Chapter 10
Field-Theoretical Approach to the Non-Relativistic Quantum Electrodynamics

We give here the field-theoretical derivation of the Hamiltonian of the non-relativistic quantum electrodynamics in the Coulomb gauge using the Lagrange formalism. It leads to the same result as the usual derivation, where one just replaces the classical vector potential in the minimal coupling of the second quantized electron Hamiltonian by the quantized one and adds the photon energy. This derivation however illustrates the proper use of the Euler–Lagrange equations and the canonical formalism that fails if one tries to quantize the classical theory of point-like particles interacting with the electromagnetic fields. In the same time it confirms the $1/c^2$ *result of the preceding chapter on states without photons.*

As one could see, building the quantum mechanics of charged particles starting from the classical model of point-like charges in the configuration space leads after a few steps into a dead end. More than the $1/c^2$ approximation cannot be achieved. The correct approach should follow a reverse order, starting from the formulation of the non-relativistic quantum electrodynamics, followed by simplifying approximations (expansion in powers of $1/c$).

In order to construct the non-relativistic quantum mechanical Hamiltonian describing the interaction between electrons and photons, we use here a way borrowed from the relativistic quantum field theory. We proceed by three steps. The first is to build up a classical Lagrangian density out of classical fields. These include besides the electric and magnetic fields also an one-electron wave function that leads to the coupled Maxwell and Schrödinger equations with the charge and current densities defined by the Schrödinger equation The second step is to choose the Coulomb gauge in order to eliminate the spurious degrees of freedom that allows one to build a classical Hamiltonian. The last step is to quantize all the physical

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fields (wave function and transverse e.m. vector potential) in the Hamiltonian. This way avoids the ill-defined theory of point-like charged particles. Of course, for the sake of stability the many-body system should contain also particles of opposite charge, but the extension of the formalism to include these is trivial.

10.1 Field Theory

In the classical field theory one defines the action $\mathscr{A}$

$$\mathscr{A} = \int d\mathbf{x} \int dt \mathscr{L}(\mathbf{x}, t)$$

by a Lagrange density $\mathscr{L}(\mathbf{x}, t)$ depending on some fields $\phi_i(\mathbf{x}, t)$ and their first time and space derivatives. The variational principle $\delta A = 0$ gives rise to the generalized Euler–Lagrange equations

$$\frac{\partial}{\partial t} \frac{\delta \mathscr{L}}{\delta \dot{\phi}_i(\mathbf{x}, t)} + \frac{\partial}{\partial x_\mu} \frac{\delta \mathscr{L}}{\delta \frac{\partial \phi_i(\mathbf{x},t)}{\partial x_\mu}} - \frac{\delta \mathscr{L}}{\delta \phi_i(\mathbf{x}, t)} = 0.$$

Here the symbol ∂ means ordinary derivative, while the symbol δ means functional derivative. Two Lagrangian densities that differ by the time derivative or by the divergence of a function give rise to the same action and therefore are considered to be equivalent, taking into account the vanishing of the fields at infinity.

Actually, we have already used this formalism in Sect. 4.2 in the treatment of the classical phonon fields on the continuum.

The generalized canonical conjugate momenta for the fields $\phi_i(\mathbf{x}, t)$ are defined by

$$\Pi_{\phi_i} = \frac{\delta \mathscr{L}}{\delta \dot{\phi}_i}$$

and the Hamiltonian density is

$$\mathscr{H}(\phi, \Pi_\phi) = -\mathscr{L} + \Pi_{\phi_i} \dot{\phi}_i,$$

provided no relations (constraints) appear between the canonical conjugate momenta. Lagrangians with constraints however have to be handled with Dirac's canonical formalism that implies also a redefinition of the Poisson bracket.

