Notes on Bound-State QED

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Based on notes 1987-91
Latex version (C/Dok/QED/Bound8791)
March 10, 2003
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Chapter 1

Semiclassical theory of radiation

1.1 Classical electrodynamics

1.1.1 Maxwell’s equations in covariant form

The Maxwell’s equations in vector form are\(^1\)

\[
\nabla \cdot \mathbf{E} = \rho / \varepsilon_0 \quad (1.1a) \quad \text{(Maxw.a)}
\]
\[
\nabla \times \mathbf{B} = \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{j} \quad (1.1b) \quad \text{(Maxw.b)}
\]
\[
\nabla \cdot \mathbf{B} = 0 \quad (1.1c) \quad \text{(Maxw.c)}
\]
\[
\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \quad (1.1d) \quad \text{(Maxw.d)}
\]

\(\rho\) is the electric charge density and \(\mathbf{j}\) the electric current density. (1.1c) gives

\[
\mathbf{B} = \nabla \times \mathbf{A},
\]

where \(\mathbf{A}\) is the vector potential. (1.1d) gives

\[
\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla \phi,
\]

where \(\phi\) is the scalar potential. (1.1a) and (1.1b) give together with (1.3) and (1.2)

\[
-\nabla^2 \phi - \frac{\partial}{\partial t} \nabla \cdot \mathbf{A} = \rho / \varepsilon_0 = \mu_0 j^0,
\]

\[
\left( \nabla^2 \mathbf{A} - \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} \right) - \nabla \left( \nabla \cdot \mathbf{A} + \frac{1}{c^2} \frac{\partial \phi}{\partial t} \right) = -\mu_0 \mathbf{j},
\]

using \(\nabla \times (\nabla \times \mathbf{A}) = \nabla (\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}\). \(j^0 = c^2 \rho\) (with \(\varepsilon_0 \mu_0 = c^{-2}\)) is the scalar or ‘time-like’ part of the four-dimensional current

\[
\mathbf{j} = j^\mu = (c^2 \rho, \mathbf{j}),
\]

\(^1\)The formulas are here given for use in a consistent unit system, like the SI system (see Appendix \(\text{ch:DimAnal}\)). Note that equations for use in a mixed system, like the Gaussian (c.g.s) unit system, used in many books, like in [1, Sect.1.2], will look differently.
where the vector part is the three-dimensional current \( j \). Similarly, the four-dimensional vector potential

\[
A = A^\mu = (\phi/c, A)
\]

has the scalar part \( \phi/c \) and the vector part \( A \). With the d’Alambertian operator, these equations can be expressed

\[
\Box \phi - \frac{\partial}{\partial t} (\nabla A) = \mu_0 j^0
\]

\[
\Box A + \nabla (\nabla A) = \mu_0 \vec{j},
\]

which leads to Maxwell’s equations in covariant form

\[
\Box A - \nabla (\nabla A) = \mu_0 \vec{j}
\]

or

\[
A^\mu - \partial^\mu (\partial^\nu A^\nu) = \mu_0 j^\mu.
\]

**Lorentz condition**

\[
\nabla A = \partial_\mu A^\mu = \nabla \cdot A + \frac{1}{c^2} \frac{\partial \phi}{\partial t} = 0
\]

\[
\Box A = \mu_0 \vec{j}
\]

\[
\nabla j = \partial_\mu j^\mu = 0
\]

**Continuity equation**

Operate on Maxwells’ equations \((1.7)\) with \(\nabla\):

\[
\nabla (\Box A) - \nabla \nabla (\nabla A) = \mu_0 \nabla j.
\]

Since \(\Box = \nabla^2\) and \(\nabla\) commute, this leads to the continuity equation

\[
\nabla j = \partial_\mu j^\mu = 0
\]

**Gauge invariance**

\(\text{Gauge transformation: } A \Rightarrow A + \nabla \Lambda \quad \Lambda \text{ scalar.}\)

Insert in \((1.7)\):

\[
\Box (\nabla \Lambda) - \nabla (\nabla \nabla \Lambda) = \Box (\nabla \Lambda) - \nabla (\Box \Lambda) = 0
\]

Maxwells’s equations are gauge invariant.

\(^2\text{Concerning covariant notations, see Appendix A.}\)
1.1.2 Interaction between electron and e-m field

The relativistic interaction between an electron of charge $-e$ and the electromagnetic field is

$$H_{\text{int}} = ec\alpha \cdot A - e\phi \quad (1.11)$$

or in covariant notations

$$H_{\text{int}} = -ec\alpha A = -ec\alpha_\mu A^\mu. \quad (1.12)$$

1.1.3 The Coulomb gauge

Transverse and longitudinal field components

The vector part of the electromagnetic field can be separated into transverse (divergence-free) and longitudinal (rotation-free) components

$$A = A_\perp + A_\parallel; \quad \nabla \cdot A_\perp = 0; \quad \nabla \times A_\parallel = 0. \quad (1.13)$$

The electric field can be similarly separated

$$E = E_\perp + E_\parallel; \quad E_\perp = -\frac{\partial A_\perp}{\partial t}; \quad E_\parallel = -\frac{\partial A_\parallel}{\partial t} - \nabla \phi,$$

while the magnetic field has only transverse components due to (1.2). The separated field equations (1.14) then become

$$\nabla^2 \phi + \frac{\partial}{\partial t} \nabla \cdot A_\parallel = -\rho/\varepsilon_0 \quad (1.14a)$$

$$\left( \nabla^2 A_\parallel - \frac{1}{c^2} \frac{\partial^2 A_\parallel}{\partial t^2} \right) - \nabla \left( \nabla \cdot A_\parallel + \frac{1}{c^2} \frac{\partial \phi}{\partial t} \right) = -\mu_0 j_\parallel \quad (1.14b)$$

$$\left( \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) A_\perp = -\mu_0 j_\perp. \quad (1.14c)$$

The longitudinal and the scalar or ‘time-like’ components ($A_\parallel, \phi$) represent the instantaneous Coulomb interaction and the transverse components ($A_\perp$) represent retardation of this interaction and all magnetic interactions, as well as the electromagnetic radiation field (see section 1.2.4).

The energy of the electromagnetic field is given by

$$E_{\text{rad}} = \frac{1}{2} \int d^3x \left[ \frac{1}{\mu_0} |B|^2 + \varepsilon_0 |E|^2 \right]$$

$$= \frac{1}{2} \int d^3x \left[ \frac{1}{\mu_0} |B|^2 + \varepsilon_0 |E_\perp|^2 \right] + \frac{1}{2} \int d^3x \varepsilon_0 |E_\parallel|^2. \quad (1.15)$$

The last term represents the energy of the instantaneous Coulomb field, which is normally already included in the Hamiltonian of the system. The first term represents the radiation energy.
Semiclassically, only the transverse part of the field is quantized, while the longitudinal part is treated classically [2, Ch. 2,3]. It should be noted that the separation into transverse and longitudinal components is not Lorentz invariant and therefore not physically justified, when relativity is taken into account. The retardation of the Coulomb interaction is represented by the transverse component (sec. 1.2.4), and therefore only the combination of transverse and longitudinal components has physical significance.

In a fully covariant treatment also the longitudinal component is quantized. The field is then represented by virtual photons with four directions of polarizations. A real photon can only have transverse polarizations.

In the Coulomb gauge we have
\[ \nabla \cdot A = 0, \]  
also known as the transversality condition. In this gauge there is no longitudinal component of \( A \), and Maxwell’s equations then reduce to
\[ \nabla^2 \phi = -\rho/\varepsilon_0. \]  
This has the solution
\[ \phi(x) = \frac{1}{4\pi\varepsilon_0} \int \frac{d^3r'}{|x-x'|} \rho(x'), \]
which is the instantaneous Coulomb interaction.

In free space the scalar potential \( \phi \) can be eliminated by a gauge transformation. Then the Lorentz condition (1.8) is automatically fulfilled in the Coulomb gauge. The field equation (1.4) then becomes
\[ \nabla^2 A - \frac{1}{c^2} \frac{\partial^2 A}{\partial t^2} = 0. \]

The relativistic interaction with an atomic electron (1.11) is in the Coulomb gage given by
\[ H_{\text{int}} = e c \alpha \cdot A_\perp \]  
and in second quantization
\[ H_{\text{int}} = \sum_{ij} c_j^\dagger \langle i|e c \alpha \cdot A_\perp |j\rangle c_j, \]
where \( c^\dagger, c \) represent creation/annihilation operators for electrons. In the interaction picture this becomes
\[ H_{\text{int},I}(t) = \sum_{ij} c_j^\dagger \langle i|e c \alpha \cdot A_\perp |j\rangle c_j e^{i(\varepsilon_i-\varepsilon_j)t/\hbar}. \]

1.2 The quantized radiation field

1.2.1 The transverse radiation field

Classically a radiation field can be represented by the vector potential [2, Eq. 2.14]
\[ A(x,t) = \sum_{k} \sum_{p=1}^{2} \left[ c_{kp} \varepsilon_p e^{i(kx-\omega t)} + c_{kp}^* \varepsilon_p e^{-i(kx-\omega t)} \right], \]
where $k$ is the wave vector, $\omega = c|k|$ the frequency, and $c_{kp} / c_{kp}^*$ represent the amplitude of the wave with the a certain $k$ vector and a certain polarization $\varepsilon_p$. The energy of this radiation can be shown to be equal to \[ E_{rad} = \varepsilon_0 \sum_{kp} \omega^2 c_{kp}^* c_{kp} = \varepsilon_0 \sum_{kp} \omega^2 (c_{kp}^* c_{kp} + c_{kp}^* c_{kp}^*) \] (1.24) 

By making the substitution

$$ c_{kp} \rightarrow \sqrt{\frac{\hbar}{2\varepsilon_0 \omega V}} a_{kp} \quad \text{and} \quad c_{kp}^* \rightarrow \sqrt{\frac{\hbar}{2\varepsilon_0 \omega V}} a_{kp}^*, $$

where $a_{kp}^*$, $a_{kp}$ are photon creation/annihilation operators, the radiation energy goes over into the Hamiltonian of a collection of harmonic oscillators

$$ H_{\text{harm, osc}} = \frac{1}{2} \sum_{kp} \hbar \omega (a_{kp} a_{kp}^* + a_{kp}^* a_{kp}). $$

Therefore, we can motivate that the quantized transverse radiation field can be represented by \[ A_{\perp}(x,t) = \sum_k \sqrt{\frac{\hbar}{2\varepsilon_0 \omega V}} \sum_{p=1}^2 \left[ a_{kp} \varepsilon_p e^{i(k \cdot x - \omega t)} + a_{kp}^* \varepsilon_p e^{-i(k \cdot x - \omega t)} \right] \] (1.25) 

### 1.2.2 The Breit interaction

\[ \text{Figure 1.1: Diagrammatic representation of the exchange of a single, transverse photon between two electrons (left). This is equivalent to a potential (Breit) interaction (right).} \]

The exchange of a single transverse photon between two electrons is illustrated by the time-ordered diagram (left) in Fig. 1.1, where one photon is emitted at the time $t_1$ and absorbed at a later time $t_2$. The second-order evolution operator for this process is given by

$$ U_{\gamma}^{(2)}(0, -\infty) = \left( \frac{-i}{\hbar} \right)^2 \int_{-\infty}^{0} dt_2 H_{\text{int},1}(t_2) \int_{-\infty}^{t_2} dt_1 H_{\text{int},1}(t_1) e^{\gamma (t_1 + t_2)} \quad (t_1 < t_2), $$

