Quantum theory of light-matter interaction: Fundamentals

Lecture 5
Quantum theory of charged particles in external fields

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BEFEKTETÉS A JÖVŐBE

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Introduction

Electrodynamics and optics deal with interactions between EM fields and charged particles. In the context of the present course the charges are atomic electrons. In the earlier lectures the motion of the charges forced by the electromagnetic fields has been described by the laws of classical mechanics. Beginning from the present lecture we shall treat this motion according to the rules of quantum mechanics, but we retain the classical description for the dynamics of the field. A more sophisticated possibility would be to work with quantized fields, but we shall not follow that approach.

We begin the description of the interaction of charged particles with electromagnetic fields at the most fundamental level, and come later to the simplifications connected with charges bound to atoms.

Hamilton's principle and Lagrange equations

Hamilton's principle states that the dynamics of a physical system is determined by a Lagrangian $L(x, \dot{x}, t)$ which is a function of the general dynamical coordinates (denoted here by x for short) and their time derivatives.The principle prescribes that the corresponding action integral $S = \int L(x, \dot{x}, t)dt$ is extremal – usually minimal – along the actual orbit $x(t)$ of the system. In classical mechanics this principle replaces Newton's second law, but it can be applied to much more general physical situations including classical and even quantized fields. As it is well known, the variational principle of getting a minimum of S is equivalent to the equation:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0$$

Free particle Lagrangian

We shall consider here first the classical dynamics of a single point charge in an external field. More generally, if we wish to include the dynamics of the field as well, then L consists of 3 parts: (1) the one giving the mechanics of a free particle, (2) the free field part and (3) the interaction term. They can be found by considerations based on general symmetry and invariance principles.

As it is known (Landau-Lifsic Vol 2, Jackson) the free particle part is with $x \to \mathbf{r}, \; \dot{\mathbf{r}} = \mathbf{v}$:

$$L_p = -mc^2\sqrt{1-\frac{\mathbf{v}^2}{c^2}} \approx (\text{ for } v \ll c) = -mc^2 + \frac{1}{2}m\mathbf{v}^2$$

From now on we restrict ourselves to the nonrelativistic limit in the dynamics of the particles, where the constant term $-mc^2$ can be trivially omitted.

Minimal couplig

A very general principle, called the *gauge principle,* requires – together with the principle of relativity – that the *coupling* between a point charge q and the field must be of the *minimal form*: *charge×four dimensional (space-time) line integral of a vector field: known as the four potential*

$$\underline{A} = \{\Phi/c, \mathbf{A}\}$$

so that the charge-field interaction is determined by the Lorentz invariant action:

$$S_i = \int L_i dt = -q \int \underline{A}(\underline{x}) d\underline{x} = \int q(\mathbf{v}\mathbf{A} - \Phi) dt$$

and accordingly

$$L_i = q\mathbf{v}\mathbf{A}(\mathbf{r}, t) - q\Phi(\mathbf{r}, t)$$

This form of the Lagrangian is called the *minimal coupling*. (In contrast to a possible nonminimal form involving the field strengths, dipole moments etc.)

Field strengths from potentials

Another consequence of the gauge priciple is that the field strengths $\mathbf{E}$ and $\mathbf{B}$, available to common physical experience should be a combination of certain derivatives of $\mathbf{A}$ and Φ. Omitting the elegant relativistic considerations (see Landau-Lifsic vol. 2.) we quote the well-known expressions of the field strengths by the potentials

$$\mathbf{B} = \nabla \times \mathbf{A}, \qquad \mathbf{E} = -\nabla\Phi - \dot{\mathbf{A}}$$

Note that in the usual approach these are considered as the consequences of the homogeneous Maxwell equations, while we follow here a reversed argument.

Problem: Starting from the above definition of the field strength show the validity of the two homogeneous Maxwell equations.

Field Lagrangian density

Finally, it can be shown that relativistic plus gauge invariance requires the free-field Lagrangian to be the volume integral of a Lagrangian density $\mathcal{L}_f$ over whole space, giving:

$$L_f = \int \mathcal{L}_f d\mathcal{V} = \frac{1}{2} \int (\epsilon_0 \mathbf{E}^2 - \mathbf{B}^2/\mu_0) d\mathcal{V}$$

The total Lagrangian is then $L_p + L_i + L_f$. We only note here that Maxwell equations can be obtained by the appropriately modified variational principle for fields from the continuous version of the Lagrangian, $\mathcal{L}_f + \mathcal{L}_i$ containing the field variables as general coordinates, where the Lagrangian density of the interaction term is $\mathcal{L}_i = \mathbf{J}\mathbf{A} - \rho\Phi$. ($\mathbf{J}$ and ρ are the current and charge densities). Note that in the derivation the dynamical variables in $\mathcal{L}_f$ as well as in $\mathcal{L}_i$ are the potentials, in terms of which $\mathbf{E}$ and $\mathbf{B}$ must be expressed.

