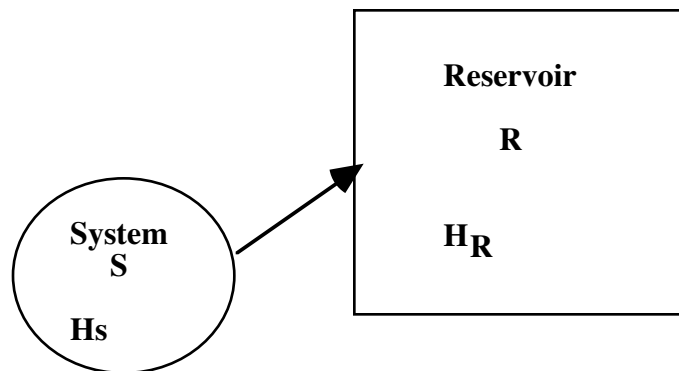


Lecture: Quantum Optics
Derivation of the Master Equation (System/Reservoir Interactions)

General Description of "Open" Quantum Systems

In our discussion of the Optical Bloch Equations we included phenomenological decay constants ($1/T_1$ and $1/T_2$). We accounted for these constants in terms of spontaneous emission, which arises from the coupling of the atom to the vacuum modes of the quantized electromagnetic field. The excitation is irreversibly emitted from the atom into the field, never again to be reabsorbed in a Rabi flop, in contrast to the interaction of an atom with a coherent light source. The evolution of an excited atom "immersed" in the vacuum of the electromagnetic field is a particular example of an "open" quantum system. That is, if all we are interested in is the evolution of the atom, we cannot describe it by a closed system with a finite number of degrees of freedom. Instead, the atom is coupled to the "outside" world (in this case the modes of the vacuum). Generally the outside world will consist of a huge number of degrees of freedom, and therefore we have no hope of following all of them. In fact we might not even know the exact state of the outside world, having only some statistical information to describe it.

One generally describes such a situation as the interaction of a "system" with a "reservoir". The system contains the (few) degrees of freedom we want to follow in detail (for example the internal state of our two level atom), while the reservoir contains the multitude of degrees of freedom associated with the outside world (for example the modes of the electromagnetic field).



We assume that there is some Hamiltonian H_S which describes the evolution of system alone, a Hamiltonian for the reservoir H_R and a Hamiltonian that describes their weak

interaction, H_{SR} , so that the Hamiltonian for the entire (closed) system+reservoir Hilbert space is

$$H_{total} = H_S + H_R + H_{SR}.$$

As the reservoir is supposed to be large it will relax on a very short time scale, and hardly "notices" that the system is interacting with it. On the other hand, the small system is profoundly effected by its coupling to the reservoir. Any excitation of the system which gets coupled to the reservoir is effectively lost forever. In this way, energy is (effectively) irreversibly dissipated into the reservoir, and the entropy of the system increases. This description is familiar in classical statistical mechanics. For example, thermal equilibrium is established when a small system is placed in contact with a "bath" or "reservoir" at some temperature T . There too, one assumes that the reservoir is barely effected by the system, relaxing back to its equilibrium in an infinitesimally short time. Of course this is an approximation. It remains one of the great unsolved problems of theoretical physics to reconcile the second law of thermodynamics, with its intrinsic arrow of time, with the microscopic time-reversible dynamical equations. The problem of dissipation in quantum mechanics has all the same ingredients. The new ingredient is that the reservoir may contain not only thermal fluctuations, but also *quantum* fluctuations associated, so even at absolute zero, the reservoir can cause decay of the excitations of the system.

Because of the dissipative nature of this problem we must turn to the density matrix for a proper description. Suppose at some initial time t the system is placed in contact with the reservoir. Up until that point S and R evolved freely with no coupling, so the total density matrix can be written simply as a product

$$\rho_{total}(t) = \rho_S(t) \otimes \rho_R(t).$$

For any nontrivial interaction, excitations of the system will get "entangled" with the excitations of the reservoir, (see lecture #3 for the definition of entangled states),

$$\rho_{total}(t + \Delta t) \neq \rho_S(t + \Delta t) \otimes \rho_R(t + \Delta t) .$$

Since we are only interested in the system degrees of freedom, without any regard to the state of the reservoir, we trace over the degrees of freedom of the reservoir. The result is a reduced density operator for the system alone,

$$\rho_S(t + \Delta t) = Tr_R(\rho_{total}(t + \Delta t)).$$

Because of the entanglement, even if the initial state of the system were a pure state, at this later time, the reduced density matrix will be a **mixed** state. Thus, the entropy of the system has increased.

Our goal in this lecture is to derive the equation of motion for the reduced density matrix for the system. We start with what we know: the closed system is Hamiltonian, and thus evolves according to the Schrödinger equation (written here in terms of the density operator)

$$\dot{\rho}_{total} = -\frac{i}{\hbar}[H_{total}, \rho_{total}] = -\frac{i}{\hbar}[H_S + H_R, \rho_{total}] - \frac{i}{\hbar}[H_{SR}, \rho_{total}].$$

The equation of motion for the reduced density matrix of the system then follows by taking the trace of this equation over the reservoir variables

$$\dot{\rho}_S = Tr_R(\dot{\rho}_{total}).$$

There are two key ingredients which will go in to our derivation

- The reservoir is large and relatively unaffected by its interaction with the system.
- Any "memory" of an effect S has on R is lost in a time scale much shorter than the time scale that S relaxes. (Stated alternatively, the reservoir is very broadband in frequency).