(1.26) 

where $\gamma$ is the parameter for the adiabatic damping of the perturbation. The interaction hamiltonians are in the Coulomb gauge given by (1.22) with the vector potential (1.25)

$$ H_{\text{int},1}(t_1) = \sum_{k_1} \sqrt{\frac{\hbar}{2\varepsilon_0 \omega_1 V}} \sum_{p_1=1}^2 c_{kp_1}^\dagger \langle \mathbf{r} | (a_{kp_1} e^{-i\mathbf{k} \cdot \mathbf{x}} e^{-i\epsilon_1} (\alpha \varepsilon_{kp} e^{-i\mathbf{k} \cdot \mathbf{x}})_{p_1=1} | a_{\mathbf{k} \cdot \mathbf{x}} e^{-i\gamma (t_1 - \mathbf{e}_1 \cdot \mathbf{x} )} / \hbar $$

\[ H_{\text{int},1}(t_2) = \sum_{k_2} \sqrt{\frac{\hbar}{2\varepsilon_0 \omega_2 V}} \sum_{p_2=1}^2 c_{kp_2}^\dagger \langle \mathbf{r} | (a_{kp_2} e^{-i\mathbf{k} \cdot \mathbf{x}} e^{-i\epsilon_2} (\alpha \varepsilon_{kp} e^{i\mathbf{k} \cdot \mathbf{x}})_{p_2=1} | a_{\mathbf{k} \cdot \mathbf{x}} e^{-i\gamma (t_2 - \mathbf{e}_2 \cdot \mathbf{x} + \hbar \omega_2)/\hbar}, \] (1.27) 

\[ \text{Hint1} \]
which leads to the evolution operator

\[
U_1^{(2)}(0, -\infty) = -c_1^\dagger c_ag c_b \sum_k e^2 e^2 \frac{e_{2}^2}{2\hbar \varepsilon_{0} V / \omega_1 \omega_2} \times \sum_{p_1 p_2} \langle rs | (a_{kp} \varepsilon_p e^{i k \cdot r_2})_2 (a_{kp}^\dagger \varepsilon_p e^{-i k \cdot r})_1 | ab \rangle \times I, \tag{1.28} \]

where \( I \) is the time integral. The contraction between the creation and annihilation operators (2.2) yields \((\omega = \omega_1 = \omega_2)\)

\[
\sum_{p_1 p_2} \langle rs | (a_{kp} \varepsilon_p e^{i k \cdot r_2})_2 (a_{kp}^\dagger \varepsilon_p e^{-i k \cdot r})_1 | ab \rangle = \sum_{p=1}^2 \langle rs | (\alpha \cdot \varepsilon_p)_2 (\alpha \cdot \varepsilon_p)_1 e^{-i k \cdot r_{12}} \rangle \tag{1.29} \]

The time integral in (1.28) is

\[
I = \int_{-\infty}^{t_2} dt_2 e^{-i H_2 (\varepsilon_b \varepsilon_r + \varepsilon_s \varepsilon_s + i \gamma)} / h \int_{-\infty}^{t_1} dt_1 e^{-i H_1 (\varepsilon_a \varepsilon_r - \hbar \omega + i \gamma)} / h \tag{1.30} \]

The result of the opposite time ordering \( t_1 > t_2 \) is obtained by the exchange \( 1 \leftrightarrow 2 \) \((\mathbf{r}_{12} \leftrightarrow -\mathbf{r}_{12})\), \( a \leftrightarrow b \), and \( r \leftrightarrow s \), and the total evolution operator, including both time-orderings, can be expressed

\[
U_1^{(2)}(0, -\infty) = c_1^\dagger c_ag c_b \sum_k e^2 e^2 \varepsilon_0 V \sum_{p=1}^2 \langle rs | (\alpha \cdot \varepsilon_p)_1 (\alpha \cdot \varepsilon_p)_2 M | ab \rangle \tag{1.31} \]

with

\[
M = \frac{e^{-i k \cdot \mathbf{r}_{12}}}{(\varepsilon_a + \varepsilon_b - \varepsilon_r - \varepsilon_s + 2i \gamma)(\varepsilon_a - \varepsilon_r - \hbar \omega + i \gamma)}
+ \frac{e^{i k \cdot \mathbf{r}_{12}}}{(\varepsilon_a + \varepsilon_b - \varepsilon_r - \varepsilon_s + 2i \gamma)(\varepsilon_a - \varepsilon_r - \hbar \omega + i \gamma)}
+ \frac{\varepsilon_a - \varepsilon_r - \varepsilon_a + \varepsilon_s}{(\varepsilon_a + \varepsilon_b - \varepsilon_r - \varepsilon_s + 2i \gamma)(\varepsilon_a - \varepsilon_r - \hbar \omega + i \gamma)}.
\tag{1.32} \]

This can be compared with the evolution operator corresponding to a potential interaction \( B_{12} \) between the electrons, as illustrated in the right diagram of Fig. 1.1,

\[
U_1^{(2)}(0, -\infty) = c_1^\dagger c_ag c_b \langle rs | B_{12} | ab \rangle \left( \frac{-i}{\hbar} \right) \int_{-\infty}^{0} dt e^{-i (\varepsilon_a \varepsilon_b - \varepsilon_r - \varepsilon_s + i \eta)} / h \tag{1.33} \]

Identification then leads to

\[
B_{12} = \frac{e^2 e^2}{2\varepsilon_0 \omega V} \sum_{kp} (\alpha_\mathrm{p} \cdot \varepsilon_p)_1 (\alpha_\mathrm{p} \cdot \varepsilon_p)_2 \times \left[ \cos (k \cdot R_{12}) \frac{\varepsilon_a + \varepsilon_b - \varepsilon_r - \varepsilon_s - 2 \hbar \omega + 2i \gamma}{(\varepsilon_a - \varepsilon_r - \hbar \omega + i \gamma)(\varepsilon_b - \varepsilon_s - \hbar \omega - i \gamma)} \right.
+ \frac{i \sin (k \cdot R_{12})}{(\varepsilon_a - \varepsilon_r - \hbar \omega + i \gamma)(\varepsilon_b - \varepsilon_s - \hbar \omega - i \gamma)}. \tag{1.34} \]

\( B_{12} \)
We assume that energy is conserved by the interaction, i.e.,
\[ \varepsilon_a - \varepsilon_r = \varepsilon_s - \varepsilon_b = \hbar \omega. \] (1.35)

Then (1.34) becomes
\[ B_{12} = -\frac{e^2 \varepsilon_0}{2 \varepsilon_0 \omega V} \sum_{kp} (\alpha \cdot \varepsilon_p)(\alpha \cdot \varepsilon_p) \left( \cos \left( k \cdot r_{12} \right) \frac{2\omega}{(cq - \omega + i\gamma)(-cq - \omega + i\gamma)} - i\sin \left( k \cdot r_{12} \right) \frac{2cq}{(cq - \omega + i\gamma)(-cq - \omega + i\gamma)} \right) \]
or
\[ B_{12} = \frac{e^2}{\varepsilon_0 V} \sum_{kp} (\alpha \cdot \varepsilon_p)(\alpha \cdot \varepsilon_p) \cos \left( k \cdot r_{12} \right) - \frac{iq/k \sin \left( k \cdot r_{12} \right)}{q^2 - k^2 + i\gamma}. \] (1.36)
with \( \omega = ck. \) Since the contribution to the sum comes from \( k \approx \pm q, \) we can replace \( q/k \) by \( \text{sgn}(q). \) In addition, it is found that the sign of the imaginary part is immaterial (see Appendix F.1), and therefore we can replace the numerator by \( e^{ik \cdot r_{12}}, \)
\[ B_{12} = \frac{e^2}{\varepsilon_0 V} \sum_{kp} (\alpha \cdot \varepsilon_p)(\alpha \cdot \varepsilon_p) \frac{e^{ik \cdot r_{12}}}{q^2 - k^2 + i\gamma}. \] (1.37)

The \( \varepsilon_p \) vectors are orthogonal unit vectors, which leads to [Sak67, Eq. 4.312]
\[ \sum_{p=1}^{3} (\alpha \cdot \varepsilon_p)(\alpha \cdot \varepsilon_p) = \alpha_1 \cdot \alpha_2. \] (1.38)
This gives
\[ \sum_{p=1}^{2} (\alpha \cdot \varepsilon_p)(\alpha \cdot \varepsilon_p) = \alpha_1 \cdot \alpha_2 - (\alpha_1 \cdot \hat{k})(\alpha_2 \cdot \hat{k}), \] (1.39)
assuming \( \varepsilon_3 = \hat{k} \) to be the unit vector in the \( k \) direction. The interaction (1.37) then becomes in the limit of continuous momenta (App. B.4)
\[ B_{12} = \frac{e^2}{\varepsilon_0} \int \frac{d^3k}{(2\pi)^3} \left[ \alpha_1 \cdot \alpha_2 - (\alpha_1 \cdot \hat{k})(\alpha_2 \cdot \hat{k}) \right] \frac{e^{ik \cdot r_{12}}}{q^2 - k^2 + i\gamma}. \] (1.40)

With the fourier transforms in Appendix F, this yields the retarded Breit interaction
\[ B_{12}^{\text{Ret}} = -\frac{e^2}{4\pi \varepsilon_0} \left[ \alpha_1 \cdot \alpha_2 \frac{e^{i|q|r_{12}}}{r_{12}} - (\alpha_1 \cdot \nabla_1)(\alpha_2 \cdot \nabla_2) \frac{e^{i|q|r_{12}} - 1}{q^2 r_{12}} \right]. \] (1.41)

Setting \( q = 0, \) we obtain the instantaneous Breit interaction (real part)
\[ B_{12}^{\text{Inst}} = -\frac{e^2}{4\pi \varepsilon_0} \left[ \alpha_1 \cdot \alpha_2 + \frac{1}{2} (\alpha_1 \cdot \nabla_1)(\alpha_2 \cdot \nabla_2) r_{12} \right] \]
or using
\[ (\alpha_1 \cdot \nabla_1)(\alpha_2 \cdot \nabla_2) r_{12} = -\frac{\alpha_1 \cdot \alpha_2}{r_{12}} + \frac{(\alpha_1 \cdot r_{12})(\alpha_1 \cdot r_{12})}{r_{12}^3} \]
we arrive at
\[ B_{12}^{\text{Inst}} = -\frac{e^2}{4\pi \varepsilon_0 r_{12}} \left[ \frac{1}{2} \alpha_1 \cdot \alpha_2 + \frac{(\alpha_1 \cdot r_{12})(\alpha_1 \cdot r_{12})}{2 r_{12}^2} \right] \] (1.42)
which is the standard form of the instantaneous Breit interaction.
1.2.3 The transverse photon propagator

We shall now consider both time-orderings of the interaction represented in the figure simultaneously. The evolution operator can then be expressed

\[ U_\gamma^{(2)}(0, -\infty) = \left( \frac{-i}{\hbar} \right)^2 \int_{-\infty}^{0} dt_2 \int_{-\infty}^{0} dt_1 T[H_{\text{int},1}(t_2) H_{\text{int},1}(t_1)] e^{-\gamma(|t_1|+|t_2|)} \],

where

\[ T[H_{\text{int},1}(t_2) H_{\text{int},1}(t_1)] = \begin{cases} H_{\text{int},1}(t_2) H_{\text{int},1}(t_1) & t_2 > t_1 \\ H_{\text{int},1}(t_1) H_{\text{int},1}(t_2) & t_1 > t_2 \end{cases} \]

In the Coulomb gauge the interaction is given by \( \text{IntCoulIP} \) and the vector potential is given by \( \text{IntCoulIP}^{(2)} \). The evolution operator for the combined interactions will then be

\[ U_\gamma^{(2)}(0, -\infty) = -c_+^e c_a c_b \frac{e^2 c^2}{\hbar^2} \times \int_{-\infty}^{0} dt_2 \int_{-\infty}^{0} dt_1 T[(\alpha \cdot A_\perp)_1 (\alpha \cdot A_\perp)_2] e^{-\imath t_1 (\epsilon_a - \epsilon_b + i\gamma)/\hbar} e^{-\imath t_2 (\epsilon_b - \epsilon_a + i\gamma)/\hbar} \]

Here

\[ T[(\alpha \cdot A_\perp)_1 (\alpha \cdot A_\perp)_2] = \sum_{k \in \mathcal{V}} \frac{\hbar}{2 \omega} (\alpha \cdot \varepsilon_p)_1 (\alpha \cdot \varepsilon_p)_2 \times \begin{cases} e^{-\imath (k_1 \cdot x_1 - \omega t_1)} e^{\imath (k_2 \cdot x_2 - \omega t_2)} & t_2 > t_1 \\ e^{-\imath (k_2 \cdot x_2 - \omega t_2)} e^{\imath (k_1 \cdot x_1 - \omega t_1)} & t_1 > t_2 \end{cases} \]

or with \( r_{12} = x_1 - x_2 \) and \( t_{12} = t_1 - t_2 \)

\[ T[(\alpha \cdot A_\perp)_1 (\alpha \cdot A_\perp)_2] = \hbar \sum_{p=1}^{2} (\alpha \cdot \varepsilon_p)_1 (\alpha \cdot \varepsilon_p)_2 \frac{1}{\mathcal{V}} \sum_{k} e^{\imath (k \cdot r_{12} - \omega t_{12})} \frac{2 \omega}{2\omega}, \]

where the upper sign is valid for \( t_2 > t_1 \). This yields

\[ U_\gamma^{(2)}(0, -\infty) = -c_+^e c_a c_b \frac{e^2 c^2}{\varepsilon_0 \hbar^2} \int_{-\infty}^{0} dt_2 \int_{-\infty}^{0} dt_1 \times \sum_{p=1}^{2} (\alpha \cdot \varepsilon_p)_1 (\alpha \cdot \varepsilon_p)_2 \frac{1}{\mathcal{V}} \sum_{k} e^{\imath (k \cdot r_{12} - \omega t_{12})} e^{-\imath \gamma t_{12}} e^{\gamma (t_1 + t_2)} \]

Figure 1.2: The two time-orderings of a single-photon exchange can be represented by a single *Feynman diagram*.
utilizing the energy conservation \(\epsilon_0\).