10.2 Classical Maxwell Equations Coupled to a Quantum Mechanical Electron

The classical Maxwell equations are two with sources

$$\nabla \times \mathbf{B} = \frac{4\pi}{c}\mathbf{j} + \frac{1}{c}\frac{\partial}{\partial t}\mathbf{E} \tag{10.1}$$

$$\nabla \mathbf{E} = 4\pi\rho \tag{10.2}$$

and two without sources

$$\nabla \mathbf{B} = 0 \tag{10.3}$$

$$\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial}{\partial t}\mathbf{B}. \tag{10.4}$$

The equations without sources are automatically satisfied by the introduction of the electromagnetic potentials

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{10.5}$$

$$\mathbf{E} = -\nabla V - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{A}. \tag{10.6}$$

Let us suppose, that the sources

$$\rho(\mathbf{x}, t) = e\psi(\mathbf{x}, t)^* \psi(\mathbf{x}, t) \tag{10.7}$$

$$\mathbf{j}(\mathbf{x}, t) = \frac{e}{2m}\psi(\mathbf{x}, t)^* \left(-\imath\hbar\nabla + \frac{e}{c}\mathbf{A}(\mathbf{x}, t)\right)\psi(\mathbf{x}, t) + c.c \tag{10.8}$$

are given by a single electron (for simplicity without spin), described by the quantum mechanical Schrödinger equation for the wave function $\psi(\mathbf{x}, t)$

$$\imath\hbar\frac{\partial}{\partial t}\psi = \left(\frac{1}{2m}\left(-\imath\hbar\nabla + \frac{e}{c}\mathbf{A}(x, t)\right)^2 + eV(x, t)\right)\psi. \tag{10.9}$$

Using only the Schrödinger equation the sources satisfy the continuity equation (required also by consistency)

$$\nabla \mathbf{j} + \frac{\partial}{\partial t}\rho = 0. \tag{10.10}$$

The electromagnetic potentials and the wave function are not uniquely defined, they allow a simultaneous gauge transformation

$$V(\mathbf{x},t) \to V(\mathbf{x},t) + \frac{1}{c}\dot{\chi}(\mathbf{x},t) \tag{10.11}$$
$$\mathbf{A}(\mathbf{x},t) \to \mathbf{A}(\mathbf{x},t) - \nabla\chi(\mathbf{x},t)$$
$$\psi(\mathbf{x},t) \to \psi(\mathbf{x},t)e^{-\frac{\imath e}{\hbar c}\chi(\mathbf{x},t)}$$

that do not change neither the Maxwell fields **B**, **E**, the sources ρ, **j** nor the whole system of equations Eqs. 10.1 to 10.10.

The source-less Maxwell equations 10.3 and 10.4 are satisfied automatically in terms of the electromagnetic potentials through Eqs. 10.5 and 10.6. Therefore, one should concentrate only on Eqs. 10.1, 10.2, and 10.9. Then the first problem is to find a Lagrangian giving rise to these equations in terms of the fields $V(\mathbf{x},t)$, $\mathbf{A}(\mathbf{x},t)$, and $\psi(\mathbf{x},t)$ as dynamical variables (generalized coordinates). Thereafter, one has to find the classical Hamiltonian (in the Coulomb gauge) and at the end quantize simultaneously the electron wave function $\psi(\mathbf{x})$ and the transverse vector potential $\mathbf{A}_\perp(\mathbf{x})$.

10.3 Classical Lagrange Density for the Maxwell Equations Coupled to a Quantum Mechanical Electron

In our case, the fields are $V(\mathbf{x},t)$, $\mathbf{A}(\mathbf{x},t)$, and $\psi(\mathbf{x},t)$. It is easy to see that the "photon" Lagrange density

$$\mathscr{L}_{ph}(\mathbf{x},t) = \frac{1}{8\pi}\left(\nabla V(\mathbf{x},t) + \frac{1}{c}\dot{\mathbf{A}}(\mathbf{x},t)\right)^2 - \frac{1}{8\pi}\left(\nabla\times\mathbf{A}(\mathbf{x},t)\right)^2 \tag{10.12}$$

through the generalized Euler–Lagrange equations for the fields $\mathbf{A}(\mathbf{x},t)$ and $V(\mathbf{x},t)$ gives rise to the Maxwell equations 10.1, respectively, Eq. 10.2, however, without sources.

