Non-relativistic QED

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Motivation

Before I give the outline of these lectures I would like to explain in non-technical terms what is non-relativistic QED. In short, it is a theory at the interface between non-relativistic Quantum Mechanics and relativistic QED.

0.1 Quantum Mechanics

Consider a Hydrogen atom described by $H = -\Delta_x - \alpha/|x|$. What quantum mechanics teaches about the spectrum of this operator is that it consists of a ground state and excited states

$$E_n = -\frac{1}{4}\frac{\alpha^2}{n^2}, \quad n = 1, 2, 3... \tag{0.1}$$

and then a continuous spectrum above zero. This means, that the electron in an excited state would stay in such an excited state forever. But experiments tell you that this is simply not true, the lines have a finite width (even at zero temperature) and thus after some time the electron relaxes to a ground state emitting photons. In the Schrödinger equation you know from Quantum Mechanics there are no terms responsible for this effect. The physical reason is coupling of the electron to the quantized electromagnetic field, which is usually not covered by introductory Quantum Mechanics courses. **Relaxation of excited atoms to the ground state is one example of a question which cannot be answered within non-relativistic Quantum Mechanics. Non-relativistic QED offers an appropriate framework to study this question**. (Relativistic QED is difficult to apply to bound state problems due to its perturbative character - see below).

0.2 Relativistic Quantum Electrodynamics

Full Quantum Electrodynamics (QED) describes interactions between electrons and positrons, described by the electric current density j, and photons, described by the electromagnetic potential A. The interaction, formally given by

$$V_{\mathrm{RQED}} = e\int d^3x\, j(x)A(x), \tag{0.2}$$

turns out to be very singular, since j and A are distributions, but we ignore these *ultraviolet problems* here for a moment. Given the interaction, the next step is to write down the scattering matrix. Rules of the game of Quantum Mechanics give

$$S = \mathrm{Texp}\Big(-i\int_{-\infty}^{\infty} dt\, V^I_{\mathrm{RQED}}(t)\Big) \tag{0.3}$$

where V^I_{RQED} is the interaction in the interaction picture. To compute the probability that a system evolves from some initial state $|\alpha\rangle$ to a final state $|\beta\rangle$ one needs to compute the scattering matrix element $\langle\alpha|S|\beta\rangle$. Let us consider Compton scattering, i.e. collision of one electron and one photon. The probability of a transition $\alpha \to \beta$ (collision cross section[1] σ) satisfies

$$\sigma \sim |\langle\alpha|S|\beta\rangle|^2. \tag{0.4}$$

$\langle\alpha|S|\beta\rangle$ can be computed as a power series in the coupling constant e and the resulting expressions can be depicted as Feynman diagrams which capture the intuitive meaning of the respective contributions. The leading contribution is given by a tree diagram (TREE DIAGRAM). Further contributions involve emission and reabsorption of virtual photons (RADIATIVE CORRECTION DIAGRAM). These contributions have the so called *infrared divergences* that is divergences at small values of the photon energy. These divergences can be traced back to vanishing mass of the photon and integration over whole space in (0.2). They have to be regularized by introducing an infrared cut-off $\lambda > 0$ (simply eliminating photons of energy smaller than λ). The resulting S-matrix element $\langle\alpha|S^\lambda|\beta\rangle$ can be computed, but $\lim_{\lambda\to 0}\langle\alpha|S^\lambda|\beta\rangle = 0$ as if there was no scattering. Thus standard rules of Quantum Mechanics give an experimentally unacceptable result: $\sigma = 0$! This is one manifestation of the **infrared problem**.

A way out, proposed by Yennie, Frautschi and Suura [3] is a serious deviation from these rules of the game. We should not consider the process $\alpha \to \beta$ alone, but a whole family of processes $\alpha \to \beta_n$, where β_n involves emission of n photons of total energe E_t in addition to particles present in β. (SOFT PHOTON EMISSION DIAGRAM). The resulting *inclusive cross-section* is given by

$$\sigma_{\mathrm{inc}}(E_t) \sim \lim_{\lambda\to 0} \sum_{n=0}^{\infty} |\langle\alpha|S^\lambda|\beta\rangle|^2, \tag{0.5}$$

which is finite and not identically zero. It gives results consistent with experiments if E_t is chosen below the sensitivity of the detector. A mathematically rigorous derivation of this formula from first principles has not been achieved in the perturbative framework of relativistic QED, in spite of many attempts [2]. **In contrast, in the framework of non-relativistic QED, there has been steady progress in understanding of the infrared problem.** Important advantage: availability of a Hamiltonian as a self-adjoint operator on a Hilbert space (and not just a formal power series).

The problem of relaxation of Hydrogen atom to the ground state is also difficult to study in the perturbative setting of relativistic QED, because electron confined in an atom cannot be considered a small perturbation of a freely moving electron.

0.3 Non-relativistic Quantum Electrodynamics

Start from the relativistic QED interaction:

$$V_{\mathrm{RQED}} = e \int d^3x\, j(x)A(x) \tag{0.6}$$

[1] $\sigma = -\frac{1}{n\Phi}\frac{d\Phi}{dz}$, where $d\Phi$ is a loss of the flux due to the event, dz is the thickness of the target material and n is the number density.

1. j and A are distributions, problems with pointlike multiplication. We need to regularize: Replace j with a convolution $j * \varphi$ for a nice function φ so that $j * \varphi$ is now also a nice function. φ plays a role of charge distribution of the electron.

2. Integral over whole $\mathbb{R}^3$ difficult to control. It helps to remove terms from j which are responsible for electron-positron pair creation. The result can be denoted as no-pairs current j_{np}.

Thus we are left with the interaction which is a controllable expression

$$V_{\mathrm{NRQED}} = \int d^3x\, (j_{\mathrm{np}} * \varphi)(x) A(x). \tag{0.7}$$

After some further steps and simplifications one obtains the standard Hamiltonian of non-relativistic QED (Pauli-Fierz Hamiltonian):

$$H_{\mathrm{NRQED}} = \sum_{j=1}^{N} \frac{1}{2m}(p_j - e(A * \varphi)(q_j))^2 + V_c(q) + H_f. \tag{0.8}$$

where (p_j, q_j) are positions and momenta of electrons, V_c is the Coulomb interaction between the electrons and H_f is the energy of photons. It is a reasonable approximation to full QED in the low energy regime, in particular below the electron-positron pair production threshold. In the next section we will obtain this Hamiltonian along a different route by quantization of classical Maxwell equations coupled to particles.

0.4 Outline of the course

1. Quantization of charged particles interacting with the electromagnetic field.

2. Pauli-Fierz Hamiltonian and other models of non-relativistic QED.

3. Fock spaces and self-adjointness of the Pauli-Fierz Hamiltonian.

4. Energy-momentum operators and their spectrum. Physical single-particle states.

5. Asymptotic photon fields and scattering matrix.

6. Infrared problems and the problem of asymptotic completeness.

1 Quantization of particles interacting with the electromagnetic field [1]

1.1 Equations of motion

Let E, B, ρ, j be the electric field, magnetic field, charge density and current density, respectively. These are functions on space-time satisfying the Maxwell equations (here we set velocity of light $c = 1$):

$$\begin{aligned} \partial_t B &= -\nabla \times E, && (1.9)\\ \partial_t E &= \nabla \times B - j, && (1.10)\\ \nabla \cdot E &= \rho, && (1.11)\\ \nabla \cdot B &= 0. && (1.12) \end{aligned}$$

We want ρ and j to describe a collection of N particles of finite extension. Thus we introduce a nice function $\varphi \in S(\mathbb{R}^3)$, s.t. $\varphi(x) = \varphi(-x)$, which models the charge distribution of each particle. Let $t \to q_j(t)$ be the trajectories. The charge and current are given by:

$$\begin{aligned} \rho(t,x) &= e \sum_{j=1}^{N} \varphi(x - q_j(t)), && (1.13)\\ j(t,x) &= e \sum_{j=1}^{N} \varphi(x - q_j(t)) \dot{q}_j(t). && (1.14) \end{aligned}$$

They obviously satisfy the charge conservation equation:

$$\partial_t \rho(t,x) + \nabla_x j(t,x) = 0. \tag{1.15}$$

The total charge of each particle is

$$Q := e \int d^3x\, \varphi(x) = (2\pi)^{3/2} e \hat{\varphi}(0). \tag{1.16}$$

If $Q \neq 0$, the particle will be called an electron. If $Q = 0$ the particle will be called an atom.

We couple this system to the Newton equations of motion

$$m\ddot{q}_j(t) = e\big(E_\varphi(t, q_j(t)) + \dot{q}_j(t) \times B_\varphi(t, q_j(t))\big), \tag{1.17}$$

where

$$E_\varphi(t,x) = (E * \varphi)(t,x) = \int d^3y\, E(t, x-y)\varphi(y), \tag{1.18}$$

and similarly for B. Clearly, for $\varphi \to \delta$ we have $E_\varphi(t,x) \to E(t,x)$ and $Q = e$ but in this limit the system of equations becomes singular. Thus in general the parameter e should be interpreted as a coupling constant, which determines the strength of interaction between the fields and the particles, rather than charge.

1.2 Electromagnetic potentials

We introduce the electromagnetic potentials ϕ, A, which satisfy

$$\begin{aligned} E &= -\partial_t A - \nabla \phi, && (1.19)\\ B &= \nabla \times A. && (1.20) \end{aligned}$$

Since $\nabla(\nabla \times A) \equiv 0$ and $(\nabla \times \nabla\phi) \equiv 0$, this guarantees

$$\nabla \cdot B = 0 \quad \text{and} \quad \partial_t B = -\nabla \times E. \tag{1.21}$$

Note that the potentials (ϕ, A) are not unique. For example, for any smooth f, the new potentials $\tilde{A}(t,x) = A(t,x) + \nabla f(x)$ and $\tilde{\phi}(t,x) = \phi(t,x)$ give rise to the same fields E, B. (Because $\nabla \times \nabla f = 0$). This is called a change of gauge of (ϕ, A). Exploiting gauge freedom, we can impose additional conditions on the potentials. For example, by choosing f s.t. $\triangle f = -\nabla \cdot A$ we obtain

$$\nabla \cdot \tilde{A} = 0. \tag{1.22}$$

In this case we say that $\tilde{A}$ satisfies the *Coulomb gauge* condition.

1.3 Lagrangian formulation

The Lagrangian is given by

$$\begin{aligned} L &= \frac{1}{2}\sum_{j=1}^{N} m\dot{q}_j^2 + \int d^3x \Big(\frac{1}{2}(E(t,x)^2 - B(t,x)^2) + j(t,x)\cdot A(t,x) - \rho(t,x)\phi(t,x)\Big) \\ &= \frac{1}{2}\sum_{j=1}^{N} m\dot{q}_j^2 + \int d^3x \Big(\frac{1}{2}(-\partial_t A - \nabla\phi)^2 - \frac{1}{2}(\nabla \times A)^2 \\ &\qquad + e\sum_{j=1}^{N}\varphi(x - q_j(t))\dot{q}_j \cdot A - e\sum_{j=1}^{N}\varphi(x - q_j(t))\phi\Big), \end{aligned} \tag{1.23}$$

where $\{q_j, \phi(x), A(x)\}$ are understood as coordinates. The Euler-Lagrange equations give the remaining equations of motion:

$$\partial_t \frac{\partial L}{\partial \dot{q}_j} - \frac{\partial L}{\partial q_j} = 0 \quad \text{gives} \quad m\ddot{q} = e\big(E_\varphi(t, q(t)) + \dot{q} \times B_\varphi(t, q(t))\big), \tag{1.24}$$

$$\partial_t \frac{\delta L}{\delta \dot{\phi}} - \frac{\delta L}{\delta \phi} = 0 \quad \text{gives} \quad \nabla E = \rho, \tag{1.25}$$

$$\partial_t \frac{\delta L}{\delta \dot{A}^i} - \frac{\delta L}{\delta A^i} = 0 \quad \text{gives} \quad \partial_t E = \nabla \times B - j. \tag{1.26}$$

Remark 1.1. *In relativistic field theory one often considers action of the form*

$$S = \int d^4x\, \mathcal{L}(\phi(x), \partial_\mu \phi(x)), \tag{1.27}$$

where x is a four-vector. Then the Euler-Lagrangian equations have the form

$$\partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)}\right) = \frac{\partial \mathcal{L}}{\partial \phi}. \tag{1.28}$$

Here $\mathcal{L}$ is a Lagrangian density (as opposed to the Lagrangian L) and therefore all the derivatives can be considered partial derivatives (as opposed to the functional derivatives $\delta/\delta\phi$ computed according to (1.34)).

Let us show (1.24): We have

$$\begin{aligned}
\frac{\partial L}{\partial \dot{q}_j^i} &= m\dot{q}_j^i + \int d^3x\, e\varphi(x - q_j(t))A^i(t,x), &(1.29)\\
\partial_t \frac{\partial L}{\partial \dot{q}_j^i} &= m\ddot{q}_j^i - \int d^3x\, e\partial_k\varphi(x - q_j(t))\dot{q}_j^k A^i(t,x)\\
&\qquad + \int d^3x\, e\varphi(x - q_j(t))\partial_t A^i(t,x), &(1.30)\\
&= m\ddot{q}_j^i + \int d^3x\, e\varphi(x - q_j(t))\dot{q}_j^k \partial_k A^i(t,x)\\
&\qquad + \int d^3x\, e\varphi(x - q_j(t))\partial_t A^i(t,x), &(1.31)\\
\frac{\partial L}{\partial q_j^i} &= -\int d^3x\, e\Big(\partial_i\varphi(x - q_j(t))\dot{q}_j^k A^k - \partial_i\varphi(x - q_j(t))\phi\Big)\\
&= \int d^3x\, e\Big(\varphi(x - q_j(t))\dot{q}_j^k \partial_i A^k - \varphi(x - q_j(t))\partial_i\phi\Big) &(1.32)
\end{aligned}$$

(Summation over index k understood). To conclude, we use

$$[\dot{q}_j \times (\nabla \times A)]^i = [\nabla(\dot{q}_j A)]^i - (\dot{q}_j \cdot \nabla)A^i = \dot{q}_j^k \partial_i A^k - \dot{q}_j^k \partial_k A^i \qquad (1.33)$$

and the property $\varphi(x) = \varphi(-x)$.

Let us now show (1.25): The functional derivative $\delta/\delta\phi$ is the 'Frechet derivative in the direction of Dirac δ'. The rule of the game is:

$$\frac{\delta\phi(t,x)}{\delta\phi(t,y)} = \delta(x - y). \qquad (1.34)$$

Thus we have

$$\begin{aligned}
\frac{\delta L}{\delta\dot{\phi}(t,y)} &= 0\\
\frac{\delta L}{\delta\phi(t,y)} &= \int d^3x\Big(- (-\partial_t A(t,x) - \nabla\phi(t,x))\nabla\delta(x - y)\\
&\qquad - e\sum_{j=1}^{N} \varphi(x - q_j(t))\delta(x - y)\Big)\\
&= \int d^3x\Big(\nabla E(t,x)\delta(x - y) - e\rho(t,x)\delta(x - y)\Big)\\
&= \nabla E(t,y) - e\sum_{j=1}^{N} \varphi(y - q_j(t)). &(1.35)
\end{aligned}$$

Finally, we show (1.26). First, we recall that

$$(\nabla \times A)^k = \varepsilon^{k\ell m}\partial_\ell A^m, \qquad (1.36)$$

where $\varepsilon^{k\ell m}$ is the completely antisymmetric Levi-Civita tensor. And therefore

$$\frac{\delta}{\delta A^i(t,y)}(\nabla \times A(t,x))^k = \varepsilon^{k\ell m}\partial_\ell \delta_{im}\delta(x-y) = \varepsilon^{k\ell i}\partial_\ell \delta(x-y) \tag{1.37}$$

$$\begin{aligned}
\frac{\delta L}{\delta \dot{A}^i(t,y)} &= -\int d^3x(-\partial_t A - \nabla\phi)\delta(x-y) = -E(t,y), &(1.38)\\
\partial_t \frac{\delta L}{\delta \dot{A}^i(t,y)} &= -\partial_t E(t,y), &(1.39)\\
\frac{\delta L}{\delta A^i(t,y)} &= \int d^3x\Big(-(\nabla\times A)^k \varepsilon^{k\ell i}\partial_\ell \delta(x-y) + e\sum_{j=1}^N \varphi(x-q_j(t))\dot{q}_j^i \delta(x-y)\Big)\\
&= \int d^3x\Big(-\varepsilon^{i\ell k}\partial_\ell(\nabla\times A)^k \delta(x-y) + e\sum_{j=1}^N \varphi(x-q_j(t))\dot{q}_j^i \delta(x-y)\Big)\\
&= -(\nabla\times(\nabla\times A))^i(t,y) + j^i(t,y)\\
&= -(\nabla\times B)^i(t,y) + j^i(t,y). &(1.40)
\end{aligned}$$

1.4 Transverse and longitudinal field components

Recall that photon has just two polarizations, whereas here we use four functions (ϕ, A) to describe the electromagnetic field. To obtain the physical Hamiltonian (energy-operator) we have to eliminate the superfluous degrees of freedom. There is a general formalism of quantisation with constraints, that could be applied here [3], but that would take us too far from the main topic of these lectures. Instead, we will make some informed guesses and in the end check that the resulting quantum theory satisfies Maxwell equations.

To start with, it is convenient to pass to the Fourier representation:

$$\widehat{E}(k) := \frac{1}{(2\pi)^{3/2}}\int d^3x\, \mathrm{e}^{-ikx}E(x), \tag{1.41}$$

$$\widehat{B}(k) := \frac{1}{(2\pi)^{3/2}}\int d^3x\, \mathrm{e}^{-ikx}B(x), \tag{1.42}$$

$$\widehat{A}(k) := \frac{1}{(2\pi)^{3/2}}\int d^3x\, \mathrm{e}^{-ikx}A(x). \tag{1.43}$$

From now on we suppress the t-dependence in the notation.

Problem: Show that $\widehat{\nabla\cdot E}(k) = ik\cdot\widehat{E}(k)$.

Now let $\hat{k} := k/|k|$ and P_k the corresponding projection. That is, for any vector $v \in \mathbb{R}^3$ we have

$$P_k v = \hat{k}(\hat{k}\cdot v). \tag{1.44}$$

(In Dirac notation from quantum mechanics: $P_k = |\hat{k}\rangle\langle\hat{k}|$). Now we can decompose the fields as follows

$$\widehat{E}(k) = P_k\widehat{E}(k) + (1 - P_k)\widehat{E}(k) = \widehat{E}_{\parallel}(k) + \widehat{E}_{\perp}(k), \tag{1.45}$$

where $\widehat{E}_{\parallel}(k)$, $\widehat{E}_{\perp}(k)$ are called the longitudinal and transverse components. (B and A are decomposed analogously). Now we note

$$\nabla \cdot B = 0 \quad \Rightarrow \quad \widehat{\nabla \cdot B} = 0 \quad \Rightarrow \quad ik \cdot \widehat{B} = 0 \quad \Rightarrow \quad \widehat{B}_{\parallel} = 0, \tag{1.46}$$

$$\nabla \cdot E = \rho \quad \Rightarrow \quad \widehat{\nabla \cdot E} = \widehat{\rho} \quad \Rightarrow \quad ik \cdot \widehat{E} = \widehat{\rho} \quad \Rightarrow \quad \widehat{E}_{\parallel} = -i\widehat{\rho}\frac{k}{|k|^2} \tag{1.47}$$

Given the second relation, we can eliminate ϕ: Note that

$$E = -\partial_t A - \nabla\phi \quad \Rightarrow \quad \widehat{E} = -\partial_t\widehat{A} - ik\widehat{\phi} \quad \Rightarrow \quad \widehat{E_{\parallel}} = -\partial_t\widehat{A_{\parallel}} - ik\widehat{\phi}. \tag{1.48}$$

Therefore,

$$k \cdot \widehat{E_{\parallel}} = -k \cdot \partial_t\widehat{A_{\parallel}} - i|k|^2\widehat{\phi} \quad \Rightarrow \quad -i\widehat{\rho} = -k \cdot \partial_t\widehat{A_{\parallel}} - i|k|^2\widehat{\phi}, \tag{1.49}$$

which gives

$$\widehat{\phi} = \frac{1}{|k|^2}\big(ik \cdot \partial_t\widehat{A_{\parallel}} + \widehat{\rho}\big). \tag{1.50}$$

Moreover,

$$\widehat{E} = \widehat{E_{\perp}} + \widehat{E_{\parallel}} = -\partial_t\widehat{A_{\perp}} - i\widehat{\rho}\frac{k}{|k|^2}, \tag{1.51}$$

$$\widehat{B} = \widehat{B_{\perp}} = \widehat{\nabla \times A_{\perp}} = ik \times \widehat{A_{\perp}}, \tag{1.52}$$

because $k \times \widehat{A_{\parallel}}$ is proportional to $k \times k = 0$.

