acts like an incoherent pumping rate associated with the applied (coherent) field.

The pumping rate R_{opt} determines two important limits:

$$R_{opt} \ll \gamma \quad \Rightarrow \quad \rho_{22} \to 0 \tag{3.78}$$

$$R_{opt} \gg \gamma \quad \Rightarrow \quad \rho_{22} \to \frac{1}{2}. \tag{3.79}$$

In the first case, the coherent field is weak, so that the atom ends up in the ground state with unit probability; in this limit, the perturbative weak-field approach is valid. In the second case the applied field leaves the atom in a statistical mixture of the ground and excited states with equal weight.

Note that the weak-field limit is sufficient but not necessary to disregard evolution of the coherences, $\dot{\rho}_{12} = 0$; we only require that $|\Omega|^2 \ll \gamma_{12}^2 + \delta^2$. Solving for ρ_{12} in this fashion is analogous to making an adiabatic approximation that the coherences follow the applied field. The resulting equations for the populations,

$$\dot{\rho}_{22} = -\gamma\rho_{22} + R_{opt}(\rho_{11} - \rho_{22}) \text{ with } \dot{\rho}_{11} = -\dot{\rho}_{22}, \tag{3.80}$$

are known as the "rate equations." They apply in situations when a coherence ρ_{12} is present, but its dynamics are unimportant. For example, the rate equations are used to describe an atom interacting with incoherent radiation, since γ_{12} is very large in this case.

Chapter 4

Stochastic Wavefunctions

This was a guest lecture given by Anders Sørensen on Oct 15, 2003

The master equation is an essential tool for studying the dynamics of a system interacting with its surroundings. In some situations, however, the complexity of the system or the subtlety of interpretation has spurred development of more sophisticated techniques for solving the master equation. One such method makes use of random processes to simulate the system state. We will derive the equations governing the evolution of these stochastic or Monte Carlo wavefunctions, and discuss appropriate applications for this technique.

The Monte Carlo wavefunction was derived simultaneously in the 1990s by two groups interested in very different questions. A group of scientists in France, Dalibard, Castin, and Mølmer, wanted to simulate laser cooling of atoms quantum mechanically in three dimensions. Their numerical solution required discretizing space into a grid of 40x40x40 positions; to implement the master equation on such a space would have required a density matrix with $\mathcal{O}(40^6)$ 10^9 entries – such calculations are beyond the scope of even modern computers. However, simulating a wavefunction with $\mathcal{O}(40^3)$ entries is quite feasible. Consequently the group sought to convert the master equation to something more like the Schrodinger equation.

At the same time, Carmichael was interested the effect that continuous monitoring would have on a system. For example, a two-level atom prepared in an equal superposition of states can decay by emitting a photon; if that photon is detected, the experimenter knows with certainty that the atom is in its ground state. But what happens 50% of the time when a photon is not detected? Certainly, after a long time has passed, the atom must be in its ground state, but how does that happen? To study these and similar questions, Carmichael wanted to incorporate the effects of continous monitoring, and understand how a measurement can cause the system state to suddenly jump into a different state.

The description on which both groups converged begins with the most general form of the master equation,

$$\frac{d\hat{\rho}_S}{dt} = \frac{1}{i\hbar}[\hat{H}_S, \hat{\rho}_S] + \mathcal{L}(\hat{\rho}_S), \tag{4.1}$$

where the Liouvillian operator can be expressed as

$$\mathcal{L}(\hat{\rho}_S) = -\sum_k \frac{\gamma_k}{2}\left(\hat{c}_k^\dagger \hat{c}_k \hat{\rho}_S + \hat{\rho}_S \hat{c}_k^\dagger \hat{c}_k - 2\hat{c}_k \hat{\rho}_S \hat{c}_k^\dagger\right). \tag{4.2}$$

It can be shown that Eq. (4.1) is the most general form for a master equation allowed by physics, and it has the added advantage that it is notationally compact. Since it is the most general form, it must contain the master equation we derived by assuming a certain kind of environment. To see this, identify the (in principle arbitrary) operators $\hat{c}_k$ with

$$\hat{c}_{2k} = \sqrt{\bar{n}+1}\hat{S}_k \tag{4.3}$$

$$\hat{c}_{2k+1} = \sqrt{\bar{n}}\hat{S}_k^\dagger, \tag{4.4}$$

in which case both the decay and absorption terms are included in Eq. (4.1).

