Lecture 16: Equations of motion of a two-level atom interacting with a quantized electromagnetic field

- Heisenberg's equations of motion
- Markov approximation

Heisenberg's equations of motion: Now that we have an idea about the basic structure behind quantizing the electromagnetic field in the presence of sources, we can look at some simple, but nevertheless important, examples. In this lecture, we will be looking at the interaction of a two-level atom with the quantized electromagnetic field. All studies of the dynamics of interactions have to begin with the Hamiltonian which we write, on recalling Eqs. (2.18) and (15.9), as

$$\hat{H} = \sum_\lambda \hbar\omega_\lambda \hat{a}_\lambda^\dagger \hat{a}_\lambda + \frac{1}{2}\hbar\omega_A\hat{\sigma}_z - \left[\hat{\sigma}^\dagger \hat{\mathbf{E}}^{(+)}(\mathbf{r}_A)\cdot\mathbf{d} + \text{h.c.}\right] . \qquad (16.1)$$

Here we have introduced the operators $\hat{\sigma} \equiv |g\rangle\langle e|$ and $\hat{\sigma}_z \equiv |e\rangle\langle e| - |g\rangle\langle g|$ where $|g\rangle$ and $|e\rangle$, the eigenstates of the Hamiltonian of the free atom, denote the ground and excited states of the two-level atom, respectively. The atomic transition frequency ω_A is just the difference between the corresponding eigenfrequencies ω_e and ω_g. Note that we kept in Eq. (16.1) only the resonant (energy-conserving) terms of the interaction Hamiltonian.

The atomic flip operators fulfil the algebra of angular momentum operators. To see that, we form the linear combinations $\hat{\sigma}_x = \hat{\sigma} + \hat{\sigma}^\dagger = |g\rangle\langle e| + |e\rangle\langle g|$ and $\hat{\sigma}_y = i(\hat{\sigma} - \hat{\sigma}^\dagger)$ $= i(|g\rangle\langle e| - |e\rangle\langle g|)$. These operators then obey the commutation rules

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k , \qquad i,j,k \in \{x,y,z\} . \qquad (16.2)$$

Other useful commutation rules are

$$[\hat{\sigma}, \hat{\sigma}_z] = 2\hat{\sigma} , \quad \left[\hat{\sigma}^\dagger, \hat{\sigma}_z\right] = -2\hat{\sigma}^\dagger , \quad \left[\hat{\sigma}, \hat{\sigma}^\dagger\right] = -\hat{\sigma}_z . \qquad (16.3)$$

The equations of motion of the atomic and photonic mode operators can be obtained from Heisenberg's equations of motion which, for an arbitrary operator $\hat{O}$, read

$$\dot{\hat{O}} = \frac{1}{i\hbar}\left[\hat{O}, \hat{H}\right] . \qquad (16.4)$$

For the operator $\hat{\sigma}_z$ (the 'population inversion' operator), we obtain

$$\dot{\hat{\sigma}}_z = \frac{1}{i\hbar}\left[\hat{\sigma}_z, \hat{H}\right] = \frac{i}{\hbar}\hat{\mathbf{E}}^{(+)}(\mathbf{r}_A)\cdot\mathbf{d}\left[\hat{\sigma}_z, \hat{\sigma}^\dagger\right] + \text{h.c.} \qquad (16.5)$$

which, on using the commutation rules (16.3) for the atomic operators, becomes

$$\boxed{\dot{\hat{\sigma}}_z = \frac{2i}{\hbar}\hat{\sigma}^\dagger \hat{\mathbf{E}}^{(+)}(\mathbf{r}_A)\cdot\mathbf{d} + \text{h.c.}}\,. \tag{16.6}$$

Similarly, we obtain for the atomic flip operator,

$$\dot{\hat{\sigma}} = \frac{1}{i\hbar}\left[\hat{\sigma},\hat{H}\right] = -\frac{i}{2}\omega_A\left[\hat{\sigma},\hat{\sigma}_z\right] + \frac{i}{\hbar}\left[\hat{\sigma},\hat{\sigma}^\dagger\right]\hat{\mathbf{E}}^{(+)}(\mathbf{r}_A)\cdot\mathbf{d} \tag{16.7}$$

which, on using the relations (16.3), becomes

$$\boxed{\dot{\hat{\sigma}} = -i\omega_A\hat{\sigma} - \frac{i}{\hbar}\hat{\sigma}_z\hat{\mathbf{E}}^{(+)}(\mathbf{r}_A)\cdot\mathbf{d}}\,. \tag{16.8}$$