For concreteness we will specialize to the problem of a two-level atom in contact with a "bath" of electromagnetic blackbody radiation at temperature T. The problem of spontaneous emission in the quantum vacuum is just the particular case T=0.

Two Level Atom Interacting with Thermal Radiation

To make contact with the discussion above we make the following associations:

- System = two level atom
- Reservoir = modes of the electromagnetic field

The total Hamiltonian for S+R is $H_{total} = H_A + H_F + H_{int}$, where

$$\begin{aligned} H_A &= \hbar\omega_{eg}|e\rangle\langle e| = \hbar\omega_{eg}S_+S_- \\ H_F &= \sum_{\mathbf{k},\lambda} \hbar\omega_{\mathbf{k}} \left(a_{\mathbf{k},\lambda}^\dagger a_{\mathbf{k},\lambda} + \frac{1}{2} \right) \\ H_{int} &= -\mathbf{d} \cdot \mathbf{E} \approx -\langle e|\mathbf{d} \cdot \mathbf{E}^{(+)}|g\rangle S_+ - \langle e|\mathbf{d} \cdot \mathbf{E}^{(-)}|g\rangle S_- . \end{aligned}$$

In the expressions above we have used the usual equivalence between our two level atom and a spin 1/2, $S_+ = |e\rangle\langle g|$, $S_- = |g\rangle\langle e|$, and in the interaction Hamiltonian we used the rotating wave approximation, with positive and negative frequency components of the field given in lecture #7. If we substitute the usual normal mode expansion for the electromagnetic field,

$$\mathbf{E}^{(+)}(\mathbf{x}) = -i \sum_{\mathbf{k},\lambda} \sqrt{\frac{2\pi\hbar\omega_{\mathbf{k}}}{V}} \vec{\epsilon}_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} e^{i\mathbf{k} \cdot \mathbf{x}},$$

and take our atom at the origin, then we can express the interaction Hamiltonian as

$$H_{int} = \hbar(FS_+ + F^\dagger S_-), \text{ where } F = -i \sum_{\mathbf{k},\lambda} \sqrt{\frac{2\pi\hbar\omega_{\mathbf{k}}}{V}} \frac{\langle e|\vec{\epsilon}_{\mathbf{k},\lambda} \cdot \mathbf{d}|g\rangle}{\hbar} a_{\mathbf{k},\lambda} = \sum_{\mathbf{k},\lambda} \frac{V_{\mathbf{k},\lambda}}{\hbar} a_{\mathbf{k},\lambda}$$

Here we've defined coupling constants, $V_{\mathbf{k},\lambda} = -i \sqrt{\frac{2\pi\hbar\omega_{\mathbf{k}}}{V}} \langle e|\vec{\epsilon}_{\mathbf{k},\lambda} \cdot \mathbf{d}|g\rangle$. Note, $V_{\mathbf{k},\lambda}$ is nothing more than the dipole interaction energy of the atom with a single photon.

Sometimes we will write $V_{\mathbf{k},\lambda} = \frac{\hbar\Omega_{\mathbf{k},\lambda}}{2}$, where $\Omega_{\mathbf{k},\lambda}$ is the single photon Rabi frequency (think about the factor of 1/2 here).

At the initial time t the atom and field are uncorrelated

$$\rho_{total}(t) = \rho_A(t) \otimes \rho_R(t),$$

The initial state of the atom $\rho_A(t)$ is arbitrary (maybe it's a pure mixture of $|e\rangle$ and $|g\rangle$), and the state of the field is to describe a thermal distribution of photons (blackbody radiation) at some temperature T ,

$$\rho_R(t) = \frac{1}{Z} \exp\left(\frac{-H_R}{k_B T}\right) = \sum_{\mathbf{k},\lambda} P(n_{\mathbf{k},\lambda}) |n_{\mathbf{k},\lambda}\rangle\langle n_{\mathbf{k},\lambda}|,$$

$$Z = Tr \left\{ \exp \left(\frac{-H_R}{k_B T} \right) \right\} = \text{Partition function ,}$$

$$P(n_{\mathbf{k},\lambda}) = \frac{e^{-\hbar\omega_{\mathbf{k}}/k_B T}}{1 - e^{-\hbar\omega_{\mathbf{k}}/k_B T}} = \text{Probability of } n_{\mathbf{k},\lambda} \text{ photons in the mode } (\mathbf{k},\lambda).$$

In other words, the state of the field is described by a canonical ensemble, which in our quantum mechanical language, is a statistical mixture of number-states, weighted by the Boltzman probability factor, normalized by the partition function. The average values of observables are calculated exactly as in classical statistical mechanics. For example, the average number of photons in a mode is,

$$\begin{aligned} \bar{n}(\omega_{\mathbf{k}}) &= Tr(\rho_R a_{\mathbf{k},\lambda}^\dagger a_{\mathbf{k},\lambda}) = \sum_{\mathbf{k},\lambda} P(n_{\mathbf{k},\lambda}) \langle n_{\mathbf{k},\lambda} | a_{\mathbf{k},\lambda}^\dagger a_{\mathbf{k},\lambda} | n_{\mathbf{k},\lambda} \rangle \\ &= \sum_{\mathbf{k},\lambda} P(n_{\mathbf{k},\lambda}) n_{\mathbf{k},\lambda} = \frac{1}{e^{\hbar\omega_{\mathbf{k}}/k_B T} - 1} \quad (\text{Planck Distribution}) \end{aligned}$$

Similarly we find,

$$Tr(\rho_R a_{\mathbf{k},\lambda}) = Tr(\rho_R a_{\mathbf{k},\lambda}^\dagger) = Tr(\rho_R a_{\mathbf{k},\lambda} a_{\mathbf{k}',\lambda'}) = Tr(\rho_R a_{\mathbf{k},\lambda}^\dagger a_{\mathbf{k}',\lambda'}^\dagger) = 0.$$

That is to say, only operators which are diagonal in the number-state basis have a nonzero expectation value. Physically, broadband thermal radiation has a completely random phase. Thus, an operator which depends on the phase has no average value in a thermal state.