The boxed part of the equation above is essentially the photon propagator (\(\text{PhotProp}\))

\[
D_F(2, 1) = \frac{1}{V} \int \frac{d^3k}{(2\pi)^3} \frac{e^{\pm i(k \cdot r_{12} - \omega t_{12})}}{2\omega} \Rightarrow \int \frac{d^3k}{(2\pi)^3} \frac{e^{\pm i(k \cdot r_{12} - \omega t_{12})}}{2\omega}.
\] (1.48) \(\text{PhotProp}\)

This can be represented by a complex integral

\[
D_F(2, 1) = i \int \frac{d^3k}{(2\pi)^3} \int \frac{dz}{2\pi} \frac{e^{itz_{12}}}{z^2 - \omega^2 + i\eta} e^{ik \cdot r_{12}},
\] (1.49) \(\text{PhotPropInt}\)

where \(\eta\) is a small, positive quantity. As before, the sign of the exponent \(ik \cdot r_{12}\) is immaterial. The integrand has poles at \(z = \pm (\omega - i\eta)\), assuming \(\omega\) to be positive. For \(t_2 > t_1\) integration over the negative half plane yields \(\int \frac{dz}{2\pi} e^{\omega t_{12}} e^{ik \cdot r_{12}}\) and for \(t_1 > t_2\) integration over the positive half plane yields \(\int \frac{dz}{2\pi} e^{-\omega t_{12}} e^{ik \cdot r_{12}}\), which is identical to (1.48).

The evolution operator (1.47) can then be expressed

\[
U^2_{\gamma}(0, -\infty) = -c_d c_d c_b \epsilon_0 \hbar \int_{-\infty}^{0} dt_2 \int_{-\infty}^{0} dt_1 \times 2 \sum_{p=1}^{2} (\alpha \cdot \epsilon_p) \sum_{p=1}^{3} (a_{kp} \alpha \cdot \epsilon_p) D_F(1, 2) e^{ik \cdot r_{12}/\hbar} e^{i(\gamma t_{12} + t_2)}.
\] (1.50) \(U2SP5\)

1.2.4 Comparison with the covariant treatment

It is illustrating to compare the quantization of the transverse photons with the fully covariant treatment, to be discussed in the next chapter. Then we simply have to replace the sum in (1.28) by the corresponding covariant expression

\[
\sum_{p_1 p_2=1}^{3} (a_{kp} \alpha \cdot \epsilon_p) (a_{kp} \alpha \cdot \epsilon_p) \Rightarrow \sum_{p_1 p_2=0}^{3} (a_{kp} \alpha \cdot \epsilon_p) (a_{kp} \alpha \cdot \epsilon_p) \Rightarrow \sum_{p_1 p_2=0}^{3} (a_{kp} \alpha \cdot \epsilon_p) (a_{kp} \alpha \cdot \epsilon_p),
\] (1.51) \(\text{eq:PolSum4}\)

The commutation relation (2.2) yields

\[
\sum_{p_1 p_2=0}^{3} (a_{kp} \alpha \cdot \epsilon_p) (a_{kp} \alpha \cdot \epsilon_p) = \alpha_1 \cdot \alpha_2 - 1.
\] (1.52) \(\text{Replace}\)

We then find that the equivalent potential interaction (1.37) becomes

\[
V_{12} = \frac{-\epsilon^2}{\epsilon_0} \int \frac{d^3k}{(2\pi)^3} \frac{(1 - \alpha_1 \cdot \alpha_2)}{q^2 - k^2 + i\gamma} e^{ik \cdot r_{12}}.
\] (1.53) \(V12\)

and with the fourier transform given in Appendix \(\text{sec:FT}\)

\[
V_{12} = \frac{\epsilon^2}{4\pi \epsilon_0 r_{12}} (1 - \alpha_1 \cdot \alpha_2) e^{i\eta |r_{12}|}.
\] (1.54) \(\text{CoulBreit}\)

We shall now compare this with the exchange of transverse photons, treated above.

We then make the decomposition

\[
1 - \alpha_1 \cdot \alpha_2 = \begin{cases} 1 - (\alpha_1 \cdot \hat{k})(\alpha_2 \cdot \hat{k}) \\ -\alpha_1 \cdot \alpha_2 + (\alpha_1 \cdot \hat{k})(\alpha_2 \cdot \hat{k}) \end{cases}.
\] (1.55) \(\text{Decompose}\)
The last part, which represents the exchange of transverse photons, is identical to (1.39), which led to the Breit interaction. The first part, which represents the exchange of longitudinal and scalar photons, corresponds to the interaction

$$V_C = -\frac{e^2}{\varepsilon_0} \int \frac{d^3k}{(2\pi)^3} \left[ 1 - (\alpha_1 \cdot \hat{k})(\alpha_2 \cdot \hat{k}) \right] \frac{e^{i\mathbf{k} \cdot \mathbf{r}_{12}}}{q^2 - k^2 + i\gamma}. \quad (1.56)$$

This Fourier transform is evaluated in Appendix \textsection F.2 and yields

$$V_C = -\frac{e^2}{\varepsilon_0} \int \frac{d^3k}{(2\pi)^3} \left[ 1 - \frac{q^2}{k^2} \right] \frac{e^{i\mathbf{k} \cdot \mathbf{r}_{12}}}{q^2 - k^2 + i\gamma} = \frac{e^2}{\varepsilon_0} \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{r}_{12}} \left( 1 - \frac{q^2}{k^2} \right), \quad (1.57)$$

provided that the orbitals are generated in a \textit{local potential}. Using the transform in Appendix \textsection F.1, this becomes

$$V_{\text{Coul}} = \frac{e^2}{4i\varepsilon_0 r_{12}}. \quad (1.58)$$

Thus, we see that \textit{the exchange of longitudinal and scalar photons corresponds to the instantaneous Coulomb interaction, while the exchange of the transverse photons corresponds to the Breit interaction}. Note that this is true only if the orbitals are generated in a \textit{local potential}.

If instead of the separation (1.55) we would separate the photons into the scalar part \((p = 0)\) and the vector part \((p = 1, 2, 3)\),

$$1 - \alpha_1 \cdot \alpha_2 = \begin{cases} 1, \\ -\alpha_1 \cdot \alpha_2, \end{cases} \quad (1.59)$$

then the result would be

$$V_{\text{Ret Coul}} = \frac{e^2}{4i\varepsilon_0 r_{12}} e^{i|q|r_{12}},$$

$$V_{\text{Ret Gaunt}} = -\frac{e^2}{4\pi\varepsilon_0 r_{12}} \alpha_1 \cdot \alpha_2 e^{i|q|r_{12}}. \quad (1.60)$$

which represents the \textit{retarded Coulomb and the retarded magnetic (Gaunt) interaction}. This implies that \textit{the longitudinal photon represents the retardation of the Coulomb interaction, which is included in the Breit interaction (1.41)}.

If we would set \(q = 0\), then we would from (1.60) retrieve the \textit{instantaneous Coulomb interaction} (1.58) and

$$-\frac{e^2}{4\pi\varepsilon_0} \alpha_1 \cdot \alpha_2, \quad (1.61)$$

which is known as the \textit{Gaunt interaction}. The Breit interaction will then turn into the instantaneous interaction (1.42). This will still have some effect of the retardation of the Coulomb interaction, although it is instantaneous.

We shall see later that the interactions (1.60) correspond to the interactions in the Feynman gauge (2.48), while the instantaneous Coulomb and Breit interactions correspond to the Coulomb gauge.
Chapter 2

Covariant theory of Quantum-ElectroDynamics

2.1 The photon propagator

The covariant electromagnetic radiation field is in analogy with (1.25) represented by the four-component vector potential

\[ A_\mu(x) = A_\mu^+(x) + A_\mu^-(x) = \sqrt{\frac{1}{2\varepsilon_0\omega V}} \sum_k \varepsilon_{\mu r} \left[ a_{kr} e^{-ikx} + a_{kr}^\dagger e^{ikx} \right], \]

where

\[ k = k^\mu = (k_0, \mathbf{k}); \quad k_0 = \omega/c = |\mathbf{k}|; \quad kx = \omega t - \mathbf{k} \cdot \mathbf{x} \]

are the covariant notations, defined in Appendix A, and \( r = (0, 1, 2, 3) \) represents the four polarization states – two transverse \( (r = 1, 2) \), one longitudinal \( (r = 3) \) and one scalar \( (r = 0) \).

The creation and annihilation operators satisfy the following commutation relation

\[ [a_{kr}, a_{kr'}^\dagger] = \delta_{kk'} \delta_{rr'} \zeta_r, \]

where \( \zeta_r = (-1, 1, 1, 1) \) for \( r = (0, 1, 2, 3) \), which leads to the relation

\[ \sum_{rr'} \left[ \varepsilon_{\mu r} a_{kr}, \varepsilon_{\nu r'} a_{k'r'}^\dagger \right] = -g_{\mu\nu} \delta_{kk'}. \]

The contraction between the photon fields is defined as the difference between the time and normal orderings

\[ A_\nu(x_2)A_\mu(x_1) = T[A_\nu(x_2)A_\mu(x_1)] - N[A_\nu(x_2)A_\mu(x_1)]. \]

Since the vacuum expectation value vanishes for every normal ordered product, it follows that the contraction is equal to the vacuum expectation of the time-ordered product

\[ A_\nu(x_2)A_\mu(x_1) = \langle 0 | T[A_\nu(x_2)A_\mu(x_1)] | 0 \rangle. \]

\(^1\)From now on we set \( \hbar = 1 \).
The **Feynman photon propagator** is defined by means of the photon-field contraction

\[ A_\nu(x_2)A_\mu(x_1) = \langle 0 | T [ A_\nu(x_2)A_\mu(x_1) ] | 0 \rangle = \frac{i}{c \varepsilon_0} D_{F\nu\mu}(x_2 - x_1). \] (2.6) **PhotPropDef**

With the radiation field (\( \mathcal{F} \)) this becomes

\[
A_\nu(x_2)A_\mu(x_1) = \langle 0 | T [ A_\nu(x_2)A_\mu(x_1) ] | 0 \rangle
\]
\[
= \langle 0 | \Theta(t_2 - t_1) A_\nu(x_2) A_\mu(x_1) + \Theta(t_1 - t_2) A_\mu(x_1) A_\nu(x_2) | 0 \rangle
\]
\[
= \sum_{k_1, \nu_{r} \nu_{r'} r_2} \frac{1}{2\varepsilon_0 V \sqrt{\omega_1 \omega_2}} \langle 0 | \Theta(t_2 - t_1) [ \varepsilon_{\mu \nu} a_{k_{\nu_{r} \nu_{r'} r_2}}, \varepsilon_{\mu \nu} a_{k_{\nu_{r} \nu_{r'} r_2}}^{\dagger} ] e^{-i(k_2 x_2 - k_1 x_1)}
\]
\[
+ \Theta(t_1 - t_2) [ \varepsilon_{\mu \nu} a_{k_{\nu_{r} \nu_{r'} r_2}}, \varepsilon_{\mu \nu} a_{k_{\nu_{r} \nu_{r'} r_2}}^{\dagger} ] e^{i(k_2 x_2 - k_1 x_1)} | 0 \rangle
\]
\[
= -g_{\nu \mu} \sum_k \frac{1}{2\varepsilon_0 V} \left[ \Theta(t_2 - t_1) e^{-i k_2 x_2 - k_1 x_1} + \Theta(t_1 - t_2) e^{i k_2 x_2 - k_1 x_1} \right]
\]
\[
= -g_{\nu \mu} \sum_k \frac{1}{2\varepsilon_0 V} e^{-i k_{12} \cdot r_2} \left[ \Theta(t_2 - t_1) e^{-i \omega(t_2 - t_1)} + \Theta(t_1 - t_2) e^{i \omega(t_2 - t_1)} \right] \] (2.7) **PhotContr1**

with \( r_{12} = x_1 - x_2 \). (The sign of \( k \) is immaterial).