On its turn, the Lagrangian density of the "electron"

$$\mathscr{L}_e(\mathbf{x},t) = -\frac{\hbar^2}{2m}\nabla\psi^*(\mathbf{x},t)\nabla\psi(\mathbf{x},t) - \frac{\imath\hbar}{2}\left(\dot{\psi}(\mathbf{x},t)^*\psi(\mathbf{x},t) - \psi(\mathbf{x},t)^*\dot{\psi}(\mathbf{x},t)\right) \tag{10.13}$$

for the field $\psi(\mathbf{x},t)^*$ gives rise to the free Schrödinger equation (uncoupled to the e.m. fields)

$$\imath\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x},t). \tag{10.14}$$

In these derivations one had to use partial integration allowed by the mentioned equivalence of Lagrangian densities.

We shall introduce the e.m. interaction between the electron and the electromagnetic field by the so-called minimal way, ensuring gauge invariance. It requires the replacements

$$\frac{\hbar}{\imath}\nabla\psi \to \left(\frac{\hbar}{\imath}\nabla + \frac{e}{c}\mathbf{A}\right)\psi \tag{10.15}$$

$$\frac{\hbar}{\imath}\frac{\partial}{\partial t}\psi \to \left(\frac{\hbar}{\imath}\frac{\partial}{\partial t} + eV\right))\psi \tag{10.16}$$

in the electron Lagrangian.

Thus, the total Lagrangian is

$$\begin{aligned}\mathscr{L} = &\frac{1}{8\pi}\left(\nabla V + \frac{1}{c}\frac{\partial}{\partial t}\mathbf{A}\right)^2 - \frac{1}{8\pi}(\nabla\times\mathbf{A})^2 \\ &- \frac{1}{2m}\left(-\frac{\hbar}{\imath}\nabla + \frac{e}{c}\mathbf{A}\right)\psi^*\left(\frac{\hbar}{\imath}\nabla + \frac{e}{c}\mathbf{A}\right)\psi \\ &- \frac{1}{2}\psi^*\left(\frac{\hbar}{\imath}\frac{\partial}{\partial t} + eV\right)\psi - \frac{1}{2}\psi\left(-\frac{\hbar}{\imath}\frac{\partial}{\partial t} + eV\right)\psi^*.\end{aligned} \tag{10.17}$$

This is obviously gauge invariant and gives rise to the correct coupled equations.

10.4 The Classical Hamiltonian in the Coulomb Gauge

Unfortunately, the above introduced Lagrangian density Eq. 10.17 is a so-called singular one. The time derivative of the variable V is not present in it and therefore the corresponding canonical momentum is vanishing, i.e., we have a constraint in the canonical formalism. Lagrangians with constraints, as we already mentioned, have to be handled with Dirac's canonical formalism that implies also a redefinition of the Poisson bracket. The simplest way out is however to use the choice of the gauge in such a way as to eliminate the spurious degrees of freedom from the Lagrangian before we could construct a Hamiltonian.

The Coulomb gauge defined by

$$\nabla\mathbf{A}(\mathbf{x}, t) = 0 \tag{10.18}$$

leaves only the physical transverse degrees of freedom of the photons and simultaneously eliminates the scalar potential in favor of the charge density

$$V(\mathbf{x}, t) = \int d\mathbf{x}'\frac{\rho(\mathbf{x}', t)}{|\mathbf{x} - \mathbf{x}'|}. \tag{10.19}$$

We shall construct the Hamiltonian the usual way, however, taking into account of the above constraint and define the canonical conjugate momenta as

$$\Pi_\psi \equiv \frac{\delta \mathscr{L}}{\delta \dot{\psi}} = \frac{\imath\hbar}{2}\psi^* \tag{10.20}$$

$$\Pi_{\psi^*} \equiv \frac{\delta \mathscr{L}}{\delta \dot{\psi}^*} = -\frac{\imath\hbar}{2}\psi \tag{10.21}$$

$$\Pi_A^\mu \equiv \frac{\mathscr{L}}{\delta \dot{A}^\mu} = \frac{1}{4\pi c}\left(\frac{\partial}{x_\mu}V + \frac{1}{c}\dot{A}\mu\right), \quad (\mu = 1,2,3) \tag{10.22}$$