1.5 Lagrangian in terms of transverse and longitudinal fields

Now we come back to the Lagrangian:

$$L = \frac{1}{2}\sum_{j=1}^{N} m\dot{q}_j^2 + \int d^3x\left(\frac{1}{2}(E(x)^2 - B(x)^2) + j(x) \cdot A(x) - \rho(x)\phi(x)\right). \tag{1.53}$$

To rewrite in terms of Fourier transformed fields, we use the Plancherel identity:

$$\int d^3x\bar{f}(x)g(x) = \int d^3k\overline{\widehat{f}}(k)\widehat{g}(k), \tag{1.54}$$

valid for square-integrable functions. Using (1.50), (1.51) and (1.52) we get

$$\begin{aligned} L \;&=\; \frac{1}{2}\sum_{j=1}^{N} m\dot{q}_j^2 + \frac{1}{2}\int d^3k\big(|\partial_t\widehat{A_{\perp}}|^2 - |k \times \widehat{A_{\perp}}|^2 + |k|^{-2}|\widehat{\rho}|^2\big) \\ &\quad + \int d^3k\,\big(\overline{\widehat{j}} \cdot \widehat{A} - |k|^{-2}|\widehat{\rho}|^2 - i|k|^{-2}\overline{\widehat{\rho}}k \cdot \partial_t\widehat{A_{\parallel}}\big). \end{aligned} \tag{1.55}$$

For example,

$$\begin{aligned}\int d^3x|E(x)|^2 &= \int d^3k|\widehat{E}(k)|^2 = \int d^3k|\partial_t\widehat{A_\perp} + i\widehat{\rho}\frac{k}{|k|^2}|^2 \\ &= \int d^3k\big(|\partial_t\widehat{A_\perp}|^2 + |k|^{-2}|\widehat{\rho}|^2\big). \qquad (1.56)\end{aligned}$$

Now we make two rearrangements of L:

(a) We use the charge conservation law (1.15):

$$\partial_t\rho + \nabla\cdot j = 0 \quad \Rightarrow \quad \partial_t\widehat{\rho} + ik\cdot\widehat{j} = 0, \qquad (1.57)$$

which gives

$$\begin{aligned}\overline{\widehat{j}}\cdot\widehat{A} - i|k|^{-2}\overline{\widehat{\rho}}(k\cdot\partial_t\widehat{A_\parallel}) &= \overline{\widehat{j}}\cdot\widehat{A_\perp} + \overline{\widehat{j}}\cdot\widehat{A_\parallel} - i|k|^{-2}\overline{\widehat{\rho}}(k\cdot\partial_t\widehat{A_\parallel}) \\ &= \overline{\widehat{j}}\cdot\widehat{A_\perp} + \overline{\widehat{j}}\cdot P_k\widehat{A_\parallel} - i|k|^{-2}\overline{\widehat{\rho}}(k\cdot\partial_t\widehat{A_\parallel}) \\ &= \overline{\widehat{j}}\cdot\widehat{A_\perp} + |k|^{-2}(\overline{\widehat{j}}\cdot k)(k\cdot\widehat{A_\parallel}) - i|k|^{-2}\overline{\widehat{\rho}}(k\cdot\partial_t\widehat{A_\parallel}) \\ &= \overline{\widehat{j}}\cdot\widehat{A_\perp} - i|k|^{-2}(\partial_t\overline{\widehat{\rho}})(k\cdot\widehat{A_\parallel}) - i|k|^{-2}\overline{\widehat{\rho}}(k\cdot\partial_t\widehat{A_\parallel}) \\ &= \overline{\widehat{j}}\cdot\widehat{A_\perp} - i|k|^{-2}\partial_t(\overline{\widehat{\rho}}(k\cdot\widehat{A_\parallel})). \qquad (1.58)\end{aligned}$$

The last term gives rise to a total time derivative contribution to L. Such terms have no effect on the Euler-Lagrange equations, thus can be skipped. Incidentally, this step eliminates $\widehat{A_\parallel}$ from the game. It is thus natural to set $\widehat{A_\parallel} = 0$ in the following. This amounts to choosing the Coulomb gauge, i.e.

$$0 = \nabla\cdot A = \widehat{\nabla\cdot A} = ik\cdot A = ik\cdot\widehat{A_\parallel}, \qquad (1.59)$$

which can be done without changing fields (E, B). (Cf. Subsection 1.2). Thus we are left with two degrees of freedom of the electromagnetic field described by $A_\perp$.

Remark 1.2. *There are two independent justifications for setting $A_\parallel = 0$: gauge freedom and freedom to add a total time derivative to the lagrangian. This is not a coincidence*[2]*: Consider the gauge-dependent part of the Lagrangian:*

$$L_I = \int d^3x(j(t,x)\cdot A(t,x) - \rho(t,x)\phi(t,x)) \qquad (1.60)$$

and make a general gauge transformation: $A(t,x) = A'(t,x) + \nabla f(t,x)$,

[2]Thanks to Vincent Beaud for pointing this out.

$\phi(t,x) = \phi'(t,x) - \partial_t f(t,x)$. Then

$$
\begin{aligned}
L_I &= \int d^3x (j(t,x)\cdot A'(t,x) - \rho(t,x)\phi'(t,x)) \\
&\quad + \int d^3x(-\nabla j(t,x) f(t,x) + \rho(t,x)\partial_t f(t,x)) \\
&= \int d^3x (j(t,x)\cdot A'(t,x) - \rho(t,x)\phi'(t,x)) \\
&\quad + \partial_t \int d^3x \rho(t,x) f(t,x).
\end{aligned}
\tag{1.61}
$$

Now we choose f s.t. $\widehat{A}'_{\|} = 0$ and $\widehat{\phi}'(t,k) = \frac{1}{|k|^2}\widehat{\rho}(t,k)$. But from (1.58) we can read off that $\widehat{f}(t,k) = -i|k|^{-2}(k\cdot \widehat{A_{\|}}(t,k))$ does the job.

(b) Now we show that the $|k|^{-2}|\widehat{\rho}|^2$ contribution gives rise to the Coulomb interaction. Let us set $V(y) = (4\pi|y|)^{-1}$. Then $\widehat{V}(k) = (2\pi)^{-3/2}|k|^{-2}$. Thus we have

$$
\begin{aligned}
V_c &= \frac{1}{2}\int d^3x d^3y\, \rho(x)V(x-y)\rho(y) = \frac{1}{2}\int d^3x\, \rho(x)(V*\rho)(x) \\
&= \frac{1}{2}\int d^3k\, \overline{\widehat{\rho}}(k)\widehat{(V*\rho)}(k) = \frac{1}{2}(2\pi)^{3/2}\int d^3k\, \overline{\widehat{\rho}}(k)\widehat{V}(k)\widehat{\rho}(k) \\
&= \frac{1}{2}\int d^3k\, |k|^{-2}|\overline{\widehat{\rho}}(k)|^2.
\end{aligned}
\tag{1.62}
$$

Since $\rho(t,x) = e\sum_{j=1}^N \varphi(x-q_j(t))$, we have

$$
V_c = \frac{1}{2}e^2\sum_{j,j'=1}^N \int d^3x d^3y\, \varphi(x)\frac{1}{4\pi|x-y+q_j(t)-q_{j'}(t)|}\varphi(y). \tag{1.63}
$$

In the limit of point charges, i.e. $\varphi \to \delta$ we get for $j \neq j'$ the expected contribution $(4\pi|q_j(t)-q_{j'}(t)|)^{-1}$. For $j = j'$ this limit diverges, however. (Infinite self-energy of a point charge).

Given (a), (b), the Lagrangian (1.55) has the form (up to total time derivative)

$$
\begin{aligned}
L &= \frac{1}{2}\sum_{j=1}^N m\dot{q}_j^2 - V_c + \frac{1}{2}\int d^3k \big(|\partial_t \widehat{A_\perp}|^2 - |k\times\widehat{A_\perp}|^2\big) + \int d^3k\, (\overline{\widehat{j}}\cdot\widehat{A_\perp}) \\
&= \frac{1}{2}\sum_{j=1}^N m\dot{q}_j^2 - V_c + \frac{1}{2}\int d^3x \big(|\partial_t A_\perp|^2 - |\nabla\times A_\perp|^2\big) + \int d^3x\, (j\cdot A_\perp).
\end{aligned}
\tag{1.64}
$$

1.6 Hamiltonian

Given formula (1.64) and recalling that $j(t,x) = e\sum_{j=1}^{N}\varphi(x - q_j(t))\dot{q}_j$, we obtain the canonical momenta:

$$
\begin{aligned}
p_j &= \frac{\partial L}{\partial \dot{q}_j} = m\dot{q}_j + eA_{\perp,\varphi}(q_j), && (1.65)\\
\Pi(y) &= \frac{\delta L}{\delta \dot{A}_\perp(y)} = \dot{A}_\perp(y) = -E_\perp(y). && (1.66)
\end{aligned}
$$

The Hamiltonian has the following form

$$
\begin{aligned}
H &= \sum_{j=1}^{N} p_j\dot{q}_j + \int d^3x\,\Pi(x)\dot{A}_\perp(x) - L\\
&= \sum_{j=1}^{N}\frac{1}{2m}(p_j - eA_{\perp,\varphi}(q_j))^2 + V_c\\
&+ \frac{1}{2}\int d^3x\,\big\{(E_\perp)^2 + (\nabla\times A_\perp)^2\big\}, && (1.67)
\end{aligned}
$$

with the canonically conjugate pairs $\{q_j, p_j\}$ and $\{A_\perp(x), -E_\perp(x)\}$. To obtain this formula, it suffices to notice that

$$
\int d^3x (j\cdot A_\perp)(x) = e\sum_{j=1}^{N}\dot{q}_j\int d^3x\,\varphi(x - q_j(t))\cdot A_\perp(x) = e\sum_{j=1}^{N}\dot{q}_j\cdot A_{\perp,\varphi}(q_j), \quad (1.68)
$$

where we made use of $\varphi(x) = \varphi(-x)$.

1.7 Formal quantization

We now proceed to a quantum theory, which means that $\{q_j, p_j\}$ and $\{A_\perp(x), -E_\perp(x)\}$ will be operators on some Hilbert space. We first forget about the fields and quantize the particles. We require that the following commutation relations hold:

$$
[q_i^\alpha, p_j^\beta] = q_i^\alpha p_j^\beta - p_j^\beta q_i^\alpha = i\delta_{\alpha,\beta}\delta_{i,j}, \quad (1.69)
$$

where we set $\hbar = 1$. Let $\mathcal{H}_p = L^2(\mathbb{R}^{3N})$ and think about distiguishable particles (otherwise we would have to restrict attention to the subspace of symmetric/antisymmetric functions). Then it is easy to see that

$$
\begin{aligned}
q_i^\alpha\psi(x_1,\dots,x_N) &:= x_i^\alpha\psi(x_1,\dots,x_N), && (1.70)\\
p_j^\beta\psi(x_1,\dots,x_N) &:= -i\partial_{j,\beta}\psi(x_1,\dots,x_N), && (1.71)
\end{aligned}
$$

satisfy (1.69).

To quantize the electromagnetic field, we will look for certain *quantum fields* $A_\perp$, $-E_\perp$ i.e. functions[3] $x \to A_\perp(x)$, $x \to -E_\perp(x)$ with values in operators

[3] More precisely distributions.

on some Hilbert space $\mathcal{F}$ (Fock space). **We stress that from now on omitted time-dependence means that the fields are evaluated at $t = 0$ i.e. $A_\perp(x) = A_\perp(t = 0, x)$.** We impose the following commutation relations:

$$[A_\perp^\alpha(x), -E_\perp^\beta(x')] = i\delta_{\alpha\beta}^\perp(x - x'), \tag{1.72}$$

$$\delta_{\alpha\beta}^\perp(x) := (2\pi)^{-3} \int d^3k\, e^{ikx}(\delta_{\alpha\beta} - \hat{k}_\alpha \hat{k}_\beta), \tag{1.73}$$

which should be understood in analogy to (1.69). We will not try to explain a priori why the transverse delta function $\delta_{\alpha\beta}^\perp(x - x')$ (and not e.g. $\delta_{\alpha\beta}\delta(x - y)$) should appear on the r.h.s. (It is plausible that this has to do with the Coulomb gauge condition $\nabla A = 0$ which we use[4]). Our strategy is to first find $A_\perp(x)$, $E_\perp(x')$ which satisfy (1.72). Then, in subsection 1.9, we will check that these quantum fields satisfy the Maxwell equations, and thus the quantization prescription (1.72) was 'correct'.

We first introduce an orthonormal basis at each $k \in \mathbb{R}^3$

$$\widehat{k} = \frac{k}{|k|},\ e_1(k),\ e_2(k), \tag{1.74}$$

which satisfies $\hat{k} \cdot e_\lambda(k) = 0$, $\lambda = 1, 2$, and $e_1(k) \cdot e_2(k) = 0$. Completeness of the basis can be expressed by

$$\widehat{k}^\alpha \widehat{k}^\beta + \sum_{\lambda=1,2} e_\lambda^\alpha(k) e_\lambda^\beta(k) = \delta_{\alpha\beta}. \tag{1.75}$$

We introduce auxiliary distributions $(k, \lambda) \to a(k, \lambda)$ and $(k, \lambda) \to a^*(k, \lambda)$ with values in operators on the Hilbert space $\mathcal{F}$ (Fock space). They are called annihilation and creation operators, respectively, and satisfy

$$[a(k, \lambda), a^*(k', \lambda')] = \delta_{\lambda,\lambda'}\delta(k - k'), \tag{1.76}$$

$$[a(k, \lambda), a(k', \lambda')] = 0, \tag{1.77}$$

$$[a^*(k, \lambda), a^*(k', \lambda')] = 0. \tag{1.78}$$

Their detailed definition is postponed to the next section, here we will only use these commutation relations. Now we define the fields $A_\perp(x)$, $E_\perp(x')$ via their Fourier transforms:

$$\widehat{A}_\perp(k) := \sum_{\lambda=1,2} \sqrt{\frac{1}{2\omega(k)}} \big(e_\lambda(k) a(k, \lambda) + e_\lambda(-k) a^*(-k, \lambda)\big), \tag{1.79}$$

$$\widehat{E}_\perp(k) := \sum_{\lambda=1,2} \sqrt{\frac{\omega(k)}{2}} \big(ie_\lambda(k) a(k, \lambda) - ie_\lambda(-k) a^*(-k, \lambda)\big), \tag{1.80}$$

[4]This form of commutation relations can be derived from a general theory of quantization with constraints, see [3].

where $\omega(k) = |k|$ is the dispersion relation (i.e. energy-momentum relation) of photons. We note that by definition $\hat{k} \cdot \widehat{A}_\perp(k) = 0$ and $\hat{k} \cdot \widehat{E}_\perp(k) = 0$ i.e. the fields are indeed transverse. In configuration space they have the form

$$\begin{aligned} A_\perp(x) &= \frac{1}{(2\pi)^{3/2}} \sum_{\lambda=1,2} \int d^3k \sqrt{\frac{1}{2\omega(k)}} e_\lambda(k) \big(\mathrm{e}^{ikx} a(k,\lambda) + \mathrm{e}^{-ikx} a^*(k,\lambda) \big), && (1.81) \\ E_\perp(x) &= \frac{1}{(2\pi)^{3/2}} \sum_{\lambda=1,2} \int d^3k \sqrt{\frac{\omega(k)}{2}} e_\lambda(k) i \big(\mathrm{e}^{ikx} a(k,\lambda) - \mathrm{e}^{-ikx} a^*(k,\lambda) \big). && (1.82) \end{aligned}$$

In order to verify the commutation relation, (1.72), we first compute

$$\begin{aligned} [\widehat{A}^\alpha_\perp(k), \widehat{E}^\beta_\perp(k')] &= \sum_{\lambda,\lambda'} \sqrt{\frac{1}{2\omega(k)}} \sqrt{\frac{\omega(k')}{2}} (-i) e^\alpha_\lambda(k) e^\beta_{\lambda'}(-k') [a(k,\lambda), a^*(-k',\lambda')] \\ &+ \sum_{\lambda,\lambda'} \sqrt{\frac{1}{2\omega(k)}} \sqrt{\frac{\omega(k')}{2}} (i) e^\alpha_\lambda(-k) e^\beta_{\lambda'}(k') [a^*(-k,\lambda), a(k',\lambda')] \\ &= \frac{1}{2}(-i)\delta(k+k') \Big(\sum_{\lambda,\lambda'} e^\alpha_\lambda(k) e^\beta_{\lambda'}(k) \delta_{\lambda\lambda'} + e^\alpha_\lambda(-k) e^\beta_{\lambda'}(-k) \delta_{\lambda\lambda'} \Big) \\ &= -i\delta(k+k')(\delta_{\alpha\beta} - \widehat{k}^\alpha \widehat{k}^\beta), && (1.83) \end{aligned}$$

where in the last step we made use of (1.75). Now we take Fourier transforms:

$$\begin{aligned} [A^\alpha_\perp(x), -E^\beta_\perp(x')] &= i(2\pi)^{-3} \int d^3k d^3k' \, e^{ikx} e^{ik'x'} \delta(k+k')(\delta_{\alpha\beta} - \widehat{k}^\alpha \widehat{k}^\beta) \\ &= i\delta^\perp_{\alpha\beta}(x-x'), && (1.84) \end{aligned}$$

which gives (1.72). By analogous computations we also obtain

$$[A^\alpha_\perp(x), A^\beta_\perp(x')] = 0, \quad [E^\alpha_\perp(x), E^\beta_\perp(x')] = 0. \qquad (1.85)$$

For example (EXERCISE IN CLASS):

$$\begin{aligned} [\widehat{A}^\alpha_\perp(k), \widehat{A}^\beta_\perp(k')] &:= \sum_{\lambda,\lambda'} \sqrt{\frac{1}{2\omega(k)}} \sqrt{\frac{1}{2\omega(k')}} \Big([e^\alpha_\lambda(k) a(k,\lambda), e^\beta_{\lambda'}(-k') a^*(-k',\lambda')] \\ &\quad + [e^\alpha_\lambda(-k) a^*(-k,\lambda), e^\beta_{\lambda'}(k') a(k',\lambda')] \Big) \\ &= \sum_\lambda \frac{1}{2\omega(k)} \delta(k+k') \Big(e^\alpha_\lambda(k) e^\beta_\lambda(k) - e^\alpha_\lambda(-k) e^\beta_\lambda(-k) \Big) \\ &= \frac{1}{2\omega(k)} \delta(k+k') \Big(\delta_{\alpha\beta} - \hat{k}^\alpha \hat{k}^\beta - (\delta_{\alpha\beta} - (-\hat{k}^\alpha)(-\hat{k}^\beta)) \Big) \\ &= 0. && (1.86) \end{aligned}$$

The full electric field also has a longitudinal component. Recall that in the Coulomb gauge $\widehat{E}_{\|} = -ik\widehat{\phi}$ and $\widehat{\phi} = |k|^{-2}\widehat{\rho}$. Therefore

$$E_{\|}(x) = \frac{1}{(2\pi)^{3/2}} \int d^3k \, e^{ikx}(-i\widehat{\rho}(k)) \frac{k}{|k|^2}, \quad \rho(x) = e \sum_{j=1}^{N} \varphi(x - q_j). \tag{1.87}$$

We have

$$\begin{aligned} \widehat{\rho}(k) &= e(2\pi)^{-3/2} \sum_{j=1}^{N} \int d^3x \, e^{-ikx} \varphi(x - q_j) \\ &= e \sum_{j=1}^{N} e^{-ikq_j} (2\pi)^{-3/2} \int d^3x \, e^{-ikx} \varphi(x) = e \sum_{j=1}^{N} e^{-ikq_j} \widehat{\varphi}(k). \end{aligned} \tag{1.88}$$

Therefore

$$E_{\|}(x) = -ie \frac{1}{(2\pi)^{3/2}} \sum_{j=1}^{N} \int d^3k \, e^{ik(x-q_j)} \widehat{\varphi}(k) \frac{k}{|k|^2}, \tag{1.89}$$

is an operator on $\mathcal{H}_p = L^2(\mathbb{R}^{3N})$. The full electric field $E(x)$ is a distribution with values in $\mathcal{H} := \mathcal{H}_p \otimes \mathcal{F}$:

$$E(x) = E_{\|}(x) \otimes 1 + 1 \otimes E_{\perp}(x). \tag{1.90}$$

For future reference, we also state the formula for the magnetic field

$$\begin{aligned} B(x) &= \nabla \times A_{\perp}(x) \\ &= \frac{1}{(2\pi)^{3/2}} \sum_{\lambda=1,2} \int d^3k \sqrt{\frac{1}{2\omega(k)}} (ik \times e_{\lambda}(k)) \big(\mathrm{e}^{ikx} a(k,\lambda) - \mathrm{e}^{-ikx} a^*(k,\lambda) \big). \end{aligned}$$

1.8 Formal quantum Hamiltonian

Recall the classical expression (1.67) for the Hamiltonian: (For clarity we denote now classical quantites by 'check'):

$$\check{H} = \sum_{j=1}^{N} \frac{1}{2m} (\check{p}_j - e\check{A}_{\perp,\varphi}(\check{q}_j))^2 + \check{V}_c + \check{H}_f, \tag{1.91}$$

$$\check{H}_f := \frac{1}{2} \int d^3x \, \big\{ (\check{E}_{\perp}(x))^2 + \frac{1}{2} (\nabla \times \check{A}_{\perp}(x))^2 \big\}. \tag{1.92}$$

We want to replace the classical quantities in the expression above by their quantum counterparts and skip 'checks'. Two problems may appear: First, multiplication of quantum quantites (operators) is not commutative - this may lead to ambiguities. Second, quantum fields are distributions, thus expressions like $(\check{E}_{\perp}(x))^2$ may be problematic. Therefore we proceed in small steps:

(a) $\check{q}_j, \check{p}_j \to q_j, p_j$, defined in (1.70),(1.71), which act on $\mathcal{H}_p := L^2(\mathbb{R}^{3N})$.

