Lecture 14: Maxwell's equations with sources

- Maxwell's equations, Coulomb gauge
- Hamiltonian in minimal coupling

<u>Maxwell's equations, Coulomb gauge</u>: So far we have concentrated on the quantized electromagnetic field in vacuum and have treated surrounding matter such as beam splitters only passively. That is to say, we assumed that the matter had no influence on the electromagnetic field. In the following lectures we will treat microscopic sources on the same level as the electromagnetic field. This is done by considering Maxwell's equations in free space in the presence of sources:

$$\nabla \cdot \mathbf{B}(\mathbf{r},t) = 0$$
 (Gauß' law), (14.1)

$$\nabla \cdot \mathbf{D}(\mathbf{r}, t) = \rho(\mathbf{r}, t)$$
 (Coulomb's law), (14.2)

 $\nabla \times \mathbf{E}(\mathbf{r}, t) = -\dot{\mathbf{B}}(\mathbf{r}, t)$ (Faraday's law), (14.3)

$$\nabla \times \mathbf{H}(\mathbf{r}, t) = \mathbf{j}(\mathbf{r}, t) + \dot{\mathbf{D}}(\mathbf{r}, t)$$
 (Amperé's law). (14.4)

The charge density $\rho(\mathbf{r}, t)$ and the current density $\mathbf{j}(\mathbf{r}, t)$ have to fulfil the continuity equation

$$\dot{\rho}(\mathbf{r},t) + \boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{r},t) = 0. \qquad (14.5)$$

If we keep Maxwell's equations (14.1)-(14.4) as they are we assume that the external charges and current are given and fixed and do not change. However, in most cases they themselves form dynamical variables and consequently have to obey some equations of motion that will depend on the electromagnetic fields.

Suppose we are given a collection of non-relativistic point-like charged particles of mass m_a and charge q_a . Then the charge and current densities are given by

$$\rho(\mathbf{r},t) = \sum_{a} q_a \delta(\mathbf{r} - \mathbf{r}_a), \qquad \mathbf{j}(\mathbf{r},t) = \sum_{a} q_a \dot{\mathbf{r}}_a \delta(\mathbf{r} - \mathbf{r}_a), \qquad (14.6)$$

where the time dependence resides in the position vectors $\mathbf{r}_a \equiv \mathbf{r}_a(t)$. The equations of motion for the position vectors are *Newton's equations* driven by the *Lorentz force*,

$$m_a \ddot{\mathbf{r}}_a = q_a \left[\mathbf{E}(\mathbf{r}_a) + \dot{\mathbf{r}}_a \times \mathbf{B}(\mathbf{r}_a) \right] \,. \tag{14.7}$$

If we introduce vector and scalar potentials as we have done previously [see Eqs. (1.9) and (1.10)], we obtain their respective wave equations as [cf. Eqs. (1.11) and (1.12)]

$$-\varepsilon_0 \left[\Delta \phi(\mathbf{r}, t) + \nabla \cdot \dot{\mathbf{A}}(\mathbf{r}, t) \right] = \rho(\mathbf{r}, t), \qquad (14.8)$$

$$\boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r},t) + \frac{1}{c^2} \ddot{\mathbf{A}}(\mathbf{r},t) + \frac{1}{c^2} \boldsymbol{\nabla} \dot{\phi}(\mathbf{r},t) = \mu_0 \mathbf{j}(\mathbf{r},t) \,. \tag{14.9}$$

In the Coulomb gauge in which the vector potential is a transverse vector function, $\nabla \cdot \mathbf{A}(\mathbf{r},t) = 0$, Eqs. (14.8) and (14.9) reduce to

$$\Delta\phi(\mathbf{r},t) = -\frac{1}{\varepsilon_0}\rho(\mathbf{r},t), \qquad (14.10)$$

$$\Delta \mathbf{A}(\mathbf{r},t) - \frac{1}{c^2} \ddot{\mathbf{A}}(\mathbf{r},t) = -\mu_0 \left[\mathbf{j}(\mathbf{r},t) - \varepsilon_0 \nabla \dot{\phi}(\mathbf{r},t) \right].$$
(14.11)