Combining Eq. (4.1) with the definition for $\mathcal{L}(\hat{\rho}_S)$, and expanding $\hat{\rho}_S = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$, we can rewrite the master equation in a suggestive form:

$$\begin{aligned} \frac{d\hat{\rho}_S}{dt} &= \tfrac{1}{i\hbar}[\hat{H}_S, \hat{\rho}_S] - \textstyle\sum_k \tfrac{\gamma_k}{2}\left(\hat{c}_k^\dagger \hat{c}_k \hat{\rho}_S + \hat{\rho}_S \hat{c}_k^\dagger \hat{c}_k - 2\hat{c}_k \hat{\rho}_S \hat{c}_k^\dagger\right) \\ &= \textstyle\sum_\alpha \Big(\tfrac{1}{i\hbar}\left(\hat{H}_S - i\hbar\sum_k \tfrac{\gamma_k}{2}\hat{c}_k^\dagger \hat{c}_k\right) p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha| \\ &\quad -\tfrac{1}{i\hbar} p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha| \left(\hat{H}_S + i\hbar\textstyle\sum_k \tfrac{\gamma_k}{2}\hat{c}_k^\dagger \hat{c}_k\right) \\ &\quad + \textstyle\sum_k p_\alpha \gamma_k \hat{c}_k |\psi_\alpha\rangle\langle\psi_\alpha| \hat{c}_k^\dagger\Big). \end{aligned} \tag{4.5}$$

The first two terms rewritten in terms of effective Hamiltonian,

$$\hat{H}_{\text{eff}} = \hat{H}_S - i\hbar\sum_k \frac{\gamma_k}{2}\hat{c}_k^\dagger \hat{c}_k, \tag{4.6}$$

so that the master equation now reads

$$\frac{d\hat{\rho}_S}{dt} = \textstyle\sum_\alpha p_\alpha \Big(\tfrac{1}{i\hbar}\left(\hat{H}_{\text{eff}}|\psi_\alpha\rangle\langle\psi_\alpha| - |\psi_\alpha\rangle\langle\psi_\alpha|\hat{H}_{\text{eff}}^\dagger\right) + \sum_k \gamma_k \hat{c}_k |\psi_\alpha\rangle\langle\psi_\alpha|\hat{c}_k^\dagger\Big). \tag{4.7}$$

The first two terms now begin to resemble the master equation for a pure state evolving according to $\hat{H}_{\text{eff}}$; the final term we will interpret as a "quantum jump" operator which changes $|\psi_\alpha\rangle$ into another state $|\tilde{\phi}_{k,\alpha}\rangle = \hat{c}_k|\psi_\alpha\rangle$ with some probability.

The Schrodinger equation corresponding to the first two terms of Eq. (4.7) is

$$i\hbar\frac{d}{dt}|\psi_\alpha\rangle = \hat{H}_{\text{eff}}|\psi_\alpha\rangle, \tag{4.8}$$

and since we are interested in using Eq. (4.7) to describe a stochastic evolution, we will write it in discrete time,

$$|\tilde{\psi}_\alpha(t+\delta t)\rangle = (1 + \frac{\hat{H}_{\text{eff}}\delta t}{i\hbar}|\psi_\alpha(t)\rangle. \tag{4.9}$$

Note that $|\tilde{\psi}_\alpha(t+\delta t)\rangle$ is not normalized because the effective Hamiltonian is not Hermitian. To lowest order in the small time δt, this state has length

$$\begin{aligned}
\langle\tilde{\psi}_\alpha(t+\delta t)|\tilde{\psi}_\alpha(t+\delta t)\rangle &= \langle\psi_\alpha|(1 - \frac{\hat{H}^\dagger_{\text{eff}}\delta t}{i\hbar})(1 + \frac{\hat{H}_{\text{eff}}\delta t}{i\hbar})|\psi_\alpha\rangle && (4.10)\\
&= \langle\psi_\alpha|\left(1 - \frac{\delta t}{i\hbar}(\hat{H}^\dagger_{\text{eff}} - \hat{H}_{\text{eff}}\right)|\psi_\alpha\rangle && (4.11)\\
&= \langle\psi_\alpha|\left(1 - \delta t\sum_k \gamma_k \hat{c}^\dagger_k \hat{c}_k\right)|\psi_\alpha\rangle. && (4.12)
\end{aligned}$$