(b) $\check{A}_\perp(x), \check{E}_\perp(x) \to A_\perp(x), E_\perp(x)$, defined in (1.81), (1.82), are **distributions** with values in operators on $\mathcal{F}$.

(c) $\check{A}_{\perp,\varphi}(x) \to A_{\perp,\varphi}(x)$ is a **function** with values in operators on $\mathcal{F}$. Explicitly, we have

$$\widehat{A}_{\perp,\varphi}(k) = \widehat{A * \varphi}(k) = (2\pi)^{3/2}\widehat{\varphi}(k)\widehat{A}(k). \tag{1.93}$$

Thus making use of $\varphi(x) = \varphi(-x)$ and therefore $\widehat{\varphi}(k) = \widehat{\varphi}(-k)$, we get

$$A_{\perp,\varphi}(x) = \sum_{\lambda=1,2} \int d^3k \, \frac{\widehat{\varphi}(k)}{\sqrt{2\omega(k)}} e_\lambda(k)\big(\mathrm{e}^{ikx} a(k,\lambda) + \mathrm{e}^{-ikx} a^*(k,\lambda)\big). \tag{1.94}$$

(d) $\check{A}_{\perp,\varphi}(q_j) \to A_{\perp,\varphi}(q_j)$ involves both particle and photon degrees of freedom. It is an operator on $\mathcal{H} := \mathcal{H}_p \otimes \mathcal{F}$, which is the full Hilbert space of the model. It is defined as

$$A_{\perp,\varphi}(q_j) = \sum_{\lambda=1,2} \int d^3k \, \frac{\widehat{\varphi}(k)}{\sqrt{2\omega(k)}} e_\lambda(k)\big(\mathrm{e}^{ikq_j} \otimes a(k,\lambda) + \mathrm{e}^{-ikq_j} \otimes a^*(k,\lambda)\big). \tag{1.95}$$

(The symbol $\otimes$ will be often omitted for brevity).

(e) $(\check{p}_j - e\check{A}_{\perp,\varphi}(\check{q}_j)) \to (p_j \otimes 1 - eA_{\perp,\varphi}(q_j))$ is an operator on $\mathcal{H} = \mathcal{H}_p \otimes \mathcal{F}$.

(f) $(\check{p}_j - e\check{A}_{\perp,\varphi}(\check{q}_j))^2 \to (p_j \otimes 1 - eA_{\perp,\varphi}(q_j))^2$ is an operator on $\mathcal{H} = \mathcal{H}_p \otimes \mathcal{F}$, but we have to be careful about ordering of operators: We have

$$\begin{aligned}(p_j \otimes 1 - eA_{\perp,\varphi}(q_j))^2 &= (p_j \otimes 1 - eA_{\perp,\varphi}(q_j))(p_j \otimes 1 - eA_{\perp,\varphi}(q_j)) \\ &= (p_j \otimes 1)^2 - e(p_j \otimes 1)A_{\perp,\varphi}(q_j) \\ &\quad - eA_{\perp,\varphi}(q_j)(p_j \otimes 1) + (eA_{\perp,\varphi}(q_j))^2.\end{aligned} \tag{1.96}$$

But if we expanded the square on the classical side, quantization could give a priori different expressions:

$$(p_j \otimes 1)^2 - 2e(p_j \otimes 1)A_{\perp,\varphi}(q_j) + (eA_{\perp,\varphi}(q_j))^2, \tag{1.97}$$
$$(p_j \otimes 1)^2 - 2eA_{\perp,\varphi}(q_j)(p_j \otimes 1) + (eA_{\perp,\varphi}(q_j))^2. \tag{1.98}$$

One could argue that (1.96) is correct, because it gives a manifestly symmetric operator (recall that given two operators A, B s.t. $A = A^*$ and $B = B^*$ then $(AB)^* = BA$ and therefore $(AB + BA)^* = (AB + BA)$). But fortunately all the expressions above turn out to be equal: Note that by $[q_i^\alpha, p_j^\beta] = i\delta_{\alpha,\beta}\delta_{i,j}$

$$[p_j^\alpha, e^{ikq_j}] = k^\alpha \mathrm{e}^{ikq_j}, \quad [p_j^\alpha, e^{-ikq_j}] = -k^\alpha \mathrm{e}^{-ikq_j}. \tag{1.99}$$

Therefore,

$$
\begin{aligned}
&[(p_j^\alpha \otimes 1), A^\alpha_{\perp,\varphi}(q_j)] \\
&= \sum_{\lambda=1,2} \int d^3k \, \frac{\widehat{\varphi}(k)}{\sqrt{2\omega(k)}} e^\alpha_\lambda(k) \big(k_j^\alpha \mathrm{e}^{ikq_j} \otimes a(k,\lambda) - k_j^\alpha \mathrm{e}^{-ikq_j} \otimes a^*(k,\lambda) \big) \\
&= 0
\end{aligned} \tag{1.100}
$$

where summation over α is understood and in the last step we made use of transversality: $e^\alpha_\lambda(k) k^\alpha = 0$. For completeness, we still have to show (1.99): (EXERCISE IN CLASS)

$$
[p_j^\alpha, e^{ikq_j}] = (p_j^\alpha - e^{ikq_j} p_j^\alpha e^{-ikq_j}) e^{ikq_j}. \tag{1.101}
$$

Now we consider a function $f(\eta) = e^{i\eta k q_j} p_j^\alpha e^{-i\eta k q_j}$ and compute

$$
\partial_\eta f(\eta) = ik^\beta e^{i\eta k q_j} [q_j^\beta, p_j^\alpha] e^{-i\eta k q_j} = ik^\beta e^{i\eta k q_j} i\delta_{\alpha\beta} e^{-i\eta k q_j} = -k^\alpha. \tag{1.102}
$$

Therefore $f(\eta) = f(0) - k^\alpha \eta = p_j^\alpha - k^\alpha \eta$, in particular $f(1) = e^{ikq_j} p_j^\alpha e^{-ikq_j} = p_j^\alpha - k^\alpha$. Substituting this to (1.101) we conclude the proof of the first identity in (1.99). Second identity follows by conjugation.

(g) $\int d^3x \, (\check{E}_\perp(x))^2 \to \int d^3x \, : (E_\perp(x))^2 :$ is an operator on $\mathcal{F}$. The 'Wick ordering' : ... : of a quadratic expression in $a^*(k,\lambda)$ and $a(k,\lambda)$ means that all creation operators should be shifted to the left of all the annihilation operators. This operation is needed to make sense of squaring distributions. We have by the Plancherel theorem:

$$
\begin{aligned}
&\int d^3x \, : (E_\perp(x))^2 : := \int d^3k \, : \widehat{E}_\perp(k)^* \cdot \widehat{E}_\perp(k) : \\
&= \sum_{\lambda,\lambda'} \int d^3k \, \frac{|k|}{2} : \big(e_\lambda(k) a^*(k,\lambda) - e_\lambda(-k) a(-k,\lambda) \big) \\
&\qquad\qquad \cdot \big(e_{\lambda'}(k) a(k,\lambda') - e_{\lambda'}(-k) a^*(-k,\lambda') \big) : \\
&= \sum_{\lambda,\lambda'} \int d^3k \, \frac{|k|}{2} \Big(e_\lambda(k) \cdot e_{\lambda'}(k) a^*(k,\lambda) a(k,\lambda') + e_\lambda(-k) \cdot e_{\lambda'}(-k) a^*(-k,\lambda) a(-k,\lambda') \\
&\qquad - e_\lambda(k) \cdot e_{\lambda'}(-k) a^*(k,\lambda) a^*(-k,\lambda') - e_\lambda(-k) \cdot e_{\lambda'}(k) a(-k,\lambda) a(k,\lambda') \Big) \\
&= \sum_\lambda \int d^3k \, |k| a^*(k,\lambda) a(k,\lambda) \\
&\qquad - \frac{1}{2} \sum_{\lambda,\lambda'} \int d^3k \, |k| \big(e_\lambda(k) \cdot e_{\lambda'}(-k) a^*(k,\lambda) a^*(-k,\lambda') + h.c. \big).
\end{aligned} \tag{1.103}
$$

Without Wick ordering we would have in addition infinite 'vacuum energy':

$$
\begin{aligned}
&\sum_{\lambda,\lambda'} \int d^3k \frac{|k|}{2} \, e_\lambda(-k) \cdot e_{\lambda'}(-k) [a(-k,\lambda), a^*(-k,\lambda')] \\
&\qquad = \sum_{\lambda,\lambda'} \int d^3k \, \frac{|k|}{2} e_\lambda(-k) \cdot e_{\lambda'}(-k) \delta(-k+k) = \infty
\end{aligned} \tag{1.104}
$$

Using Wick ordering one can 'prove' many things. For example

$$\delta(k-k') =: \delta(k-k') :=: [a(k), a^*(k')] :=: (a(k)a^*(k') - a^*(k')a(k)) := 0 \tag{1.105}$$

By integrating we even get $1 = 0$. Therefore it is sometimes useful to have a more precise definition: Let Ω be the vacuum vector which satisfies $a(k)\Omega = 0$ and $\eta_n \to \delta$ be a smooth delta-approximating sequence. We have

$$: E_\perp(x)^2 := \lim_{n\to\infty} \Big((E * \eta_n)(x)E(x) - \langle \Omega, (E*\eta_n)(x)E(x)\Omega\rangle \Big). \tag{1.106}$$

With this representation the problems above would not appear. It is also clear that one can apply the Plancherel theorem.

(h) $\int d^3x\, (\nabla \times \check{A}_\perp(x))^2 \to \int d^3x\, : (\nabla \times A_\perp(x))^2 :$. Again, by the Plancherel theorem

$$\int d^3x : (\nabla \times A_\perp(x))^2 := \int d^3k\ : (k \times \widehat{A}_\perp(k))^* \cdot (k \times \widehat{A}_\perp(k)) : \tag{1.107}$$

Now we recall that $a(b\times c) = b(c \times a)$ and $a \times (b \times c) = b(a\cdot c) - c(a \cdot b)$. Therefore, since $\widehat{A}_\perp(k), \widehat{A}_\perp(k')$ commute,

$$\begin{aligned} : (k \times \widehat{A}_\perp(k)^*) \cdot (k \times \widehat{A}_\perp(k)) : &= k : \cdot (\widehat{A}_\perp(k) \times (k \times \widehat{A}_\perp(k)^*)) : \\ &= k \cdot \big(k : (\widehat{A}_\perp(k)^* \cdot \widehat{A}_\perp(k)) : \\ &\quad - : \widehat{A}_\perp(k)^* (k \cdot \widehat{A}_\perp(k)) : \big) \\ &= |k|^2 : (\widehat{A}_\perp(k)^* \cdot \widehat{A}_\perp(k)) :, \end{aligned} \tag{1.108}$$

where we made use of the transversality condition. Thus we have

$$\begin{aligned} &\int d^3k\, |k|^2 : (\widehat{A}_\perp(k)^* \cdot \widehat{A}_\perp(k)) : \\ &= \frac{1}{2} \int d^3k\, |k| \sum_{\lambda,\lambda'} : \big(e_\lambda(k) a^*(k,\lambda) + e_\lambda(-k) a(-k,\lambda) \big) \\ &\qquad \cdot \big(e_{\lambda'}(k) a(k,\lambda') + e_{\lambda'}(-k) a^*(-k,\lambda') \big) : \\ &= \sum_\lambda \int d^3k\, |k| a^*(k,\lambda) a(k,\lambda) \\ &\quad + \frac{1}{2} \sum_{\lambda,\lambda'} \int d^3k\, |k| \big(e_\lambda(k) \cdot e_{\lambda'}(-k) a^*(k,\lambda) a^*(-k,\lambda') + h.c. \big) \end{aligned} \tag{1.109}$$

(i) $\check{H}_f \to H_f := \sum_\lambda \int d^3k\, |k| a^*(k,\lambda) a(k,\lambda)$ which is an operator on $\mathcal{F}$. (Follows from (g) (h) above). The corresponding contribution to the Hamiltonian is $1 \otimes H_f$ as an operator on $\mathcal{H} = \mathcal{H}_p \otimes \mathcal{F}$.

Altogether, the quantum Hamiltonian has the form:

$$H = \sum_{j=1}^{N} \frac{1}{2m}(p_j \otimes 1 - eA_{\perp,\varphi}(q_j))^2 + V_c(q) \otimes 1 + 1 \otimes H_f, \tag{1.110}$$

Usually we will just skip $\otimes$ and write like in the classical case

$$H = \sum_{j=1}^{N} \frac{1}{2m}(p_j - eA_{\perp,\varphi}(q_j))^2 + V_c(q) + H_f. \tag{1.111}$$

1.9 Quantum Maxwell-Newton equations

Given the Hamiltonian, we can define the time-evolution of the quantum fields in the Heisenberg picture

$$E(t,x) := e^{itH}\big((1 \otimes E_\perp(x)) + (E_\parallel(x) \otimes 1)\big)e^{-itH}, \tag{1.112}$$
$$A(t,x) := e^{itH}(1 \otimes A_\perp(x))e^{-itH}, \tag{1.113}$$
$$B(t,x) := e^{itH}\big(1 \otimes (\nabla \times A_\perp(x))\big)e^{-itH}, \tag{1.114}$$
$$\rho(t,x) := e^{itH}(\rho(x) \otimes 1)e^{-itH}. \tag{1.115}$$

There is still one quantity missing, namely the current: Recall the classical current:

$$\check{j}(t,x) = e\sum_{j=1}^{N} \varphi(x - q_j(t))\dot{q}_j(t). \tag{1.116}$$

(EXERCISE IN CLASS: QUANTIZE). We first define the velocity operator

$$v_j^\alpha := \frac{1}{m}(p_j \otimes 1 - eA_{\perp,\varphi}(q_j))^\alpha. \tag{1.117}$$

and then set

$$j(x) := \frac{1}{2}\sum_j \Big(ev_j(\varphi(q_j - x) \otimes 1) + h.c.\Big), \tag{1.118}$$
$$j(t,x) = e^{itH}j(x)e^{-itH}. \tag{1.119}$$

This is a symmetric quantization of the classical current (1.116).

1.9.1 Verification of $\nabla \cdot B = 0$ and $\nabla \cdot E = \rho$

We have

$$\nabla B(t,x) = e^{itH}\big(1 \otimes \nabla \cdot (\nabla \times A_\perp(x))\big)e^{-itH} = 0, \tag{1.120}$$
$$\nabla E(t,x) = e^{itH}(\nabla E_\parallel(x) \otimes 1)e^{-itH} = e^{itH}(\rho(x) \otimes 1)e^{-itH} = \rho(t,x), \tag{1.121}$$

where we made use of the relation:

$$E_\parallel(x) = \frac{1}{(2\pi)^{3/2}}\int d^3k\, e^{ikx}(-i\widehat{\rho}(k))\frac{k}{|k|^2}. \tag{1.122}$$

1.9.2 Verification of $\partial_t B = -\nabla \times E$

Now we verify the dynamical equations. We have

$$\partial_t B(t,x) = e^{itH} i[H, \big(1 \otimes (\nabla \times A_\perp(x))\big)] e^{-itH}. \tag{1.123}$$

Thus we have to verify commutators with the Hamiltonian. We have

$$[p_j \otimes 1, 1 \otimes (\nabla \times A_\perp(x))] = 0, \tag{1.124}$$

$$[A_{\perp,\varphi}(q_j), 1 \otimes (\nabla \times A_\perp(x))]$$
$$= (\nabla_x \times) \int d^3y\, (\varphi(q_j - y) \otimes 1)(1 \otimes [A_\perp(y), A_\perp(x)]) = 0, \tag{1.125}$$

where we made use of (1.85). Therefore

$$[(p_j \otimes 1 - eA_{\perp,\varphi}(q_j))^2, (\nabla \times A_\perp(x))] = 0. \tag{1.126}$$

Now we note (POSSIBLE EXERCISE IN CLASS):

$$[H_f, \widehat{A}_\perp(k)]$$
$$= \sum_{\lambda,\lambda'} \int d^3k' |k'| \, [a^*(k',\lambda')a(k',\lambda'), \frac{1}{\sqrt{2|k|}}\big(e_\lambda(k)a(k,\lambda) + e_\lambda(-k)a^*(-k,\lambda)\big)]$$
$$= \sum_{\lambda,\lambda'} \int d^3k' \sqrt{\frac{|k'|}{2}} \big(- e_\lambda(k')a(k',\lambda)\delta(k-k')\delta_{\lambda\lambda'} + e_\lambda(-k)a^*(k',\lambda')\delta(k+k')\delta_{\lambda\lambda'}\big)$$
$$= \sum_{\lambda} \sqrt{\frac{|k|}{2}} \big(- e_\lambda(k)a(k,\lambda) + e_\lambda(-k)a^*(-k,\lambda)\big) = i\widehat{E}_\perp(k). \tag{1.127}$$

Hence

$$i[H_f, A_\perp(x)] = -E_\perp(x), \tag{1.128}$$

$$i[H_f, \nabla \times A_\perp(x)] = -\nabla \times E_\perp(x) = -\nabla \times E(x), \tag{1.129}$$

and we get

$$\partial_t B(t,x) = -\nabla \times E(t,x). \tag{1.130}$$

1.9.3 Verification of $\partial_t E = \nabla \times B - j$

We write

$$\partial_t E(t,x) = e^{itH} i[H, (1 \otimes E_\perp(x))] e^{-itH} + e^{itH} i[H, (E_\parallel(x) \otimes 1)] e^{-itH} \tag{1.131}$$

We consider first the commutator involving $E_\perp$. We have (SECOND COMMUTATOR - POSSIBLE EXERCISE IN CLASS)

$$[p_j \otimes 1, 1 \otimes E_\perp(x)] = 0, \tag{1.132}$$

$$[A^\alpha_{\perp,\varphi}(q_j), 1 \otimes E^\beta_\perp(x)] = \int d^3y\, (\varphi(q_j - y) \otimes 1)(1 \otimes [A^\alpha_\perp(y), E^\beta_\perp(x)])$$
$$= -i \int d^3y\, \varphi(q_j - y)\delta^\perp_{\alpha\beta}(y-x) \otimes 1. \tag{1.133}$$

Consequently,

$$\begin{aligned}
&[(p_j \otimes 1 - eA_{\perp,\varphi}(q_j))^2, 1 \otimes E_\perp^\beta(x)] \\
&= -e(p_j \otimes 1 - eA_{\perp,\varphi}(q_j))^\alpha [A^\alpha_{\perp,\varphi}(q_j), 1 \otimes E^\beta_\perp(x)] \\
&\quad - e[A^\alpha_{\perp,\varphi}(q_j), 1 \otimes E^\beta_\perp(x)](p_j \otimes 1 - eA_{\perp,\varphi}(q_j))^\alpha \\
&= iemv_j^\alpha \big(\int d^3y\, \varphi(q_j - y)\delta^\perp_{\alpha\beta}(y-x) \otimes 1\big) + h.c., \qquad (1.134)
\end{aligned}$$

with summation over α and definition of the velocity operator

$$v_j^\alpha := \frac{1}{m}(p_j \otimes 1 - eA_{\perp,\varphi}(q_j))^\alpha. \qquad (1.135)$$

Now we look at the commutator with the photon energy:

$$\begin{aligned}
&[H_f, \widehat{E}_\perp(k)] \\
&= \sum_{\lambda,\lambda'} \int d^3k' |k'|\, [a^*(k',\lambda')a(k',\lambda'), \sqrt{\frac{|k|}{2}}\big(ie_\lambda(k)a(k,\lambda) - ie_\lambda(-k)a^*(-k,\lambda)\big)] \\
&= \sum_{\lambda,\lambda'} \int d^3k' \frac{|k'|^{3/2}}{\sqrt{2}} \Big(-ie_\lambda(k)\delta(k-k')a(k',\lambda')\delta_{\lambda\lambda'} - ie_\lambda(-k)\delta(k+k')a^*(k',\lambda')\delta_{\lambda\lambda'}\Big) \\
&= (-i)\sum_\lambda \frac{|k|^{3/2}}{\sqrt{2}} \Big(e_\lambda(k)a(k,\lambda) + e_\lambda(-k)a^*(-k,\lambda)\Big). \qquad (1.136)
\end{aligned}$$

We show that the r.h.s. equals $(-i)\widehat{\nabla \times B}$. We have

$$\begin{aligned}
&\widehat{\nabla \times B}(k) = \nabla \widehat{\times \nabla} A_\perp(k) = -(k \times (k \times \widehat{A}_\perp(k))) \\
=\;& -k(k\cdot \widehat{A}_\perp(k)) + k^2\widehat{A}_\perp(k) = k^2 \widehat{A}_\perp(k) \\
=\;& \sum_\lambda \frac{|k|^{3/2}}{\sqrt{2}} \Big(e_\lambda(k)a(k,\lambda) + e_\lambda(-k)a^*(-k,\lambda)\Big). \qquad (1.137)
\end{aligned}$$

Thus indeed we get

$$i[H_f, E_\perp(x)] = \nabla \times B(x). \qquad (1.138)$$

Altogether, the result for the transversal part is

$$\begin{aligned}
i[H, 1 \otimes E^\beta_\perp(x)] &= (\nabla \times B)^\beta(x) \\
&\quad - \frac{1}{2}\sum_j \big(ev_j^\alpha\big(\int d^3y\, \varphi(q_j - y)\delta^\perp_{\alpha\beta}(y-x) \otimes 1\big) + h.c.\big). \qquad (1.139)
\end{aligned}$$