Equation of motion for the reduced matrix

In order to remove the trivial free evolution of the atom and field from our problem will we transform into the "interaction picture" via the unitary operator,

$$U^{(I)} = \exp \left\{ -\frac{i}{\hbar} (H_A + H_F) t \right\}. \text{ The density operator, and interaction operator in this picture}$$

are

$$\begin{aligned} \rho_{total}^{(I)}(t) &= U^{(I)\dagger} \rho_{total} U^{(I)} \\ H_{int}^{(I)}(t) &= U^{(I)\dagger} H_{int} U^{(I)} = \hbar \left(F^{(I)}(t) S_+^{(I)}(t) + F^{(I)\dagger}(t) S_-^{(I)}(t) \right), \end{aligned}$$

with $F^{(I)}(t) = \sum_{\mathbf{k}, \lambda} \frac{V_{\mathbf{k}, \lambda}}{\hbar} a_{\mathbf{k}, \lambda} e^{-i\omega_{\mathbf{k}} t}$, $S_+^{(I)}(t) = S_+ e^{-i\omega_{eg} t}$. Using these definitions, and the Liouville equation in the Schrodinger picture, we arrive at the Liouville equation in the interaction picture,

$$\dot{\rho}_{total}^{(I)} = -\frac{i}{\hbar} [H_{int}^{(I)}(t), \rho_{total}^{(I)}(t)]$$

If we integrate this equation from $t \rightarrow t + \Delta t$, we obtain the formal solution,

$$\rho_{total}^{(I)}(t + \Delta t) = \rho^{(I)}(t) - \frac{i}{\hbar} \int_t^{t+\Delta t} dt' [H_{int}^{(I)}(t'), \rho_{total}^{(I)}(t')].$$

This can be iterated over and over to get an infinite series solution. If we terminate this series at some point we get a perturbation solution, good to some order in H_{int} . Since the coupling between the system and reservoir is assumed to be weak will expand only up to second order

$$\begin{aligned} \rho_{total}^{(I)}(t + \Delta t) = & \rho_{total}^{(I)}(t) - \frac{i}{\hbar} \int_t^{t+\Delta t} dt' [H_{int}^{(I)}(t'), \rho_{total}^{(I)}(t)] \\ & - \frac{1}{\hbar^2} \int_t^{t+\Delta t} dt' \int_t^{t'} dt'' [H_{int}^{(I)}(t'), [H_{int}^{(I)}(t''), \rho_{total}^{(I)}(t)]] \end{aligned}$$

Henceforth we will drop the superscript (I), with the understanding that we are operating in the interaction picture.

We seek the dynamics of the reduced density matrix for the atom alone, having traced over the modes of the electromagnetic field,

$$\begin{aligned} \rho_A(t + \Delta t) = & Tr_R(\rho_{total}(t + \Delta t)) \\ = & \rho_A(t) - \frac{i}{\hbar} \int_t^{t+\Delta t} dt' Tr_R([H_{int}(t'), \rho_A(t)\rho_R(t)]) \\ & - \frac{1}{\hbar^2} \int_t^{t+\Delta t} dt' \int_t^{t'} dt'' Tr_R([H_{int}(t'), [H_{int}(t''), \rho_A(t)\rho_R(t)]] \end{aligned}$$

Here we have used the fact that at the initial time the atom and field are uncorrelated so that the total density matrix is a product of the two subsystems. Substituting for $H_{int}(t)$ given

on page 5, we arrive at the following expression, after some tedious algebra, making use of the cyclic property of the trace $\text{Tr}(ABC)=\text{Tr}(CAB)=\text{Tr}(BCA)$,

$$\begin{aligned} \rho_A(t + \Delta t) - \rho_A(t) = & -i \int_t^{t+\Delta t} dt' \left([S_+(t'), \rho_A(t)] \langle F(t') \rangle_R + [S_-(t'), \rho_A(t)] \langle F^\dagger(t') \rangle_R \right) \\ & - \int_t^{t+\Delta t} dt' \int_t^{t'} dt'' \left\{ \left(S_-(t') S_+(t'') \rho_A(t) - S_+(t'') \rho_A(t) S_-(t') \right) \langle F^\dagger(t') F(t'') \rangle_R \right. \\ & + \left(S_+(t') S_-(t'') \rho_A(t) - S_-(t'') \rho_A(t) S_+(t') \right) \langle F(t') F^\dagger(t'') \rangle_R \\ & \left. + H.c. \right\} \\ & + \text{Terms proportional to } \langle F(t_a) F(t_b) \rangle \text{ or } \langle F^\dagger(t_a) F^\dagger(t_b) \rangle. \end{aligned}$$

(Whew!!).