Finally, for the photonic mode operators we get [recall the mode expansion for the electric field, Eq. (2.13)]

$$\boxed{\dot{\hat{a}}_\lambda = -i\omega_\lambda\hat{a}_\lambda + \frac{\omega_\lambda}{\hbar}\mathbf{A}_\lambda^*(\mathbf{r}_A)\cdot\mathbf{d}^*\hat{\sigma}}\,. \tag{16.9}$$

The three equations (16.6), (16.8) and (16.9) are the basis of everything that follows from now on. They are coupled differential operator equations and not solvable in closed form. Instead, we have to resort to approximations.

Markov approximation: We can attempt to solve Eq. (16.9) by formally integrating it,

$$\hat{a}_\lambda(t) = e^{-i\omega_\lambda t}\hat{a}_\lambda + \frac{\omega_\lambda}{\hbar}\mathbf{A}_\lambda^*(\mathbf{r}_A)\cdot\mathbf{d}^*\int_0^t dt'\, e^{-i\omega_\lambda(t-t')}\hat{\sigma}(t')\,. \tag{16.10}$$

The first term in Eq. (16.10) is the free evolution of the photonic mode operator whereas the second term describes the influence of the interaction. The temporal integral is of course tricky since we do not know the temporal evolution of the atomic flip operators. Nevertheless, we can approximate the integral using the rotating-wave approximation in which we assume that the flip operators consist of a slowly varying part and a rapidly oscillating contribution that evolves with ω_A [see Eq. (16.8)], $\hat{\sigma}(t') = \tilde{\hat{\sigma}}(t')e^{-i\omega_A t'}$. Then we take the slow envelope $\tilde{\hat{\sigma}}$ out of the integral at the upper time t and replace it with its full operator function, $\tilde{\hat{\sigma}}(t) = e^{i\omega_A t}\hat{\sigma}(t)$,

$$\int_0^t dt'\, e^{-i\omega_\lambda(t-t')}\hat{\sigma}(t') = \int_0^t dt'\, e^{-i\omega_\lambda(t-t')}e^{-i\omega_A t'}\tilde{\hat{\sigma}}(t')$$

$$\approx \tilde{\hat{\sigma}}(t)\int_0^t dt'\, e^{-i\omega_\lambda(t-t')}e^{-i\omega_A t'} = \hat{\sigma}(t)\int_0^t dt'\, e^{i(\omega_A-\omega_\lambda)(t-t')}\,. \tag{16.11}$$

Such an approximation in which information of past times has been erased and only information about the present time is kept is also called the *Markov approximation*.

The integral itself can be easily solved and gives

$$\int_0^t dt'\, e^{i(\omega_A-\omega_\lambda)(t-t')} = \frac{\sin(\omega_A-\omega_\lambda)t}{\omega_A-\omega_\lambda} + i\frac{[1-\cos(\omega_A-\omega_\lambda)t]}{\omega_A-\omega_\lambda} \equiv s(\omega_A-\omega_\lambda)+ic(\omega_A-\omega_\lambda)$$

which we have for convenience split into its real and imaginary parts. The function $s(\omega_A-\omega_\lambda)$ is sharply peaked at $\omega_A=\omega_\lambda$ (see Fig. 22). Away from this value it oscillates rapidly. If all

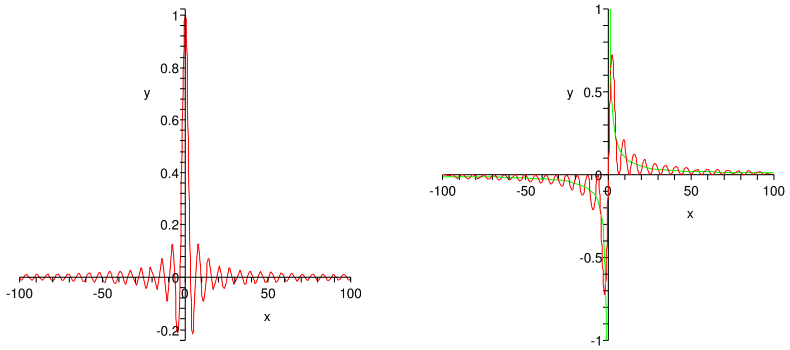

FIG. 22: Functions $s(x)=\sin x/x$ (left figure) and $c(x)=(1-\cos x)/x$ (right figure) showing how they can be approximated by the functions $\pi\delta(x)$ and $\mathcal{P}(1/x)$, respectively.

quantities that contain this function are averaged (or cannot be resolved) over sufficiently long times, then $s(\omega_A-\omega_\lambda)$ can be replaced by $\pi\delta(\omega_A-\omega_\lambda)$ whereby introducing only little error. Similarly, the function $c(\omega_A-\omega_\lambda)$ can be replaced by $\mathcal{P}(\omega_A-\omega_\lambda)^{-1}$ where $\mathcal{P}$ denotes the principal value.