Now we look at the longitudinal part: We recall

$$E_\parallel(x) = -ie\frac{1}{(2\pi)^{3/2}} \sum_{j'=1}^N \int d^3k\, e^{ik(x-q_{j'})}\widehat{\varphi}(k)\frac{k}{|k|^2}. \qquad (1.140)$$

Since we know that $[p_j^\alpha, e^{-ikq_j}] = -k^\alpha \mathrm{e}^{-ikq_j}$ we have

$$[p_j^\alpha, E_\parallel^\beta(x)] = ie\frac{1}{(2\pi)^{3/2}}\int d^3k\, e^{ik(x-q_j)}\widehat{\varphi}(k)\frac{k^\alpha k^\beta}{|k|^2}. \qquad (1.141)$$

To compute the last expression, we use $\check{fg} = (2\pi)^{-3/2}\check{f} * \check{g}$ with $f(k) = e^{-ikq_j}\widehat{\varphi}(k)$ and $g(k) = k^\alpha k^\beta/|k|^2$ and

$$\check{f}(x) = \varphi(x - q_j), \qquad (1.142)$$
$$\check{g}(x) = \frac{1}{(2\pi)^{3/2}}\int d^3k\, e^{ikx}k^\alpha k^\beta/|k|^2 = (2\pi)^{3/2}(\delta_{\alpha\beta}\delta(x) - \delta^\perp_{\alpha\beta}(x)). \qquad (1.143)$$

Therefore,

$$[p_j^\alpha, E_\parallel^\beta(x)] = (ie)\int d^3y\, \varphi(q_j - y)(\delta_{\alpha\beta}\delta(y-x) - \delta^\perp_{\alpha\beta}(y-x)), \qquad (1.144)$$

where we made use of symmetry of all the integrated functions. Since $E_\parallel^\beta(x)$ depends only on q, we have

$$[A_{\perp,\varphi}(q_j), E_\parallel(x)\otimes 1] = 0. \qquad (1.145)$$

Consequently,

$$\begin{aligned} & i[(p_j\otimes 1 - eA_{\perp,\varphi}(q_j))^2, E_\parallel^\beta(x)\otimes 1] = \big(mv_j^\alpha(i[p_j^\alpha, E_\parallel^\beta(x)]\otimes 1) + h.c.\big) \\ & = (-e)\Big(mv_j^\alpha(\int d^3y\, \varphi(q_j-y)(\delta_{\alpha\beta}\delta(y-x) - \delta^\perp_{\alpha\beta}(y-x))\otimes 1) + h.c.\Big) \end{aligned} \qquad (1.146)$$

Since $[1\otimes H_f, E_\parallel^\beta(x)\otimes 1] = 0$, we get

$$\begin{aligned} & i[H, E_\parallel^\beta(x)\otimes 1] \\ & = -\frac{1}{2}\sum_j \Big(ev_j^\alpha(\int d^3y\, \varphi(q_j-y)(\delta_{\alpha\beta}\delta(y-x) - \delta^\perp_{\alpha\beta}(y-x))\otimes 1) + h.c.\Big). \end{aligned} \qquad (1.147)$$

Thus, together with (1.139), we obtain

$$\begin{aligned} i[H, E^\beta(x)] &= (\nabla\times B)^\beta(x) - \frac{1}{2}\sum_j \Big(ev_j^\alpha(\int d^3y\, \varphi(q_j-y)\delta_{\alpha\beta}\delta(y-x)\otimes 1) + h.c.\Big) \\ &= (\nabla\times B)^\beta(x) - \frac{1}{2}\sum_j \Big(ev_j^\beta(\varphi(q_j-x)\otimes 1) + h.c.\Big) \end{aligned} \qquad (1.148)$$

Thus writing

$$j(x) := \frac{1}{2}\sum_j \Big(ev_j(\varphi(q_j - x)\otimes 1) + h.c.\Big) \qquad (1.149)$$

and $j(t,x) := e^{itH} j(x) e^{-itH}$ we obtain

$$\partial_t E(t,x) = (\nabla \times B)(t,x) - j(t,x). \tag{1.150}$$

We recall that (1.149) is a 'symmetric' quantization of the classical current

$$\check{j}(t,x) = e \sum_{j=1}^{N} \varphi(x - q_j(t)) \dot{q}_j(t). \tag{1.151}$$

1.9.4 Verification of the Newton equations

Recall that the velocity operator of the j-th particle at $t = 0$ is

$$v_j^\beta := \frac{1}{m}(p_j \otimes 1 - eA_{\perp,\varphi}(q_j))^\beta. \tag{1.152}$$

We have $v_j^\beta(t) = e^{iHt} v_j^\beta e^{-iHt}$, and therefore

$$m\dot{v}_j^\beta(t) = me^{iHt} i[H, v_j^\beta] e^{-iHt}. \tag{1.153}$$

Let us compute the relevant commutators. We note that $H = \frac{1}{2}\sum_{\ell,\alpha} m v_\ell^\alpha v_\ell^\alpha + V_c + 1 \otimes H_f$. (Up to now all the commutators involving $V_c(q)$ were vanishing. Now they will be important). It is convenient to first evaluate $[v_\ell^\alpha, v_j^\beta]$. We have

$$[A_{\perp,\varphi}(q_\ell)^\alpha, A_{\perp,\varphi}(q_j)^\beta] = 0 \tag{1.154}$$

because $[q_\ell, q_j] = 0$ and $[A_\perp(x), A_\perp(y)] = 0$. Moreover,

$$\begin{aligned}
[p_\ell^\alpha \otimes 1, A_{\perp,\varphi}(q_j)^\beta] &= \int d^3y \, [p_\ell^\alpha \otimes 1, \varphi(q_j - y) \otimes A_\perp^\beta(y)] \\
&= \int d^3y \, [p_\ell^\alpha, \varphi(q_j - y)] \otimes A_\perp^\beta(y) \\
&= \delta_{\ell,j} \int d^3y \, (+i)(\partial_{y^\alpha}\varphi)(q_j - y) \otimes A_\perp^\beta(y) \\
&= \delta_{\ell,j} \int d^3y \, (-i)\varphi(q_j - y) \otimes \partial_\alpha A_\perp^\beta(y) \\
&= (-i)\delta_{\ell,j} \partial_\alpha A_{\perp,\varphi}^\beta(q_j).
\end{aligned} \tag{1.155}$$

Thus

$$\begin{aligned}
[v_\ell^\alpha, v_j^\beta] &= -\frac{e}{m^2}[p_\ell^\alpha \otimes 1, A_{\perp,\varphi}(q_j)^\beta] - \frac{e}{m^2}[A_{\perp,\varphi}(q_\ell)^\alpha, p_j^\beta \otimes 1] \\
&= i\frac{e}{m^2}\delta_{\ell,j}\Big(\partial_\alpha A_{\perp,\varphi}^\beta(q_j) - \partial_\beta A_{\perp,\varphi}^\alpha(q_j)\Big) \\
&= i\frac{e}{m^2}\delta_{\ell,j}\varepsilon^{\alpha\beta\gamma} B_\varphi^\gamma(q_j).
\end{aligned} \tag{1.156}$$

(Comment, non-commutative geometry). In the last step we used

$$\begin{aligned}\varepsilon^{\alpha\beta\gamma}B^\gamma_\varphi(q_j) &= \varepsilon^{\alpha\beta\gamma}\varepsilon_{\gamma\alpha'\beta'}\partial_{\alpha'}A^{\beta'}_{\perp,\varphi}(q_j)\\ &= (\delta_{\alpha\alpha'}\delta_{\beta\beta'}-\delta_{\alpha\beta'}\delta_{\beta\alpha'})\partial_{\alpha'}A^{\beta'}_{\perp,\varphi}(q_j)\\ &= (\partial_\alpha A^\beta_{\perp,\varphi}-\partial_\beta A^\alpha_{\perp,\varphi})(q_j). \end{aligned}\tag{1.157}$$

Now we compute

$$\begin{aligned}\frac{1}{2}\sum_{\ell,\alpha} mi[v^\alpha_\ell v^\alpha_\ell, v^\beta_j] &= \frac{1}{2}\sum_{\ell,\alpha} m(v^\alpha_\ell i[v^\alpha_\ell, v^\beta_j]+i[v^\alpha_\ell, v^\beta_j]v^\alpha_\ell)\\ &= \frac{1}{2}\frac{e}{m}\big(-v^\alpha_j\varepsilon^{\alpha\beta\gamma}B^\gamma_\varphi(q_j)+h.c.\big)\\ &= \frac{1}{2}\frac{e}{m}\big(\varepsilon^{\beta\alpha\gamma}v^\alpha_j B^\gamma_\varphi(q_j)-\varepsilon^{\beta\gamma\alpha}B^\gamma_\varphi(q_j)v^\alpha_j\big)\\ &= \frac{1}{2}\frac{e}{m}\big((v_j\times B_\varphi(q_j))^\beta-(B_\varphi(q_j)\times v_j)^\beta\big). \end{aligned}\tag{1.158}$$

Now we focus on the term $1\otimes H_f$ from the Hamiltonian. We know that

$$i[H_f, A_\perp(x)] = -E_\perp(x). \tag{1.159}$$

Therefore,

$$\begin{aligned} i[1\otimes H_f, A_{\perp,\varphi}(q_j)] &= \int d^3x\, i[1\otimes H_f, \varphi(q_j-x)\otimes A_\perp(x)]\\ &= \int d^3x\,\varphi(q_j-x)(1\otimes i[H_f, A_\perp(x)])\\ &= -\int d^3x\,\varphi(q_j-x)(1\otimes E_\perp(x)) = -E_{\perp,\varphi}(q_j). \end{aligned}\tag{1.160}$$

Hence

$$i[1\otimes H_f, v^\beta_j] = i[1\otimes H_f, \frac{1}{m}(p_j\otimes 1 - eA_{\perp,\varphi}(q_j))^\beta] = \frac{e}{m}E_{\perp,\varphi}(q_j). \tag{1.161}$$

Finally, we compute the commutator with the Coulomb interaction:

$$i[V_c(q)\otimes 1, v^\beta_j] = i\frac{1}{m}[V_c(q), p^\beta_j]\otimes 1 = -(\partial_{q^\beta_j}V_c)(q). \tag{1.162}$$

We have, since $\widehat{\rho}(t,k) = e\sum_{j=1}^N e^{-ikq_j}\widehat{\varphi}(k)$,

$$V_c(q) = \frac{1}{2}\int d^3k\,|k|^{-2}|\widehat{\rho}(k)|^2 = \frac{1}{2}\sum_{\ell,\ell'=1}^N e^2\int d^3k\,|k|^{-2}e^{-ik(q_\ell-q_{\ell'})}|\widehat{\varphi}(k)|^2 \tag{1.163}$$

and therefore

$$
\begin{aligned}
(\partial_{q_j^\beta} V_c)(q) &= \frac{1}{2}\sum_{\ell,\ell'=1}^{N} e^2 \int d^3k\, |k|^{-2} e^{-ik(q_\ell - q_{\ell'})}(-ik^\beta \delta_{j,\ell} + ik^\beta \delta_{j,\ell'})|\widehat{\varphi}(k)|^2 \\
&= -\frac{1}{2}e\sum_{\ell}\int d^3k\, |k|^{-2}\overline{\widehat{\rho(k)}}e^{-ikq_\ell} ik^\beta \delta_{j,\ell}\widehat{\varphi}(k) + \frac{1}{2}e\sum_{\ell'}\int d^3k\, |k|^{-2}\widehat{\rho(k)}e^{ikq_{\ell'}} ik^\beta \delta_{j,\ell'}\overline{\widehat{\varphi}(k)} \\
&= -\frac{1}{2}e\int d^3k\, |k|^{-2}\overline{\widehat{\rho(k)}}e^{-ikq_j} ik^\beta \widehat{\varphi}(k) + \frac{1}{2}\int d^3k\, |k|^{-2}\widehat{\rho(k)}e^{ikq_j} ik^\beta \overline{\widehat{\varphi}(k)} \\
&= e\int d^3k\, |k|^{-2}\widehat{\rho(k)}e^{ikq_j} ik^\beta \widehat{\varphi}(k), \qquad (1.164)
\end{aligned}
$$

where we made use of the fact that $\overline{\widehat{\rho(k)}} = \widehat{\rho}(-k)$ and $\widehat{\varphi}(k) = \widehat{\varphi}(-k) = \overline{\varphi}(k)$. We recall that

$$
E_{\|}^{\beta}(x) = -\frac{1}{(2\pi)^{3/2}}\int d^3k\, e^{ikx} i\widehat{\rho}(k)\frac{k}{|k|^2}. \qquad (1.165)
$$

Therefore

$$
\begin{aligned}
eE_{\|,\varphi}^{\beta}(q_j) &= e\int d^3y\, \varphi(q_j - y)E_{\|}^{\beta}(y) \\
&= -e\int d^3k\, e^{ikq_j}\widehat{\varphi}(k) i\widehat{\rho}(k)\frac{k^\beta}{|k|^2} = -(\partial_{q_j^\beta} V_c)(q). \qquad (1.166)
\end{aligned}
$$

(Making use of

$$
\widehat{\rho}(k) = e\sum_{j=1}^{N} e^{-ikq_j}\widehat{\varphi}(k) \qquad (1.167)
$$

it is easy to see that $E_{\|,\varphi}^{\beta}(q_j) = 0$ for one particle. Thus particles do not interact with their own Coulomb field). We have established

$$
i[V_c(q) \otimes 1, v_j^\beta] = eE_{\|,\varphi}^{\beta}(q_j). \qquad (1.168)
$$

Summing up all the contributions we get the Newton equations with the Lorentz force

$$
m\dot{v}_j = eE_\varphi(q_j) + \frac{1}{2}e\big((v_j \times B_\varphi(q_j)) - (B_\varphi(q_j) \times v_j)\big). \qquad (1.169)
$$

2 Self-adjointness of the Pauli-Fierz Hamiltonian

2.1 Fock space

The single-particle space has the form $\mathfrak{h} := L^2(\mathbb{R}^3) \otimes \mathbb{C}^2 = L^2(\mathbb{R}^3 \times \{1,2\}) =: L^2(\underline{\mathbb{R}}^3)$ with the scalar product

$$
\langle f_1, f_2\rangle = \sum_{\lambda=1,2}\int d^3k \bar{f}_1(k,\lambda) f_2(k,\lambda) =: \int d^3\underline{k} \bar{f}_1(\underline{k}) f_2(\underline{k}). \qquad (2.1)
$$

We have for $n \in \mathbb{N}$

$$\begin{aligned} \otimes^n \mathfrak{h} &= \mathfrak{h} \otimes \cdots \otimes \mathfrak{h} = L^2(\underline{\mathbb{R}}^{3n}), & (2.2)\\ \otimes_s^n \mathfrak{h} &= S_n(\mathfrak{h} \otimes \cdots \otimes \mathfrak{h}) = L_s^2(\underline{\mathbb{R}}^{3n}), & (2.3)\\ \otimes_s^0 \mathfrak{h} &:= \mathbb{C}\Omega, \text{ where } \Omega \text{ is called the vacuum vector.} & (2.4) \end{aligned}$$

Here $\underline{\mathbb{R}}^{3n}$ should be read $(\underline{R}^3)^n = \underline{R}^3 \times \cdots \times \underline{R}^3$ and S_n is the symmetrization operator defined by

$$S_n = \frac{1}{n!} \sum_{\sigma \in P_n} \sigma, \text{ where } \sigma(f_1 \otimes \cdots \otimes f_n) = f_{\sigma(1)} \otimes \cdots \otimes f_{\sigma(n)}, \tag{2.5}$$

P_n is the set of all permutations and $L_s^2(\underline{\mathbb{R}}^{3n})$ is the subspace of symmetric (w.r.t. permutations of variables $\underline{k}_i = (k_i, \lambda_i)$) square integrable functions. The (symmetric) Fock space is given by

$$\Gamma(\mathfrak{h}) := \oplus_{n \geq 0} \otimes_s^n \mathfrak{h} = \oplus_{n \geq 0} L_s^2(\underline{\mathbb{R}}^{3n}). \tag{2.6}$$

For brevity we will sometimes write $\mathcal{F} := \Gamma(\mathfrak{h})$ and $\mathcal{F}^{(n)} := \Gamma^{(n)}(\mathfrak{h}) := L_s^2(\underline{\mathbb{R}}^{3n})$. We can write $\Psi, \Phi \in \Gamma(\mathfrak{h})$ in terms of its Fock space components $\Psi = \{\Psi^{(n)}\}_{n \geq 0}$, $\Phi = \{\Phi^{(n)}\}_{n \geq 0}$ and the scalar product in $\Gamma(\mathfrak{h})$ is given by

$$\langle \Psi, \Phi \rangle = \sum_{n=0}^{\infty} \langle \Psi^{(n)}, \Phi^{(n)} \rangle = \sum_{n=0}^{\infty} \int d^{3n}\underline{k}\, \bar{\Psi}^{(n)}(\underline{k}_1, \ldots, \underline{k}_n) \Phi^{(n)}(\underline{k}_1, \ldots, \underline{k}_n). \tag{2.7}$$

We define a dense subspace $\Gamma_{\text{fin}}(\mathfrak{h}) \subset \Gamma(\mathfrak{h})$ consisting of such Ψ that $\Psi^{(n)} = 0$ except for finitely many n. Next, we define a domain

$$D := \{ \Psi \in \Gamma_{\text{fin}}(\mathfrak{h}) \,|\, \Psi^{(n)} \in S(\underline{\mathbb{R}}^{3n}) \text{ for all } n \}. \tag{2.8}$$

Now, for each $\underline{q} \in \underline{\mathbb{R}}^3$ we define an operator $a(\underline{q}) : D \to \Gamma(\mathfrak{h})$ by

$$\begin{aligned} &(a(\underline{q})\Psi)^{(n)}(\underline{k}_1, \ldots, \underline{k}_n) = \sqrt{n+1}\Psi^{(n+1)}(\underline{q}, \underline{k}_1, \ldots, \underline{k}_n),\\ &\text{In particular } a(\underline{q})\Omega = 0. \end{aligned} \tag{2.9}$$

We will also use the notation $a(q, \lambda)$ for $a(\underline{q})$, if convenient. Note that the adjoint of $a(q)$ is not densely defined, since formally

$$(a^*(\underline{q})\Psi)^{(n)}(\underline{k}_1, \ldots, \underline{k}_n) = \frac{1}{\sqrt{n}} \sum_{\ell=1}^{n} \delta(\underline{q} - \underline{k}_\ell) \Psi^{(n-1)}(\underline{k}_1, \ldots, \underline{k}_{\ell-1}, \underline{k}_{\ell+1}, \ldots, \underline{k}_n) \tag{2.10}$$

where $\delta(\underline{q} - \underline{k}_\ell) = \delta(q - k)\delta_{\lambda,\lambda'}$ for $\underline{q} = (q, \lambda)$ and $\underline{k} = (k, \lambda')$. So, becuase of the presence of deltas (which are not square integrable) the r.h.s. is not in the Hilbert space $\Gamma(\mathfrak{h})$ if it is non-zero. Let us now justify (2.10): For $\Phi, \Psi \in D$ we have:

$$
\begin{aligned}
\langle \Phi, a^*(\underline{q})\Psi\rangle &= \langle a(\underline{q})\Phi, \Psi\rangle = \sum_{n=0}^{\infty} \langle (a(\underline{q})\Phi)^{(n)}, \Psi^{(n)}\rangle \\
&= \sum_{n=0}^{\infty} \int d^{3n}\underline{k}\, \overline{(a(\underline{q})\Phi)}^{(n)}(\underline{k}_1, \ldots, \underline{k}_n)\Psi^{(n)}(\underline{k}_1, \ldots, \underline{k}_n) \\
&= \sum_{n=0}^{\infty} \sqrt{n+1} \int d^{3n}\underline{k}\, \overline{\Phi}^{(n+1)}(\underline{q}, \underline{k}_1, \ldots, \underline{k}_n)\Psi^{(n)}(\underline{k}_1, \ldots, \underline{k}_n) \\
&= \sum_{n=0}^{\infty} \sqrt{n+1} \int d^{3n}\underline{k} d^3\underline{k}_0\, \overline{\Phi}^{(n+1)}(\underline{k}_0, \underline{k}_1, \ldots, \underline{k}_n)\delta(\underline{q}-\underline{k}_0)\Psi^{(n)}(\underline{k}_1, \ldots, \underline{k}_n) \\
&= \sum_{n'=1}^{\infty} \sqrt{n'} \int d^{3(n'-1)}\underline{k} d^3\underline{k}_0\, \overline{\Phi}^{(n')}(\underline{k}_0, \underline{k}_1, \ldots, \underline{k}_{n'-1})\delta(\underline{q}-\underline{k}_0)\Psi^{(n'-1)}(\underline{k}_1, \ldots, \underline{k}_{n'-1}) \\
&= \sum_{n'=1}^{\infty} \sqrt{n'} \int d^{3n'}\underline{k}'\, \overline{\Phi}^{(n')}(\underline{k}'_1, \underline{k}'_2, \ldots, \underline{k}'_{n'})\delta(\underline{q}-\underline{k}'_1)\Psi^{(n'-1)}(\underline{k}'_2, \ldots, \underline{k}'_{n'}) \\
&= \sum_{n'=1}^{\infty} \sqrt{n'}\frac{1}{n'} \sum_{\ell=1}^{n'} \int d^{3n'}\underline{k}'\, \overline{\Phi}^{(n')}(\underline{k}'_1, \underline{k}'_2, \ldots, \underline{k}'_{n'})\delta(\underline{q}-\underline{k}'_\ell)\Psi^{(n'-1)}(\underline{k}'_1, \ldots, \underline{k}'_{\ell-1}, \underline{k}'_{\ell+1}, \ldots, \underline{k}'_{n'}).
\end{aligned}
\tag{2.11}
$$