Here, H.c. stands for the Hermitian conjugate to the preceding terms, and $\langle \rangle_R$ is a short hand for the expectation value of some field operator take in the state $\rho_R(t)$ given on page 4, $\langle O \rangle_R \equiv \text{Tr}(O \rho_R)$. Using the definition of $F(t)$, and the fact that the average value of any field operator which depends on the phase of the field vanishes we have,

$$\langle F(t') \rangle_R \equiv \text{Tr}(F(t') \rho_R(t)) = \sum_{\mathbf{k}, \lambda} \frac{V_{\mathbf{k}, \lambda}}{2} e^{-i\omega_{\mathbf{k}} t'} \text{Tr}(\rho_R(t) a_{\mathbf{k}, \lambda}) = 0.$$

Similarly, we find $\langle F^\dagger(t') \rangle_R = \langle F(t_a) F(t_b) \rangle_R = \langle F^\dagger(t_a) F^\dagger(t_b) \rangle_R = 0$. Thus we are left only with the second order terms proportional to $\langle F^\dagger(t_a) F(t_b) \rangle_R$ or $\langle F(t_a) F^\dagger(t_b) \rangle_R$.

Reservoir Correlation Function and the Markov Approximation

Let us define

$$K(t', t'') \equiv \left\langle F^\dagger(t') F(t'') \right\rangle_R,$$

known as the reservoir **correlation function**. Physically this measures how an excitation of the reservoir at time t' is correlated with the excitation at t'' . From general principles, we can immediately see some properties of K .

- Stationary correlations

For a reservoir describing thermal equilibrium the correlations should not depend on any origin of time. That is if we ask how an excitation at t' is correlated with an excitation at $t''=t'+\tau$, the result should only depend on the time difference τ ,

$$K(t', t'') = K(t' - t'') = \left\langle F^\dagger(t' - t'') F(0) \right\rangle_R$$

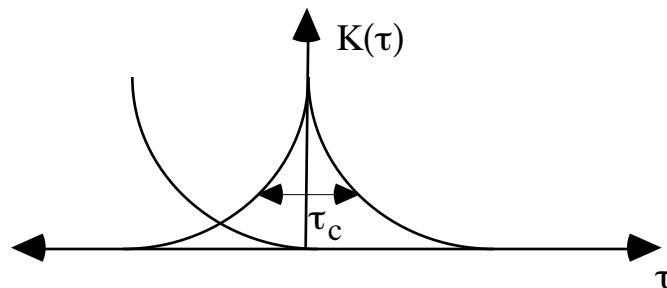
- Time reversal

From the properties of stationarity and the Hermitian conjugate we have

$$K(t'' - t') = \left\langle F^\dagger(t'') F(t') \right\rangle_R = K^*(t' - t'').$$

Thus, the real part of K is symmetric in its argument: $\text{Re}(K(-\tau)) = \text{Re}(K(\tau))$.

From these properties we can make a rough sketch of the of the correlation function



For sufficiently large values of $|\tau|$, the correlation function should approach zero. The characteristic temporal width τ_c is known as the **correlation time**. Physically, it sets the scale of time over which the reservoir relaxes back to thermal equilibrium given some excitation. Figuratively, one often speaks of the correlation time as the time scale over which the reservoir has "memory". After this time the reservoir is back to equilibrium and effectively has no memory that there was any excitation.

One can also define a spectral density of the correlation function by as the Fourier transform

$$S(\omega) \equiv \int d\tau K(\tau) e^{i\omega\tau}.$$

The bandwidth of the reservoir, $\Delta\omega_R$, given by the characteristic width of $S(\omega)$, is related to the correlation time by the usual Fourier duality

$$\tau_c \sim \frac{1}{\Delta\omega_R}.$$

As $\Delta\omega_R \rightarrow \infty$, (i.e. the reservoir is "white noise"), the correlation time $\tau_c \rightarrow 0$. The real part of the correlation function is then proportional to a delta function

$$\text{Re}(K(\tau)) \sim \delta(\tau).$$

Thus a "white-noise" reservoir has no memory; it instantaneously relaxes to its equilibrium value. In general, the correlation time will be very small, but not exactly zero.

The other important time scale in the problem is the time for the system to relax to its equilibrium value as it dissipates energy to the reservoir. If we call this rate of relaxation Γ , then it will generally be the case that $\Gamma \ll \Delta\omega_R$, or equivalently $\tau_c \ll 1/\Gamma$. Furthermore, this inequality is generally so extreme that the reservoir correlation time is effectively zero when compared with the system decay time. We want to study the evolution of the reduced density matrix for the system alone, which changes on a time scale $1/\Gamma$. Thus, we want to look on time scales $\Delta t \ll 1/\Gamma$. On the other hand, this time scale may still be very large compared to the reservoir correlation time. Therefore, we have

$$\tau_c \ll \Delta t \ll 1/\Gamma.$$

Stated alternatively, we want to study the dynamics of the reduced density matrix for the system "coarse-grained" over the reservoir correlation time. In this way we approximate the reservoir as have no memory, and is thus "delta-correlated". Such an approximation is known as the **Markov approximation**. This approximation will allow us to take the time-reversible equations of motion into irreversible equation which give rise to dissipation.