The rhs of Eq. (14.11) is in fact the definition of the transverse current density $\mathbf{j}^{\perp}(\mathbf{r}, t)$. Poisson's equation (14.10) can be integrated to give the (longitudinal) scalar potential

$$\phi(\mathbf{r},t) = \frac{1}{4\pi\varepsilon_0} \int d^3 r' \frac{\rho(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{4\pi\varepsilon_0} \sum_a \frac{q_a}{|\mathbf{r}-\mathbf{r}_a(t)|}$$
(14.12)

where in the last equation we have inserted the charge density from Eq. (14.6). Note also that the transverse current density can be written solely in terms of the total current by using the continuity equation (14.5),

$$\mathbf{j}^{\perp}(\mathbf{r},t) = \mathbf{j}(\mathbf{r},t) + \boldsymbol{\nabla} \int d^3 r' \frac{\boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{r}',t)}{4\pi |\mathbf{r} - \mathbf{r}'|} \,.$$
(14.13)

We have derived the wave equation for the vector potential [Eq. (14.11)] which now contains a driving term on its rhs given by the transverse current density. If we were to quantize this theory as we did in the free theory by using mode expansions, the time evolutions of the photonic amplitude operators will certain not be the same as in the free-field case. The interaction with the charged particles will changes the time evolution dramatically. **Hamiltonian in minimal coupling**: We now attempt to construct a Hamiltonian (or total energy) which we can then use to quantize our fields. The Hamiltonian represents the total energy of the combined system of electromagnetic field and charged particles. Hence, one part of the Hamiltonian is certainly the free-field Hamiltonian

$$H_F = \frac{1}{2} \int d^3r \left\{ \varepsilon_0 \mathbf{E}^2(\mathbf{r}, t) + \frac{1}{\mu_0} \left[\boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r}, t) \right]^2 \right\} \,. \tag{14.14}$$

The Hamiltonian of the charged particles is the sum of their kinetic and the Coulomb energy,

$$H_A = \sum_{a} \frac{\mathbf{p}_a^2(t)}{2m_a} + \frac{1}{2} \int d^3 r \,\rho(\mathbf{r}, t) \phi(\mathbf{r}, t) = \sum_{a} \frac{\mathbf{p}_a^2(t)}{2m_a} + \frac{1}{8\pi\varepsilon_0} \sum_{\substack{a,a'\\a\neq a'}} \frac{q_a q_{a'}}{|\mathbf{r}_a - \mathbf{r}_{a'}|} \,. \tag{14.15}$$

Finally, there is an interaction energy associated with the coupling between the electromagnetic field and the charged particles

$$H_{\text{int}} = -\sum_{a} \frac{q_a}{m_a} \mathbf{p}_a(t) \cdot \mathbf{A}(\mathbf{r}_a, t) + \sum_{a} \frac{q_a^2}{2m_a} \mathbf{A}^2(\mathbf{r}_a, t) \,. \tag{14.16}$$

The three parts of the classical Hamiltonian function, Eqs. (14.14)—(14.16), can be combined to the total *minimal coupling* Hamiltonian

$$H = H_F + H_A + H_{\text{int}}$$

$$= \frac{1}{2} \int d^3 r \left\{ \varepsilon_0 \mathbf{E}^2(\mathbf{r}, t) + \frac{1}{\mu_0} \left[\boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r}, t) \right]^2 \right\} + \sum_a \frac{1}{2m_a} \left[\mathbf{p}_a(t) - q_a \mathbf{A}(\mathbf{r}_a, t) \right]^2 + W_C$$
(14.17)

Note that the canonical particle momentum

$$\mathbf{p}_a(t) = m_a \dot{\mathbf{r}}_a(t) + q_a \mathbf{A}(\mathbf{r}_a, t) \tag{14.18}$$

is different from the *mechanical momentum* $m_a \dot{\mathbf{r}}_a(t)$ due to the interaction with the electromagnetic field.

In many situations, in particular in the quantum-optical settings we are interested in, the term quadratic in the vector potential can be disregarded with respect to the $\mathbf{p} \cdot \mathbf{A}$ term. The ratio between these two terms is, forgetting about vector characters and phases,

$$\frac{q_a^2}{2m_a} \left[\mathbf{A}(\mathbf{r}_a) \right]^2 / \frac{q_a}{m_a} \mathbf{p}_a \cdot \mathbf{A}(\mathbf{r}_a) \simeq \frac{qA}{2p} = \frac{q\omega A}{2p\omega} = \frac{qE}{2p\omega} = \frac{qE}{2m\omega^2 r}$$
(14.19)