If we insert the formal solution (16.10) in the Markov approximation back into the mode expansion for the electric field we get

$$\hat{\mathbf{E}}^{(+)}(\mathbf{r}_A,t) = \hat{\mathbf{E}}^{(+)}_{\text{free}}(\mathbf{r}_A,t) + i\sum_\lambda \frac{\omega_\lambda^2}{\hbar}\left[\mathbf{A}_\lambda(\mathbf{r}_A)\otimes\mathbf{A}^*_\lambda(\mathbf{r}_A)\right]\cdot\mathbf{d}^*\hat{\sigma}(t)\left[s(\omega_A-\omega_\lambda)+ic(\omega_A-\omega_\lambda)\right] \tag{16.12}$$

where $\hat{\mathbf{E}}_{\text{free}}(\mathbf{r}_A,t)$ denotes the freely evolving electric field operator. Finally, we insert Eq. (16.12) into the equations of motion for the atomic operators and we obtain

$$\dot{\hat{\sigma}}_z = -\Gamma\left(1+\hat{\sigma}_z\right) + \frac{2i}{\hbar}\hat{\sigma}^\dagger\hat{\mathbf{E}}^{(+)}_{\text{free}}(\mathbf{r}_A)\cdot\mathbf{d} - \frac{2i}{\hbar}\hat{\sigma}\hat{\mathbf{E}}^{(-)}_{\text{free}}(\mathbf{r}_A)\cdot\mathbf{d}^* \tag{16.13}$$

and

$$\dot{\hat{\sigma}} = -i(\omega_A + \delta\omega)\hat{\sigma} - \frac{\Gamma}{2}\hat{\sigma} - \frac{i}{\hbar}\hat{\sigma}_z \hat{\mathbf{E}}^{(+)}_{\text{free}}(\mathbf{r}_A) \cdot \mathbf{d} \,. \tag{16.14}$$

Here we have defined the symbols

$$\boxed{\Gamma = \frac{2\pi}{\hbar^2} \sum_\lambda \omega_\lambda^2 |\mathbf{A}_\lambda(\mathbf{r}_A) \cdot \mathbf{d}|^2 \delta(\omega_A - \omega_\lambda)} \tag{16.15}$$

and

$$\boxed{\delta\omega = \frac{1}{\hbar^2} \sum_\lambda \mathcal{P}\left(\frac{\omega_\lambda^2}{\omega_A - \omega_\lambda}\right) |\mathbf{A}_\lambda(\mathbf{r}_A) \cdot \mathbf{d}|^2} \tag{16.16}$$

whose significance we will discuss soon.

The Eqs. (16.13) and (16.14) are effective equations of motion for the atomic flip operators which do not depend on the photonic variables anymore. The operators $\hat{\mathbf{E}}^{(+)}_{\text{free}}(\mathbf{r}_A)$ describe freely evolving fields such as external laser fields that are used to manipulate the atom.

Lecture 17: Spontaneous decay and the Lamb shift

- Spontaneous decay
- Lamb shift
- Modified spontaneous decay

Spontaneous decay: We have seen that, after employing the Markov approximation to eliminate the photonic variables, the equation of motion of the population inversion operator in the absence of any external electromagnetic fields reads

$$\dot{\hat{\sigma}}_z = -\Gamma\left(1+\hat{\sigma}_z\right) . \tag{17.1}$$

Recall that $\hat{\sigma}_z = |e\rangle\langle e| - |g\rangle\langle g|$ and that the identity operator in the atomic Hilbert space is just $\hat{I} = |e\rangle\langle e| + |g\rangle\langle g|$. Hence, the projection operator onto the excited state is $|e\rangle\langle e| \equiv \hat{\sigma}_{ee} = (\hat{I}+\hat{\sigma}_z)/2$ and Eq. (17.1) can be written as