The expression in the square brackets of (2.7) can as in (1.49) be written as a complex integral

\[
I = \Theta(t_2 - t_1) e^{-i \omega(t_2 - t_1)} + \Theta(t_1 - t_2) e^{i \omega(t_2 - t_1)} = 2i \omega \int_{-\infty}^{\infty} \frac{dz}{2\pi} \frac{e^{-iz(t_2 - t_1)}}{z^2 - \omega^2 + i\eta}. \] (2.8) **ComplInt**

Thus,

\[
\langle 0 | T [ A_\nu(x_2)A_\mu(x_1) ] | 0 \rangle = -g_{\nu \mu} \frac{i}{\varepsilon_0 V} \sum_{k_1, \nu_{r} \nu_{r'} r_2} e^{i k_{12} \cdot r_2} \int_{-\infty}^{\infty} \frac{dz}{2\pi} \frac{e^{-iz(t_2 - t_1)}}{z^2 - \omega^2 + i\eta}
\]
\[
- g_{\nu \mu} \frac{i}{\varepsilon_0 V} \int \frac{d^3k}{(2\pi)^3} e^{i k_{12} \cdot r_2} \int_{-\infty}^{\infty} \frac{dz}{2\pi} \frac{e^{-iz(t_2 - t_1)}}{z^2 - \omega^2 + i\eta}, \] (2.9) **PhotProp0**

and the photon propagator (2.6) becomes (c.f (1.49))

\[
D_{F\nu\mu}(x_2 - x_1) = -g_{\nu \mu} c \int \frac{d^3k}{(2\pi)^3} e^{i k_{12} \cdot r_2} \int_{-\infty}^{\infty} \frac{dz}{2\pi} \frac{e^{-iz(t_2 - t_1)}}{z^2 - \omega^2 + i\eta}. \] (2.10) **PhotProp**

With \( z = ck_0, \omega^2 = c^2 k^2, k^2 = k_0^2 - k^2 \) this becomes in four-component form

\[
D_{F\nu\mu}(x_2 - x_1) = -g_{\nu \mu} \int \frac{d^4k}{(2\pi)^4} \frac{e^{-ik(x_2 - x_1)}}{k^2 + i\eta}. \] (2.11) **PhotProp4**

The photon propagator (2.10) can be expressed

\[
D_{F\nu\mu}(x_2 - x_1) = \int \frac{dz}{2\pi} e^{-iz(t_2 - t_1)} D_{F\nu\mu}(x_2, x_1; z), \] (2.12)
where $D_{F\nu}(x_2, x_1; z)$ is the *fourier transform* with respect to time

$$D_{F\nu}(x_2, x_1; z) = -g_{\nu\mu} c \int \frac{d^3k}{(2\pi)^3} \frac{e^{ik\cdot r_{12}}}{z^2 - c^2 k^2 + i\eta} \tag{2.13}$$

The photon propagator (2.13) can also be expressed

$$\langle x_2 | D_{F\nu}(z) | x_1 \rangle = -g_{\nu\mu} c \frac{|ks\rangle \langle ks|}{z^2 - c^2 k^2 + i\eta} \tag{2.14}$$

where

$$|ks\rangle = (2\pi)^{-3/2} u_s(k) e^{ik \cdot x}$$

is the momentum eigenfunction (5.35) and summation over $s$ and integration over $k$ are understood. (2.14) is the coordinate representation (see section 5.3) of the operator

$$D_{F\nu}(z) = -g_{\nu\mu} c \frac{|ks\rangle \langle ks|}{z^2 - c^2 k^2 + i\eta}. \tag{2.15}$$

The corresponding *momentum representation* is

$$\langle p_2 r_2 | D_{F\nu}(z) | p_1 r_1 \rangle = -g_{\nu\mu} c \frac{\langle p_2 r_2 | ks \rangle \langle ks | p_1 r_1 \rangle}{z^2 - c^2 k^2 + i\eta} = -g_{\nu\mu} c \frac{\delta_{s,s'} \delta_{r,r'} \delta^3(p_2 - k)}{z^2 - c^2 k^2 + i\eta}, \tag{2.16}$$

which leads to

$$\langle p_2 r_2 | D_{F\nu}(z) | p_1 r_1 \rangle = -g_{\nu\mu} c \frac{\delta^3(p_2 - p_1)}{z^2 - c^2 p^2 + i\eta}, \tag{2.17}$$

where $p = p_1 = p_2$. The corresponding *fourier transform* is according to (5.38)

$$\sum_{r_1 r_2} u_{r_2}(p_2) \langle p_2 r_2 | D_{F\nu}(z) | p_1 r_1 \rangle u_{r_1}^+(p_1) = D_{F\nu}(p_2, p_1; z) = -g_{\nu\mu} c \frac{\delta^3(p_2 - p_1)}{z^2 - c^2 p^2 + i\eta}. \tag{2.18}$$

### 2.2 The electron propagator

The electron field is in the *bound-interaction picture* given by

$$\psi(x) = \sum_j c_j(t) \phi_j(x), \quad \psi^\dagger(x) = \sum_j c_j^\dagger(t) \phi_j^\dagger(x), \tag{2.19}$$

where $\{\phi_j\}$ is a complete set of single-electron orbitals – with positive as well as negative energy – and $c_j(t), c_j^\dagger(t)$ are the corresponding time-dependent annihilation and creation operators. The orbitals are generated by the Dirac hamiltonian in the field of the nucleus (with charge $Z$) and with an additional potential $U$

$$\hat{h}_D \phi_a(x) = \left( c \alpha \cdot \hat{p} + \beta m c^2 - \frac{Ze^2}{4\pi\varepsilon_0 r} + U \right) \phi_a(x) = \varepsilon_a \phi_a(x), \tag{2.20}$$

where $\varepsilon_a$ is the orbital energy eigenvalue. The operators have in this picture the time dependence

$$c_j(t) = c_j e^{-i\varepsilon_j t} \quad ; \quad c_j^\dagger(t) = c_j^\dagger e^{i\varepsilon_j t}, \tag{2.21}$$

where $c_j, c_j^\dagger$ are the time-independent operators.
The **Feynman electron propagator** is defined by means of the *contraction* between the electron field operators in analogy with (2.6)

$$\psi(x)\psi^\dagger(x') = \langle 0 | T[\psi(x)\psi^\dagger(x')] | 0 \rangle = i S_F(x_2, x_1).$$ (2.22)  

It should be noted that the propagator is a matrix with the elements defined by

$$i S_F(x_2, x_1)_{\alpha, \beta} = \langle 0 | T[\psi(x_2)\psi^\dagger(x')] | 0 \rangle_{\alpha, \beta} = \langle 0 | T[\psi(x)\alpha\psi^\dagger(x')\beta] | 0 \rangle.$$ (2.23)

The time-independent operators satisfy the **fermion anti-commutation rule** [1, Eq.4.39]

$$\{c_i, c_j^\dagger\} = c_i c_j^\dagger + c_j^\dagger c_i = \delta_{i,j}. \quad (2.24)$$  

We then get in analogy with (2.7) for $t_1 \neq t_2$ ($t_1 = t_2$ will be considered below)

$$\psi(x_2)\psi^\dagger(x_1) = \langle 0 | T[\psi(x_2)\psi^\dagger(x_1)] | 0 \rangle \quad \text{(2.25)}$$

$$\begin{align*}
\langle 0 | T[\Theta(t_2 - t_1)\psi(x_2)\psi^\dagger(x_1) - \Theta(t_1 - t_2)\psi^\dagger(x_1)\psi(x_2)] | 0 \rangle \\
= \langle 0 | T[\Theta(t_2 - t_1)\{\psi_+(x_2), \psi_+^\dagger(x_1)\} - \Theta(t_1 - t_2)\{\psi_-(x_1), \psi_-(x_2)\}] | 0 \rangle \\
= \langle 0 | T[\Theta(t_2 - t_1) \sum_{p,p'} \{c_p, c_{p'}^\dagger\} e^{-i\varepsilon_p t_2} e^{i\varepsilon_{p'} t_1} \phi_p(x_2)\phi_{p'}^\dagger(x_1) \\
- \Theta(t_1 - t_2) \sum_{h,h'} \{c_h, c_{h'}^\dagger\} e^{i\varepsilon_h t_1} e^{-i\varepsilon_{h'} t_2} \phi_h(x_2)\phi_{h'}^\dagger(x_1)] | 0 \rangle \\
= \Theta(t_2 - t_1)e^{-i\varepsilon_p(t_2 - t_1)}\phi_p(x_2)\phi_{p'}^\dagger(x_1) - \Theta(t_1 - t_2) \sum_h e^{-i\varepsilon_h(t_2 - t_1)}\phi_h(x_2)\phi_h^\dagger(x_1).  
\end{align*}$$

Here, $\psi_\pm(x_1)$ represent the electron field operators for particles and holes, respectively, and $p, h$ represent particles and holes in the single-particle picture. The contraction above can now be expressed as a complex integral in analogy with (1.49)

$$\langle 0 | T[\psi(x_1)\psi^\dagger(x_1)] | 0 \rangle = i \sum_j \int \frac{dz}{2\pi} \frac{\phi_j(x_2)\phi_j^\dagger(x_1)}{z - \varepsilon_j + i\eta_j} e^{-iz(t_2-t_1)}, \quad (2.26)$$

where $\eta_j$ is a small real quantity with the same sign as $\varepsilon_j$. This gives the **electron propagator** [1, Eq.22]

$$S_F(x_2, x_1) = \sum_j \int \frac{dz}{2\pi} \frac{\phi_j(x_2)\phi_j^\dagger(x_1)}{z - \varepsilon_j + i\eta_j} e^{-iz(t_2-t_1)} \quad (2.27)$$

Here, $j$ runs over positive and negative energy states, and $\eta$ is a small positive quantity.

The contraction has so far been defined only for $t_1 \neq t_2$. For the bound-state problem it is necessary to consider also equal-time contractions. We then define the time-ordering for equal time as

$$T[\psi(x_2)\psi^\dagger(x_1)] = \frac{1}{2} \left[ \psi(x_2)\psi^\dagger(x_1) - \psi^\dagger(x_1)\psi(x_2) \right] \quad (t_1 = t_2) \quad (2.28)$$
\[
\psi(x_2)\psi^\dagger(x_1) = \left\langle 0 \middle| T[\psi(x_2)\psi^\dagger(x_1)] \middle| 0 \right\rangle = \frac{1}{2} \left\langle 0 \middle| \psi(x_2)\psi^\dagger(x_1) - \psi^\dagger(x_1)\psi(x_2) \middle| 0 \right\rangle \\
= \frac{1}{2} \sum_p \phi_p(x_2) \phi_p^\dagger(x_1) - \frac{1}{2} \sum_h \phi_h(x_2) \phi_h^\dagger(x_1) = \frac{1}{2} \sum_j \text{sgn}(\varepsilon_j) \phi_j(x_2) \phi_j^\dagger(x_1), \tag{2.29}
\]

where \(j\) as before runs over particles and holes. This can still be expressed by the integral above, as can be seen from the relation
\[
\frac{1}{\varepsilon_j - z - i\varepsilon_j \eta} = \frac{\varepsilon_j - z}{(\varepsilon_j - z)^2 + (\varepsilon_j \eta)^2} + \frac{i\varepsilon_j \eta}{(\varepsilon_j - z)^2 + (\varepsilon_j \eta)^2} = P - \frac{1}{\varepsilon_j - z} + i\pi \text{sgn}(\varepsilon_j) \delta(\varepsilon_j - z). \tag{2.30}
\]

\(P\) stands for the principal-value integration, which does not contribute here. Therefore, the electron propagator \((2.27)\) is valid also for equal times.

The Fourier transform with respect to time of the electron propagator \((2.27)\) is
\[
S_F(x_2, x_1; z) = \sum_j \phi_j(x_2) \phi_j^\dagger(x_1) \frac{1}{z - \varepsilon_j + i\eta_j}. \tag{2.31}
\]

This can be regarded as the coordinate representation
\[
S_F(x_2, x_1; z) = \langle x_2|S_F(z)|x_1 \rangle = \frac{\langle x_2|j \rangle \langle j|x_1 \rangle}{z - \varepsilon_j + i\eta_j} \tag{2.32}
\]

of the operator
\[
\hat{S}_F(z) = \frac{|j\rangle \langle j|}{z - \varepsilon_j (1 - i\eta)}. \tag{2.33}
\]

Using the relation \((2.30)\), this can also be expressed
\[
\hat{S}_F(z) = \frac{1}{z - \hat{h}_D (1 - i\eta)}, \tag{2.34}
\]

where \(\hat{h}_D\) is the Dirac hamiltonian \((2.20)\), \(\hat{h}_D |j\rangle = \varepsilon_j |j\rangle\). The corresponding momentum representation is
\[
S_F(p_2 \hat{r}_2, p_1 \hat{r}_1; z) = \langle p_2 \hat{r}_2|S_F(z)|p_1 \hat{r}_1 \rangle = \frac{\langle p_2 \hat{r}_2|j \rangle \langle j|p_1 \hat{r}_1 \rangle}{z - \varepsilon_j + i\eta_j}. \tag{2.35}
\]

### 2.3 Single-photon exchange

The exchange of a single photon between two electrons is represented by the Feynman diagram in Fig. 2.1, and the scattering amplitude is given by \(\langle cd|S^{(2)}|ab\rangle\), where \(S^{(2)}\) is the second-order S-matrix [1, Eq.7.1]
\[
S^{(2)} = -\frac{1}{2} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \text{T}[H_{\text{int},1}(t_2) H_{\text{int},1}(t_1)] e^{-\eta_1 |t_1| - \eta_2 |t_2|} \\
= -\frac{1}{2} \int d^4x_1 d^4x_2 \text{T}[H_{\text{int},1}(x_2) H_{\text{int},1}(x_1)] e^{-\eta_1 |t_1| - \eta_2 |t_2|}. \tag{2.36}
\]
The time integral is

\[
\int dt_1 dt_2 e^{it_1(\varepsilon_d-\varepsilon_b)} e^{it_2(\varepsilon_c-\varepsilon_a)} e^{iz(t_1-t_2)} e^{-\eta_1|t_1|-\eta_2|t_2|}
\]

\[
= 2\pi \Delta_{\eta_1}(\varepsilon_a - \varepsilon_c - z) \Delta_{\eta_2}(\varepsilon_b - \varepsilon_d + z),
\]

Figure 2.1: The Feynman representation of the exchange of a single, virtual photon between two electrons. The heavy lines represent electronic states in the bound-interaction picture.