which one recognizes as the ratio between electrostatic and centrifugal forces of a particle with charge q and mass m orbiting around a central potential at a distance r. Inserting typical values such as the electron charge and mass, $|q| = 1.6 \cdot 10^{-19}$ As and $m = 9.1 \cdot 10^{-31}$ kg, the Bohr radius $r = 5.2 \cdot 10^{-11}$ m, and a typical optical frequency $\omega = 10^{15}$ Hz, we find that the term quadratic in the vector potential can be neglected for electric-field strengths that are weak compared to intra-atomic field strengths, $|E| \ll 10^9$ Vm⁻¹ (this is violated for very short and intense laser pulses). The notion minimal coupling refers to the fact that the charged particles are treated microscopically and individually in terms of their position and momentum variables. Solving the equations of motion for one particle is hard enough, but for large systems of charged particles this approach becomes close to impossible. In many circumstances, for instance when considering bound charges in atoms or molecules, one is only interested in global properties of the system of particles. It then makes sense to introduce a charge density

$$\rho_A(\mathbf{r},t) = \left(\sum_a q_a\right) \delta(\mathbf{r} - \mathbf{r}_A(t)) \tag{14.20}$$

of the coarse-grained system at position \mathbf{r}_A The difference between the actual charge distribution $\rho(\mathbf{r}, t)$ and the coarse-grained one is combined into a microscopic polarization field

$$\nabla \cdot \mathbf{P}_A(\mathbf{r}, t) = -\rho(\mathbf{r}, t) + \rho_A(\mathbf{r}, t)$$
(14.21)

so that Coulomb's law (14.2) becomes

$$\nabla \cdot [\varepsilon_0 \mathbf{E}(\mathbf{r}, t) + \mathbf{P}_A(\mathbf{r}, t)] = \rho_A(\mathbf{r}, t). \qquad (14.22)$$

For globally neutral systems we have $\rho_A(\mathbf{r}, t) = 0$, and the displacement field $\mathbf{D}(\mathbf{r}, t) = \varepsilon_0 \mathbf{E}(\mathbf{r}, t) + \mathbf{P}_A(\mathbf{r}, t)$ is transverse. The Hamiltonian then transforms into a function that, instead of the vector potential $\mathbf{A}(\mathbf{r}, t)$ and the current density $\mathbf{j}(\mathbf{r}, t)$, depends on the new variables $\mathbf{P}_A(\mathbf{r}, t)$ and the fields $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$. This so-called *Power-Zienau* transformation [E.A. Power and S. Zienau, Phil. Trans. R. Soc. A**251**, 427 (1959)] leads to the *multipolar-coupling* Hamiltonian.

Field quantization: Let us return to the minimal-coupling Hamiltonian (14.17) which we will now quantize. The vector potential and the electric field are again expanded in terms of monochromatic modes, $\hat{\mathbf{A}}(\mathbf{r}) = \sum_{\lambda} \mathbf{A}_{\lambda}(\mathbf{r})\hat{a}_{\lambda} + \text{h.c.}$ and $\hat{\mathbf{E}}^{\perp}(\mathbf{r}) = i \sum_{\lambda} \omega_{\lambda} \mathbf{A}_{\lambda}(\mathbf{r})\hat{a}_{\lambda} + \text{h.c.}$. The coordinates and momenta of the charged particles, however, are quantized in the usual way by postulating canonical commutation relations for the operators $\hat{\mathbf{r}}_{a}$ and $\hat{\mathbf{p}}_{a}$ associated with them,

$$[\hat{r}_{ka}(t), \hat{p}_{k'a'}(t)] = i\hbar\delta_{kk'}\delta_{aa'}.$$
(14.23)

Lecture 15: Approximate interaction Hamiltonians and Heisenberg's equations of motion

- electric-dipole Hamiltonian, rotating-wave approximation, two-level Hamiltonian
- Heisenberg's equations of motion

Everything we said so far about quantizing the electromagnetic field in the presence of sources was very general and exact. Unfortunately, the equations of motions resulting from the corresponding Hamiltonians are far too complicated to yield analytical solutions. So we need suitable approximations that reveal the physics behind the interactions.

The first approximation we will look at is the *electric-dipole approximation*. The interaction part of the (yet classical) Hamiltonian (14.17) reads

$$H_{\text{int}} = -\sum_{a} \frac{q_a}{m_a} \mathbf{p}_a \cdot \mathbf{A}(\mathbf{r}_a) + \sum_{a} \frac{q_a^2}{2m_a} \left[\mathbf{A}(\mathbf{r}_a)\right]^2 \,. \tag{15.1}$$