Master Equation in the Markov Approximation

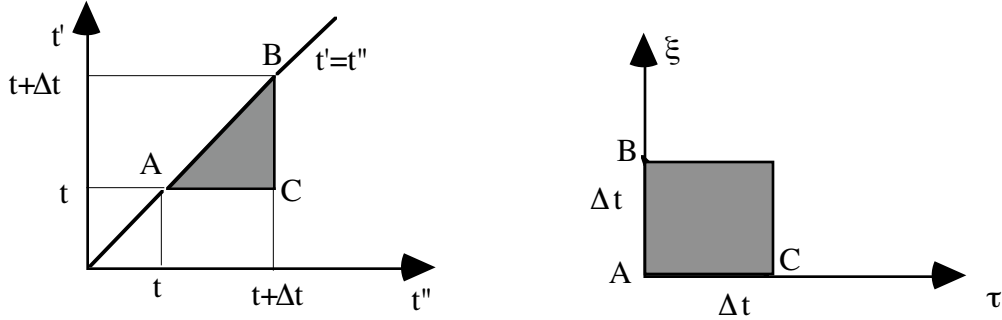
With our characterization of the correlation function for the reservoir forcing function, we make the following change of variables so that, only time differences appear,

$$\tau \equiv t'' - t', \quad \xi \equiv t'' - t.$$

The Jacobian for the change of area element for our two dimensional integral is

$$\frac{\partial(\xi, \tau)}{\partial(t', t'')} = \det \begin{bmatrix} \frac{\partial \xi}{\partial t'} & \frac{\partial \xi}{\partial t''} \\ \frac{\partial \tau}{\partial t'} & \frac{\partial \tau}{\partial t''} \end{bmatrix} = \det \begin{bmatrix} 0 & 1 \\ -1 & 1 \end{bmatrix} = 1.$$

To get the limits of integration we must map the two dimension integration region in the $\{t', t''\}$ plane to the (τ, ξ) plane



Thus, $\int_t^{t+\Delta t} dt' \int_t^{t'} dt'' \rightarrow \int_0^{\Delta t} d\xi \int_0^{\Delta t} d\tau$. The equation for the reduced density operator for the atom

in these new variables becomes

$$\begin{aligned} \rho_A(t + \Delta t) - \rho_A(t) = & - \int_0^{\Delta t} d\xi \int_0^{\Delta t} d\tau \left\{ \left(S_- S_+ \rho_A(t) - S_+ \rho_A(t) S_- \right) e^{i\omega_{eg}\tau} \left\langle F^\dagger(0) F(\tau) \right\rangle_R \right. \\ & + \left(S_+ S_- \rho_A(t) - S_- \rho_A(t) S_+ \right) e^{-i\omega_{eg}\tau} \left\langle F(0) F^\dagger(\tau) \right\rangle_R \\ & \left. + \text{H.c.} \right\}. \end{aligned}$$

Here we have substituted for S_+ and S_- in terms of their simple exponential time dependence.

Now we invoke the Markov approximation. According to the discussion above, the integrand will be nonnegligible only for times τ smaller than the correlation time. As we are coarse graining the dynamics on time scales $\Delta t \gg t_c$, the upper limit of integration over τ is effectively infinity, ($\Delta t \rightarrow \infty$, τ integral). On the other hand, the coarse grained time step is chosen to be much much smaller than the rate at which ρ_A changes, as is therefore, effectively a differential. Under the Markov approximation we have

$$\begin{aligned} \frac{d\rho_A}{dt} &\approx \left(-S_- S_+ \rho_A(t) + S_+ \rho_A(t) S_- \right) \int_0^\infty d\tau e^{i\omega_{eg}\tau} \left\langle F^\dagger(0) F(\tau) \right\rangle_R \\ &+ \left(-S_+ S_- \rho_A(t) + S_- \rho_A(t) S_+ \right) \int_0^\infty d\tau e^{-i\omega_{eg}\tau} \left\langle F(0) F^\dagger(\tau) \right\rangle_R \\ &+ \text{H.c.} \end{aligned}$$

The Fluctuation-Dissipation Theorem

We are left to evaluate the Fourier transforms of the correlation functions. Substituting for the reservoir forcing function $F(t)$ on page 4, gives.

$$\int_0^\infty d\tau e^{i\omega_{eg}\tau} \left\langle F^\dagger(0) F(\tau) \right\rangle_R = \sum_{\mathbf{k}, \lambda, \mathbf{k}', \lambda'} \frac{V_{\mathbf{k}, \lambda}^* V_{\mathbf{k}', \lambda'}}{\hbar^2} \left\langle a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}', \lambda'} \right\rangle_R \int_0^\infty d\tau e^{-i(\omega_{\mathbf{k}} - \omega_{eg})\tau}.$$

We found on page 5, $\left\langle a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}', \lambda'} \right\rangle_R = \bar{n}(\omega_{\mathbf{k}}) \delta_{\mathbf{k}, \mathbf{k}'} \delta_{\lambda, \lambda'}$, so that

$$\int_0^\infty d\tau e^{i\omega_{eg}\tau} \left\langle F^\dagger(0) F(\tau) \right\rangle_R = \sum_{\mathbf{k}, \lambda} \frac{|V_{\mathbf{k}, \lambda}|^2}{\hbar^2} \bar{n}(\omega_{\mathbf{k}}) \int_0^\infty d\tau e^{-i(\omega_{\mathbf{k}} - \omega_{eg})\tau}.$$

The next step in obtaining irreversible equations of motion is to let the reservoir consist of an uncountable infinite (i.e. continuous) number of degrees of freedom. Under this approximation the sum over reservoir modes goes to an integral over the density of modes $D(\omega_{\mathbf{k}})$,

$$\int_0^\infty d\tau e^{i\omega_{eg}\tau} \left\langle F^\dagger(0) F(\tau) \right\rangle_R = \sum_{\lambda} \int d\omega_{\mathbf{k}} \frac{|V_{\lambda}(\omega_{\mathbf{k}})|^2}{\hbar^2} D(\omega_{\mathbf{k}}) \bar{n}(\omega_{\mathbf{k}}) \int_0^\infty d\tau e^{-i(\omega_{\mathbf{k}} - \omega_{eg})\tau}.$$