Here, \( H_{\text{int},1}(t) \) is the interaction hamiltonian (c.f. Eq. 1.12)

\[
H_{\text{int},1}(t) = c \int d^3x \, H_{\text{int}}(x)
\]

with

\[
H_{\text{int},1}(x) = -ec \psi(x) \alpha^\mu A_\mu(x) \psi(x).
\] (2.37)

\( \eta_1, \eta_2 \) are adiabatic damping coefficients, which eventually go to zero. \( \psi(x) \) and \( \psi^\dagger(x) \) are the electron-field operators in the bound-interaction picture (2.24). (Note that the interaction (2.37) is defined without the normal-ordering in order to allow for equal-time contractions discussed above). The exchange of a virtual photon represents a contraction between the photon fields (2.35)

\[
S^{(2)} = -\frac{e^2c^2}{2} \int d^4x_1 d^4x \, T \left[ (\psi(x) \alpha^\nu A_\nu(x) \psi(x))_2 (\psi^\dagger(x) \alpha^\mu A_\mu(x) \psi(x))_1 \right] e^{-\eta_1|t_1|-\eta_2|t_2|}
\]

\[
= -\frac{e^2c^2}{2} \sum_{abcd} \int d^4x_1 d^4x_2 \left[ c^\dagger_d c^\dagger_b \phi^\dagger_b(x) \alpha^\nu c_a \phi_b(x) \right]_2 \langle 0|T[A_\nu(x_2)A_\mu(x_1)]|0 \rangle
\]

\times \left[ c^\dagger_c c^\dagger_a \alpha^\mu c_a \phi_a(x) \right]_1 e^{-\eta_1|t_1|-\eta_2|t_2|}.
\] (2.38)

Identification with the second-quantized form

\[
S^{(2)} = \frac{i}{2} \sum_{abcd} c^\dagger_d c^\dagger_b \langle \mathbf{c}d | S^{(2)} | ab \rangle c_b c_a
\] (2.39)

gives

\[
\langle \mathbf{cd} | S^{(2)} | ab \rangle = -e^2c^2 \int d^4x_1 d^4x_2 \left[ c^\dagger_d c^\dagger_b \phi^\dagger_b(x) \alpha^\nu \phi_b(x) \right]_2 \langle 0|T[A_\nu(x_2)A_\mu(x_1)]|0 \rangle
\]

\times \left[ \phi^\dagger_a(x) \alpha^\mu \phi_a(x) \right]_1 e^{-\eta_1|t_1|-\eta_2|t_2|}.
\] (2.40)

Using the definition of the photon propagator (2.6) this becomes

\[
\langle \mathbf{cd} | S^{(2)} | ab \rangle = -\frac{ie^2c}{\varepsilon_0} \int d^4x_1 d^4x_2 \left[ \phi^\dagger_b(x) \alpha^\nu \phi_b(x) \right]_2 \mathcal{D}_{F\nu\mu}(x_2-x_1) \left[ \phi^\dagger_a(x) \alpha^\mu \phi_a(x) \right]_1 e^{-\eta_1|t_1|-\eta_2|t_2|}.
\] (2.41)

The time integral is

\[
\int dt_1 dt_2 e^{it_1(\varepsilon_d-\varepsilon_b)} e^{it_2(\varepsilon_c-\varepsilon_a)} e^{iz(t_1-t_2)} e^{-\eta_1|t_1|-\eta_2|t_2|}
\]

\[
= 2\pi \Delta_{\eta_1}(\varepsilon_a - \varepsilon_c - z) \Delta_{\eta_2}(\varepsilon_b - \varepsilon_d + z),
\] (2.42)
where the $\Delta$ function is defined in Appendix B.1.

Integration over $z$ gives $z = \varepsilon_a - \varepsilon_c = \varepsilon_d - \varepsilon_b = cq$ and the scattering amplitude (2.44)

\[
\langle \text{cd} | S^{(2)} | ab \rangle = -2\pi i \Delta_{n_1+n_2}(\varepsilon_c+\varepsilon_d-\varepsilon_a-\varepsilon_b) \times \frac{e^2c}{\varepsilon_0} \int d^3x_1 d^3x_2 \left[ \phi_d^\dagger(x) \alpha^\mu \phi_b(x) \right] \left[ \phi_c^\dagger(x) \alpha^\mu \phi_a(x) \right] D_{F\mu}(x_2-x_1; cq) \left[ \phi_c^\dagger(x) \alpha^\mu \phi_a(x) \right]_1. \tag{2.43} \]

With the photon propagator in the Feynman gauge (2.13) this becomes

\[
\langle \text{cd} | S^{(2)} | ab \rangle = 2\pi i \Delta_{n_1+n_2}(\varepsilon_a+\varepsilon_b-\varepsilon_c-\varepsilon_d) \times \frac{e^2c}{\varepsilon_0} \int d^3x_1 d^3x_2 \left[ \phi_d^\dagger(x) \alpha^\mu \phi_b(x) \right] \left[ \phi_c^\dagger(x) \alpha^\mu \phi_a(x) \right] \int \frac{d^3k}{(2\pi)^3} e^{ik\cdot r_{12}}. \tag{2.44} \]

The time integration leads – in the limit $\eta \to 0$ – to energy conservation at each vertex with $z$ treated as the energy parameter of the propagator.

![Figure 2.2: The single-photon exchange is compared with the scattering of a potential, $V_{12}$.](Fig:SingPot)

The single-photon exchange can be compared with the scattering by an energy-dependent potential interaction, $V_{12}(cq)$, (see Fig. 2.2) with the scattering amplitude

\[
\langle \text{cd} | S^{(2)} | ab \rangle = -2\pi i \Delta_{n_1+n_2}(\varepsilon_c+\varepsilon_d-\varepsilon_a-\varepsilon_b) \langle \text{cd} | V_{12}(cq) | ab \rangle. \tag{2.45} \]

Identification then gives

\[
\langle \text{cd} | V_{12}(cq) | ab \rangle = -\frac{e^2}{\varepsilon_0} \int d^3x_1 d^3x_2 \left[ \phi_d^\dagger(x_2) \alpha^\mu \phi_b(x_2) \right] \left[ \phi_c^\dagger(x_1) \alpha^\mu \phi_a(x_1) \right] \int \frac{d^3k}{(2\pi)^3} e^{ik\cdot r_{12}}. \tag{2.46} \]

Thus, with $\alpha_1^\mu \alpha_2^\mu = 1 - \alpha_1 \cdot \alpha_2$, the equivalent potential in the Feynman gauge becomes

\[
V_{12}^F(cq) = -\frac{e^2}{\varepsilon_0} (1 - \alpha_1 \cdot \alpha_2) \int \frac{d^3k}{(2\pi)^3} e^{ik\cdot r_{12}}. \tag{2.47} \]

which is identical to the previous result (11.53). The Fourier transform then yields

\[
V_{12}^F = (1 - \alpha_1 \cdot \alpha_2) \frac{e^2}{4\pi \varepsilon_0 r_{12}} e^{i|q| r_{12}}. \tag{2.48} \]
which is the retarded Coulomb and Gaunt interactions \( \text{CoulGauntRet} \).

In calculating the first-order energy shift, corresponding to the exchange of a single photon, we employ the Gell-Mann-Low-Sucher \( \text{GML51,Su57} \) prescription and set all \( \eta \) equal to \( \eta \).

Then the energy shift in the (closed-shell) state \( \Phi \) is given by

\[
\Delta E = \lim_{\eta \to 0} \frac{i\eta}{2} \sum n \langle \Phi | S^{(n)} | \Phi \rangle \langle \Phi | S | \Phi \rangle, \tag{2.49} \]

which in lowest order becomes

\[
\Delta E = \lim_{\eta \to 0} \eta \langle \Phi | S^{(2)} | \Phi \rangle. \tag{2.50} \]

Using (I.9), we get from (I.12)

\[
\lim_{\eta_1 + \eta_2 \to 0} \frac{i(\eta_1 + \eta_2)}{2} \langle cd | S^{(2)} | ab \rangle = \delta_{\varepsilon_c + \varepsilon_d, \varepsilon_a + \varepsilon_b} \langle cd | V_{12}(cq) | ab \rangle
\]

and the first-order energy shift becomes

\[
\Delta E = \langle \Phi | V_{12}(cq) | \Phi \rangle = \langle ab | V_{12}(cq) | ab \rangle - \langle ba | V_{12}(cq) | ab \rangle, \tag{2.51} \]

where \( \Phi \) is the \text{antisymmetricized}, unperturbed state \(|\{ab\}\rangle\). This result is consistent with the interpretation of \( V_{12} \) as an equivalent perturbing potential.

Due to the energy conservation of the scattering process, only diagonal (on-the-energy-shell) matrix elements of the potential are obtained from the analysis of the single-photon exchange. \text{Off-diagonal elements} are obtained from the analysis of the \text{two-photon exchange} \( \text{Li89} \).

### 2.4 The bound-electron self energy

#### 2.4.1 General

![Figure 2.3: Diagram representing the first-order self-energy of a bound electron.](Fig:SE)

With the rules given in Appendix \( \text{Feynman} \), the first-order electron self energy in the state \( |a\rangle \) is (see Fig. 2.3)

\[
\Delta_{\text{SE}}(a) = i \int d^3 x_1 d^3 x_2 \phi_d^\dagger(x_2) \text{i} e \alpha^\nu \int \frac{dx}{2\pi} i S_F(x_2, x_1; \varepsilon_a - z) \times \frac{i}{c \varepsilon_0} D_{\nu \mu}(x_2 - x_1; z) \text{i} e \alpha^\mu \phi_a(x_1), \tag{2.52} \]

20
where the orbitals are generated by the Dirac equation \( \text{DiracEq} \). \( S_F(x_2, x_1; \varepsilon_a - z) \) is the electron propagator (\( \text{PhotPropFT} \)), \( D_{F	ext{pot}}(x_2 - x_1; z) \) is the photon propagator (\( \text{ch:CoordMom} \)).

With the notations of Appendix B, the self energy can be written

\[
\Delta_{SE}(a) = \langle a | \Sigma(\varepsilon_a) | a \rangle = \langle a | x_2 \rangle \langle \Sigma(\varepsilon_a) | x_1 \rangle \langle x_1 | a \rangle ,
\]

where

\[
\langle x_2 | \Sigma(\varepsilon_a) | x_1 \rangle = \frac{i e^2 c \alpha^\nu}{\varepsilon_0} \int \frac{dz}{2\pi} S_F(x_2, x_1; \varepsilon_a - z) D_{F\text{pot}}(x_2 - x_1; z) \alpha^\mu
\]

\[
= -\frac{e^2 c^2}{\varepsilon_0} \int \frac{dz}{2\pi} \int \frac{d^3k}{(2\pi)^3} \frac{\langle x_2 | \alpha_{\mu} e^{i k \cdot x} | t \rangle \langle \alpha_{\nu} e^{-i k \cdot x} | x_1 \rangle}{(\varepsilon_a - \varepsilon_x - c k \text{sgn}(\varepsilon_x)) (\varepsilon_x^2 - c^2 k^2 + i\eta)}
\]

is the coordinate representation of the electron self-energy operator, \( \Sigma(\varepsilon_a) \). This is a mass operator, which should be added to the Dirac Hamiltonian in order to include the electron self energy – together with a counter term to take care of the renormalization.