Clearly, $a^*(\underline{q})$ is well defined as a quadratic form on $D \times D$. Moreover, expressions

$$
a(g) = \int d^3\underline{q}\, a(\underline{q})\overline{g(\underline{q})}, \quad a^*(g) = \int d^3\underline{q}\, a^*(\underline{q})g(\underline{q}), \quad g \in S(\underline{\mathbb{R}}^3), \tag{2.12}
$$

defined first as weak integrals, give rise to well-defined operators on D which can be extended to $\Gamma_{\mathrm{fin}}(\mathfrak{h})$. On this domain they act consistently with (2.9):

$$
(a(g)\Psi)^{(n)}(\underline{k}_1, \ldots, \underline{k}_n) = \sqrt{n+1} \int d^3\underline{q}\, \overline{g}(\underline{q})\Psi^{(n+1)}(\underline{q}, \underline{k}_1, \ldots, \underline{k}_n), \tag{2.13}
$$

$$
(a^*(g)\Psi)^{(n)}(\underline{k}_1, \ldots, \underline{k}_n) = \frac{1}{\sqrt{n}} \sum_{\ell=1}^{n} g(\underline{k}_\ell)\Psi^{(n-1)}(\underline{k}_1, \ldots, \underline{k}_{\ell-1}, \underline{k}_{\ell+1}, \ldots, \underline{k}_n). \tag{2.14}
$$

(In this sense $a(\underline{q}), a^*(\underline{q})$ are operator valued distributions). These expressions can be used to define $a(g), a^*(g)$ for $g \in L^2(\underline{\mathbb{R}}^3)$ and note that by (2.12) we have $a(g)^* = a^*(g)$ on $\Gamma_{\mathrm{fin}}(\mathfrak{h})$. Since these operators leave $\Gamma_{\mathrm{fin}}(\mathfrak{h})$ invariant, one can compute on this domain:

$$
[a(f), a^*(g)] = \langle f, g\rangle 1 \tag{2.15}
$$

for $f, g \in L^2(\underline{\mathbb{R}}^3)$. Formally, this follows from $[a(p,\lambda), a^*(q,\lambda')] = \delta(p-q)\delta_{\lambda\lambda'}$, but this computational rule does not make much sense without smearing (not even as quadratic forms). Thus let us give a formal proof of (2.15):

$$(a(f)a^*(g)\Psi)^{(n)}(\underline{k}_1,\dots,\underline{k}_n) = \sqrt{n+1}\int d^3\underline{q}\,\overline{f}(\underline{q})(a^*(g)\Psi)^{(n+1)}(\underline{q},\underline{k}_1,\dots,\underline{k}_n)$$
$$= \int d^3\underline{q}\,\overline{f}(\underline{q})g(\underline{q})\Psi^{(n)}(\underline{k}_1,\dots,\underline{k}_n) + \sum_{\ell=1}^{n}\int d^3\underline{q}\,\overline{f}(\underline{q})g(\underline{k}_\ell)\Psi^{(n)}(\underline{q},\underline{k}_1,\dots,\underline{k}_{\ell-1},\underline{k}_{\ell+1},\dots,\underline{k}_n).$$

The sum on the r.h.s. above is cancelled by

$$\begin{aligned}(a^*(g)a(f)\Psi)^{(n)}(\underline{k}_1,\dots,\underline{k}_n) &= \frac{1}{\sqrt{n}}\sum_{\ell=1}^{n} g(\underline{k}_\ell)(a(f)\Psi)^{(n-1)}(\underline{k}_1,\dots,\underline{k}_{\ell-1},\underline{k}_{\ell+1},\dots,\underline{k}_n)\\ &= \sum_{\ell=1}^{n} g(\underline{k}_\ell)\int d^3\underline{q}\,\overline{f}(\underline{q})\Psi^{(n)}(\underline{q},\underline{k}_1,\dots,\underline{k}_{\ell-1},\underline{k}_{\ell+1},\dots,\underline{k}_n),\end{aligned}$$

which concludes the proof of (2.15).

With the above definitions, the transverse electromagnetic potential and electric field, given by:

$$A_\perp(x) = \frac{1}{(2\pi)^{3/2}}\sum_{\lambda=1,2}\int d^3k\sqrt{\frac{1}{2\omega(k)}}e_\lambda(k)\big(\mathrm{e}^{ikx}a(k,\lambda)+\mathrm{e}^{-ikx}a^*(k,\lambda)\big), \quad (2.16)$$
$$E_\perp(x) = \frac{1}{(2\pi)^{3/2}}\sum_{\lambda=1,2}\int d^3k\sqrt{\frac{\omega(k)}{2}}e_\lambda(k)i\big(\mathrm{e}^{ikx}a(k,\lambda)-\mathrm{e}^{-ikx}a^*(k,\lambda)\big). \quad (2.17)$$

can be understood as operator-valued distributions. Indeed, for $f, g \in S(\mathbb{R}^3)$ we have as weak integrals

$$\begin{aligned}A_\perp(f) &= \int d^3x A_\perp(x)f(x)\\ &= \sum_{\lambda=1,2}\int d^3k\sqrt{\frac{1}{2\omega(k)}}e_\lambda(k)\big(\widehat{f}(-k)(a(k,\lambda)+\widehat{f}(k)a^*(k,\lambda)\big), \quad (2.18)\\ E_\perp(g) &= \int d^3x E_\perp(x)g(x)\\ &= \sum_{\lambda=1,2}\int d^3k\sqrt{\frac{\omega(k)}{2}}e_\lambda(k)i\big(\widehat{g}(-k)a(k,\lambda)-\widehat{g}(k)a^*(k,\lambda)\big). \quad (2.19)\end{aligned}$$

By our earlier considerations we know that $A_\perp(f)$ and $E_\perp(g)$ extend to operators on $\Gamma_{\mathrm{fin}}(\mathfrak{h})$.

Consider a unitary operator u on $\mathfrak{h}$. Then, its 'second quantization' is the following operator on the Fock space:

$$\Gamma(u)|_{\Gamma^{(n)}(\mathfrak{h})} = u\otimes\cdots\otimes u, \quad (2.20)$$
$$\Gamma(u)\Omega = \Omega. \quad (2.21)$$

where $\Gamma^{(n)}(\mathfrak{h})$ is the n-particle subspace. We have the useful relations:

$$\Gamma(u)a^*(h)\Gamma(u)^* = a^*(uh), \quad \Gamma(u)a(h)\Gamma(u)^* = a(uh). \tag{2.22}$$

Let us show the latter formula in the special case where $u = u(\underline{k})$ is a multiplication operator. We set $U_n(\underline{k}_1, \dots, \underline{k}_n) := u(\underline{k}_1) \dots u(\underline{k}_n)$ and compute

$$\begin{aligned}
&(\Gamma(u)a(h)\Gamma(u)^*\Psi)^{(n)}(\underline{k}_1, \dots, \underline{k}_n) = U_n(\underline{k}_1, \dots, \underline{k}_n)(a(h)\Gamma(u)^*\Psi)^{(n)}(\underline{k}_1, \dots, \underline{k}_n) \\
&= U_n(\underline{k}_1, \dots, \underline{k}_n)\sqrt{n+1} \int d^3\underline{k}\, \overline{h}(\underline{k})(\Gamma(u)^*\Psi)^{(n+1)}(\underline{k}, \underline{k}_1, \dots, \underline{k}_n) \\
&= U_n(\underline{k}_1, \dots, \underline{k}_n)\sqrt{n+1} \int d^3\underline{k}\, \overline{h}(\underline{k})\overline{U}_{n+1}(\underline{k}, \underline{k}_1, \dots, \underline{k}_n)(\Psi)^{(n+1)}(\underline{k}, \underline{k}_1, \dots, \underline{k}_n) \\
&= \sqrt{n+1} \int d^3\underline{k}\, \overline{h}(\underline{k})\overline{u}(\underline{k})\Psi^{(n+1)}(\underline{k}, \underline{k}_1, \dots, \underline{k}_n) = (a(uh)\Psi)^{(n)}(\underline{k}_1, \dots, \underline{k}_n).
\end{aligned} \tag{2.23}$$

Consider a self-adjoint operator b on $\mathfrak{h}$ with domain D_b. Then, its 'second quantization' is the following operator on the Fock space:

$$\mathrm{d}\Gamma(b)|_{\Gamma^{(n)}(\mathfrak{h})} = \sum_{i=1}^{n} 1 \otimes \cdots b \cdots \otimes 1, \tag{2.24}$$

$$\mathrm{d}\Gamma(b)\Omega = 0, \tag{2.25}$$

whose domain of essential self-adjointness[5] is $\Gamma_{\mathrm{fin}}(D_b)$. (In the definition above b is on the i-th tensor factor in each term in the sum). Suppose that $b = b(\underline{k})$ is a multiplication operator in momentum space on $\mathfrak{h} = L^2(\underline{\mathbb{R}}^3)$. Then as an equality of quadratic forms on $D \times D$ we have

$$\mathrm{d}\Gamma(b) = \int d^3\underline{q}\, b(\underline{q})a^*(\underline{q})a(\underline{q}) = \sum_{\lambda \in 1,2} \int d^3q\, b(q,\lambda)a^*(q,\lambda)a(q,\lambda). \tag{2.26}$$

Indeed, let us compute for $\Psi, \Phi \in D$: (POSSIBLE EXERCISE IN CLASS)

$$\begin{aligned}
&\int d^3\underline{q}\, b(\underline{q})\langle \Psi, a^*(\underline{q})a(\underline{q})\Phi\rangle = \int d^3\underline{q}\, b(\underline{q})\langle a(\underline{q})\Psi, a(\underline{q})\Phi\rangle \\
&= \int d^3\underline{q}\, b(\underline{q}) \sum_{n=0}^{\infty} \int d^{3n}\underline{k}\, \overline{(a(\underline{q})\Psi)}^{(n)}(\underline{k}_1, \dots, \underline{k}_n)(a(\underline{q})\Phi)^{(n)}(\underline{k}_1, \dots, \underline{k}_n) \\
&= \int d^3\underline{q}\, b(\underline{q}) \sum_{n=0}^{\infty}(n+1) \int d^{3n}\underline{k}\, \overline{\Psi}^{(n+1)}(\underline{q}, \underline{k}_1, \dots, \underline{k}_n)\Phi^{(n+1)}(\underline{q}, \underline{k}_1, \dots, \underline{k}_n) \\
&= \sum_{n=0}^{\infty} \int d^{3(n+1)}\underline{k} \sum_{\ell=1}^{n+1} \overline{\Psi}^{(n+1)}(\underline{k}_1, \dots, \underline{k}_\ell, \dots, \underline{k}_{n+1})b(\underline{k}_\ell)\Phi^{(n+1)}(\underline{k}_1, \dots, \underline{k}_\ell, \dots, \underline{k}_{n+1}),
\end{aligned} \tag{2.27}$$

[5]See Subsection 2.2.

and it is easy to see that the last expression is $\langle \Psi, \mathrm{d}\Gamma(b)\Phi\rangle$.

Finally, suppose that $u(t) = e^{itb}$. Then

$$\Gamma(u(t)) = e^{it\overline{\mathrm{d}\Gamma(b)}}, \tag{2.28}$$

where $\overline{\mathrm{d}\Gamma(b)}$ is the unique self-adjoint extension of $\mathrm{d}\Gamma(b)$. (See e.g. Homework Sheet 3 of my AQFT lectures).

Example: Time evolution of the free electric field. The Hamiltonian which governs the time evolution of the free electromagnetic field is given by

$$H_f = \int d^3\underline{q}\,\omega(q) a^*(\underline{q}) a(\underline{q}) = \mathrm{d}\Gamma(\omega), \quad \omega(q) := |q|. \tag{2.29}$$

Moreover, we have for $g \in S(\mathbb{R}^3)$ real-valued

$$\begin{aligned} E_\perp(g) &= \int d^3x E_\perp(x) g(x) \\ &= \sum_{\lambda=1,2} \int d^3k \sqrt{\frac{\omega(k)}{2}} e_\lambda(k) i \big(\widehat{g}(-k) a(k,\lambda) - \widehat{g}(k) a^*(k,\lambda)\big) \\ &= a(\widetilde{g}) + a^*(\widetilde{g}), \text{ where } \widetilde{g}(k,\lambda) := -\sqrt{\frac{\omega(k)}{2}} e_\lambda(k) i \widehat{g}(k). \end{aligned} \tag{2.30}$$

The time-evolved, smeared electric field is given by

$$\begin{aligned} E_\perp(t,g) &= e^{itH_f} E_\perp(g) e^{-itH_f} = e^{it\overline{\mathrm{d}\Gamma(\omega)}} E_\perp(g) e^{-it\overline{\mathrm{d}\Gamma(\omega)}} \\ &= \Gamma(e^{it\omega})(a(\widetilde{g}) + a^*(\widetilde{g}))\Gamma(e^{-it\omega}) = a(e^{it\omega}\widetilde{g}) + a^*(e^{it\omega}\widetilde{g}), \end{aligned} \tag{2.31}$$

where we made use of (2.28) and (2.22).

We define the non-smeared time evolved free electric field as the operator valued distribution:

$$E_\perp(t,x) = \frac{1}{(2\pi)^{3/2}} \sum_{\lambda=1,2} \int d^3k \sqrt{\frac{\omega(k)}{2}} e_\lambda(k) i \big(\mathrm{e}^{-i\omega(k)t + ikx} a(k,\lambda) - \mathrm{e}^{i\omega(k)t - ikx} a^*(k,\lambda)\big). \tag{2.32}$$

With $E_\perp(t,g)$ given by (2.31), we have

$$E_\perp(t,g) = \int d^3x\, E_\perp(t,x) g(x). \tag{2.33}$$

Of course analogous facts hold for $A_\perp$ and $B = \nabla \times A_\perp$.

2.2 Self-adjointness: basic concepts

A reference for this subsection is Chapter VIII of [4].

Consider an unbounded operator A on a dense domain $D(A) \subset \mathcal{H}$. Define the graph of A (denoted $\mathrm{Gr}(A)$) as the set of pairs $(\varphi, A\varphi)$, $\varphi \in D(A)$. This is a subset of $\mathcal{H} \times \mathcal{H}$ which is a Hilbert space with the product:

$$\langle (\varphi_1, \psi_1), (\varphi_2, \psi_2)\rangle = \langle \varphi_1, \varphi_2\rangle + \langle \psi_1, \psi_2\rangle. \tag{2.34}$$

1. We say that $(A, D(A))$ is a closed operator if $\mathrm{Gr}(A)$ is closed.

2. We say that A_1 is an extension of A if $\mathrm{Gr}(A_1) \supset \mathrm{Gr}(A)$.

3. We say that A is closable if it has a closed extension. The smallest closed extension is called the closure $\overline{A}$.

4. If A is closable, then $\mathrm{Gr}(\overline{A}) = \overline{\mathrm{Gr}(A)}$.

Define $D(A^*)$ as the set of all $\varphi \in \mathcal{H}$, for which there exists $\eta \in \mathcal{H}$ s.t.

$$\langle A\psi, \varphi \rangle = \langle \psi, \eta \rangle \text{ for all } \psi \in D(A). \tag{2.35}$$

For such $\varphi \in D(A^*)$ we define $A^*\varphi = \eta$. Fact: $(A, D(A))$ is closable if and only if $D(A^*)$ is dense in which case $\overline{A} = A^{**}$.

1. We say that $(A, D(A))$ is self-adjoint if $A = A^*$ and $D(A) = D(A^*)$.
   Fact: Self-adjointness is equivalent to $(A \pm i)D(A) = \mathcal{H}$.

2. Let $(A, D(A))$ be a self-adjoint operator. We define its spectrum $\sigma(A)$ as the set of all $\lambda \in \mathbb{C}$ s.t. $(\lambda - A)$ does not have a bounded inverse. We have $\sigma(A) \subset \mathbb{R}$. If $\sigma(A) \subset [0, \infty)$, we say that A is positive. This is equivalent to $\langle \psi, A\psi \rangle \geq 0$ for all $\psi \in D(A)$.

3. We say that $(A, D(A))$ is symmetric if $D(A) \subset D(A^*)$ and $A\psi = A^*\psi$ for $\psi \in D(A)$.
   Fact : Any symmetric operator is closable.

4. We say that symmetric A is essentially self adjoint if $\overline{A}$ is self-adjoint. In this case $D(A)$ is called *the core* of $\overline{A}$. (We stress that $D(A)$ is usually smaller than $D(\overline{A})$).
   Fact 1: If A is essentially self-adjoint then it has exactly one self-adjoint extension.
   Fact 2: Essential self-adjointness is equivalent to $(A \pm i)D(A)$ being dense.

2.3 Measure theory: basic concepts and results

The theory of self-adjoint operators relies heavily on measure theory. Here we recall several basic concepts and facts which will be useful in the remaining part of this section. Proofs can be found in the first two chapters of [6].

1. Let X be a topological space (a set with topology). A family $\mathcal{M}$ of subsets of X is a σ-algebra in X if it has the following properties:

   - $X \in \mathcal{M}$,
   - $A \in \mathcal{M} \Rightarrow A^c \in \mathcal{M}$,
   - $A_n \in \mathcal{M}$, $n \in \mathbb{N}$, $\Rightarrow A := \bigcup_{n=1}^{\infty} A_n \in \mathcal{M}$.

If $\mathcal{M}$ is a σ-algebra in X then X is called a *measurable space* and elements of $\mathcal{M}$ are called *measurable sets*.

2. Let X be a measure space and Y a topological space. Then a map $f : X \to Y$ is called *measurable* if for any open $V \subset Y$ the inverse image $f^{-1}(V)$ is a measurable set.

3. A (positive) measure is a function $\mu : \mathcal{M} \to [0, \infty]$ s.t. for any countable family of disjoint sets $A_i \in \mathcal{M}$ we have

$$\mu(\bigcup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} \mu(A_i). \tag{2.36}$$

   Also, we assume that $\mu(A) < \infty$ for at least one $A \in \mathcal{M}$. Moreover, we say that a *measure space* is a measurable space whose σ-algebra of measurable sets carries a positive measure.

4. We denote by $\mathcal{L}^p(X, \mu)$, $1 \le p < \infty$ the space of measurable functions $f : X \to \mathbb{C}$ s.t.

$$\|f\|_p := \left(\int_X |f(x)|^p d\mu(x) \right)^{1/p} < \infty. \tag{2.37}$$

   We denote by $L^p(X, \mu)$ the space of equivalence classes of functions from $\mathcal{L}^p(X, \mu)$ which are equal almost everywhere w.r.t. μ. Space $L^p(X, \mu)$ is a Banach space with the norm (2.37) (Riesz-Fisher theorem).

Theorem 2.1. *(Riesz-Markov-Kakutani). Let X be a locally compact Hausdorff space*[6] *and $C_c(X)$ the space of continuous compactly supported functions on X. Let $\Lambda : C_c(X) \to \mathbb{C}$ be a positive linear functional*[7]*. Then there exists a σ-algebra $\mathcal{M}$ in X and a positive measure on $\mathcal{M}$ s.t.*

$$\Lambda(f) = \int_X f(x) d\mu(x) \text{ for any } f \in C_c(X). \tag{2.38}$$

Theorem 2.2. *(Dominated convergence). Let f_n be a sequence of complex, measurable functions on X s.t.*

$$f(x) = \lim_{n\to\infty} f_n(x) \tag{2.39}$$

exists for any x. If there exists a function $g \in \mathcal{L}^1(X, \mu)$ s.t.

$$|f_n(x)| \le g(x) \text{ for all } n \in \mathbb{N}, x \in X, \tag{2.40}$$

then $f \in \mathcal{L}^1(X, \mu)$. Moreover,

$$\lim_{n\to\infty} \int_X f_n(x) d\mu(x) = \int_X f(x) d\mu(x). \tag{2.41}$$

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[6] i.e. a topological space s.t. any two distinct points have disjoint neighbourhoods and any point has a compact neighbourhood.

[7] i.e. if f takes values in $[0, \infty]$ then $\Lambda(f) \ge 0$.

Theorem 2.3. *(Monotone convergence). Let f_n be a sequence of measurable functions and suppose that*

(a) $0 \leq f_1(x) \leq f_2(x) \leq \cdots \leq \infty$ *for all* $x \in X$.

(b) $f_n(x) \to f(x)$ *for all* $x \in X$.

Then f is measurable and

$$\lim_{n\to\infty} \int_X f_n(x) d\mu(x) = \int_X f(x) d\mu(x). \tag{2.42}$$

2.4 Self-adjointness: basic results

Now we use the above results in measure theory to study self-adjointness questions. A reference for this subsection is [4, 5].