To simplify notation, we define

$$\begin{aligned}
\delta p_{k,\alpha} &= \delta t \gamma_k \langle\psi\alpha|\hat{c}^\dagger_k \hat{c}_k|\psi\alpha\rangle && (4.13)\\
\delta p_\alpha &= \delta t \sum_k \gamma_k \langle\psi\alpha|\hat{c}^\dagger_k \hat{c}_k|\psi\alpha\rangle, && (4.14)
\end{aligned}$$

so that the length of the unnormalized state becomes

$$\langle\tilde{\psi}_\alpha(t+\delta t)|\tilde{\psi}_\alpha(t+\delta t)\rangle = 1 - \sum_k \delta p_{k,\alpha} = 1 - \delta p_\alpha. \tag{4.15}$$

We now know the proper normalization for the state at time $t + \delta t$:

$$|\psi_\alpha(t+\delta t)\rangle = \frac{1 + \hat{H}_{\text{eff}}\delta t/i\hbar}{\sqrt{1-\delta p_\alpha}}|\psi_\alpha(t)\rangle. \tag{4.16}$$

This normalized state corresponds the state of a system evolving solely under the influence of the first two terms in the master equation, i.e. a system which has never jumped into one of the $|\tilde{\phi}_{k,\alpha}\rangle$.

As we found for $|\tilde{\psi}_\alpha\rangle$, the "quantum jump" states $|\tilde{\phi}_{k,\alpha}\rangle$ are not normalized, since

$$\langle\tilde{\phi}_{k,\alpha}|\tilde{\phi}_{k,\alpha}\rangle = \langle\psi\alpha|\hat{c}_k^\dagger\hat{c}_k|\psi_\alpha\rangle = \frac{\delta p_{k,\alpha}}{\gamma_k\delta t}. \tag{4.17}$$

Again, we will define a normalized state

$$|\phi_{k,\alpha}\rangle = \sqrt{\frac{\gamma_k\delta t}{\delta p_{k,\alpha}}}|\tilde{\phi}_{k,\alpha}\rangle \tag{4.18}$$

to explicitly keep track of probability conservation.

Like the Schrodinger equation, the master equation may be written for discrete times δt,

$$\hat{\rho}_S(t+\delta t) = \sum_\alpha p_\alpha\Big(|\tilde{\psi}_\alpha(t+\delta t)\rangle\langle\tilde{\psi}_\alpha(t+\delta t)| + \delta t\sum_k \gamma_k|\tilde{\phi}_{k,\alpha}\rangle\langle\tilde{\phi}_{k,\alpha}|\Big), \tag{4.19}$$

and expressed in terms of the normalized states $|\psi_\alpha(t+\delta t)\rangle$ and $|\phi_{k,\alpha}\rangle$,

$$\begin{aligned}\hat{\rho}_S(t+\delta t) \quad = \quad & \textstyle\sum_\alpha p_\alpha\Big((1-\delta p_\alpha)|\psi_\alpha(t+\delta t)\rangle\langle\psi_\alpha(t+\delta t)| \\ & + \textstyle\sum_k \delta p_{k,\alpha}|\phi_{k,\alpha}\rangle\langle\phi_{k,\alpha}|\Big).\end{aligned} \tag{4.20}$$

By rewriting the master equation in this form, we can use a probability interpretation to gain intuition – and develop numerics – for the resulting system dynamics. Eq. (4.20) has two terms, which lead to two possible outcomes after a time δt :

(1) with probability $(1-\delta p_\alpha)$, the system evolves according to $\hat{H}_{\text{eff}}$, and remains in state $|\psi_\alpha\rangle$

(2) with probability δp_α, the system jumps into another state; in particular it jumps into state $|\phi_{k,\alpha}\rangle$ with probability $\delta p_{k,\alpha}$.
This statistical picture of a state vector evolution provides a clear procedure for simulation which only requires computation of the state vector (rather than density matrix) elements. A sample algorithm is summarized in Table (4.1).

As an example of the Monte Carlo Wavefunction method, consider a two level system which starts out in a pure state $|\psi(0)\rangle = a_1|1\rangle + a_2|2\rangle$, and decays at a rate γ so that $\hat{c} = |1\rangle\langle 2|$. In a time δt, the probability that the system jumps out of the superposition state is

$$\begin{aligned}\delta p \quad &= \quad \delta t\gamma\langle\psi|\hat{c}^\dagger\hat{c}|\psi\rangle & (4.21)\\ &= \quad \delta t\gamma|a_2^2|. & (4.22)\end{aligned}$$