The second term will be dropped by assuming that the applied electric fields are sufficiently weak. In the first term, we Taylor expand the positions of the charges $\hat{\mathbf{r}}_a$ around \mathbf{r}_A so that $\hat{H}_{\text{int}} \approx -\sum_a (q_a/m_a)\hat{\mathbf{p}}_a \cdot \hat{\mathbf{A}}(\mathbf{r}_A)$. This is similar to the treatment that led to the multipolarcoupling Hamiltonian where a system of (bound) charges at the coarse-grained position \mathbf{r}_A was considered. The assumption here is that the size of the atomic system is much smaller than the wavelength of the relevant electromagnetic fields. We define the *dipole operator*

$$\hat{\mathbf{d}} = \sum_{a} q_a \left(\hat{\mathbf{r}}_a - \mathbf{r}_A \right) \tag{15.2}$$

that in fact does not depend on \mathbf{r}_A for globally neutral systems. Recall that the part of the Hamiltonian associated with the free particles is $\hat{H}_A = \sum_a \hat{\mathbf{p}}_a^2/(2m_a) + \hat{W}_C$. Using the commutation rule (14.23) for the position and momentum operators, we see that $[\hat{\mathbf{r}}_a, \hat{\mathbf{p}}_a^2] = 2i\hbar\hat{\mathbf{p}}_a$, so that we can replace the momentum operator $\hat{\mathbf{p}}_a$ in the interaction Hamiltonian (15.1) by the commutator between the dipole operator (15.2) and the free atomic Hamiltonian \hat{H}_A . The interaction Hamiltonian (15.1) in the electric-dipole approximation is then

$$\hat{H}_{\text{int}} \approx \frac{i}{\hbar} \left[\hat{\mathbf{d}}, \hat{H}_A \right] \cdot \hat{\mathbf{A}}(\mathbf{r}_A) \,.$$
 (15.3)

We define the eigenstates of the free atomic Hamiltonian as $\hat{H}_A|i\rangle = \hbar \omega_i |i\rangle$, and use the fact that they form a complete orthonormal set of state vectors. Hence, we can expand both

the dipole moment $\hat{\mathbf{d}}$ as well as \hat{H}_A as

$$\hat{H}_A = \sum_i \hbar \omega_i |i\rangle \langle i|, \qquad \hat{\mathbf{d}} = \sum_{k,l} |k\rangle \langle k| \hat{\mathbf{d}} |l\rangle \langle l| = \sum_{k,l} \mathbf{d}_{kl} |k\rangle \langle l| = \sum_{k,l} \mathbf{d}_{kl} \hat{\sigma}_{kl}$$
(15.4)

where we have defined the dipole-moment matrix elements $\mathbf{d}_{kl} = \langle k | \hat{\mathbf{d}} | l \rangle$ and the atomic transition operators $\hat{\sigma}_{kl} = |k\rangle \langle l|$. Using the atomic transition frequencies $\omega_{kl} = \omega_k - \omega_l$, we can finally write the electric-dipole Hamiltonian (15.3) as

$$\hat{H}_{\text{int}} = -i \sum_{i,j} \omega_{ij} \hat{\sigma}_{ij} \mathbf{d}_{ij} \cdot \hat{\mathbf{A}}(\mathbf{r}_A) = -i \sum_{i,j} \sum_{\lambda} \omega_{ij} \hat{\sigma}_{ij} \mathbf{d}_{ij} \cdot \mathbf{A}_{\lambda}(\mathbf{r}_A) \hat{a}_{\lambda} + \text{h.c.}$$
(15.5)

This interaction Hamiltonian couples the photonic amplitude operators \hat{a}_{λ} to the atomic flip operators $\hat{\sigma}_{ij}$ where the coupling strength is determined by the atomic transition frequencies, the dipole-moment matrix elements and the mode functions. The *i*, *j*-sums run over all atomic levels and the sum over λ runs over all modes of the electromagnetic field. For a two-level atom, the Hamiltonian (15.5) contains terms $\propto (\hat{\sigma}_{12} + \hat{\sigma}_{21}) (\hat{a}_{\lambda} + \hat{a}_{\lambda}^{\dagger})$.

Rotating-wave approximation, two-level Hamiltonian: For resonant interactions in which a particular mode frequency ω_{λ} is close to one of the atomic transition frequencies ω_{ij} , we can approximate the Hamiltonian (15.5) even further. Let us assume that narrow-band light with mid-frequency ω_{λ} impinges on an atom close to one of its resonances ω_{ij} (see figure). Since the free photonic amplitude operators evolve as $\hat{a}_{\lambda}(t) = e^{-i\omega_{\lambda}t}\hat{a}_{\lambda}$ and the free



atomic flip operators as $\hat{\sigma}_{ij}(t) = e^{i\omega_{ij}t}\hat{\sigma}_{ij}$, their combined time evolution is $e^{i(\omega_{ij}-\omega_{\lambda})t} \approx 1$ for $t \ll |\omega_{ij} - \omega_{\lambda}|^{-1}$. Other atomic transitions $\omega_{i'j'}$ then do not contribute on this time scale as $e^{i(\omega_{i'j'}-\omega_{\lambda})t}$ averages to zero. That is, in this *rotating-wave approximation* we keep the resonant interactions and neglect the non-resonant ones. If only two atomic levels are resonant, we get the dipole Hamiltonian in the *two-level approximation*