Example: [4, Chapter VIII, Proposition 2] Let f be a real valued, measurable, finite a.e. function on a measure space (X, μ). Then the corresponding multiplication operator T_f on $L^2(X, \mu)$ (acting by $\psi(x) \mapsto f(x)\psi(x)$) defined on the domain

$$D(T_f) := \{ \psi \in L^2(X, \mu) \,|\, \int d\mu(x) \, |f(x)\psi(x)|^2 < \infty \} \tag{2.43}$$

is self-adjoint. To prove this, we compute $D((T_f)^*)$: Suppose that $\psi \in D((T_f)^*)$ and let χ_n be the characteristic function of $\{|f(x)| \leq n\}$. We denote the corresponding multiplication operator by $\chi_n(x)$. Then making use of the monotone convergence (or dominated convergence) theorem in the first step:

$$\begin{aligned} \|(T_f)^*\psi\| &= \lim_{n\to\infty} \|\chi_n(x)(T_f)^*\psi\| \\ &= \lim_{n\to\infty} \sup_{\|\phi\|=1} |\langle \phi, \chi_n(x)(T_f)^*\psi \rangle| \\ &= \lim_{n\to\infty} \sup_{\|\phi\|=1} |\langle T_f \chi_n(x)\phi, \psi \rangle| \\ &= \lim_{n\to\infty} \sup_{\|\phi\|=1} |\langle \phi, \chi_n(x) f(x)\psi \rangle| = \lim_{n\to\infty} \|\chi_n(x) f(x)\psi\|. \end{aligned} \tag{2.44}$$

From the last equality and the monotone convergence theorem we conclude that $f(x)\psi(x)$ is square integrable and therefore $D((T_f)^*) = D(T_f)$.

It turns out that any self-adjoint operator can be represented as a multiplication operator on some measure space:

Theorem 2.4. *(Spectral theorem, multiplication operator variant). Let A be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$ with domain $D(A)$. Then there is a measure space (X, μ) with μ a finite measure, a unitary operator $U : \mathcal{H} \to L^2(X, d\mu)$ and a real-valued, measurable function f on X which is finite almost everywhere, s.t.*

(a) $\psi \in D(A)$ *iff* $f(\,\cdot\,)(U\psi)(\,\cdot\,) \in L^2(X, d\mu)$.

(b) If $\phi \in U[D(A)]$, *then* $(UAU^*\phi)(x) = f(x)\phi(x)$.

There is another variant of the spectral theorem, using the concept of spectral measures:

Definition 2.5. *Let* X *be a measurable space with a* σ*-algebra* $\mathcal{M}$. *We say that* $\mathcal{M} \ni \Delta \to E(\Delta) \in B(\mathcal{H})$ *is a spectral measure if:*

- *Each* $E(\Delta)$ *is an orthogonal projection.*
- $E(\emptyset) = 0$, $E(X) = 1$.
- *If* $\Delta = \bigcup_{n=1}^{N} \Delta_n$, *with* $\Delta_n \cap \Delta_m = \emptyset$ *for* $n \neq m$, *then*

$$E(\Delta) = \text{s}-\lim_{N\to\infty} \sum_{n=1}^{N} E(\Delta_n). \tag{2.45}$$

- $E(\Delta_1)E(\Delta_2) = E(\Delta_1 \cap \Delta_2)$.

For any $\psi \in \mathcal{H}$ the expression $\Delta \to \langle \psi, E(\Delta)\psi \rangle$ is a positive measure and the formula

$$\langle \psi, A\psi \rangle = \int x \, \langle \psi, dE(x)\psi \rangle \tag{2.46}$$

defines a self-adjoint operator A on the domain

$$D(A) = \{\psi \in \mathcal{H} \,|\, \int |x|^2 \langle \psi, dE(x)\psi \rangle < \infty \}. \tag{2.47}$$

It turns out that also the converse is true:

Theorem 2.6. *(Spectral theorem, spectral measure variant). For any self-adjoint operator* $(A, D(A))$ *there exists a spectral measure* E *on (a* σ*-algebra of measurable sets) on* $\mathbb{R}$ *s.t.*

$$A = \int_{\sigma(A)} x dE(x), \tag{2.48}$$

where the last relation means that (2.46), (2.47) hold.

Idea of proof: Let A be bounded, for simplicity. Consider a map $g \to \langle \psi, g(A)\psi \rangle$ defined first for polynomials and then extended, using the Stone-Weierstrass theorem to continuous functions. Then we get by the Riesz-Markov-Kakutani theorem a measure space (X_ψ, μ_ψ) s.t.

$$\langle \psi, g(A)\psi \rangle = \int_{X_\psi} g(x) d\mu_\psi(x) \tag{2.49}$$

and we can extend this expression to measurable functions g. In particular, we set $E(\Delta) := \chi_\Delta(A)$ and it is easy to check that this gives a spectral measure. □

Spectral theorem (multiplication operator form) has the following corollary which is useful when dealing with tensor products:

Corollary 2.7. *[5, Theorem VIII.33] Let A_k be a self-adjoint operator on $\mathcal{H}_k$ and let $P(x_1,\dots,x_N)$ be a polynomial with real coefficients of degree n_k in the k-th variable and suppose that D^e_k is the domain of essential self-adjointness of for A^{n_k}. Then $P(A_1,\dots A_N)$ is essentially self-adjoint on*

$$D^e = \otimes_{k=1}^N D^e_k. \tag{2.50}$$

(The polynomial involves tensor products of different operators. For example, if $P(x_1,x_2,x_3) = x_1x_2^3 + x_3$ then $P(A_1,A_2,A_3) = A_1 \otimes A_2^3 \otimes 1 + 1 \otimes 1 \otimes A_3$). Moreover, we have the spectral mapping property:

$$\sigma(\overline{P(A_1,\dots A_N)}) = \overline{P(\sigma(A_1),\dots \sigma(A_n))}. \tag{2.51}$$

Example: Let $\omega(k) = |k|$ be a multiplication operator on $\mathfrak{h} = L^2(\underline{\mathbb{R}}^3)$ defined on the domain

$$D(\omega) = \{\psi \in L^2(\underline{\mathbb{R}}^3) \,|\, \int d^3\underline{k}\, |\omega(k)\psi(\underline{k})|^2 < \infty\}. \tag{2.52}$$

We know from the example above, that $(\omega, D(\omega))$ is self-adjoint. In fact we can also show this by checking that

$$(\omega \pm i)D(\omega) = \mathfrak{h}. \tag{2.53}$$

For this purpose pick an arbitrary $\psi \in \mathfrak{h}$ and note that $k \to (\omega(k) \pm i)^{-1}\psi(k)$ is an element of $D(\omega)$. Therefore we can write

$$\psi = (\omega \pm i)(\omega \pm i)^{-1}\psi \in (\omega \pm i)D(\omega). \tag{2.54}$$

Example: Now let $H_f := \mathrm{d}\Gamma(\omega)$ and $D(H_f) = \Gamma_{\mathrm{fin}}(D(\omega))$. Let us show that $(H_f, D(H_f))$ is an essentially self-adjoint operator: Let $\mathrm{d}\Gamma^{(n)}(\omega) = \omega \otimes \cdots \otimes 1 + \cdots + 1 \otimes \cdots \otimes \omega$ be the restriction of $\mathrm{d}\Gamma(\omega)$ to $\Gamma^{(n)}(D(\omega))$, where

$$\Gamma^{(n)}(D(\omega)) = S_n(D(\omega) \otimes \cdots \otimes D(\omega)), \tag{2.55}$$

and S_n is the symmetrization operator. Denote be $\mathrm{d}\Gamma^{(n)}_{us}(\omega)$ the corresponding operator on the unsymmetrized tensor product space:

$$\Gamma^{(n)}_{us}(D(\omega)) = D(\omega) \otimes \cdots \otimes D(\omega). \tag{2.56}$$

By Corollary 2.7, $\mathrm{d}\Gamma^{(n)}_{us}(\omega)$ is essentially self-adjoint on $\Gamma^{(n)}_{us}(D(\omega))$ which means that the sets

$$X_n := (\mathrm{d}\Gamma^{(n)}_{us}(\omega) \pm i)\Gamma^{(n)}_{us}(D(\omega)) \tag{2.57}$$

are dense in $\Gamma^{(n)}_{us}(\mathfrak{h})$. Since $\mathrm{d}\Gamma^{(n)}_{us}(\omega)$ commutes with the projection S_n on the symmetric subspace, we have (by decomposing each X_n into a direct sum of orthogonal subspaces $S_n X_n \oplus (1-S_n)X_n$ which must be then separately dense in $S_n\Gamma^{(n)}_{us}(D(\omega))$ and $(1-S_n)\Gamma^{(n)}_{us}(D(\omega))$, respectively) that the sets

$$(\mathrm{d}\Gamma^{(n)}(\omega) \pm i)\Gamma^{(n)}(D(\omega)) \tag{2.58}$$

are dense in $\Gamma^{(n)}(\mathfrak{h})$. Now we want to show from (2.58) that

$$(\mathrm{d}\Gamma(\omega) \pm i)\Gamma_{\mathrm{fin}}(D(\omega)) \tag{2.59}$$

is dense: Let $\Psi_{\mathrm{fin}} = \sum_{n\in\mathbb{N}_{\mathrm{fin}}} \Psi^{(n)}$ be an arbitrary element of $\Gamma_{\mathrm{fin}}(D(\omega))$ i.e. $\Psi^{(n)}$ are arbitrary elements of $\Gamma^{(n)}(D(\omega))$ and $\mathbb{N}_{\mathrm{fin}}$ is an arbitrary finite subset of $\mathbb{N}$. We have

$$(\mathrm{d}\Gamma(\omega) \pm i)\Psi_{\mathrm{fin}} = \sum_{n\in\mathbb{N}_{\mathrm{fin}}} (\mathrm{d}\Gamma(b) \pm i)\Psi^{(n)}. \tag{2.60}$$

By (2.58) we can approximate any element of $\Gamma_{\mathrm{fin}}(\mathfrak{h})$ with such vectors, which concludes the proof of essential self-adjointness of $(H_f, D(H_f))$.

Lemma 2.8. *The operator $H_0 = \frac{p^2}{2m} \otimes 1 + 1 \otimes H_f$ is essentially self-adjoint on $D(p^2) \otimes D(H_f)$. Its closure $\overline{H}_0$ is a positive self-adjoint operator on some domain $D(\overline{H}_0)$.*

Proof. Essential self-adjointness follows from Lemma 2.7 and from essential self-adjointness of p^2, $\mathrm{d}\Gamma(\omega)$. Positivity of p^2 and ω is obvious (by checking positivity of the matrix elements $\langle\psi, \cdot\,\psi\rangle$). Then positivity of $\mathrm{d}\Gamma(\omega)$ and H_0 follows from the spectral mapping property from Corollary 2.7. □

So we have H_0 i.e. the non-interacting part of the Pauli-Fierz Hamiltonian (with one electron[8]), under control. The full Hamiltonian has the form

$$H = H_0 + H_1, \quad H_1 = -\frac{e}{m} p \cdot A_{\perp,\varphi}(q) + \frac{e^2}{2m} A_{\perp,\varphi}(q)^2. \tag{2.61}$$

To obtain essential self-adjointness of H we will follow a strategy which can be called perturbation theory of linear operators. It consists in decomposing a self-adjoint operator A into $A = A_0 + A_1$, where A_0 is 'simple' and A_1 is 'small'. More precisely:

Definition 2.9. *Let A_0 and A_1 be densely defined linear operators on a Hilbert space $\mathcal{H}$. Suppose that:*

(a) $D(A_1) \supset D(A_0)$

(b) For some $a, b \in \mathbb{R}$ and all $\phi \in D(A_0)$

$$\|A_1\phi\| \le a\|A_0\phi\| + b\|\phi\|. \tag{2.62}$$

Then A_1 is said to be A_0-bounded. The infimum of such a is called the relative bound of A_1 w.r.t. A_0.

[8]From now on we consider only the Pauli-Fierz Hamiltonian with one electron

Theorem 2.10. *(Kato-Rellich). Let A_0 be self-adjoint, A_1 symmetric and A_0-bounded with a relative bound $a < 1$. Then $A_0 + A_1$ is self-adjoint on $D(A_0)$ and essentially self-adjoint on any core of A_0. Further, if A_0 is bounded below by M then $A_0 + A_1$ is bounded below by $M - \max\{b/(1-a), a|M| + b\}$.*

Proof. We follow [5]. We will show that $(A_0 + A_1 \pm i\mu)D(A_0) = \mathcal{H}$ for some $\mu_0 > 0$, which implies self-adjointness. For $\phi \in D(A_0)$ we have

$$\|(A_0 + i\mu)\phi\|^2 = \|A_0\phi\|^2 + \mu^2\|\phi\|^2. \tag{2.63}$$

Letting $\phi = (A_0 + i\mu)^{-1}\psi$, where $\psi \in \mathcal{H}$ is arbitrary, we have

$$\|\psi\|^2 = \|A_0(A_0 + i\mu)^{-1}\psi\|^2 + \mu^2\|(A_0 + i\mu)^{-1}\psi\|^2. \tag{2.64}$$

We conclude from this that $\|A_0(A_0 + i\mu)^{-1}\| \leq 1$ and $\|(A_0 + i\mu)^{-1}\| \leq \mu^{-1}$. Therefore, applying (2.62) with $\phi = (A_0 + i\mu)^{-1}\psi$, we get

$$\|A_1(A_0 + i\mu)^{-1}\psi\| \leq a\|A_0(A_0 + i\mu)^{-1}\psi\| + b\|(A_0 + i\mu)^{-1}\psi\| \leq (a + b/\mu)\|\psi\|. \tag{2.65}$$

Hence, for μ large, $C := A_1(A_0 + i\mu)^{-1}$ has norm less than one, since $a < 1$. This implies that $-1 \notin \sigma(C)$, so $\mathrm{Ran}(I + C) = \mathcal{H}$. (Since $(I + C)^{-1}$ exists, I can write $\psi = (I + C)(I + C)^{-1}\psi$ for any $\psi \in \mathcal{H}$). Since A_0 is self-adjoint, also $\mathrm{Ran}(A_0 + i\mu) = \mathcal{H}$. So the equation

$$(I + C)(A_0 + i\mu)\phi = (A_0 + A_1 + i\mu)\phi, \text{ for } \phi \in D(A_0) \tag{2.66}$$

implies that $\mathrm{Ran}(A_0 + A_1 + i\mu) = \mathcal{H}$. The proof that $\mathrm{Ran}(A_0 + A_1 - i\mu) = \mathcal{H}$ is the same.

Let D_0 be a core of A_0. Then, we claim that by the bound (2.62),

$$D(\overline{(A_0 + A_1)|D_0}) \supset D(\overline{A_0|D_0}) = D(A_0) = D(A_0 + A_1). \tag{2.67}$$

Let us prove the inclusion above: Suppose $\psi \in D(\overline{A_0|D_0})$. This means that $(\psi, \overline{A_0|D_0}\psi) \in \mathrm{Gr}(\overline{A_0|D_0}) = \overline{\mathrm{Gr}(A_0|D_0)}$. Hence, there is a sequence $\psi_n \in D_0$ s.t. $(\psi_n, A_0\psi_n) \to (\psi, \overline{A_0|D_0}\psi)$, that is

$$\psi_n \to \psi, \quad A_0\psi_n \to \overline{A_0|D_0}\psi. \tag{2.68}$$

We will show that $\psi \in D(\overline{(A_0 + A_1)|D_0})$, i.e. $(\psi, \overline{(A_0 + A_1)|D_0}\psi) \in \mathrm{Gr}(\overline{(A_0 + A_1)|D_0}) = \overline{\mathrm{Gr}((A_0 + A_1)|D_0)}$ i.e. that there is a sequence $\psi'_n \in D_0$ s.t. $(\psi'_n, (A_0 + A_1)\psi'_n)$ converges. (Then the limit can be called $\overline{(A_0 + A_1)|D_0}\psi$). We check that the sequence from (2.68), i.e. $\psi'_n = \psi_n$, does the job. Namely, we verify the Cauchy criterion:

$$\begin{aligned} \|(A_0 + A_1)(\psi_{n_1} - \psi_{n_2})\| &\leq \|A_0(\psi_{n_1} - \psi_{n_2})\| + \|A_1(\psi_{n_1} - \psi_{n_2})\| \\ &\leq (1 + a)\|A_0(\psi_{n_1} - \psi_{n_2})\| + b\|(\psi_{n_1} - \psi_{n_2})\| \to 0, \end{aligned} \tag{2.69}$$

where in the last step we used (2.68). This gives $\psi \in D(\overline{(A_0 + A_1)|D_0})$. (We skip the proof of semi-boundedness). □

The Kato-Relich theorem gives rather concrete information about domains, but the estimate (2.62) is somewhat difficult to verify in examples. We state below a different result, the KLMN theorem, where the relevant bound is much easier to check, but the information about the domains is less explicit. For this we need the concept of quadratic forms:

Definition 2.11. *A quadratic form is a map $Q(q) \times Q(q) \to \mathbb{C}$, (where $Q(q)$ is a dense linear subset of $\mathcal{H}$), which is antilinear in the first argument and linear in the second argument.*

1. *If $q(\phi, \psi) = \overline{q(\psi, \phi)}$, we say that the form is symmetric.*
2. *If $q(\phi, \phi) \geq 0$ for $\phi \in Q(q)$ we say that the form is positive.*
3. *If $q(\phi, \phi) \geq -M\|\phi\|^2$ for some $M \geq 0$ and all $\phi \in Q(q)$ we say that the form is semibounded.*
4. *If q is semibounded and $Q(q)$ is complete under the norm $\|\psi\|_{+,1} := \sqrt{q(\psi, \psi) + (M+1)\|\psi\|^2}$, we say that q is closed*[9]*.*
5. *If there is a self adjoint operator $(A, D(A))$, s.t.*
$$q(\phi, \psi) = \langle \phi, A\psi \rangle, \quad Q(q) = D(|A|^{1/2}), \tag{2.70}$$
then we say that q is the quadratic form of this self-adjoint operator. (Strictly speaking, we mean $q(\phi, \psi) = \langle |A|^{1/2}\phi, \mathrm{sgn}(A)|A|^{1/2}\psi \rangle$, where $x \to \mathrm{sgn}(x)$ is the sign function). If this form is semibounded, then it is closed.
6. *Given a self-adjoint operator $(A, D(A))$ as above, we write $Q(A) := Q(q) = D(|A|^{1/2})$.*

The fundamental relation between quadratic forms and self-adjoint operators is given by the following theorem:

Theorem 2.12. *([4], Theorem VIII.15). Let q be a closed, semibounded quadratic form. Then q is the quadratic form of a unique self-adjoint operator.*

Theorem 2.13. *(KLMN, [5], Theorem X.17). Let A_0 be a positive self-adjoint operator. Let $\beta(\psi, \phi)$ be a symmetric quadratic form defined for all $\psi, \phi \in Q(A_0) = D(A_0^{1/2})$ s.t. for some constants $0 \leq a < 1$, $0 \leq b < \infty$*
$$|\beta(\psi, \psi)| \leq a\langle \psi, A_0\psi \rangle + b\langle \psi, \psi \rangle \tag{2.71}$$
for all $\psi \in Q(A_0)$. Then there exists a unique self-adjoint operator A with $Q(A) = Q(A_0)$ s.t.
$$\langle \psi, A\phi \rangle = \langle \psi, A_0\phi \rangle + \beta(\psi, \phi) \tag{2.72}$$
for all $\psi, \phi \in Q(A)$. Moreover, A is bounded from below by $-b$.