$$\Pi_V \equiv 0 \tag{10.23}$$

and the Hamiltonian density is

$$\begin{aligned}\mathscr{H} &= -\mathscr{L} + \Pi_{A_\mu}\dot{A}_\mu + \Pi_\psi\dot{\psi} + \Pi_{\psi^*}\dot{\psi}^* \\ &= -\frac{1}{8\pi}\left(\nabla V + \frac{1}{c}\dot{\mathbf{A}}\right)^2 + \frac{1}{8\pi}(\nabla \times \mathbf{A})^2 + \frac{1}{4\pi c}\dot{\mathbf{A}}\left(\nabla V + \frac{1}{c}\dot{\mathbf{A}}\right) \\ &+ \frac{1}{2m}\left(-\frac{\hbar}{\imath}\nabla\psi^* + \frac{e}{c}\mathbf{A}\psi^*\right)\left(\frac{\hbar}{\imath}\nabla\psi + \frac{e}{c}\mathbf{A}\psi\right) + eV\psi^*\psi,\end{aligned} \tag{10.24}$$

or (underlining also by the notation $\mathbf{A}_\perp$ the transverse character of the vector potential)

$$\begin{aligned}\mathscr{H} &= \frac{1}{8\pi}\left(\nabla V + \frac{1}{c}\dot{\mathbf{A}}_\perp\right)^2 + \frac{1}{8\pi}(\nabla \times \mathbf{A}_\perp)^2 - \frac{1}{4\pi}\nabla V\left(\nabla V + \frac{1}{c}\dot{\mathbf{A}}_\perp\right) \\ &+ \frac{1}{2m}\left(-\frac{\hbar}{\imath}\nabla\psi^* + \frac{e}{c}\mathbf{A}_\perp\psi^*\right)\left(\frac{\hbar}{\imath}\nabla\psi + \frac{e}{c}\mathbf{A}_\perp\psi\right) + eV\psi^*\psi.\end{aligned}$$

In the Hamiltonian

$$H = \int d\mathbf{x}\mathscr{H}(\mathbf{x})$$

one may use a partial integration in order to obtain

$$\begin{aligned}H = \int d\mathbf{x}\Bigg[&\frac{1}{8\pi}\left(\nabla V + \frac{1}{c}\dot{\mathbf{A}}_\perp\right)^2 + \frac{1}{8\pi}(\nabla \times \mathbf{A}_\perp)^2 + \frac{1}{4\pi}V\nabla\left(\nabla V + \frac{1}{c}\dot{\mathbf{A}}_\perp\right) \\ &+ \frac{1}{2m}\left(-\frac{\hbar}{\imath}\nabla\psi^* + \frac{e}{c}\mathbf{A}_\perp\psi^*\right)\left(\frac{\hbar}{\imath}\nabla\psi + \frac{e}{c}\mathbf{A}_\perp\psi\right) + eV\psi^*\psi\Bigg].\end{aligned}$$

Due to the transversality of the vector potential and expressing the scalar potential through the charge density Eq. 10.19, one gets

$$H = \int d\mathbf{x} \left[\frac{1}{8\pi} \left(\nabla V + \frac{1}{c}\dot{\mathbf{A}}_\perp \right)^2 + \frac{1}{8\pi} \left(\nabla \times \mathbf{A}_\perp \right)^2 + \frac{1}{2m} \left(-\frac{\hbar}{\imath}\nabla\psi^* + \frac{e}{c}\mathbf{A}_\perp\psi^* \right) \left(\frac{\hbar}{\imath}\nabla\psi + \frac{e}{c}\mathbf{A}_\perp\psi \right) \right],$$

or

$$H = \int d\mathbf{x} \left[\frac{1}{8\pi} \left(\mathbf{E}^2 + \mathbf{B}^2 \right) + \frac{1}{2m} \left(-\frac{\hbar}{\imath}\nabla\psi^* + \frac{e}{c}\mathbf{A}_\perp\psi^* \right) \left(\frac{\hbar}{\imath}\nabla\psi + \frac{e}{c}\mathbf{A}_\perp\psi \right) \right].$$