Finally, it remains to evaluate the integral over τ . In order to do this we add convergence factor $e^{-\varepsilon\tau}$, and then take the limit as $\varepsilon \rightarrow 0$,

$$\begin{aligned}\lim_{\varepsilon \rightarrow 0} \int_0^{\infty} d\tau e^{-i(\omega_{\mathbf{k}} - \omega_{eg} - i\varepsilon)\tau} &= \lim_{\varepsilon \rightarrow 0} \frac{1}{i(\omega_{\mathbf{k}} - \omega_{eg}) + \varepsilon} \\ &= \lim_{\varepsilon \rightarrow 0} \frac{\varepsilon}{(\omega_{\mathbf{k}} - \omega_{eg})^2 + \varepsilon^2} - i \lim_{\varepsilon \rightarrow 0} \frac{\omega_{\mathbf{k}} - \omega_{eg}}{(\omega_{\mathbf{k}} - \omega_{eg})^2 + \varepsilon^2}.\end{aligned}$$

The real part is a Lorentzian, which in the limit $\varepsilon \rightarrow 0$, becomes a delta function whose area is π ,

$$\lim_{\varepsilon \rightarrow 0} \frac{\varepsilon}{(\omega_{\mathbf{k}} - \omega_{eg})^2 + \varepsilon^2} = \pi \delta(\omega_{\mathbf{k}} - \omega_{eg}).$$

In this limit, the imaginary part become Cauchy's "principle part",

$$\lim_{\varepsilon \rightarrow 0} \frac{\omega_{\mathbf{k}} - \omega_{eg}}{(\omega_{\mathbf{k}} - \omega_{eg})^2 + \varepsilon^2} = \mathbf{P} \left(\frac{1}{\omega_{\mathbf{k}} - \omega_{eg}} \right),$$

defined, like the delta function, by its effect integration

$$\int dx \mathbf{P} \left(\frac{1}{x} \right) f(x) \equiv \lim_{\varepsilon \rightarrow 0} \left[\int_{-\infty}^{-\varepsilon} dx + \int_{\varepsilon}^{\infty} dx \right] \frac{f(x)}{x}.$$

In other words, the principle part allows one to exclude the singularity at $x=0$. Thus,

$$\int_0^{\infty} d\tau e^{-i(\omega_{\mathbf{k}} - \omega_{eg})\tau} = \pi \delta(\omega_{\mathbf{k}} - \omega_{eg}) - i \mathbf{P} \left(\frac{1}{\omega_{\mathbf{k}} - \omega_{eg}} \right).$$

Plugging this into the equation of motion for the reduced density matrix

$$\begin{aligned}\int_0^{\infty} d\tau e^{i\omega_{eg}\tau} \left\langle F^\dagger(0)F(\tau) \right\rangle_R &= \frac{1}{2} \sum_{\lambda} \frac{2\pi}{\hbar^2} |V_{\lambda}(\omega_{eg})|^2 D(\omega_{eg}) \bar{n}(\omega_{eg}) \\ &\quad - \frac{i}{\hbar} \mathbf{P} \int d\omega_{\mathbf{k}} \frac{|V_{\lambda}(\omega_{\mathbf{k}})|^2}{\hbar\omega_{\mathbf{k}} - \hbar\omega_{eg}} D(\omega_{\mathbf{k}}) \bar{n}(\omega_{\mathbf{k}}).\end{aligned}$$

We recognize the real part of this expression as the transition rate for the perturbation Hamiltonian as given by Fermi's Golden rule. In fact, if we separate off the factor $\bar{n}(\omega_{eg})$,

then the remaining coefficient is nothing more than the spontaneous emission coefficient (the Einstein A-coefficient) calculated in lecture #8!

$$\Gamma = \sum_{\lambda} \frac{2\pi}{\hbar^2} |V_{\lambda}(\omega_{eg})|^2 D(\omega_{eg}).$$

The imaginary part consists of a square of the coupling strength divided by an energy denominator. This is recognizable as the correction to the energy levels of the free atom due to the light field as given by second order perturbation theory,

$$\delta E_{light} = P \int d\omega_{\mathbf{k}} \frac{|V_{\lambda}(\omega_{\mathbf{k}})|^2}{\hbar\omega_{\mathbf{k}} - \hbar\omega_{eg}} D(\omega_{\mathbf{k}}) \bar{n}(\omega_{\mathbf{k}}).$$

This energy shift is known as the "light-shift" and will typically be a small fraction of the energy separation between the ground and excited states. Putting this all together,

$$\int_0^{\infty} d\tau e^{i\omega_{eg}\tau} \langle F^{\dagger}(0)F(\tau) \rangle_R = \frac{1}{2} \bar{n} \Gamma - \frac{i}{\hbar} \delta E_{light},$$

where \bar{n} is the Planck distribution evaluated at the resonance frequency of the atom and temperature of the reservoir,

$$\bar{n} \equiv \bar{n}(\omega_{eg}) = \frac{1}{\exp(\hbar\omega_{eg} / k_B T) - 1}.$$

The calculation for the Fourier transform of the correlation function $\langle F(0)F^{\dagger}(\tau) \rangle_R$ follows in exactly the same manner. The only difference is that when we substitute for the reservoir function in terms of the normal mode expansion we have the reservoir average,

$$\langle a_{\mathbf{k},\lambda} a_{\mathbf{k}',\lambda'}^{\dagger} \rangle_R = (\bar{n}(\omega_{\mathbf{k}}) + 1) \delta_{\mathbf{k},\mathbf{k}'} \delta_{\lambda,\lambda'}.$$