Integration over \( z \) then yields

\[
\langle x_2 | \Sigma(\varepsilon_a) | x_1 \rangle = -\frac{e^2 c^2}{\varepsilon_0} \int \frac{d^3k}{(2\pi)^3} \frac{1}{k} \frac{\langle x_2 | \alpha_{\mu} e^{i k \cdot x} | t \rangle \langle \alpha_{\nu} e^{-i k \cdot x} | x_1 \rangle}{\varepsilon_a - \varepsilon_x - c k \text{sgn}(\varepsilon_x)},
\]

where \( k = |k| \). Integration over the angular part of \( k \) yields

\[
\langle x_2 | \Sigma(\varepsilon_a) | x_1 \rangle = -\frac{e^2 c^2}{4\pi \varepsilon_0 r_{12}} \langle x_2 | \alpha_{\mu} | t \rangle \int_0^\infty \frac{dk \sin k r_{12}}{\varepsilon_a - \varepsilon_x - c k \text{sgn}(\varepsilon_x)} \langle \alpha_{\nu} | x_1 \rangle,
\]

where \( r_{12} = |x_1 - x_2| \). This yields the following expression for the self-energy operator itself

\[
\Sigma(\varepsilon_a) = -\frac{e^2 c^2}{4\pi \varepsilon_0 r_{12}} \langle x_2 | \alpha_{\mu} | t \rangle \int_0^\infty \frac{dk \sin k r_{12}}{\varepsilon_a - \varepsilon_x - c k \text{sgn}(\varepsilon_x)} \langle \alpha_{\nu} | x_1 \rangle.
\]

Note that the self energy depends on the energy \( \varepsilon_a \) of the state \( |a\rangle \).

### 2.4.2 Renormalization in the nonrelativistic limit (Bethe’s treatment)

For small \( k \) values and positive intermediate states, \( \Sigma(\varepsilon_a) \) reduces to

\[
\Sigma(\varepsilon_a) = -\frac{e^2 c^2}{4\pi \varepsilon_0} \alpha_{\mu} | t \rangle \int_0^\infty \frac{k dk}{\varepsilon_a - \varepsilon_x - c k} \langle t | \alpha_{\nu} \rangle.
\]

The scalar part of \( \alpha_{\mu} \alpha_{\nu} \) cancels in the renormalization, leaving only the vector part to be considered,

\[
\Sigma(\varepsilon_a) = \frac{e^2 c^2}{4\pi \varepsilon_0} \alpha_{\mu} | t \rangle \int_0^\infty \frac{k dk}{\varepsilon_a - \varepsilon_x - c k} \langle t | \alpha_{\nu} \rangle.
\]

The corresponding operator for a free electron in the state \( p_+ \) (see Fig. 2) is

\[
\Sigma^\text{Free}(p_+) = \frac{e^2 c^2}{4\pi \varepsilon_0} \alpha_{\mu} | q_+ \rangle \int_0^\infty \frac{k dk}{\varepsilon_{p_+} - \varepsilon_{q_+} - c k} \langle q_+ | \alpha_{\nu} \rangle.
\]

restricting the intermediate states to positive energies. In the momentum representation this becomes

\[
\langle p'_+ | \Sigma^\text{Free}(p_+) | p_+ \rangle = \frac{e^2 c^2}{4\pi \varepsilon_0} \langle p'_+ | \alpha_{\mu} | q_+ \rangle \int_0^\infty \frac{k dk}{\varepsilon_{p'_+} - \varepsilon_{q_+} - c k} \langle q_+ | \alpha_{\nu} | p_+ \rangle.
\]
But since $\alpha$ is diagonal with respect to the momentum, we must have $q = p = p'$. Thus,

$$\langle p' + | \Sigma^\text{Free}(p_+)| p_+ \rangle = -\delta^3 \delta^3 \frac{e^2}{4\pi^2 \varepsilon_0} |\langle p_+ | \alpha | p_+ \rangle|^2 \int_0^\infty dk \ .$$ \hspace{1cm} (2.62) \hspace{1cm} \text{SEFreeMom2}

Obviously, this quantity is infinite. Inserting a set of complete states (2.51), this becomes

$$\langle p' + | \Sigma^\text{Free}(p_+)| p_+ \rangle = -\delta^3 \delta^3 \frac{e^2}{4\pi^2 \varepsilon_0} \langle p_+ | \alpha | t \rangle \cdot \langle t | \alpha | p_+ \rangle \int_0^\infty dk \ .$$ \hspace{1cm} (2.63) \hspace{1cm} \text{SEFreeMom3}

The free-electron self-energy operator can then be expressed

$$\Sigma^\text{Free}(p_+) = -\delta^3 \delta^3 \frac{e^2}{4\pi^2 \varepsilon_0} \alpha | t \rangle \cdot \int_0^\infty dk \langle t | \alpha \rangle ,$$ \hspace{1cm} (2.64) \hspace{1cm} \text{SEFreeOp}

which should be subtracted from the bound-electron self-energy operator (2.52). We can assume the intermediate states $\{| j \rangle \}$ to be identical to those in the bound case. This gives the \textbf{renormalized self-energy operator}

$$\Sigma^\text{Renorm}(\varepsilon_a) = \frac{e^2}{4\pi^2 \varepsilon_0} \alpha | t \rangle \cdot \int_0^\infty dk \frac{\varepsilon_a - \varepsilon_t - ck}{\varepsilon_a - \varepsilon_t} \langle t | \alpha \rangle.$$ \hspace{1cm} (2.65) \hspace{1cm} \text{SE0pRen}

The expectation value of this operator in a bound state $| a \rangle$ yields the renormalized bound-electron self energy in this approximation, i.e., the corresponding contribution to the physical \textbf{Lamb shift},

$$\langle a | \Sigma^\text{Renorm}(\varepsilon_a) | a \rangle = \frac{e^2}{4\pi^2 \varepsilon_0} \frac{\varepsilon_a - \varepsilon_t}{\varepsilon_a - \varepsilon_t - ck} \langle a | \alpha | t \rangle \cdot \langle t | \alpha | a \rangle \int_0^\infty dk \frac{\varepsilon_a - \varepsilon_t}{\varepsilon_a - \varepsilon_t - ck} .$$ \hspace{1cm} (2.66) \hspace{1cm} \text{BetheSE1}

This result is derived in a covariant Feynman gauge, where the quantized radiation has transverse as well as longitudinal components. In the Coulomb gauge only the former are quantized. Since all three vector components above yield the same contribution, we will get the result in the Coulomb gauge by multiplying by 2/3. Furthermore, in the non-relativistic limit we have $\alpha \rightarrow p/c$, which leads to

$$\langle a | \Sigma^\text{Renorm}(\varepsilon_a) | a \rangle = \frac{e^2}{4\pi^2 \varepsilon_0} \frac{\varepsilon_a - \varepsilon_t}{\varepsilon_a - \varepsilon_t - ck} \frac{\varepsilon_a - \varepsilon_t}{\varepsilon_a - \varepsilon_t - ck} ,$$ \hspace{1cm} (2.67) \hspace{1cm} \text{BetheSE}

which is essentially the result of Bethe.

\textbf{2.4.3 Relativistic renormalization}

For the renormalization in the general case we use the momentum representation of the electron self energy

$$\Delta_{SE}(a) = \langle a | pr \rangle \langle pr | \Sigma(\varepsilon_a) | p'r' \rangle \langle p'r'|a \rangle ,$$ \hspace{1cm} (2.68) \hspace{1cm} \text{SECoord2}

where the self-energy operator in the momentum representation is obtained by transforming the coordinate representation (2.50)

$$\langle pr | \Sigma(\varepsilon_a) | p'r' \rangle = \langle pr | x \rangle \langle x | \Sigma(\varepsilon_a) | x' \rangle \langle x' | p'r' \rangle$$ \hspace{1cm} (2.69) \hspace{1cm} \text{SEMom1}

or
cancel, making the expression only logarithmically divergent.

The last two expressions contain some linearly divergent terms, which can be shown to cancel, making the expression only logarithmically divergent [1, p. 225].

\[
\langle \mathbf{p}|\Sigma(\varepsilon_a)|\mathbf{p}'\rangle = -\frac{e^2 c}{2\varepsilon_0} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \delta^3(\mathbf{p} - \mathbf{p}') \delta_{rr'} \alpha_{\mu} \sum_s \frac{d^3 \mathbf{k}}{k} u_s(\mathbf{p} - \mathbf{k}) \nonumber
\]
\[
\times \frac{1}{\varepsilon_{p,r} - \varepsilon_{p-k,s} - ck \text{sgn}(s)} u_{r'}^\dagger(\mathbf{p} - \mathbf{k}) \alpha^\mu u_r(\mathbf{p}').
\]

The corresponding expression for a free electron in the state \( \mathbf{p}, r \) is obtained by replacing the bound-electron energy \( \varepsilon_a \) by the free-electron energy \( \varepsilon_{p,r} \) and letting the intermediate states run over free-electron states,

\[
\langle \mathbf{p}|\Sigma^{\text{Free}}|\mathbf{p}'\rangle = -\frac{e^2 c}{2\varepsilon_0} \delta^3(\mathbf{p} - \mathbf{p}') \delta_{rr'} \alpha_{\mu} \sum_s \frac{d^3 \mathbf{k}}{k} u_s(\mathbf{p} - \mathbf{k}) \nonumber
\]
\[
\times \frac{1}{\varepsilon_{p,r} - \varepsilon_{p-k,s} - ck \text{sgn}(s)} u_{r'}^\dagger(\mathbf{p} - \mathbf{k}) \alpha^\mu u_r(\mathbf{p}').
\]

The renormalized self-energy operator is the difference between the bound-state and the free-electron operators

\[
\langle \mathbf{p}|\Sigma^{\text{Renorm}}|\mathbf{p}'\rangle = \langle \mathbf{p}|\Sigma(\varepsilon_a) - \Sigma^{\text{Free}}|\mathbf{p}'\rangle
\]
\[
= -\frac{e^2 c}{2\varepsilon_0} u_s^\dagger(\mathbf{p}) \alpha_{\mu} \sum_{ss'} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{1}{k} u_s(\mathbf{p} - \mathbf{k}) \nonumber
\]
\[
\times \left[ \frac{(\mathbf{p} - \mathbf{k}, s|t)\langle \mathbf{p}'|\mathbf{p}' - \mathbf{k}, s'|\rangle}{\varepsilon_a - \varepsilon_t - ck \text{sgn}(\varepsilon_t)} - \frac{\delta^3(\mathbf{p} - \mathbf{p}')}{\varepsilon_{p,r} - \varepsilon_{p-k,s} - ck \text{sgn}(s)} \right] u_{s'}(\mathbf{p} - \mathbf{k}) \alpha^\mu u_r(\mathbf{p}').
\]

Using the relation (2.25) we can rewrite this as

\[
\langle \mathbf{p}|\Sigma^{\text{Renorm}}|\mathbf{p}'\rangle = -\frac{e^2 c}{2\varepsilon_0} u_s^\dagger(\mathbf{p}) \alpha_{\mu} \sum_{ss'} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{1}{k} u_s(\mathbf{p} - \mathbf{k}) \langle \mathbf{p} - \mathbf{k}, s|t\rangle \nonumber
\]
\[
\times \left[ \frac{1}{\varepsilon_a - \varepsilon_t - ck \text{sgn}(\varepsilon_t)} - \frac{1}{\varepsilon_{p,r} - \varepsilon_{p-k,s} - ck \text{sgn}(s)} \right] \langle \mathbf{p}' - \mathbf{k}, s'|\rangle u_{s'}^\dagger(\mathbf{p} - \mathbf{k}) \alpha^\mu u_r(\mathbf{p}).
\]
The renormalized self energy is the average of this operator in the state $a$,

$$\Delta_{SE}^{\text{Renorm}} = \sum_{pp'r'} \langle a|pr\rangle \langle pr|\Sigma^{\text{Renorm}}|p'r'\rangle \langle p'r'|a \rangle. \quad (2.74) \quad \text{SERenAv}$$

![Diagram](image)

Figure 2.5: Graphical illustration of the renormalization of the first-order electron $\Sigma^{\text{Ren}}$. The second diagram represents the average of the free-electron self-energy in the bound state $|a\rangle$.