Apparently the Coulomb interaction disappeared, but actually it is contained in the energy of the longitudinal electric field. Since under the integral

$$\mathbf{E}^2 = (\nabla V)^2 + (\frac{1}{c}\dot{\mathbf{A}}_\perp)^2$$

and after a partial integration

$$(\nabla V)^2 \rightarrow -V\nabla^2 V$$

we get

$$H = \int d\mathbf{x} \left[\frac{1}{8\pi} \left(\mathbf{E}_\perp^2 + \mathbf{B}^2 \right) + \frac{1}{2} e\psi^*\psi V + \frac{1}{2m} \left(-\frac{\hbar}{\imath}\nabla\psi^* + \frac{e}{c}\mathbf{A}_\perp)\psi^* \right) \left(\frac{\hbar}{\imath}\nabla\psi + \frac{e}{c}\mathbf{A}_\perp\psi \right) \right]. \tag{10.25}$$

The first term represents the energy of the transverse "photon" field.

10.5 Quantization of the Hamiltonian

Starting from our classical Hamiltonian in Coulomb gauge Eq. 10.26, after the usual equal-time quantization of the anti-commuting electron wave functions

$$[\psi(\mathbf{x}, t), \psi^+(\mathbf{x}', t)]_+ = \delta(\mathbf{x} - \mathbf{x}')$$

and the introduction of the creation and annihilation operators $b^+_{\mathbf{q},\lambda}$ and $b_{\mathbf{q},\lambda}$ of photons of polarization λ and momentum $\mathbf{q}$, one defines the quantized transverse e.m. vector potential

$$\mathbf{A}_\perp(\mathbf{x}) = \sum_{\lambda=1,2} \sqrt{\frac{\hbar c}{\Omega}} \sum_{\mathbf{q}} \frac{1}{\sqrt{|\mathbf{q}|}} \mathbf{e}_{\mathbf{q}}^{(\lambda)} e^{-\imath \mathbf{q}\mathbf{x}} \left(b_{\mathbf{q},\lambda} + b^+_{-\mathbf{q},\lambda} \right) \tag{10.26}$$

taken with periodical boundary conditions. This definition brings the photon part of the Hamiltonian to a diagonal form. Here the bosonic commutators are

$$\left[b_{\mathbf{q},\lambda}, b^+_{\mathbf{q}',\lambda'} \right] = \delta'_{\mathbf{q},\mathbf{q}} \delta_{\lambda\lambda'}$$

and the unit vectors $\mathbf{e}_{\mathbf{q}}^{(\lambda)}$ are orthogonal to the wave vector $\mathbf{q}$ and to each other

$$\mathbf{q}\mathbf{e}_{\mathbf{q}}^{(\lambda)} = 0; \qquad \mathbf{e}_{\mathbf{q}}^{(\lambda)} \mathbf{e}_{\mathbf{q}}^{(\lambda')} = \delta_{\lambda\lambda'}; \qquad \mathbf{e}_{\mathbf{q}}^{(\lambda)} = \mathbf{e}_{-\mathbf{q}}^{(\lambda)}; \qquad (\lambda, \lambda' = 1, 2).$$

With these ingredients and the normal ordering of the operators, one gets the non-relativistic QED Hamiltonian

$$\begin{aligned} H^{QED} &= \sum_{\mathbf{q},\lambda} \hbar\omega_q b^+_{\mathbf{q},\lambda} b_{\mathbf{q},\lambda} \\ &+ \int d\mathbf{x} N \left[\frac{1}{2m} \left(-\frac{\hbar}{\imath} \nabla \psi^+(\mathbf{x}) + \frac{e}{c} \mathbf{A}_\perp(\mathbf{x}) \psi^+(\mathbf{x}) \right) \left(\frac{\hbar}{\imath} \nabla \psi(\mathbf{x}, t) + \frac{e}{c} \mathbf{A}_\perp(\mathbf{x}) \psi(\mathbf{x}) \right) \right] \\ &+ \frac{1}{2} \int d\mathbf{x} \int d\mathbf{x}' \psi^+(\mathbf{x}) \psi^+(\mathbf{x}') \frac{e^2}{|\mathbf{x} - \mathbf{x}'|} \psi(\mathbf{x}') \psi(\mathbf{x}), \end{aligned} \tag{10.27}$$