$$\hat{H}_{\text{int}} \approx -i \sum_{\lambda} \omega_{21} \hat{\sigma}_{21} \mathbf{d}_{21} \cdot \mathbf{A}_{\lambda}(\mathbf{r}_{A}) \hat{a}_{\lambda} + \text{h.c.} \approx -\hat{\sigma}_{21} \mathbf{d}_{21} \cdot \hat{\mathbf{E}}^{\perp(+)}(\mathbf{r}_{A}) + \text{h.c.}, \qquad (15.6)$$

where the terms $\propto \hat{\sigma}_{21} \hat{a}^{\dagger}_{\lambda}$ and $\propto \hat{\sigma}_{12} \hat{a}_{\lambda}$ have been omitted. Recall that this approximation is only valid if there is a one-photon resonance. For far off-resonant interactions, approximating

the electric-field strength only by the resonant part as in (15.6) may not be enough, and the neglected \hat{A}^2 -term in the minimal-coupling Hamiltonian may become relevant.

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. (2.17) and (15.6), as

$$\hat{H} = \sum_{\lambda} \hbar \omega_{\lambda} \hat{a}^{\dagger}_{\lambda} \hat{a}_{\lambda} + \frac{1}{2} \hbar \omega_{A} \hat{\sigma}_{z} - \left[\hat{\sigma}^{\dagger} \hat{\mathbf{E}}^{(+)}(\mathbf{r}_{A}) \cdot \mathbf{d} + \text{h.c.} \right] .$$
(15.7)

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. (15.7) 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 obey the (angular-momentum) commutation rules

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k, \qquad i, j, k \in \{x, y, z\}.$$
(15.8)

Other useful commutation relations are

$$\left[\hat{\sigma}, \hat{\sigma}_z\right] = 2\hat{\sigma}, \quad \left[\hat{\sigma}^{\dagger}, \hat{\sigma}_z\right] = -2\hat{\sigma}^{\dagger}, \quad \left[\hat{\sigma}, \hat{\sigma}^{\dagger}\right] = -\hat{\sigma}_z.$$
(15.9)

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

$$\dot{\hat{O}} = \frac{1}{i\hbar} \left[\hat{O}, \hat{H} \right] \,. \tag{15.10}$$

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

$$\dot{\hat{\sigma}}_{z} = \frac{1}{i\hbar} \left[\hat{\sigma}_{z}, \hat{H} \right] = \frac{i}{\hbar} \hat{\mathbf{E}}^{(+)}(\mathbf{r}_{A}) \cdot \mathbf{d} \left[\hat{\sigma}_{z}, \hat{\sigma}^{\dagger} \right] + \text{h.c.}$$
(15.11)

which, on using the commutation rules (15.9) for the atomic operators, becomes

$$\dot{\hat{\sigma}}_z = \frac{2i}{\hbar} \hat{\sigma}^{\dagger} \hat{\mathbf{E}}^{(+)}(\mathbf{r}_A) \cdot \mathbf{d} + \text{h.c.} \qquad (15.12)$$

Similarly, we obtain for the atomic flip operator,

$$\dot{\hat{\sigma}} = \frac{1}{i\hbar} \left[\hat{\sigma}, \hat{H} \right] = -\frac{i}{2} \omega_A \left[\hat{\sigma}, \hat{\sigma}_z \right] + \frac{i}{\hbar} \left[\hat{\sigma}, \hat{\sigma}^\dagger \right] \hat{\mathbf{E}}^{(+)}(\mathbf{r}_A) \cdot \mathbf{d}$$
(15.13)

which, on using the relations (15.9), becomes

$$\dot{\hat{\sigma}} = -i\omega_A \hat{\sigma} - \frac{i}{\hbar} \hat{\sigma}_z \hat{\mathbf{E}}^{(+)}(\mathbf{r}_A) \cdot \mathbf{d} \,. \tag{15.14}$$

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

$$\dot{\hat{a}}_{\lambda} = -i\omega_{\lambda}\hat{a}_{\lambda} + \frac{\omega_{\lambda}}{\hbar}\mathbf{A}_{\lambda}^{*}(\mathbf{r}_{A})\cdot\mathbf{d}^{*}\hat{\sigma} . \qquad (15.15)$$

The three equations (15.12), (15.14) and (15.15) 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 again to some approximation.