Problem: Recall the derivation of the Maxwell equations from the Lagrangian density $\mathcal{L}_f + \mathcal{L}_i$ (Landau-Lifsic, Jackson)

Equation of motion

From now on we wish to find the equation of motion of the charged particle in a given external field so we restrict ourselves to the Lagrangian

$$L(\mathbf{r}, \mathbf{v}) = L_p + L_i = \frac{1}{2}m\mathbf{v}^2 + q\mathbf{v}\mathbf{A}(\mathbf{r},t) - q\Phi(\mathbf{r},t)$$

and omit L_f that contains only the field variables.

Problem: Derive the equation of motion of the charge in external field:

$$m\frac{d\mathbf{v}}{dt} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

from this L. Make use of the rule: $\frac{df(\mathbf{r},t)}{dt} = \frac{\partial f}{\partial t} + (\mathbf{v}\nabla)f$.

This proves a posteriori the validity of the assumptions leading to the above Lagrangian.

Gauge transformations and invariance

As it is well known, the potentials $\mathbf{A}$ and Φ are not unique, there is a freedom determined by the *gauge transfomation of the second kind:*

$$\tilde{\mathbf{A}} = \mathbf{A} + \nabla\chi, \qquad \tilde{\Phi} = \Phi - \dot{\chi} \tag{GT2}$$

where $\chi((r,t)$ is a completely arbitrary (smooth) function.

Problem: Check that the gauge transformation adds only a constant term to S_i*, thus leaving invariant the corresponding equation of motion.*

L_f itself is also invariant with respect to GT2 , as according to

$$\mathbf{B} = \nabla \times \mathbf{A}, \qquad \mathbf{E} = -\nabla\Phi - \dot{\mathbf{A}}$$

the transformed quantities $\tilde{\mathbf{A}}$ and $\tilde{\Phi}$ yield the same $\mathbf{E}$ and $\mathbf{B}$ as do $\mathbf{A}$ and Φ. So Maxwell equations and Lorentz force are invariant with respect to (GT2). This gives us a certain freedom to choose the potentias in a way that fits most to a given problem.
We shall discuss the gauge principle below in the framework of quantum mechanics in a little more detail.

Hamiltonian

The *canonical momentum* $\mathbf{P} = \frac{\partial L}{\partial \mathbf{v}}$ and the *kinetic momentum* $\mathbf{p} = m\mathbf{v}$ are connected by

$$m\mathbf{v} = \mathbf{p} = \mathbf{P} - q\mathbf{A} \qquad \text{(mom)}$$

The Hamiltonian defined as $H = \mathbf{P}\mathbf{v} - L$ results in

$$H(\mathbf{P}, \mathbf{r}) = \frac{1}{2m}(\mathbf{P} - q\mathbf{A})^2 + q\Phi \qquad \text{(HEM)}$$

The $\mathbf{r}$ dependence of the Hamiltonian is contained in the potentials. Note that H is not gauge invariant, as it depends on the choice of $\mathbf{A}$ and Φ.

Problem: Show that the canonical equations derived from this H yield the Lorentz force equation of motion.

Schrödinger equation in EM field

The Schrödinger equation for a single particle of charge q (for an electron we have $q < 0$), in external field is the following

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi = \left(\frac{1}{2m}(\mathbf{P}-q\mathbf{A})^2 + q\Phi\right)\Psi = $$
$$= \left(\frac{1}{2m}(-i\hbar\nabla-q\mathbf{A})^2 + q\Phi\right)\Psi(\mathbf{r},t)$$

where we use coordinate representation, thus Ψ is a function of the coordinate as $\mathbf{A}$ and Φ are operators as much as they depend on the particle location $\mathbf{R}$ considered to be an operator here. Note that it is the canonical momentum and not the kinetic one (!) that is replaced by $-i\hbar\nabla$, as the canonical commutation relation $[X_i, P_j] = i\hbar\delta_{ij}$ is prescribed for $\mathbf{P}$ and not for $\mathbf{p}$. The equation is written here in a particular gauge given by $\mathbf{A}$ and Φ. One can easily see that by performing a gauge transformation, the Schrödinger equation takes a different form, thus at first sight it seems to be gauge dependent.

Gauge transformation of the first kind

This is not the case, however, if together with the transformation (GT2) we prescribe the gauge transformation of the first kind, which is a local phase change of the wave function:

$$\tilde{\Psi}(\mathbf{r},t) = \Psi(\mathbf{r},t)\exp\left[i\frac{q}{\hbar}\chi(\mathbf{r},t)\right] \tag{GT1}$$

Problem: Show that the simultaneous transformations (GT1), (GT2) *yield the same form for the Schrödinger equation, i.e. quantum dynamics is gauge invariant.*

(GT1) is a unitary tarnsformation therefore all physically relevant quantities, expectaion values, transition probabilities, etc. are invariant with respect of this transformation of Ψ, which means that quantum mechanics is gauge invariant, in general.