**So far, no approximations have been made.** Let us now assume that the bound states $|t\rangle$ contain only positive free-electron components when $\varepsilon_t > 0$ and vice versa, i.e., $\text{sgn}(\varepsilon_t) = \text{sgn}(s)$. Then

$$\langle pr|\Sigma^{\text{Renorm}}|p'r'\rangle = -\frac{e^2 c}{2\varepsilon_0} u_k^\dagger(p) \alpha_\mu \sum_s \int \frac{d^3 k}{(2\pi)^3} \frac{1}{k} u_s(p-k) \langle p-k, s|t \rangle$$

$$\times \left[ \frac{1}{\varepsilon_a - \varepsilon_t + ck \text{sgn}(s)} - \frac{1}{\varepsilon_{p,r} - \varepsilon_{p,k,s} - ck \text{sgn}(s)} \right] \langle t|p' - k, s \rangle u_k^\dagger(p' - k) \alpha_\mu u_{r'}(p'). \quad (2.75) \quad \text{SERen2}$$

or using (2.39)

$$\langle pr|\Sigma^{\text{Renorm}}|p'r'\rangle = -\frac{e^2 c}{2\varepsilon_0} u_k^\dagger(p) \alpha_\mu \sum_s \int \frac{d^3 k}{(2\pi)^3} \frac{1}{k} u_s(p-k)$$

$$\times \left[ \frac{1}{\varepsilon_a - \varepsilon_t - ck \text{sgn}(s)} - \frac{1}{\varepsilon_{p,r} - \varepsilon_{p,k,s} - ck \text{sgn}(s)} \right] \langle p' - k, s|u_k^\dagger(p' - k) \alpha_\mu u_{r'}(p'). \quad (2.76) \quad \text{SERen3}$$

As a test of the general treatment, we let $k \to 0$ and neglect negative energy contributions. Then $u_s(p)|p, s|t \rangle$ in (2.74) becomes the fourier component $|p|t\rangle$

$$\langle pr|\Sigma^{\text{Renorm}}|p'r'\rangle = -\frac{e^2 c}{2\varepsilon_0} u_k^\dagger(p) \alpha_\mu \int \frac{d^3 k}{(2\pi)^3} \frac{1}{k} \langle p|t \rangle$$

$$\times \left[ \frac{1}{\varepsilon_a - \varepsilon_t - ck} + \frac{1}{ck} \right] (t|p') \alpha_\mu u_{r'}(p'). \quad (2.77)$$

and after integrating over the angular part of $k$ (see Appendix $\text{Fh:FT}$) and eliminating the scalar part of $\alpha_\mu \alpha^\mu$ we retrieve the Bethe result (2.66)

$$\langle p|\Sigma^{\text{Renorm}}|p'\rangle = -\frac{e^2}{2\varepsilon_0} \int \frac{d^3 k}{(2\pi)^3} \frac{1}{k^2} \alpha_\mu(|p|t) \left[ \frac{\varepsilon_a - \varepsilon_t}{\varepsilon_a - \varepsilon_t - ck} \right] \langle t|p'\rangle \alpha^\mu$$

$$= \frac{e^2}{4\pi^2 \varepsilon_0 r_1 2} \int dk \alpha \cdot \langle p|t \rangle \left[ \frac{\varepsilon_a - \varepsilon_t}{\varepsilon_a - \varepsilon_t - ck} \right] \langle t|p'\rangle \alpha_0. \quad (2.78)$$
In order to make contact with other treatment we will split the operator difference in (2.76) into two parts. In the first part we replace $\varepsilon_p r$ by $\varepsilon_a$, giving

$$\frac{1}{\varepsilon_a - \hat{h}_D - ck \text{sgn}(s)} - \frac{1}{\varepsilon_p r - \hat{h}_D - ck \text{sgn}(s)} = \frac{1}{\varepsilon_a - \hat{h}_D - ck \text{sgn}(s)} U \frac{1}{\varepsilon_a - \hat{h}_D - ck \text{sgn}(s)} = \frac{U}{\varepsilon_a - \hat{h}_D - ck \text{sgn}(s)} \frac{1}{\varepsilon_a - \hat{h}_D - ck \text{sgn}(s)} + \frac{1}{\varepsilon_a - \hat{h}_D - ck \text{sgn}(s)} U \frac{1}{\varepsilon_a - \hat{h}_D - ck \text{sgn}(s)} \frac{1}{\varepsilon_a - \hat{h}_D - ck \text{sgn}(s)}.$$  

The second part corrects for the difference,

$$\frac{1}{\varepsilon_a - \hat{h}_D - ck \text{sgn}(s)} - \frac{1}{\varepsilon_p r - \hat{h}_D - ck \text{sgn}(s)} = \frac{1}{\varepsilon_a - \hat{h}_D - ck \text{sgn}(s)} \frac{\varepsilon_p r - \varepsilon_a}{\varepsilon_p r - \hat{h}_D - ck \text{sgn}(s)} U \frac{1}{\varepsilon_p r - \hat{h}_D - ck \text{sgn}(s)}.$$  

25
The first part becomes after transforming to the coordinate representation

\[
\Delta_{SE;1}^{\text{Renorm}} = -\frac{e^2 c}{2\varepsilon_0} \langle a|\alpha_\mu|x\rangle \int \frac{d^3k}{(2\pi)^3} \frac{1}{k} e^{i k \cdot (x-x')} \\
\times \left| \frac{1}{\varepsilon_a - h_D - ck \text{sgn}(s)} \right| U \left| \frac{1}{\varepsilon_a - h_D^{\text{Free}} - ck \text{sgn}(s)} \right| \langle x'|\alpha_\mu|a\rangle \langle a|\alpha_\mu|x\rangle (2.81) \]

The second part represents the difference between the free-electron self energy inserted on a free-electron line and a bound-electron line.
Appendix A

Notations

A.1 Four-component vector notations

Contravariant vector: \( x = x^\mu = (x^0, \mathbf{x}) = (ct, \mathbf{x}) \)  
(\( \mu = 0,1,2,3 \) and \( \mathbf{x} \) is the three-dimensional coordinate vector)

Covariant vector: \( x_\mu = g_{\mu\nu} x^\nu = (x_0, -\mathbf{x}) = (ct, -\mathbf{x}) \)  
(Summation over repeated indices.)

Four-dimensional differential:  
\[ d^4x = cdt - d^3\mathbf{x} \quad \text{and} \quad d^3\mathbf{x} = dx dy dz \]

Metric tensor: \( g_{ij} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \)

Scalar product: \( ab = a^\mu b_\mu = a^0 b_0 - \mathbf{a} \cdot \mathbf{b} \)

Gradient operator (covariant): \( \partial_\mu = \frac{\partial}{\partial x^\mu} = \left( \frac{1}{c} \frac{\partial}{\partial t}, \mathbf{\nabla} \right) \)

Gradient operator (contravariant): \( \partial^\mu = \frac{\partial}{\partial x_\mu} = \left( \frac{1}{c} \frac{\partial}{\partial t}, -\mathbf{\nabla} \right) \)

Four-dimensional divergence: \( \partial_\mu A^\mu = \frac{1}{c} \frac{\partial A^0}{\partial t} + \mathbf{\nabla} \cdot \mathbf{A} = \mathbf{\nabla} A \)

d’Alembertian operator: \( \Box = \partial^\mu \partial_\mu = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \mathbf{\nabla}^2 = \mathbf{\nabla}^2 \)
A.2 Alpha and gamma matrices

The alpha matrices are related to the standard gamma matrices by

\[ \gamma^\mu = \gamma^0 \alpha^\mu ; \quad \alpha^\mu = (1, \alpha) ; \quad \gamma^0 = \beta ; \quad \alpha = \gamma^0 \gamma = -\gamma \gamma^0 \]

where \( \alpha, \beta \) are the Dirac matrices.

\[ \hat{\mu} = a_\mu \gamma^\mu = a_0 \gamma^0 - \mathbf{a} \cdot \mathbf{\gamma} \]
Appendix B

Representations of states and operators

B.1 The Dirac delta function

We consider the integral
\[
\int_{-L/2}^{L/2} dx \, e^{ikx} .
\] (B.1)

Assuming periodic boundary conditions, \( e^{-iLx/2} = e^{iLx/2} \), limits the possible \( k \) values to \( k = k_n = 2\pi n/L \). Then
\[
\frac{1}{L} \int_{-L/2}^{L/2} dx \, e^{ik_n x} = \delta_{k_n, 0} = \delta(k_n, 0),
\] (B.2)

where \( \delta_{n,m} \) is the Kronecker delta factor
\[
\delta_{n,m} = \begin{cases} 
1 & \text{if } m = n \\
0 & \text{if } m \neq n.
\end{cases}
\] (B.3)

If we let \( L \to \infty \), then we have to add a ’damping factor’ \( e^{-\eta|x|} \), where \( \eta \) is a small positive number, in order to make the integral meaningful,
\[
\int_{-\infty}^{\infty} dx \, e^{ikx} e^{-\eta|x|} = \frac{2\eta}{k^2 + \eta^2} = 2\pi \Delta_\eta(k) .
\] (B.4)

In the limit \( \eta \to 0 \), we have
\[
\lim_{\eta \to 0} \Delta_\eta(k) = \lim_{\eta \to 0} \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \, e^{ikx} e^{-\eta|x|} = \delta(k),
\] (B.5)

which can be regarded as a definition of the Dirac delta function, \( \delta(k) \). Formally, we write this relation as
\[
\frac{1}{2\pi} \int_{-\infty}^{\infty} dx \, e^{ikx} = \delta(k)
\] (B.6)

\( ^1 \)This may for typographical reasons sometimes be written \( \delta(n, m) \), not to be confused by the delta function \( \delta(x) \).
The $\Delta$ function also has the following properties

$$\lim_{\eta \to 0} \pi \eta \Delta_\eta(x) = \delta_{x,0}$$

$$\int_\infty^\infty dx \, \Delta_\eta(x-a)\Delta_\kappa(x-b) = \Delta_\eta+\kappa(a-b). \quad \text{(B.7)}$$

In three dimensions equation (IntL B.2) goes over into

$$\frac{1}{V} \int_V d^3x \, e^{ik_n \cdot x} = \delta^3(k_n,0) = \delta(k_{nx},0) \delta(k_{ny},0) \delta(k_{nz},0). \quad \text{(B.8)}$$

In the limit where the integration is extended over the entire three-dimensional space, we have in analogy with (IntL B.6)

$$\int d^3x \, e^{ik \cdot x} = \delta^3(k) \quad \text{(B.9)}$$

### B.2 Dirac notations

The *ket vector* $|a\rangle$ is a *vector representation* of the state $a$ in a certain basis,

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}. \quad \text{(B.10)}$$

The corresponding *bra vector* $\langle a|$ is

$$\langle a| = (a_1^*, a_2^*, \cdots). \quad \text{(B.11)}$$

The basis states are represented by unit vectors $|j\rangle$

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix} \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ \vdots \end{pmatrix} \quad \text{etc.} \quad \text{(B.12)}$$

The basis set need not be numerable but can also form a *continuum*.

The *scalar product* of two vectors is denoted $\langle a|b\rangle$ and defined

$$\langle a|b\rangle = \sum_t a_t^* b_t. \quad \text{(B.13)}$$

It follows from the definitions that

$$a_t = \langle t|a\rangle \quad \text{and} \quad a_t^* = \langle a|t\rangle. \quad \text{(B.14)}$$

Then the scalar product (B.13) can also be expressed

$$\langle a|b\rangle = \sum_t \langle a|t\rangle \langle t|b\rangle = \langle a|t\rangle \langle t|b\rangle. \quad \text{(B.15)}$$
With the Dirac notations, a summation over intermediate states will always be understood. Since the relation (B.15) holds for arbitrary vectors, we have the formal identity

\[ |t⟩⟨t| \equiv 1 \]  \hspace{1cm} \text{(B.16) Id}

which is known as the resolution of the identity.

The coordinate representation of the ket vector |a⟩ is denoted ⟨x|a⟩ and is identical to the state (Schrödinger) function

\[ ⟨x|a⟩ = Ψ_a(x); \quad ⟨a|x⟩ = Ψ_a^*(x) \]  \hspace{1cm} \text{(B.17) StateFcn}

(assuming for simplicity that there is only a single particle in the system). In analogy with (B.15) the scalar product becomes

\[ ⟨a|b⟩ = \int d^3x \langle a|x⟩⟨x|b⟩ = \int d^3x Ψ_a^*(x) Ψ_b(x). \]  \hspace{1cm} \text{(B.18) ScalProd3}

Also here we shall assume that an integration is always understood, i.e.,

\[ ⟨a|b⟩ = ⟨a|x⟩⟨x|b⟩, \]  \hspace{1cm} \text{(B.19) ScalProd3}

which leads to the formal identity

\[ |x⟩⟨x| ≡ 1 \]  \hspace{1cm} \text{(B.20) Id2}

From the closure property we have

\[ \sum_t φ_t^*(x)φ_t(x') = ⟨x|t⟩⟨t|x'⟩ = ⟨x|I|x'⟩ = δ^3(x - x'), \]  \hspace{1cm} \text{(B.21) ClosProp}

which with the identity (B.16) leads to the formal identity

\[ ⟨x|x'⟩ = δ^3(x - x') \]  \hspace{1cm} \text{(B.22) ClosProp2}

This is also the coordinate representation of the identity operator (B.16). Note that here there is no integration over the space coordinates. Setting \(x = x'\) and integrating, leads to unity on both sides.

The results above hold also when the basis states form a continuum, as can be illustrated by the momentum eigenstates (B.27),

\[ ⟨x|pr⟩⟨pr|x'⟩ = \sum_r \int d^3p \ φ_r^*(x) φ_{pr}(x') = \sum_r u_r^J(p) u_r(p) \int \frac{d^3p}{(2π)^3} e^{ip(x-x')}, \]  \hspace{1cm} \text{(B.23) PlaneW}

which using (B.30) and (B.9) leads to

\[ |pr⟩⟨pr| ≡ 1 \]  \hspace{1cm} \text{(B.24) Id3}

Here, a summation over \(r\) and an integration over \(p\) is understood.