$$\dot{\hat{\sigma}}_{ee} = -\Gamma\hat{\sigma}_{ee} \tag{17.2}$$

with the solution

$$\hat{\sigma}_{ee}(t) = e^{-\Gamma(t-t')}\hat{\sigma}_{ee}(t') . \tag{17.3}$$

If the atom at some initial time t' had been prepared in its excited state $|e\rangle$, it will decay into its ground state $|g\rangle$ on a time scale $1/\Gamma$. Hence, we call Γ is the *rate of spontaneous decay*. It is important to note that the atom will lose its excitation despite the fact that there is no driving field. However, the atom is coupled to the electromagnetic vacuum which, as we have seen earlier, is a state of infinite energy with a certain amount of fluctuations contained in it. Let us follow this line of thought further and rewrite the spontaneous decay rate (16.15) as

$$\Gamma = \frac{2\pi}{\hbar^2}\int d\omega\, \mathbf{d}\cdot\langle 0|\hat{\mathbf{E}}^{(+)}(\mathbf{r}_A,\omega)\otimes\hat{\mathbf{E}}^{(-)}(\mathbf{r}_A,\omega_A)|0\rangle\cdot\mathbf{d}^* \tag{17.4}$$

where the electric-field strength operators have to be evaluated at the atomic transition frequency. Equation (17.4) tells us that the rate of spontaneous decay is proportional to the strength of the vacuum fluctuations of the electromagnetic field. In other words, we can say that spontaneous decay is actually stimulated emission driven by the vacuum fluctuations of the electromagnetic field. Therefore, the process of spontaneous decay is proof of the existence of the quantum vacuum.

The spontaneous decay rate can be easily computed from the plane-wave expansion in which case Eq. (16.15) becomes

$$\begin{aligned}
\Gamma &= \frac{2\pi}{\hbar^2}\sum_\lambda \omega_\lambda^2 |\mathbf{A}_\lambda(\mathbf{r}_A)\cdot\mathbf{d}|^2\delta(\omega_A-\omega_\lambda) \\
&= \frac{2\pi}{\hbar^2}\sum_\sigma \int_0^\infty \frac{\omega^2 d\omega}{c^3(2\pi)^3}\int d\Omega\,\frac{\hbar\omega}{2\varepsilon_0}|\mathbf{e}_\sigma\cdot\mathbf{d}|^2\delta(\omega_A-\omega) \\
&= \frac{\omega_A^3 d^2}{3\pi\hbar\varepsilon_0 c^3}\,, \qquad (17.5)
\end{aligned}$$

where σ labels the two possible orthogonal polarizations and $d\Omega$ is the solid angle.

Note that the spontaneous decay rate can alternatively be computed by using *Fermi's Golden Rule* which states that the transition probability per unit time from a state $|\psi_i\rangle$ to a continuum of states $|\psi_f\rangle$ in an infinitesimally small energy interval $(E-dE, E+dE)$ is

$$p_{i\mapsto f} = (2\pi/\hbar)|V_{fi}|^2\rho_f(E)\,. \qquad (17.6)$$

This result follows from standard first-order time-dependent perturbation theory. The matrix element V_{fi} of the perturbation is nothing but the dipole moment matrix element, and the density of final states, $\rho_f(E)$, has to be associated with the strength of the vacuum fluctuations of the electromagnetic field.

Lamb shift: When going back to the effective equation of motion for the transition operators $\hat{\sigma}$, Eq. (16.14), which in the absence of external fields reduces to

$$\dot{\hat{\sigma}} = -i(\omega_A+\delta\omega)\hat{\sigma} - \frac{\Gamma}{2}\hat{\sigma}\,, \qquad (17.7)$$

we note that the atomic transition frequency ω_A has been altered to $\omega_A+\delta\omega$ with $\delta\omega$ being given by Eq. (16.16). This so-called *Lamb shift* is also purely a vacuum effect. The Lamb shift is measurable by high-precision spectroscopy. Table II summarizes experimental data for the hydrogen atom taken from [M. Weitz, A. Huber, F. Schmidt–Kaler, and T.W. Hänsch, Phys. Rev. Lett. **72**, 328 (1994)]. The Nobel Prize in Physics 2005 was awarded, amongst others, to Theodor W. Hänsch for his contributions to high-precision spectroscopy.