On the gauge principle

It is a good place here to point out that the celebrated *gauge principle*, quoted above is actually a reversed argument. Thus starting from the Schrödinger equation with $\mathbf{A} = 0$, $\Phi = 0$, for a certain $\Psi(\mathbf{r}, t)$ one requires its invariance when introducing the local phase change (GT1) for a charged particle with an arbitrary χ.

One can show that this is only possible if one introduces new dynamical variables $\mathbf{A}$ and Φ, which are to be transformed by (GT2) simultaneously with (GT1), which compensate the effect of the phase change and keep the Schrödinger equation invariant.

Problem: Prove the above statement

Coulomb gauge

It is convenient to write the Schrödinger equation as

$$i\hbar\frac{\partial\Psi_g}{\partial t}=H_g\Psi_g$$

where the label g refers to the particular gauge chosen.
A specific and frequently used gauge is the one defined by

$$\nabla\mathbf{A}=0\quad\text{called Coulomb gauge,}$$

known also as radiation, or transverse gauge. The condition $\nabla\mathbf{A}=0$ is not invariant with respect to Lorentz transformations, but has several advantages in nonrelativistic calculations in atomic physics. In this gauge the operators $\mathbf{P}$ and $\mathbf{A}(\mathbf{R},t)$ commute and the Schrödinger equation can be written for an appropriately chosen $\Psi_C(\mathbf{r},t)$ (subscript refers to Coulomb gauge) as

$$i\hbar\frac{\partial\Psi_C}{\partial t}=-\frac{\hbar^2}{2m}\Delta\Psi_C(\mathbf{r},t)+i\hbar\frac{q}{m}\mathbf{A}_C(\mathbf{r},t)\nabla\Psi_C(\mathbf{r},t)+\left(\frac{q^2}{2m}\mathbf{A}_C^2+q\Phi_C\right)\Psi_C(\mathbf{r},t)\tag{Coul}$$

Coulomb gauge II

We see that we have now

$$H = H_0 + K_c(t)$$

$$H_0 = -\frac{\hbar^2}{2m}\Delta + q\Phi_C$$

and the interaction term is

$$K_C(t) = -\frac{q}{m}\mathbf{A}_C\mathbf{P} + \frac{q^2}{2m}\mathbf{A}_\mathbf{C}^\mathbf{2} = i\hbar\frac{q}{m}\mathbf{A}_C\nabla + \frac{q^2}{2m}\mathbf{A}_C^2$$

For weak fields one sometimes omits the $\mathbf{A}^2$ term as a small correction to the one linear in $\mathbf{A}$.

As we shall see below this is not always necessary, however.

Dipole approximation, B of the field is neglected

In optical problems the wavelength of electromagnetic field $\lambda \sim 500$ nm is at least three orders of magnitude larger than the atomic size, which is of the order of the Bohr radius $a_0 \sim 0.1$ nm. Therefore the spatial variation of the electromagnetic field is negligible. Accordingly we assumme here that the electric field strength is a sum of two terms $\mathbf{E} = \mathbf{E}_s(\mathbf{r}) + \mathbf{E}_w(t)$. The first term is the static Coulomb field of the atom, assumed to be curl free, while the second one is the external field of the electromagnetic wave depending only on time and not on the spatial variable. In such a case the magnetic field is at most a constant due to the Maxwell equations, and it must be chosen $\mathbf{B}$ =0 at the place of the atom. This is consistent only for weak electromagnetic fields not accelerating the charge up to relativistic velocities, because then the magnetic part of the Lorentz force is negligible if compared with the electric part. This is because in a plane wave $|\mathbf{B}| = |\mathbf{E}|/c$ and therefore one can neglect the $\mathbf{v} \times \mathbf{B}$ part of the force for electron velocities $v \ll c$.

Potentials in the velocity gauge

One of the possible pair of potentials reproducing the field strengths $\mathbf{E} = \mathbf{E_s}(\mathbf{r}) + \mathbf{E_w}(t)$, $\mathbf{B}$ =0 are:

$$\mathbf{A}_v(t) = -\int_{-\infty}^{t} \mathbf{E}_w(t')dt', \qquad \Phi_s(\mathbf{r}) = -\int_{\infty}^{\mathbf{r}} \mathbf{E_s}(\mathbf{r}')d\mathbf{r}' \tag{1}$$

The latter being the usual definition of the static potential in terms of a path independent line integral. In case of a Hydrogen atom e.g. $\Phi_s(\mathbf{R}) = \frac{q^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{R}|}$.
These potentials represent one particular Coulomb gauge as $\nabla \mathbf{A}_v$=0 trivially. This choice is called the *velocity gauge* or PA gauge, or sometimes simply P gauge because the Hamiltonian contains the combination $(\mathbf{P} - q\mathbf{A}_v)/m$ explicitly, which is the operator of the particle velocity according to $m\mathbf{v} = \mathbf{p} = \mathbf{P} - q\mathbf{A}$ see (mom).
One can substitute these potentials into the Schrödinger Eq. as in (Coul), and obtain the corresponding equation to be solved.