[9]This definition looks quite different than closedness of an operator A, given by closedness of $\mathrm{Gr}(A)$. But the latter definition can be reformulated as completeness of $D(A)$ under the norm $\psi \to \|\psi\| + \|A\psi\|$

Remark 2.14. *To construct the quadratic form* β *we will first write* $\beta(\psi, \phi) := \langle\psi, A_1\phi\rangle$ *on some 'nice' domain and then extend to the domain required in the theorem.* $\langle\phi, A_1\phi\rangle$ *is easier to estimate than* $\|A_1\phi\| = \langle\phi, A_1^2\phi\rangle^{1/2}$ *appearing in the Kato-Rellich theorem.*

Proof. Define a form $\gamma(\varphi, \psi) = \langle\varphi, A_0\psi\rangle + \beta(\varphi, \psi)$ on $Q(A_0)$. By the bound (2.71) we have

$$\beta(\varphi, \varphi) \geq -a\langle\varphi, A_0\varphi\rangle - b\langle\varphi, \varphi\rangle \tag{2.73}$$

and therefore

$$\gamma(\varphi, \varphi) \geq (1-a)\langle\varphi, A_0\varphi\rangle - b\|\varphi\|^2 \geq -b\|\varphi\|^2, \tag{2.74}$$

since A_0 is positive and $0 \leq a < 1$. Thus γ is bounded from below by $-b$. Moreover,

$$\begin{aligned} (1-a)\langle\varphi, A_0\varphi\rangle + \|\varphi\|^2 &\leq \gamma(\varphi, \varphi) + (b+1)\|\varphi\|^2 \\ &= \langle\varphi, A_0\varphi\rangle + \beta(\varphi, \varphi) + (b+1)\|\varphi\|^2 \\ &\leq (1+a)\langle\varphi, A_0\varphi\rangle + (2b+1)\|\varphi\|^2. \end{aligned} \tag{2.75}$$

This means that the norms $\|\cdot\|_{+1,A_0}$ and $\|\cdot\|_{+1,\gamma}$ are equivalent on $Q(A_0)$. Since $Q(A_0)$ is closed under $\|\cdot\|_{+1,A_0}$, it is closed under $\|\cdot\|_{+1,\gamma}$. Thus γ is a semibounded, closed quadratic form on $Q(A_0)$ and the existence of A now follows from Theorem 2.12. □

2.5 Self-adjointness of the Pauli-Fierz Hamiltonian

For concreteness we study the Pauli-Fierz Hamiltonian with one electron. We recall the definition of the Pauli-Fierz Hamiltonian:

$$H = \frac{1}{2m}(p \otimes 1 - eA_{\perp,\varphi}(q))^2 + 1 \otimes H_f. \tag{2.76}$$

We write

$$H_0 = \frac{1}{2m}(p^2 \otimes 1) + 1 \otimes H_f, \tag{2.77}$$

$$H_1 = -\frac{e}{m}p \cdot A_{\perp,\varphi}(q) + \frac{e^2}{2m}A_{\perp,\varphi}(q)^2. \tag{2.78}$$

To apply the KLMN theorem we first have to know that $\overline{H}_0$ is positive, self-adjoint. This was checked in Lemma 2.8. Then we have to check that H_1 defines a symmetric quadratic form on $D(\overline{H}_0^{1/2}) \times D(\overline{H}_0^{1/2})$ s.t. for some constants $0 \leq a < 1$, $0 \leq b < \infty$ and $\psi \in D(\overline{H}_0^{1/2})$

$$|\langle\psi, H_1\psi\rangle| \leq a\langle\psi, \overline{H}_0\psi\rangle + b\langle\psi, \psi\rangle. \tag{2.79}$$

We check it in a series of lemmas:

Lemma 2.15. *Let $\psi \in D(H_f) = \Gamma_{\mathrm{fin}}(D(\omega))$ and $h \in L^2(\underline{\mathbb{R}}^3)$ s.t. $\omega^{-1/2}h \in L^2(\underline{\mathbb{R}}^3)$. Then*

$$\|a(h)\psi\| \leq \|\omega^{-1/2}h\|_2 \, \langle\psi, H_f\psi\rangle^{1/2}, \tag{2.80}$$
$$\|a(h)^*\psi\| \leq \|\omega^{-1/2}h\|_2 \, \langle\psi, H_f\psi\rangle^{1/2} + \|h\|_2\|\psi\|. \tag{2.81}$$

Proof. First, we recall

$$(a(h)\psi)^{(n)}(\underline{k}_1, \ldots, \underline{k}_n) \quad = \quad \sqrt{n+1}\int d^3\underline{q}\, \overline{h}(\underline{q})\psi^{(n+1)}(\underline{q}, \underline{k}_1, \ldots, \underline{k}_n). \tag{2.82}$$

Now to prove (2.80) we first compute for $\psi \in \Gamma_{\mathrm{fin}}(D(\omega)) = D(H_f)$:

$$\begin{aligned}
&\|a(h)\psi\|^2 \\
&\leq \sum_{n=0}^{\infty}(n+1)\int d^{3n}\underline{k}\int d^3\underline{q}_1 d^3\underline{q}_2\, |\omega^{-1/2}(q_1)h(\underline{q}_1)\omega^{-1/2}(q_2)\overline{h}(\underline{q}_2) \\
&\times\omega^{1/2}(q_1)\overline{\psi}^{(n+1)}(\underline{q}_1, \underline{k}_1, \ldots, \underline{k}_n)\omega^{1/2}(q_2)\psi^{(n+1)}(\underline{q}_2, \underline{k}_1, \ldots, \underline{k}_n)| \\
&\leq \sum_{n=0}^{\infty}(n+1)\int d^{3n}\underline{k}\left(\int d^3\underline{q}_1 d^3\underline{q}_2\, |\omega^{-1/2}(q_1)h(\underline{q}_1)\omega^{-1/2}(q_2)\overline{h}(\underline{q}_2)|^2\right)^{1/2} \\
&\times\left(\int d^3\underline{q}_1 d^3\underline{q}_2 |\omega^{1/2}(q_1)\overline{\psi}^{(n+1)}(\underline{q}_1, \underline{k}_1, \ldots, \underline{k}_n)\omega^{1/2}(q_2)\psi^{(n+1)}(\underline{q}_2, \underline{k}_1, \ldots, \underline{k}_n)|^2|\right)^{1/2} \\
&\leq \|\omega^{-1/2}h\|_2^2\sum_{n=0}^{\infty}(n+1)\int d^{3n}\underline{k}\, d^3\underline{q}\, \omega(q)|\psi^{(n+1)}(\underline{q}, \underline{k}_1, \ldots, \underline{k}_n)|^2 \\
&= \|\omega^{-1/2}h\|_2^2\langle\psi, H_f\psi\rangle.
\end{aligned} \tag{2.83}$$

Relation (2.81) now easily follows from the canonical commutation relations:

$$\|a(h)^*\psi\|^2 = \langle\psi, a(h)a(h)^*\psi\rangle = \|h\|^2\|\psi\|^2 + \langle\psi, a(h)^*a(h)\psi\rangle \tag{2.84}$$

and the previous bound. □

Now we write

$$A_{\perp,\varphi}(q) = a(f_q) + a^*(f_q), \tag{2.85}$$

where $f_q(k,\lambda) = \widehat{\varphi}(k)\sqrt{1/(2\omega(k))}e_\lambda(k)\mathrm{e}^{-ikq}$. It is also convenient to define $f'(k) = \widehat{\varphi}(k)\sqrt{1/(2\omega(k))}$. It has to be kept in mind that q is here an operator so (2.85) is an abuse of notation. In the proof of the next lemma we will first proceed as if q was a number, and then explain why this is legitimate.

Lemma 2.16. *For $\Psi, \Phi \in L^2(\mathbb{R}^3) \otimes \Gamma_{\mathrm{fin}}(D(\omega))$ we have*

$$\langle\Psi, A_{\perp,\varphi}(q)^2\Psi\rangle \leq 18\|\omega^{-\frac{1}{2}}f'\|_2^2\langle\Psi, (1 \otimes H_f)\Psi\rangle + 12\|f'\|_2^2\|\Psi\|^2. \tag{2.86}$$

For $\Psi \in D(p^2) \otimes \Gamma_{\mathrm{fin}}(D(\omega))$

$$|\langle\Psi, p \cdot A_{\perp,\varphi}(q)\Psi\rangle| \leq \frac{1}{2}\langle\Psi, p^2\Psi\rangle + \frac{1}{2}\langle\Psi, A_{\perp,\varphi}(q)^2\Psi\rangle. \tag{2.87}$$

Proof. We obtain for $\Psi \in L^2(\mathbb{R}^3) \otimes D(H_f^{1/2})$

$$\begin{aligned}
\langle \Psi, (a(f_q^i) + a^*(f_q^i))^2 \Psi \rangle &= |\langle \Psi, a(f_q^i) a(f_q^i) \Psi \rangle + \langle \Psi, a(f_q^i) a^*(f_q^i) \Psi \rangle \\
&\quad \langle \Psi, a^*(f_q^i) a(f_q^i) \Psi \rangle + \langle \Psi, a^*(f_q^i) a^*(f_q^i) \Psi \rangle| \\
&\leq \|a(f_q^i)\Psi\| \, \|a^*(f_q^i)\Psi\| + \|a^*(f_q^i)\Psi\| \, \|a^*(f_q^i)\Psi\| \\
&\quad + \|a(f_q^i)\Psi\| \, \|a(f_q^i)\Psi\| + \|a^*(f_q^i)\Psi\| \, \|a(f_q^i)\Psi\| \\
&\leq \frac{1}{2}\big(4\|a(f_q^i)\Psi\|^2 + 4\|a^*(f_q^i)\Psi\|^2\big), \qquad (2.88)
\end{aligned}$$

where we made use of $ab \leq \frac{1}{2}(a^2 + b^2)$. Now, by Lemma 2.15, we have

$$\begin{aligned}
\|a(f_q^i)\Psi\|^2 &\leq \|\omega^{-1/2} f^i\|_2^2 \, \|(H_f)^{1/2}\Psi\|^2, \qquad (2.89) \\
\|a^*(f_q^i)\Psi\|^2 &\leq \big(\|\omega^{-1/2} f^i\|_2 \, \|(H_f)^{1/2}\Psi\| + \|f^i\|_2 \|\Psi\|\big)^2 \qquad (2.90) \\
&\leq 2\big(\|\omega^{-1/2} f^i\|_2^2 \, \|(H_f)^{1/2}\Psi\|^2 + \|f^i\|_2^2 \|\Psi\|^2\big), \qquad (2.91)
\end{aligned}$$

where in the last step we made use of $(a+b)^2 \leq 2(a^2 + b^2)$. Therefore

$$\begin{aligned}
\langle \Psi, A_{\perp,\varphi}(q)^2 \Psi \rangle &= \sum_{i=1}^{3} \langle \Psi, (a(f_q^i) + a^*(f_q^i))^2 \Psi \rangle \\
&\leq 6 \sum_{i=1}^{3} \|\omega^{-1/2} f^i\|_2^2 \, \|(H_f)^{1/2}\Psi\|^2 + 4 \sum_{i=1}^{3} \|f^i\|_2^2 \|\Psi\|^2 \\
&\leq 18\|\omega^{-1/2} f'\|_2^2 \, \|(H_f)^{1/2}\Psi\|^2 + 12\|f'\|_2^2 \|\Psi\|^2. \qquad (2.92)
\end{aligned}$$

Let us now make a clarification concerning the notation $a(f_q)$ (given that q is an operator): We defined the Hilbert space of the system as $\mathcal{H} = L^2(\mathbb{R}^3_{(p)}) \otimes \mathcal{F}$, where (p) reminds that we mean wave-functions in momentum representation. We have the following standard isomorphisms:

$$\mathcal{H} = L^2(\mathbb{R}^3_{(p)}) \otimes \mathcal{F} \simeq L^2(\mathbb{R}^3_{(q)}) \otimes \mathcal{F} \simeq L^2(\mathbb{R}^3_{(q)}; \mathcal{F}), \qquad (2.93)$$

where the first equality is the Plancherel theorem and the last space contains square-integrable functions of q' with values in $\mathcal{F}$. In this last representation we have $\Psi = \{\Psi_{q'}\}_{q' \in \mathbb{R}^3}$ and we can write, for example

$$\langle \Psi, a^*(f_q^i) a(f_q^i) \Psi \rangle_{\mathcal{H}} = \int d^3 q' \, \langle \Psi_{q'}, a^*(f_{q'}^i) a(f_{q'}^i) \Psi_{q'} \rangle_{\mathcal{F}}, \qquad (2.94)$$

$$\|\Psi\|_{\mathcal{H}}^2 = \int d^3 q' \, \|\Psi_{q'}\|_{\mathcal{F}}^2. \qquad (2.95)$$

Our computations in the first part of the proof above should be considered a short-hand notation for this.

Finally, we note that by Cauchy-Schwarz:

$$\begin{aligned}
|\langle \Psi, p \cdot A_{\perp,\varphi}(q) \Psi \rangle)| &= |\langle p_i \Psi, A^i_{\perp,\varphi}(q) \Psi \rangle| \leq \|p_i \Psi\| \, \|A^i_{\perp,\varphi}(q)\Psi\| \\
&\leq \frac{1}{2}\langle \Psi, p^2 \Psi \rangle + \frac{1}{2}\langle \Psi, A_\varphi(q)^2 \Psi \rangle, \qquad (2.96)
\end{aligned}$$

which concludes the proof. □

Recall the definitions

$$H_0 = \frac{1}{2m}(p^2 \otimes 1) + 1 \otimes H_f, \tag{2.97}$$

$$H_1 = -\frac{e}{m} p \cdot A_{\perp,\varphi}(q) + \frac{e^2}{2m} A_{\perp,\varphi}(q)^2. \tag{2.98}$$

Lemma 2.17. *(a) For $\Psi \in D(p^2) \otimes \Gamma_{\text{fin}}(D(\omega))$ and $\|\omega^{-\frac{1}{2}} f'\|_2, \|f'\|_2 < \infty$ we have:*

$$|\langle \Psi, H_1 \Psi \rangle| \leq a(e)\langle \Psi, H_0 \Psi \rangle + b(e)\langle \Psi, \Psi \rangle, \tag{2.99}$$

where $a(e) \to 0$ as $e \to 0$.
(b) The quadratic form $\beta(\Psi, \Phi) := \langle \Psi, H_1 \Phi \rangle$, defined first on the domain specified above, extends to $D(\overline{H}_0^{1/2}) \times D(\overline{H}_0^{1/2})$.
(c) For $\Psi \in D(\overline{H}_0^{1/2})$ we have

$$|\beta(\Psi, \Psi)| \leq a(e)\langle \Psi, \overline{H_0} \Psi \rangle + b(e)\langle \Psi, \Psi \rangle. \tag{2.100}$$

Remark 2.18. *Properties (b) and (c) above are assumptions of the KLMN theorem.*

Proof. We first derive an auxiliary estimate for $\Psi, \Phi \in D(p^2) \otimes \Gamma_{\text{fin}}(D(\omega))$. Lemma 2.16 gives:

$$\begin{aligned}
|\langle \Psi, H_1 \Phi \rangle| &\leq c_1(e)|\langle \Psi, p \cdot A_{\perp,\varphi}(q)\Phi \rangle| + c_2(e)|\langle \Psi, A_{\perp,\varphi}(q)^2 \Phi \rangle| \\
&\leq c_1(e)\langle \Psi, p^2 \Psi \rangle^{1/2} \langle \Phi, A_{\perp,\varphi}(q)^2 \Phi \rangle^{1/2} \\
&\quad + c_2(e)\langle \Psi, A_{\perp,\varphi}(q)^2 \Psi \rangle^{1/2} \langle \Phi, A_{\perp,\varphi}(q)^2 \Phi \rangle^{1/2} \\
&\leq c_1(e)\langle \Psi, p^2 \Psi \rangle^{1/2} \langle \Phi, A_{\perp,\varphi}(q)^2 \Phi \rangle^{1/2} \\
&\quad + c_2'(e)(\langle \Psi, H_f \Psi \rangle + \|\Psi\|^2)^{1/2} (\langle \Phi, H_f \Phi \rangle + \|\Phi\|^2)^{1/2} \\
&\leq c_1'(e)\langle \Psi, H_0 \Psi \rangle^{1/2} (\langle \Phi, H_0 \Phi \rangle + \|\Phi\|^2)^{1/2} \\
&\quad + c_2'(e)(\langle \Psi, H_0 \Psi \rangle + \|\Psi\|^2)^{1/2} (\langle \Phi, H_0 \Phi \rangle + \|\Phi\|^2)^{1/2} \\
&\leq c_2''(e)(\langle \Psi, H_0 \Psi \rangle + \|\Psi\|^2)^{1/2} (\langle \Phi, H_0 \Phi \rangle + \|\Phi\|^2)^{1/2},
\end{aligned} \tag{2.101}$$

where $c_2''(e) \to 0$ for $e \to 0$.

Now suppose that $\Psi, \Phi \in D(\overline{H}_0)$. This means that $(\Phi, \overline{H}_0 \Phi) \in \text{Gr}(\overline{H}_0) = \overline{\text{Gr}(H_0)}$ so there is a sequence of $\Phi_n \in D(H_0) = D(p^2) \otimes \Gamma_{\text{fin}}(D(\omega))$ s.t. $(\Phi_n, H_0 \Phi_n) \to (\Phi, \overline{H}_0 \Phi)$ and similarly for Ψ. In other words:

$$\Phi_n \to \Phi, \quad H_0 \Phi_n \to \overline{H_0} \Phi, \tag{2.102}$$

$$\Psi_n \to \Psi, \quad H_0 \Psi_n \to \overline{H_0} \Psi. \tag{2.103}$$

We can define the quadratic form β on $D(\overline{H}_0) \times D(\overline{H}_0)$ by the formula

$$\beta(\Psi, \Phi) := \lim_{n \to \infty} \langle \Psi_n, H_1 \Phi_n \rangle. \tag{2.104}$$

We check that the limit exists[10] using the Cauchy criterion and the bound (2.101):

$$|\langle \Psi_{n_1}, H_1 \Phi_{n_1}\rangle - \langle \Psi_{n_2}, H_1 \Phi_{n_2}\rangle| \le |\langle (\Psi_{n_1} - \Psi_{n_2}), H_1 \Phi_{n_1}\rangle| + |\langle \Psi_{n_2}, H_1(\Phi_{n_1} - \Phi_{n_2})\rangle| \tag{2.105}$$

It suffices to consider one of the two terms: By (2.101), (2.102), (2.103) we have

$$\begin{aligned} |\langle (\Psi_{n_1} - \Psi_{n_2}), H_1 \Phi_{n_1}\rangle| \le c_2''(e)\big(\langle (\Psi_{n_1} - \Psi_{n_2}), H_0(\Psi_{n_1} - \Psi_{n_2})\rangle + \|\Psi_{n_1} - \Psi_{n_2}\|^2\big)^{1/2} \\ \times \big(\langle \Phi_{n_1}, H_0 \Phi_{n_1}\rangle + \|\Phi_{n_1}\|^2\big)^{1/2} \to 0. \end{aligned} \tag{2.106}$$

Now we check that the bound (2.101) extends to $D(\overline{H}_0) \times D(\overline{H}_0)$: We have

$$\begin{aligned} |\beta(\Psi, \Phi)| &= \lim_{n\to\infty} |\langle \Psi_n, H_1 \Phi_n\rangle| \\ &\le \lim_{n\to\infty} c_2''(e)(\langle \Psi_n, H_0 \Psi_n\rangle + \|\Psi_n\|^2)^{1/2}(\langle \Phi_n, H_0 \Phi_n\rangle + \|\Phi_n\|^2)^{1/2} \\ &= c_2''(e)(\langle \Psi, \overline{H}_0 \Psi\rangle + \|\Psi\|^2)^{1/2}(\langle \Phi, \overline{H}_0 \Phi\rangle + \|\Phi\|^2)^{1/2}. \end{aligned} \tag{2.107}$$

Finally, we extend β to $\Psi, \Phi \in D(\overline{H}_0^{1/2})$: Let $\Psi_n := \chi(\overline{H}_0 \le n)\Psi$, $\Phi_n := \chi(\overline{H}_0 \le n)\Phi$. We set

$$\beta(\Psi, \Phi) := \lim_{n\to\infty} \beta(\Psi_n, \Phi_n). \tag{2.108}$$

We check the Cauchy criterion and make use of the bound (2.107). For $n_2 \ge n_1$

$$|\beta(\Psi_{n_1}, \Phi_{n_1}) - \beta(\Psi_{n_2}, \Phi_{n_2})| \le |\beta(\Psi_{n_2} - \Psi_{n_1}, \Phi_{n_1})| + |\beta(\Psi_{n_2}, \Phi_{n_2} - \Phi_{n_1})|. \tag{2.109}$$

It suffices to consider one of these terms. We have by (2.107)

$$\begin{aligned} |\beta(\Psi_{n_2} - \Psi_{n_1}, \Phi_{n_1})| \le\ & c_2''(e)\big(\langle (\Psi_{n_2} - \Psi_{n_1}), \overline{H}_0(\Psi_{n_2} - \Psi_{n_1})\rangle + \|\Psi_{n_2} - \Psi_{n_1}\|^2\big)^{1/2} \\ & \times(\langle \Phi_{n_1}, \overline{H}_0 \Phi_{n_1}\rangle + \|\Phi_{n_1}\|^2)^{1/2}. \end{aligned} \tag{2.110}$$

We note that $\Psi_{n_2} - \Psi_{n_1} = \chi(n_1 < \overline{H}_0 \le n_2)\Psi$. Now we have by the spectral theorem:

$$\begin{aligned} \langle (\Psi_{n_2} - \Psi_{n_1}), \overline{H}_0(\Psi_{n_2} - \Psi_{n_1})\rangle &= \int \lambda\, \chi(n_1 < \lambda \le n_2)\langle \Psi, dE(\lambda)\Psi\rangle \\ &\le \int \lambda\, \chi(n_1 < \lambda)\langle \Psi, dE(\lambda)\Psi\rangle \to 0. \end{aligned} \tag{2.111}$$

where dE is the spectral measure of $\overline{H}_0$ and in the last step we used dominated convergence: For any fixed λ

$$\lim_{n_1\to\infty} \lambda\, \chi(n_1 < \lambda) = 0. \tag{2.112}$$

[10] One should also check that the resulting expression is a quadratic form and that it does not depend on the choice of the approximating sequences. We leave this part to the reader.

Moreover, $\lambda\,\chi(n_1 < \lambda) \leq \lambda$ and, since dE is supported on the spectrum of $\overline{H}_0$, which is a subset of $\mathbb{R}_+$, and $\Psi \in D(\overline{H}_0)$

$$\int \lambda\langle\Psi, dE(\lambda)\Psi\rangle = \langle\Psi, \overline{H}_0\Psi\rangle = \langle\overline{H}_0^{1/2}\Psi, \overline{H}_0^{1/2}\Psi\rangle < \infty, \tag{2.113}$$

By similar and simpler arguments we complete verification of the Cauchy criterion.

Finally we extend the bound (2.107) to $D(\overline{H}_0^{1/2}) \times D(\overline{H}_0^{1/2})$. We have

$$\begin{aligned} |\beta(\Psi,\Phi)| &:= \lim_{n\to\infty} |\beta(\Psi_n,\Phi_n)| \\ &\leq \lim_{n\to\infty} c_2''(e)(\langle\overline{H}_0^{1/2}\Psi, \chi(\overline{H}_0 \leq n)\overline{H}_0^{1/2}\Psi\rangle + \|\chi(\overline{H}_0 \leq n)\Psi\|^2)^{1/2} \\ &\quad \times(\langle\overline{H}_0^{1/2}\Phi, \chi(\overline{H}_0 \leq n)\overline{H}_0^{1/2}\Phi\rangle + \|\chi(\overline{H}_0 \leq n)\Phi\|^2)^{1/2} \\ &\leq c_2''(e)(\langle\Psi, \overline{H}_0\Psi\rangle + \|\Psi\|^2)^{1/2}(\langle\Phi, \overline{H}_0\Phi\rangle + \|\Phi\|^2)^{1/2}, \end{aligned} \tag{2.114}$$

where we made use of the spectral theorem and the fact that $\Psi, \Phi \in D(\overline{H}_0^{1/2})$. $\Box$

From Lemma 2.17, Lemma 2.8 and the KLMN theorem we obtain:

Theorem 2.19. *For $|e| > 0$ sufficiently small and $\|\omega^{-\frac{1}{2}}f'\|_2, \|f'\|_2 < \infty$ there exists a unique self-adjoint operator H with $Q(H) = Q(\overline{H}_0)$ s.t.*

$$\langle\Phi, H\Psi\rangle = \langle\Phi, \overline{H}_0\Psi\rangle + \beta(\Phi,\Psi), \text{ for } \Phi, \Psi \in Q(\overline{H}_0) \tag{2.115}$$

and $\beta(\Phi,\Psi)$ extends the quadratic form $\langle\Phi, H_1\Psi\rangle$ as described in Lemma 2.17.