Table 4.1: **Monte Carlo Procedure**

(1) Pick initial state $|\psi_\alpha\rangle$
(2) Pick a random number r
(3) For an appropriate time interval δt, calculate δp_α. If $\delta p_\alpha < r$, replace $|\psi_\alpha\rangle$ by $(1 - i\delta t\hat{H}_{\text{eff}}/\hbar)|\psi_\alpha\rangle/\sqrt{1-\delta p_\alpha}$.
If $\sum_{k=1}^{K} \delta p_{k,\alpha} \leq r < \sum_{k=1}^{K+1} \delta p_{k,\alpha}$, replace $|\psi_\alpha\rangle$ by $|\phi_{k,\alpha}\rangle$
(4) Repeat steps (2) and (3) for the desired length of time.
(5) Repeat steps (1) through (4) N times, i.e. until sufficient statistics have been gathered.
(6) If necessary, repeat steps (1) through (5) for all possible initial states $|\psi_\alpha\rangle$.
(7) Density matrix evolution: $\hat{\rho}_S(t) = \sum_\alpha p_\alpha |\psi_\alpha(t)\rangle\langle\psi_\alpha(t)|/N$.

Since δp is just the probability to emit a photon while decaying from $|2\rangle$ to $|1\rangle$, it makes sense that it is equal to the probability to be in the excited state multiplied by the probability for that excited state to decay. If the state does not decay, it evolves according to the effective Hamiltonian

$$\hat{H}_{\text{eff}} = \Delta|2\rangle\langle 2| + \frac{i\gamma}{2}\hat{c}^\dagger\hat{c}. \tag{4.23}$$

Solving the Schrodinger equation,

$$\frac{d}{dt}|\psi\rangle = -\left(\frac{\gamma}{2} + i\Delta\right)|2\rangle \tag{4.24}$$

we may easily find the time-dependent state,

$$|\psi(t)\rangle = \frac{1}{\sqrt{|a_1^2| + |a_2|^2 e^{-\gamma t}}}\left(a_1|1\rangle + a_2 e^{-(\gamma/2+i\Delta)t}|2\rangle\right). \tag{4.25}$$

Due to the normalization terms in the denominator, the probability to be in state $|2\rangle$ decays more slowly than $e^{-\gamma t}$; however, at each step along the way, there is a finite probability to emit a photon and collapse definitely into the ground state. If one averages over all such trajectories, following the Monte Carlo algorithm, one can show that the average population in the excited state does indeed decay as $e^{-\gamma t}$.

However, this picture has physical meaning beyond the statistical average, because it provides an answer to Carmichael's original question: What happens if the atom does not emit a photon? The above analysis shows that *not* detecting a photon is also a measurement on the system, because it causes the state to evolve in a certain way. Due to the normalization condition, at long times the system will always end up in $|1\rangle$ even if it never emits a photon.

Although the statistical wavefunction approach can provide some intuition and computational power, it is only useful in a small subset of calculations. In particular, it is advantageous to use the Monte Carlo method for simulations when

(1) The Hilbert space is so large that density matrix calculations are impossible

(2) One wishes to incorporate measurement-dependent feedback into the system.

Feedback terms are difficult to incorporate into the master equation, but trivial to implement in the Monte Carlo Wavefunction algorithm.

4.1 Non-Hermitian Hamiltonian evolution: summary

The stochastic wavefunction method has two fundamental parts: (1) evolution via the effective, non-Hermitian Hamiltonian, and (2) quantum jumps which occur randomly in time. Although the two parts are easily combined in numerical algorithms, only the first can be simply solved by hand. Nevertheless, in the limit that quantum jumps are very improbable, one might hope to accurately model a system using only the non-Hermitian Hamiltonian evolution. We will often treat a system by solving a non-Hermitian Schrodinger equation and subsequently showing that the integrated probability for a quantum jump is negligible during the time interval under consideration.

For example, consider a two-level system initially in the ground state and illuminated by a weak field Ω. The probability of a quantum jump in this system is $\int dt \gamma \rho_{22} \propto |\Omega|^2$, so to lowest order in the applied field we can neglect quantum jumps and treat the system using the Schrodinger equation with a non-Hermitian Hamiltonian. For this two-level system, the equations of motion obtained from the non-Hermitian Hamiltonian exactly mirror the master equation except for one term: the increase in ρ_{11} due to decay from the excited state is missing. By adding non-Hermitian terms to the Hamiltonian, we have effectively described loss from the system, but we cannot account for where the lost population ends up. To fix this inconsistency quantum jumps are required.