Another velocity gauge

Problem: Perform a gauge transformation from the v gauge to a v' gauge with

$$\chi_{vv'}(\mathbf{r}, t) = \frac{q}{2m} \int_{-\infty}^{t} \mathbf{A}_v^2(t')dt'$$

$$\mathbf{A}_{v',t} = \mathbf{A}_{v,t}, \qquad \Phi_{v'}(\mathbf{r}) = \Phi_s(\mathbf{r}) - \frac{q}{2m}\mathbf{A}_v^2$$

Show that the corresponding Schrödinger equation for

$$\Psi_{v',t} = \Psi_v \exp\left[i\frac{q^2}{2m\hbar} \int_{-\infty}^{t} \mathbf{A}_v^2(t')dt'\right]$$

leads to an interaction operator without the A^2 term. This v' gauge is also called sometimes as a velocity gauge, but it is different from the v gauge.

Potentials in the length gauge

Another possibility emerges by performing a gauge transformation from the v gauge to a new one with the generating function

$$\chi_{vl}(\mathbf{r},t) = -\mathbf{r}\mathbf{A}_v(t) = \mathbf{r}\int_{-\infty}^{t} \mathbf{E}_w(t')dt'$$

resulting in

$$\mathbf{A}_l(t) := \mathbf{A}_v(t) + \nabla\chi_{vl}(\mathbf{r},t) = 0$$

$$\Phi_l(\mathbf{r}) := \Phi_s(\mathbf{r}) - \dot{\chi}_{vl}(\mathbf{r},t) = \Phi_s(\mathbf{r}) + \mathbf{r}\dot{\mathbf{A}}_v(t) = \Phi_s(\mathbf{r}) - \mathbf{r}\mathbf{E}_w(t) \qquad \text{(lgauge)}$$

This is another sort of a Coulomb gauge, called the *length gauge*, where $\mathbf{A}_l(t) \equiv 0$, (obviously $\nabla\mathbf{A}_l{=}0$) and the time dependence of the field is carried now by the $-\mathbf{r}\mathbf{E_w}(t)$ part of the scalar potential.
!Note the frequent occurence of the incorrect terminology calling the nonvanishing quantitity $-\int_{-\infty}^{t}\mathbf{E}_w(t')dt' \neq \mathbf{A}_l(t)$ as the vector potential when using the length gauge, which is to be avoided!

Dipole interaction

The length gauge is also called **r** gauge or **rE** gauge, or sometimes as Goeppert-Mayer gauge (see next slide).
In the length gauge the time-dependent Schrödinger equation for the wave function

$$\Psi_l = \Psi_v \exp\left[i\frac{q}{\hbar}\mathbf{r}\int_{-\infty}^{t}\mathbf{E}_w(t')dt'\right]$$

can be shown to be:

$$\begin{aligned} i\hbar\frac{\partial\Psi_l}{\partial t} &= H_l\Psi_l = -\frac{\hbar^2}{2m}\Delta\Psi_l(\mathbf{r},t) + q\Phi_s(\mathbf{r})\Psi_l(\mathbf{r},t) - q\mathbf{r}\mathbf{E}(t)\Psi_l(\mathbf{r},t) = \\ &= (H_0 - \mathbf{D}\mathbf{E}(t))\Psi_l(\mathbf{r},t) \end{aligned} \qquad \text{(ScheL)}$$

where **D** is the dipole moment operator of the electron $q\mathbf{R}$ ($q\mathbf{r}$ in coordinate rep.).
Problem: Show by directly substituting Ψ_l *into the Schrödinger equation the validity of* (ScheL).
Note that the term with $\mathbf{A}^2$ could be eliminated in the length gauge.

Maria Goeppert-Mayer

It is worth to note here an interesting fact from the history of 20-th century physics. The **r** gauge was first applied by Maria Göppert in 1929 in the theory of two-photon processes. She is the second woman so far who received the Nobel prize in physics (in 1963) after Marie Curie, and the only one awarded for a theoretical work. She explained the role of the spin-orbit interaction in nuclear shell model and the stability of nuclei with "magic" numbers of nucleons in 1950. The German born Göppert worked first with M. Born in Göttingen. Later she married the American physicist J. Mayer, and lived in the USA. She obtained there a permanent physics professorship only in 1960, when she was already very close to the Nobel prize. Her name is cited as Goeppert-Mayer in the English literature.