where according to the general recipe of second quantization a normal ordering $N(\ldots)$ had to be introduced also with respect to the photon creation and annihilation operators $b^+_{\mathbf{q},\lambda}$, $b_{\mathbf{q}}$ in the Hamiltonian, and the photon frequency is $\omega_q = c|q|$.

This non-relativistic QED Hamiltonian coincides with the standard one obtained directly from the second quantized Hamilton operator of electrons interacting with a classical electromagnetic field in the Coulomb gauge, after the quantization of the transverse vector potential and adding the energy of the photons.

Our derivation has shown, how a field-theoretical treatment allows the use of the Lagrange formalism in deriving a non-relativistic quantum mechanical many-body theory of charged particles interacting with photons avoiding the problems linked to point-like classical charges.

10.6 Derivation of the $1/c^2$ Hamiltonian

In this framework one can show that the tedious construction of Chap. 9 is indeed equivalent to the $1/c^2$ approximation of the non-relativistic QED on states without photons. Then, if we want to retain only contributions up to order $1/c^2$, we may omit from the beginning the “seagull” term $\frac{e^2}{c^2} \int \psi^+ \psi AA$. Being itself of order $1/c^2$, it

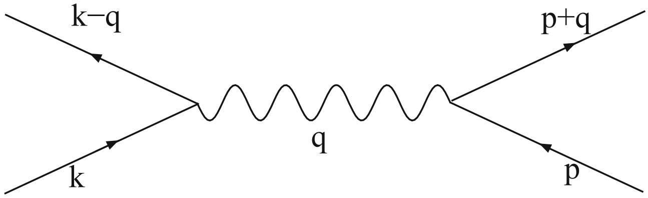

Fig. 10.1 The basic current–current (transverse photon exchange) graph in QED

may have only even higher order non-vanishing matrix elements in this subspace and besides the standard Coulomb term one is left only with the photon-current interaction $-\frac{1}{c}\int i_{\perp} A$.

In the S-matrix theory of adiabatic perturbations within this subspace, any Feynman diagram may be constructed using only the Coulomb vertex Fig. 3.3 and the basic graph having four electron legs and two current-photon vertices connected by a photon propagator as shown in Fig. 10.1. This graph differs from that of Fig. 3.3 by two features: the wavy line corresponds to the transverse photon propagator in the 4-dimensional Fourier space ω, $\mathbf{q}$

$$\frac{1}{q^2 - \omega^2/c^2 - \imath 0}(\delta_{\mu,\nu} - \frac{q_\mu q_\nu}{q^2}); \qquad (\mu, \nu = 1, 2, 3)$$

and the vertices contain momentum factors $-\imath \frac{e\hbar}{m} p_\mu, \quad -\imath \frac{e\hbar}{m} p_\nu$ due to the replacement of the charge densities by the currents. After neglecting the term $-\omega^2/c^2$ in the denominator of the photon propagator (i.e., ignoring retardation and implicitly eliminating corrections of higher order as $1/c^2$ already contained in the vertex parts), the photon propagator looks as

$$\frac{1}{q^2}(\delta_{\mu,\nu} - \frac{q_\mu q_\nu}{q^2}); \qquad (\mu, \nu = 1, 2, 3).$$

Since no pole survived, the $-\imath 0$ term could have been also ignored. Then one may convince oneself that this graph coincides with the basic vertex of the S-matrix of the $1/c^2$ theory including the transverse current–current interaction of the previous section.

Strange enough, although the non-relativistic QED and its correct $1/c^2$ approximation were well-known already in the sixties of the last century, they were used only in the treatment of the optical phenomena and completely ignored in the treatment of magnetism.