The factor of 1 comes from the commutator of $a_{\mathbf{k},\lambda}$ and $a_{\mathbf{k}',\lambda'}^{\dagger}$, and thus represents the effects of *vacuum fluctuations*. After carrying through the calculation one finds,

$$\int_0^{\infty} d\tau e^{-i\omega_{eg}\tau} \left\langle F(0)F^\dagger(\tau) \right\rangle_R = \frac{1}{2}(\bar{n} + 1)\Gamma + \frac{i}{\hbar}\delta E_{light} + \frac{i}{\hbar}\delta E_{vac},$$

where $\delta E_{vac} = \mathcal{P} \int d\omega_{\mathbf{k}} \frac{|V_\lambda(\omega_{\mathbf{k}})|^2}{\hbar\omega_{\mathbf{k}} - \hbar\omega_{eg}} D(\omega_{\mathbf{k}})$ is the energy shift due to the vacuum. This is one of the contributions to the famous Lamb shift of quantum electrodynamics. We do not get the full Lamb shift in this calculation as we have treated the atom in a nonrelativistically.

If we look at the real part of the correlation functions is time, we have

$$\begin{aligned} \text{Re} \left\langle F^\dagger(0)F(\tau) \right\rangle_R &= \frac{1}{2}\Gamma\bar{n}\delta(\tau), \\ \text{Re} \left\langle F(0)F^\dagger(\tau) \right\rangle_R &= \frac{1}{2}\Gamma(\bar{n} + 1)\delta(\tau). \end{aligned}$$

These have the characteristic "delta-correlations" associated with the Markov approximation as discussed above. In addition we see that the "strength" of the correlations, given by the area under the correlation function is proportional to the decay constant Γ . This is an important result, originally derived by Einstein in the context of classical Brownian motion, which relates the strength of the fluctuations of the reservoir to the damping constant of the system. This is known as the **fluctuation-dissipation** theorem.

The Master Equation for thermal radiation

Having determined the Fourier transform of the correlation functions we can write the equation of motion for the reduced density matrix. Recall that were operating in the interaction picture. We return to the Schrodinger picture at this state by restoring the free atom evolution. Plugging in for the correlation functions, and including the H.c. terms,

$$\begin{aligned} \frac{d\rho_A}{dt} &= -\frac{i}{\hbar}[H'_A, \rho_A] - \frac{\Gamma}{2}\bar{n}\{S_-S_+, \rho_A\} + \Gamma\bar{n}S_+\rho_AS_- \\ &\quad - \frac{\Gamma}{2}(\bar{n} + 1)\{S_+S_-, \rho_A\} + \Gamma(\bar{n} + 1)S_-\rho_AS_+. \end{aligned}$$

Here $\{ , \}$ is the anticommutator, and

$$H'_A = (\hbar\omega_{eg} - \delta E_{light})S_+S_- + (\delta E_{light} + \delta E_{vac})S_-S_+$$

$$= (\hbar\omega_{eg} - \delta E_{light})|e\rangle\langle e| + (\delta E_{light} + \delta E_{vac})|g\rangle\langle g|$$

is the renormalized atomic Hamiltonian, including the energy level shifts due to the light-shift and the vacuum shift. Using the definition of the S_+ and S_- we can write the equations of motion for the matrix elements of ρ_A ,

$$\begin{aligned}\dot{\rho}_{ee} &= \langle e|\dot{\rho}_A|e\rangle = -\Gamma(\bar{n} + 1)\rho_{ee} + \Gamma\bar{n}\rho_{gg} \\ \dot{\rho}_{gg} &= \langle g|\dot{\rho}_A|g\rangle = -\Gamma\bar{n}\rho_{gg} + \Gamma(\bar{n} + 1)\rho_{ee} \\ \dot{\rho}_{eg} &= \langle e|\dot{\rho}_A|g\rangle = -i(\omega'_{eg} - i\frac{\Gamma}{2}(\bar{n} + 1))\rho_{eg}\end{aligned}$$

Note that $\dot{\rho}_{ee} + \dot{\rho}_{gg} = 0$, so the trace of the density matrix is preserved. The first two equations are nothing more than Einstein's rate equation, with the contributions of stimulated absorption and emission, as well as spontaneous emission evident. The third equation tells us how the coherence in the superposition of excited and ground states decays. The steady state solution is immediately found by setting the right hand side to zero,

$$\begin{aligned}\rho_{eg} &= 0 \\ \frac{\rho_{ee}}{\rho_{gg}} &= \frac{\bar{n}}{\bar{n} + 1} = \left(\frac{1}{\exp(\hbar\omega_{eg}/k_B T) - 1} \right) \left(\frac{1}{\exp(\hbar\omega_{eg}/k_B T) - 1} + 1 \right)^{-1} = \exp(-\hbar\omega_{eg}/k_B T)\end{aligned}$$

The coherences decay to zero, while the populations reach a steady state distribution which is a thermal Boltzmann distribution

$$\frac{\rho_{ee}}{\rho_{gg}} = \frac{e^{-E_e/k_B T}}{e^{-E_g/k_B T}} = e^{-(E_e - E_g)/k_B T} = e^{-\hbar\omega_{eg}/k_B T}.$$

Thus, we come to the physically appealing solution that, in steady state, the atom comes into thermal equilibrium with the "bath" of thermal radiation, and can be written as a canonical ensemble at the same temperature T as the reservoir.

$$\text{Steady State: } \rho_A = \frac{e^{-H_A/k_B T}}{Z}.$$

We have come full circle to the solution derived by Einstein. He assumed a thermal distribution and rate equations, and was able to derive a relation between the spontaneous

and stimulated emission coefficients. We assume only fundamental interactions of absorption and emission, and were able to derive the coefficients, and the steady state thermal distribution which results.