Our calculations imply that the 'bare' atomic transition frequency ω_A is not measurable in an experiment because the atom is always coupled to the quantized electromagnetic vacuum and thus always experiences the Lamb shift. What we call ω_A would be the transition frequency calculated quantum-mechanically for an isolated atom. Note, however, that our

atomic level in hydrogen	Lamb shift $\delta\omega$/MHz
$^1S_{1/2}$	8173.12
$^2S_{1/2}$	1045.043
$^2P_{1/2}$	-12.8354
$^4S_{1/2}$	131.6804

TABLE II: Lamb shift $\delta\omega$ for particular levels of the hydrogen atom.

simplified calculations would not result in the measured data shown in Table II as we have neglected non-rotating terms.

In addition to the Lamb shift, the off-diagonal elements of the atomic density matrix decay, but with the rate $\Gamma/2$, exactly half the rate than the excitation itself.

Modified spontaneous decay: Let us return to the expression (17.4) for the spontaneous decay in terms of the vacuum fluctuations of the electric field. This relation can be used to generalize the theory of spontaneous decay from free space to situations in which the quantized electromagnetic field is modified by the presence of dielectric materials. In connection with the Casimir effect we realized that boundary conditions change the structure of the quantum vacuum, and we can expect spontaneous decay properties to change as well. As a simple example, let us consider an atom in front of an ideal mirror. The two-level atom can be viewed as a dipole that can be oriented in different ways with respect to the mirror (see Fig. 23).

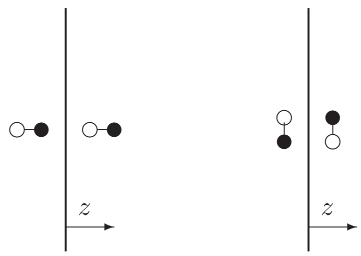

FIG. 23: A dipole (at $z > 0$) in front of a mirror generates an image (at $z < 0$). Depending on the dipole orientation, the spontaneous decay rate changes as $z \to 0$.

If the dipole in oriented in z-direction, i.e. perpendicular to the mirror surface, the dipole and its image effectively form a dipole with double its original strength when brought close to the mirror. In contrast, a dipole oriented parallel to the mirror surface, the two dipole cancel one another when they come close. In this case, the spontaneous decay drops to zero as $z \to 0$. Close here means that the distance z is smaller than the wavelength of the atomic transition, $z \ll \lambda_A = 2\pi c/\omega_A$.

Reality, however, is very different. There exists no ideal mirror, each metal has a finite resistivity. If an atom comes close to a metallic surface, it can lose its excitation due to short-range van der Waals interaction to the vast amount of dipoles that make up the mirror. The Coulomb interaction of a single dipole falls off at a distance r as $1/r^3$, and therefore the interaction energy between two dipoles falls off as $1/r^6$. Summing, or rather integrating, over the volume of the mirror material, leaves one with an effective interaction energy and $1/z^3$ which swamps the effects that we have described above to the extent that the suppression of spontaneous decay for a z-oriented dipole has never been observed.

Add-on: In order to describe the effect of dielectric materials on spontaneous decay, we would need a theory of the electromagnetic field in dielectrics. Without giving any proof, such a theory can be quantized as well, and its vacuum fluctuations are determined by the imaginary part of the Green tensor as

$$\langle 0|\hat{\mathbf{E}}(\mathbf{r},\omega)\otimes\hat{\mathbf{E}}^\dagger(\mathbf{r}',\omega')|0\rangle = \frac{\hbar\omega^2}{\pi\varepsilon_0 c^2}\mathrm{Im}\,\boldsymbol{G}(\mathbf{r},\mathbf{r}',\omega)\delta(\omega-\omega')\,.$$

This is an instance of the linear fluctuation-dissipation theorem which states that the correlations of a fluctuating quantity are related to the imaginary part of the causal response function.

The modified spontaneous decay rate then reads

$$\Gamma = \frac{2\omega_A^2}{\hbar\varepsilon_0 c^2}\mathbf{d}\cdot\mathrm{Im}\,\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_A,\omega_A)\cdot\mathbf{d} \qquad (17.8)$$

where $\mathbf{r}_A$ and ω_A are the location and the transition frequency of the atom, respectively. Needless to say that, when the Green tensor of free space, $\boldsymbol{G}^{(0)}(\mathbf{r},\mathbf{r}',\omega)$, is used, the free-space decay rate (17.5) is recovered. In all other cases, the expression (17.8) can be used to determine the effect of the presence of dielectric bodies or metals on the decay properties of a two-level atom.