This theorem gives self-adjointness of the Pauli-Fierz Hamiltonian, but the information about domains is somewhat indirect. To improve on that, one verifies by more cumbersome analysis (we skip the details) that

$$\begin{aligned} \|H_1\Psi\| &\leq c_1(e)\|p\cdot A_{\perp,\varphi}(q)\Psi\| + c_2(e)\|A_{\perp,\varphi}(q)^2\Psi\|, \\ &\leq c_1(e)\|\overline{H}_0\Psi\| + c_2\|\Psi\| \end{aligned} \tag{2.116}$$

where $c_1(e) \to 0$ as $e \to 0$. This gives:

Theorem 2.20. *For $|e| > 0$ sufficiently small and $\|\omega^{-\frac{1}{2}}f'\|_2, \|f'\|_2 < \infty$ the operator $H = \overline{H_0} + H_1$ is self-adjoint on $D(\overline{H}_0)$.*

3 Elements of scattering theory

In this section we will give an overview of scattering theory for Pauli-Fierz Hamiltonians. In contrast to the previous section, we will not pay much attention to 'domain questions'. Nevertheless, ideas of some proofs will be given.

3.1 Total momentum operators and fiber Hamiltonians

The following lemma expresses translation-invariance of the Pauli-Fierz Hamiltonians.

Lemma 3.1. *The total momentum operators*

$$P := p \otimes 1 + 1 \otimes P_f, \quad P_f = \mathrm{d}\Gamma(k), \tag{3.1}$$

commute (strongly) with the Pauli-Fierz Hamiltonian.

Proof. We give only the computational part of the proof, which implies vanishing of a commutator on some 'nice' domain. For methods of improving this weak commutativity to strong commutativity (i.e. commutation of spectral measures) interested reader may consult [7].

Recall that $H = H_0 + H_1$, where

$$H_0 = \frac{1}{2m}(p^2 \otimes 1) + 1 \otimes \mathrm{d}\Gamma(\omega), \tag{3.2}$$

$$H_1 = -\frac{e}{m} p \cdot A_{\perp,\varphi}(q) + \frac{e^2}{2m} A_{\perp,\varphi}(q)^2. \tag{3.3}$$

We have $i[\mathrm{d}\Gamma(k), \mathrm{d}\Gamma(\omega)] = \mathrm{d}\Gamma([k, \omega]) = 0$. So it suffices to show that

$$[P, A_{\perp,\varphi}(q)] = 0. \tag{3.4}$$

Clearly, this follows from $e^{iP\cdot y} A_{\perp,\varphi}(q) e^{-iP\cdot y} = A_{\perp,\varphi}(q)$, which in turn is equivalent to

$$e^{ip\cdot y} A_{\perp,\varphi}(q) e^{-ip\cdot y} = e^{-iP_f\cdot y} A_{\perp,\varphi}(q) e^{iP_f\cdot y}. \tag{3.5}$$

We recall that for $f_q(k, \lambda) = \widehat{\varphi}(k)\sqrt{1/(2\omega(k))}e_\lambda(k)\mathrm{e}^{-ikq}$

$$\begin{aligned} A_{\perp,\varphi}(q) &= a(f_q) + a^*(f_q) && (3.6)\\ &= \sum_{\lambda=1,2} \int d^3k \, \frac{\widehat{\varphi}(k)}{\sqrt{2\omega(k)}} e_\lambda(k) \big(\mathrm{e}^{ik\cdot q} a(k, \lambda) + \mathrm{e}^{-ik\cdot q} a^*(k, \lambda)\big). && (3.7) \end{aligned}$$

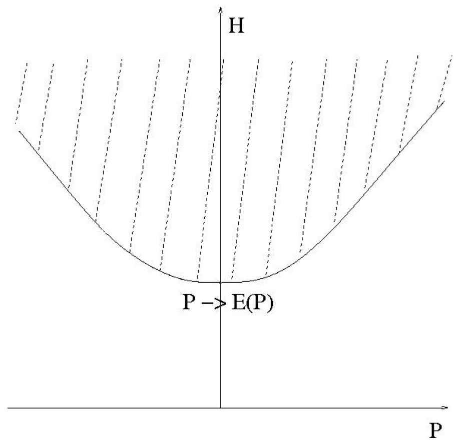
Clearly, $e^{ip\cdot y} q e^{-ip\cdot y} = q + y$. Therefore

$$\begin{aligned} &e^{ip\cdot y} A_{\perp,\varphi}(q) e^{-ip\cdot y} \\ &= \sum_{\lambda=1,2} \int d^3k \, \frac{\widehat{\varphi}(k)}{\sqrt{2\omega(k)}} e_\lambda(k) \big(\mathrm{e}^{ik\cdot q} e^{ik\cdot y} a(k, \lambda) + \mathrm{e}^{-ik\cdot q} e^{-ik\cdot y} a^*(k, \lambda)\big). \end{aligned} \tag{3.8}$$

Now consider

$$\begin{aligned} e^{-iP_f\cdot y} A_{\perp,\varphi}(q) e^{iP_f\cdot y} &= e^{-i\mathrm{d}\Gamma(k)\cdot y}(a(f_q) + a^*(f_q))e^{i\mathrm{d}\Gamma(k)\cdot y} = \Gamma(e^{-ik\cdot y})(a(f_q) + a^*(f_q))\Gamma(e^{ik\cdot y}) \\ &= a(e^{-ikq} f_q) + a^*(e^{-ikq} f_q) \end{aligned} \tag{3.9}$$

which proves (3.5), □



Thus we have a family of four commuting self-adjoint operators (H, P^1, P^2, P^3) and we draw their joint spectrum. For small values of the coupling constant e and for $H \leq \Sigma$, for some constant $\Sigma > \inf \sigma(H)$ its shape is, schematically depicted on the figure. Namely, the lower boundary of the spectrum $\xi \mapsto E(\xi)$ is a small perturbation of the non-interacting dispersion relation $\xi \to \xi^2/(2m)$ [8]. The restriction to energies less that Σ is needed to ensure that the electron moves slower than photons. For higher energies other interesting effects arrise, e.g. Cherenkov radiation, which are outside the scope of these notes.

For a more detailed discussion of this spectrum it is convenient to introduce the fiber Hamiltonians:

Proposition 3.2. *The Pauli-Fierz Hamiltonian*

$$H = \frac{1}{2m}(p - eA_{\perp,\varphi}(q))^2 + H_f \tag{3.10}$$

has the following direct integral representation

$$H = V^* \int^{\oplus} d^3\xi \, H(\xi)V, \quad H(\xi) = \frac{1}{2m}(\xi - P_f - eA_{\perp,\varphi})^2 + H_f, \tag{3.11}$$

where the 'fiber Hamiltonians' $H(\xi)$ are self-adjoint operators on (a domain in) $\mathcal{F}$, $A_{\perp,\varphi} := A_{\perp,\varphi}(0)$ and the unitary

$$V : \left(L^2(\mathbb{R}^3_{(q)}) \otimes \mathcal{F} \simeq L^2(\mathbb{R}^3_{(q)}; \mathcal{F})\right) \to \left(L^2(\mathbb{R}^3_{(\xi)}; \mathcal{F}) \simeq \int^{\oplus} d^3\xi \, \Gamma(\mathfrak{h})\right) \tag{3.12}$$

is given by $V = Fe^{iP_f \cdot q}$, where F is the Fourier transform in variables (ξ, q), that is

$$(Ff)(\xi) = (2\pi)^{-3/2} \int e^{-i\xi \cdot q} f(q) d^3q. \tag{3.13}$$

Proof. As a preliminary computation, let us first consider a general expression $\{G(-i\nabla_q)\}_{q\in\mathbb{R}^3}$, which is understood as an operator on $L^2(\mathbb{R}^3_{(q)};\mathcal{F})$. Then, by the properties of the Fourier transform we have

$$F\{G(-i\nabla_q)\}_{q\in\mathbb{R}^3}F^* = \{G(\xi)\}_{\xi\in\mathbb{R}^3} = \int^{\oplus} d^3\xi\, G(\xi). \tag{3.14}$$

As a second preliminary computation, we write

$$\begin{aligned} \mathrm{e}^{iP_f\cdot q}p\mathrm{e}^{-iP_f\cdot q} &= \mathrm{e}^{iP_f\cdot q}(-i\nabla_q)\mathrm{e}^{-iP_f\cdot q} \\ &= \mathrm{e}^{iP_f\cdot q}\mathrm{e}^{-iP_f\cdot q}(-i)^2P_f + \mathrm{e}^{iP_f\cdot q}\mathrm{e}^{-iP_f\cdot q}(-i\nabla_q) = p - P_f. \end{aligned} \tag{3.15}$$

As a third preliminary computation we obtain from (3.9) that

$$\begin{aligned} \mathrm{e}^{iP_f\cdot q}A_{\perp,\varphi}(q)\mathrm{e}^{-iP_f\cdot q} &= \mathrm{e}^{iP_f\cdot q}(a^*(e^{-ikq}f) + a(e^{-ikq}f))\mathrm{e}^{-iP_f\cdot q} \\ &= a^*(f) + a(f) = A_{\perp,\varphi}(0), \end{aligned} \tag{3.16}$$

where we decomposed $f_q = e^{-ikq}f$. From the three observations above we obtain

$$\begin{aligned} V(p - A_{\perp,\varphi}(q))V^* &= F(p - P_f - A_{\perp,\varphi})F^* = \{(\xi - P_f - A_{\perp,\varphi})\}_{\xi\in\mathbb{R}^3} \\ &= \int^{\oplus} d^3\xi\,(\xi - P_f - A_{\perp,\varphi}), \end{aligned} \tag{3.17}$$

and analogous result holds for $(p - A_{\perp,\varphi}(q))^2$. Also, since $[H_f, P_f] = 0$,

$$VH_fV^* = F(\{H_f\}_{q\in\mathbb{R}^3})F^* = \{H_f\}_{\xi\in\mathbb{R}^3} = \int^{\oplus} d\xi\, H_f, \tag{3.18}$$

which concludes the proof. □

3.2 Conventional scattering theory and its limitations

We denoted the lower boundary of the joint spectrum of the energy-momentum operators by $\xi \to E(\xi)$. Since the lower boundary of the spectrum corresponds to configurations of the system of lowest possible energy, this quantity is in fact the dispersion relation (energy-momentum relation) of the 'physical massive particle[11]' (as opposed to the 'bare massive-particle' whose dispersion relation is $\xi \to \xi^2/(2m)$). With the help of the fiber Hamiltonians we can write

$$E(\xi) = \inf\, \sigma(H(\xi)). \tag{3.19}$$

A decisive question for scattering theory is whether $E(\xi)$ is an eigenvalue or not (for sufficiently many ξ).

If this is the case, then, denoting by ψ_ξ the corresponding normalized eigenvector of $H(\xi)$, we can form wave-packets

$$\psi_g = V^* \int^{\oplus} d^3\xi\, g(\xi)\psi_\xi \in L^2(\mathbb{R}^3) \otimes \mathcal{F}, \tag{3.20}$$

[11] I deliberately avoid the term 'electron' here as it suggests non-zero electric charge. See below.

for square-integrable g supported in $E(\xi) \leq \Sigma$. Such vectors (in the defining Hilbert space of the model) describe a propagating massive particle in empty space (that is just massive particle and no photons). It is easy to see that it satisfies

$$e^{-itH}\psi_g = e^{-itE(P)}\psi_g, \tag{3.21}$$

where $E(P)$ is the function $\xi \to E(\xi)$ of the momentum operator. We call the subspace of all such vectors $\mathcal{H}_{\mathrm{sp}} \subset \chi(H \leq \Sigma)\mathcal{H}$.

Unfortunately, $\mathcal{H}_{\mathrm{sp}} = \{0\}$ for electrically charged particles This fact is known as the **infraparticle problem**, and was shown in non-relativistic QED in [10].To be more precise, recall that the interaction

$$A_{\perp,\varphi}(q) = a^*(f_q) + a(f_q) \tag{3.22}$$

involves $f_q(k,\lambda) = \widehat{\varphi}(k)\sqrt{1/(2\omega(k))}e_\lambda(k)\mathrm{e}^{-ikq}$ and φ has the interpretation of the charge distribution of the particle. So the total charge of the particle is given by

$$Q = \int d^3x\, \varphi(x) = (2\pi)^{3/2}\widehat{\varphi}(0) \tag{3.23}$$

and $\widehat{\varphi}(0) \neq 0$ implies that $E(\xi)$ is not an eigenvalue whenever $\nabla E(\xi) \neq 0$ [10]. This result has a partial converse, namely if $\widehat{\varphi}(k) \sim |k|^\delta$ near zero for some $\delta > 0$ one can show that $\mathcal{H}_{\mathrm{sp}} \neq \{0\}$ [8]. This is the situation in which conventional scattering theory, described below, can be applied. It covers electrically neutral particles, as for example a small dipole, hydrogen atom in its ground state etc. For charged particles more complicated infraparticle scattering theory is available [9] but will not be discussed here.

To construct states describing incoming and outgoing configurations of the massive particle and photons, we need the concept of asymptotic creation and annihilation operators:

Lemma 3.3. *[16] For $\psi \in \chi(H \leq \Sigma)\mathcal{H}$ the following limits exist*

$$a_+^{(*)}(h)\psi = \lim_{t\to\infty} e^{itH}a^{(*)}(e^{-it|k|}h)e^{-itH}\psi \tag{3.24}$$

and are called the asymptotic (outgoing) creation and annihilation operators. They satisfy

$$[a_+(h_1), a_+^*(h_2)] = \langle h_1, h_2\rangle, \tag{3.25}$$

$$a_+(h)\psi_g = 0, \tag{3.26}$$

for vectors $\psi_g \in \mathcal{H}_{\mathrm{sp}}$. The incoming creation and anninhilation operators $a_-^{(*)}(h)$ are defined analogously by taking the limit $t \to \infty$ in (3.24)

Given this, scattering states describing one massive particle and n photons are defined as follows

$$\Psi_{n,g}^+ = a_+^*(h_1)\dots a_+^*(h_n)\psi_g. \tag{3.27}$$

Due to properties (3.25), (3.26), the scalar product of two such vectors is analogous as for the corresponding vectors from $\mathcal{F} \otimes \mathcal{H}_{\mathrm{sp}}$:

$$\langle \Psi'^{+}_{n',g'}, \Psi^{+}_{n,g} \rangle = \delta_{n,n'} \langle \Psi_{g'}, \Psi_{g} \rangle \sum_{\sigma \in S_n} \langle h'_1, h_{\sigma(1)} \rangle \dots \langle h'_n, h_{\sigma(n)} \rangle, \tag{3.28}$$

therefore they can be interpreted as asymptotic configurations of independent particles.

Of course incoming scattering states Ψ^- are defined analogously and one can define scattering matrix elements $\langle \Psi^+, \Psi'^- \rangle$, and transition probabilities $|\langle \Psi^+, \Psi'^- \rangle|^2$ of physical processes.

The problem of **asymptotic completeness** is the question if scattering states of the form (3.27) span the entire subspace $\chi(H \leq \Sigma)\mathcal{H}$. In spite of some progress [11–15], this problem is largely open to date, especially for models with massless photons (as the one we study). Important fact for the study of asymptotic completeness is the existence of a closed-form formula for the wave-operator[12], whose range is spanned by the scattering states (3.27). Let us recall the construction [17].

Define the extended Fock space $\Gamma^{\mathrm{ex}}(\mathfrak{h}) = \Gamma(\mathfrak{h}) \otimes \Gamma(\mathfrak{h})$. Let $U : \Gamma(\mathfrak{h} \oplus \mathfrak{h}) \to \Gamma(\mathfrak{h}) \otimes \Gamma(\mathfrak{h})$ be the canonical identification given by

$$U a^*(h) = (a^*(h) \otimes 1 + 1 \otimes a^*(h))U, \quad U\Omega = \Omega \otimes \Omega. \tag{3.29}$$

Let c_0, c_∞ be operators on $\mathfrak{h}$ and define $c : \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h}$ which acts by $ch = (c_0 h, c_\infty h)$. Then

$$\check{\Gamma}(c) := U\Gamma(c) \tag{3.30}$$

is a mapping $\Gamma(\mathfrak{h}) \to \Gamma^{\mathrm{ex}}(\mathfrak{h})$. Note that $\Gamma(c) : \Gamma(\mathfrak{h}) \to \Gamma(\mathfrak{h} \oplus \mathfrak{h})$, acting by

$$\Gamma(c)|_{\Gamma^{(n)}(\mathfrak{h})} = c \otimes \dots \otimes c, \tag{3.31}$$

is a generalization of the map introduced before in the context of second quantization.

Now define the extended Hilbert space

$$\mathcal{H}^{\mathrm{ex}} = \mathcal{H} \otimes \Gamma(\mathfrak{h}) = L^2(\mathbb{R}^3) \otimes \Gamma(\mathfrak{h}) \otimes \Gamma(\mathfrak{h}) \tag{3.32}$$

and the extended Hamiltonian

$$H^{\mathrm{ex}} = H \otimes 1 + 1 \otimes H_f. \tag{3.33}$$

We define a tentative wave operator $\widetilde{W}^+ : \mathcal{H}^{\mathrm{ex}} \to \mathcal{H}$,

$$\widetilde{W}^+ := \lim_{t \to \infty} e^{itH} \check{\Gamma}(1,1)^* e^{-itH^{\mathrm{ex}}} \chi(H^{\mathrm{ex}} \leq \Sigma), \tag{3.34}$$

[12]Recall that in quantum mechanics $H = -\Delta + V(x)$, $H_0 = -\Delta$ and the wave-operator is $W_+ = \lim_{t\to\infty} e^{iHt} e^{-iH_0 t}$

where $\check{\Gamma}(1,1)^*$ is naturally extended from $\Gamma^{\mathrm{ex}}(\mathfrak{h})$ to $\mathcal{H}^{\mathrm{ex}}$. It is easy to see that the existence of the limit follows from Lemma 3.3. The actual wave operator is given by

$$W^+ := \widetilde{W}^+ \restriction (\mathcal{H}_{\mathrm{sp}} \otimes \Gamma(\mathfrak{h})) \tag{3.35}$$

and it is easy to see that vectors from the range of this operator are scattering states of the form (3.27).

In the language of the wave operators, the problem of asymptotic completeness amounts to invertibility of W^+. But it is easy to find a candidate for this inverse, namely

$$M^+ := \lim_{t\to\infty} e^{itH^{\mathrm{ex}}} \check{\Gamma}(c_{0,t}, c_{1,t}) e^{-itH} \chi(H \leq \Sigma), \tag{3.36}$$

where $c_{0,t} + c_{\infty,t} = 1$ and apart from this can be arbitrary[13]. Then, if M^+ exists and maps into the domain of W^+, we can write for any $\psi \in \operatorname{Ran} \chi(H \leq \Sigma)$

$$W^+ M^+ \psi = \lim_{t\to\infty} e^{itH} \check{\Gamma}(1,1)^* e^{-itH^{\mathrm{ex}}} e^{itH^{\mathrm{ex}}} \check{\Gamma}(q_{0,t}, q_{1,t}) e^{-itH} \psi = \psi, \tag{3.37}$$

since $\check{\Gamma}(1,1)^* \check{\Gamma}(q_{0,t}, q_{1,t}) = \Gamma(1,1)^* \Gamma(q_{0,t}, q_{1,t}) = 1$. Therefore any such ψ is in the range of the wave-operator and therefore a scattering state. Thus we could reduce the problem of density of scattering states (which does not look very tractable) to the problem of existence of the limit in (3.36) (which is still difficult, but much more concrete). One difficulty with proving asymptotic completeness in relativistic (algebraic) QFT is the absence of such a closed-form formula for the wave operator. The above considerations suggest that the split property should be relevant in this context [18].

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[13] Common choices are $c_{0,t} = c_0((x-y)/t)$, $c_{\infty,t} = c_\infty((x-y)/t)$, where $x-y$ is the relative distance between the massive particle and the photon, and c_0 is an approximate characteristic function of a neighbourhood of zero. Then the role of $\check{\Gamma}(c_{0,t}, c_{1,t})$ is to cut a given physical state into two pieces: First $(c_{0,t})$ where the relative velocity between the massive particle and the photon is small. This piece is put on the first factor of the extended Hilbert space $\mathcal{H} \otimes \Gamma(\mathfrak{h})$ and contributes to the wave packet of the physical particle. Second (c_∞), where the relative velocity between the massive particle and the photon is large. This is put on the second factor of $\mathcal{H} \otimes \Gamma(\mathfrak{h})$ and contributes to freely propagating photons.

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