The connection between system-reservoir interactions and quantum measurement

We see that even if the initial state of the atom were a pure state coherent superposition of excited and ground states, in steady state it will "decohere", i.e. decay, into a statistically mixed state with no phase coherence. Phase coherence was lost in the $|e\rangle |g\rangle$ basis because of the form of the S-R coupling and the fact that the state reservoir had a random phase. The loss of phase coherence due the interaction with the reservoir is the central feature of this problem. In general a measuring device, in Bohr's sense of a macroscopic classical apparatus, can be thought of as a reservoir, which will thus act to decohere a pure state into a mixed state. The mixed state is a classical ensemble of possibilities, "e" or "g" as opposed to the quantum superposition where the atom has the "potential" for being measured "e" or "g". This decoherence can be thought of as the mystical "collapse" of the wave function, which projects a wave function onto an eigenstate of a the observable being measured. Here the collapse is seen as a decoherence from a pure state to a mixed state. We can never, within the confines of the quantum mechanical formalism, describe the evolution of an individual member of the ensemble. Thus this result must only be interpreted in a statistical sense of the evolution of an ensemble.

The Master Equation for an Atom in the Vacuum, with a Coherent Driving Field

The case of the atomic damping due to the electromagnetic vacuum is already contained in our solution. It is the particular case of a zero temperature reservoir with zero average photon number $\bar{n} = 0$. In the absence of any other field, the Master equation becomes

$$\begin{aligned} \frac{d\rho_A}{dt} &= -\frac{i}{\hbar}[H'_A, \rho_A] - \frac{\Gamma}{2}\{S_+S_-, \rho_A\} + \Gamma S_- \rho_A S_+ \\ &= -i\omega'_{eg}[S_+S_-, \rho_A] - \frac{\Gamma}{2}\{S_+S_-, \rho_A\} + \Gamma S_- \rho_A S_+. \end{aligned}$$

The evolution of the matrix elements can be written immediately,

$$\begin{aligned} \dot{\rho}_{ee} &= -\dot{\rho}_{gg} = -\Gamma\rho_{ee} \\ \dot{\rho}_{eg} &= \dot{\rho}_{ge}^* = -i(\omega'_{eg} - \frac{\Gamma}{2})\rho_{eg}. \end{aligned}$$

Thus we have justified our phenomenological decay constants $1/T_1$ and $1/T_2$ from lecture 5.

Notice that the anticommutator term in the Master equation has the same form as the atomic Hamiltonian term. It is sometimes useful to define an effective *nonHermitian* atomic Hamiltonian

$$H_A^{eff} \equiv \left(\hbar\omega'_{eg} - i\frac{\Gamma}{2} \right) S_+ S_- = \left(\hbar\omega'_{eg} - i\frac{\Gamma}{2} \right) |e\rangle\langle e|.$$

The master equation can then be written,

$$\frac{d\rho_A}{dt} = -\frac{i}{\hbar} [H_A^{eff}, \rho_A]' + \Gamma S_- \rho_A S_+,$$

where $[H_A^{eff}, \rho_A]' \equiv H_A^{eff} \rho_A - \rho_A H_A^{eff\dagger}$, so that ρ_A is Hermitian. Thus, the anticommutator term accounts for decay of the excited state, while the second is a "feeding" term which accounts for the replenishing of the ground state when the atom makes a "quantum jump" from the excited state into the ground state. This division of the relaxation effects into decay and quantum jumps is useful for numerical solutions to the master equation. One can simulate the "trajectory" of the atom initially in the excited state by a deterministic decay by the nonHermitian Hamiltonian, followed by a quantum jump. Averaging over many realization of this random event gives the solution. This method is known as the **quantum Monte-Carlo wave function simulation** and very useful for extremely large problems where there are too many matrix elements to solve for using more traditional techniques.

If we want to study the evolution of the atom in the presence of a classical, coherent, driving field, such as a monochromatic laser, but also including spontaneous emission, we need only include the dipole Hamiltonian for the atom-field interaction H_{int} ,

$$\frac{d\rho_A}{dt} = -\frac{i}{\hbar} [H'_A, \rho_A] - \frac{i}{\hbar} [H_{int}, \rho_A] - \frac{\Gamma}{2} \{S_+ S_-, \rho_A\} + \Gamma S_- \rho_A S_+.$$

Then in the rotating frame, and using the rotating-wave approximation, we arrive at the equations for the evolution of the matrix elements,

$$\begin{aligned} \dot{\rho}_{ee} &= -\dot{\rho}_{gg} = -\Gamma \rho_{ee} + i\frac{\Omega}{2} (\tilde{\rho}_{ge} - \tilde{\rho}_{eg}) \\ \dot{\tilde{\rho}}_{ge} &= \dot{\tilde{\rho}}_{eg}^* = -i(\Delta - i\frac{\Gamma}{2}) \rho_{eg} + i\frac{\Omega}{2} (\rho_{ee} - \rho_{gg}). \end{aligned}$$

This is the standard master equation for the two level atom that we have been studying for many weeks.