Similarly, we find

\[ ⟨pr|I|pr'⟩ = ⟨pr|x⟩⟨x|I|x'⟩⟨x'|p'⟩ = \frac{1}{(2π)^3} \int d^3x d^3x' δ^3(x - x') e^{ixr(p-p')} = δ_{rr'} δ^3(p - p'), \]  \hspace{1cm} \text{(B.25) ClosProp4}

using (B.21) and (B.9).
B.3 Momentum eigenfunctions

(See also Appendix sec:Dirac)

The Dirac eqn for a free particle
\[ (c\alpha \cdot \hat{p} + \beta m c^2) \phi_{pr}(x) = \varepsilon_{pr} \phi_{pr}(x) \]  
(B.26)  
Dirac

has the normalized plane-wave solutions
\[ \phi_{pr}(x) = \sqrt{\frac{1}{V}} u_r(p) e^{i p \cdot x} \rightarrow (2\pi)^{-3/2} e^{i p \cdot x} u_r(p), \]  
(B.27)  
PlaneW

which are eigenfunctions of the momentum operator
\[ \hat{p} = -i \nabla; \phantom{.} \hat{p} \phi_{pr}(x) = p \phi_{pr}(x). \]

\( r = + \) or \( - \) correspond to positive and negative energies, respectively. The momentum operator \( \hat{p} \) should be distinguished from the momentum vector \( p \).

According to (uq C.10) we have
\[ u_+(p) = N \left( \frac{p_0 + mc}{\sigma \cdot p} \right); \quad u_-(p) = N \left( \frac{-\sigma \cdot p}{p_0 + mc} \right); \quad N = \frac{1}{\sqrt{2p_0(p_0 + mc)}} \]  
(B.28)  
up

\[ E_{pr} = |\varepsilon_{pr}| = cp_0; \quad p_0 = \sqrt{p^2 + m^2 c^2} \]  
(B.29)  
NormII

With the normalization (C.24b) we have
\[ u_r^\dagger(p) u_{r'}(p) = \delta_{rr'} \]  
(B.30)  
I2

The projection operators are with this normalization (udag C.33a), (vdag C.33b)
\[ \Lambda_+(p) = u_+(p) u_+^\dagger(p) = \frac{p_0 + \alpha \cdot p + \beta mc}{2p_0} \]  
(B.31a)  
\[ \Lambda_-(p) = u_-(p) u_-^\dagger(p) = \frac{p_0 - \alpha \cdot p - \beta mc}{2p_0} \]  
(B.31b)  
\[ \sum_r u_r(p) u_r^\dagger(p) = u_+(p) u_+^\dagger(p) + u_-(p) u_-^\dagger(p) = I (4 \times 4). \]  
(B.32)  
uID

Note that \( \Lambda_\pm(p) \) are functions of the momentum \( p \) and act as projection operators only when operating on momentum eigenfunctions. The true projection operators, \( \Lambda_\pm(\hat{p}) \), are obtained by replacing \( p \) by the operator \( \hat{p} \).

B.4 Representation of states

Coordinate representation of a state \( |a\rangle \): \( \phi_a(x) = \langle x | a \rangle \)

Momentum representation of a state \( |a\rangle \): \( \phi_a(p) = \langle pr | a \rangle \)
The momentum representation is the expansion coefficient of the state in momentum eigenfunctions

\[ \phi_{pr}(x) = \langle x|pr \rangle = \sqrt{\frac{1}{V}} u_r(p) e^{ip \cdot x} \quad \text{(B.33)} \]

\[ \langle x|a \rangle = \sum_{pr} \langle x|pr \rangle \langle pr|a \rangle \quad \text{(B.34)} \]

\[ \langle pr|a \rangle = \int d^3x \langle pr|x\rangle \langle x|a \rangle = \sqrt{\frac{1}{V}} \int d^3x e^{-ip \cdot x} u^\dagger_r(p) \phi_a(x). \quad \text{(B.35)} \]

In the limit of continuous momenta, \( \sum_{pr} \) is replaced by \( \int \frac{d^3p}{(2\pi)^3} \) and \( \sqrt{\frac{1}{V}} \) by \( (2\pi)^{-3/2} \).

The momentum representation is distinct from the Fourier transform. The latter is defined as

\[ \langle p|a \rangle = \sum_r u_r(p) \langle pr|a \rangle = \sqrt{\frac{1}{V}} \int d^3x e^{-ip \cdot x} \phi_a(x) \]

\[ \rightarrow (2\pi)^{3/2} \int d^3x e^{-ip \cdot x} \phi_a(x), \quad \text{(B.36)} \]

using the identity \( p \mapsto \hat{p} \).

### B.5 Representation of Operators

**Coordinate representation** of an operator \( \hat{O} : O(x_2, x_1) = \langle x_2|\hat{O}|x_1 \rangle \)

**Momentum representation** of an operator \( \hat{O} : \hat{O}(p_2 r_2, p_1 r_1) = \langle p_2 r_2|\hat{O}|p_1 r_1 \rangle \). Transformation between the representations

\[ \langle p_2 r_2|O|p_1 r_1 \rangle = \int d^3x_2 d^3x_1 \langle p_2 r_2|x_2\rangle \langle x_2|O|x_1\rangle \langle x_1|p_1 r_1 \rangle. \quad \text{(B.37)} \]

The corresponding Fourier transform is according to \( \text{FT} \)

\[ \sum_{r_1 r_2} u_{r_2}(p_2) \langle p_2 r_2|O|p_1 r_1 \rangle u^\dagger_{r_1}(p_1). \quad \text{(B.38)} \]

Any operator with a complete set of eigenstates can be expanded as

\[ \hat{O} = |j\rangle \varepsilon_j \langle j| \quad \text{where} \quad \hat{O}|j\rangle = \varepsilon_j |j\rangle, \quad \text{(B.39)} \]

using the summation convention \( \text{OpExp} \). This gives the coordinate and momentum representations

\[ \langle x_2|O|x_1 \rangle = \langle x_2|j \rangle \varepsilon_j \langle j|x_1 \rangle \quad \text{(B.40a)} \]

\[ \langle p_2 r_2|\hat{O}|p_1 r_1 \rangle = \langle p_2, r_2|j \rangle \varepsilon_j \langle j|p_1 r_1 \rangle. \quad \text{(B.40b)} \]

The identity operator \( \text{Ident} \)

\[ I = |j\rangle \langle j| \quad \text{(B.41)} \]

has the coordinate and momentum representations

\[ \langle x_2|I|x_1 \rangle = \langle x_2|j \rangle \langle j|x_1 \rangle = \delta^3(x_2 - x_1) \quad \text{(B.42a)} \]

\[ \langle p_2 r_2|I|p_1 r_1 \rangle = \langle p_2 r_2|j \rangle \langle j|p_1 r_1 \rangle = \delta^3(p' - p) \delta_{r',r}. \quad \text{(B.42b)} \]
Appendix C

Dirac free particle

C.1 Solutions to the Dirac equation

The time-dependent Dirac eqn for a free particle is

$$i \frac{\partial \psi_q(x)}{\partial t} = (c \alpha \cdot \hat{p} + \beta m_e c^2) \psi_q(x)$$  \hfill (C.1) \text{DiracFree}

or

$$\left(\frac{i \beta}{c} \frac{\partial}{\partial t} - \beta \alpha \cdot \hat{p} - m_e c\right) \psi_q(x) = 0$$

$$(\gamma^0 \hat{p}_0 - \gamma \cdot \hat{p} - m_e c) \psi_q(x) = 0,$$ \hfill (C.2) \text{DiracFree2}

where (see Chapter \text{ch:Not})

$$\hat{p} = \gamma^\mu \hat{p}_\mu = \gamma^0 \hat{p}_0 - \gamma \cdot \hat{p}; \quad \hat{p}_0 = \frac{i}{c} \frac{\partial}{\partial t}; \quad \hat{p} = -i \nabla$$

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}; \quad \beta = \gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \gamma = \gamma^0 \alpha = \begin{pmatrix} 0 & \sigma \\ -\sigma & 0 \end{pmatrix}$$

$$\alpha = \gamma^0 \gamma = -\gamma^0$$

Separation of the wave function into space and time parts

$$\psi_q(x) = \phi_q(x) e^{-i \varepsilon_q t}$$  \hfill (C.3) \text{DiracSp}

leads to the time-independent eqn

$$\hat{h}_D^{\text{free}}(\hat{p}) \phi_q(x) = (c \alpha \cdot \hat{p} + \beta m_e c^2) \phi_q(x) = \varepsilon_q \phi_q(x)$$  \hfill (C.4) \text{DiracP}

or

$$(\gamma^0 \varepsilon_q/c - \gamma \cdot \hat{p} - m_e c) \phi_q(x) = 0.$$ \hfill (C.5) \text{Dirac3}

\(\phi_q(x)\) is a four-component wave function, which can be represented by

$$\phi_q(x) \propto \frac{1}{\sqrt{V}} u_r(q) e^{i q \cdot x}; \quad \hat{p} \phi_q(x) = q \phi_q(x).$$  \hfill (C.6) \text{MomFcn}
\( q \) is a momentum vector (to be distinguished from the momentum operator \( \hat{p} \)) and \( u_r(q) \) is a four-component vector function of the momentum \( q \). For each \( q \) there are four independent solutions \( (r = 1, 2, 3, 4) \) to the Dirac eqn. The parameter \( q \) in \( \phi_q \) and \( \varepsilon_q \) represents \( q \) and \( r \) or, more explicitly,

\[
\phi_q(x) = \phi_{q,r}(x); \quad \varepsilon_q = \varepsilon_{q,r}
\]

With the wave function \( \text{MomFcn} \), Eq. (C.3) Dirac leads to

\[
(\gamma^0 \varepsilon_q/c - \gamma \cdot q - m_e c) u_r(q) = 0
\]

or

\[
\begin{pmatrix}
\varepsilon_q/c - m_e c & -\boldsymbol{\sigma} \cdot \boldsymbol{q} \\
\boldsymbol{\sigma} \cdot \boldsymbol{q} & -\varepsilon_q/c - m_e c
\end{pmatrix}

u_r(q) = 0,
\]

(C.7) Dirac

where each element is a \( 2 \times 2 \) matrix. This eqn has two solutions for each \( q \):

\[
u_+ (q) = N_+ \begin{pmatrix}
\varepsilon_q/c + m_e c \\
\boldsymbol{\sigma} \cdot \boldsymbol{q}
\end{pmatrix}; 
\quad u_- (q) = N_- \begin{pmatrix}
-\varepsilon_q/c + m_e c \\
-\boldsymbol{\sigma} \cdot \boldsymbol{q}
\end{pmatrix}
\]

(C.8) DiracSol

corresponding to positive \( (r = 1, 2) \) and negative \( (r = 3, 4) \) eigenvalues, respectively. Defining \( q_0 \) by

\[
|\varepsilon_q| = E_q = cq_0; \quad q_0 = \sqrt{q^2 + m_e c^2}
\]

(C.9) \( q_0 \)
gives

\[
u_+ (q) = N_+ \begin{pmatrix}
q_0 + m_e c \\
\boldsymbol{\sigma} \cdot \boldsymbol{q}
\end{pmatrix}; 
\quad u_- (q) = N_- \begin{pmatrix}
-q_0 + m_e c \\
-\boldsymbol{\sigma} \cdot \boldsymbol{q}
\end{pmatrix}
\]

(C.10) \( u_q \)
The corresponding eigenfunctions \( \text{MomFcn} \) are

\[
\phi_{q,+} (x) \propto \frac{1}{\sqrt{V}} u_+ (q) e^{iq \cdot x}; \quad \phi_{q,-} (x) \propto \frac{1}{\sqrt{V}} u_- (q) e^{iq \cdot x}.
\]

(C.11) \( \text{MomFcn2} \)

Note that the equation

\[
(\hat{p} - m_e c) \phi_q, (x) = (\gamma^0 \hat{p}_0 - \gamma \cdot \hat{p} - m_e c) \phi_q, (x) 
\]

\[
= (\gamma^0 q_0 - \gamma \cdot q - m_e c) \phi_q, (x) = 0
\]

(C.12a) \( \text{MomPos} \)

with \( \hat{p}_0 = \sqrt{\hat{p}^2 + m_e c^2} \) is satisfied by the positive energy solutions only, although the corresponding time-dependent eqn (C.2) is valid for all solutions, when is defined as a time derivative. The corresponding negative energy solutions satisfy the

\[
(\gamma^0 \hat{p}_0 - \gamma \cdot \hat{p} - m_e c) \phi_q, (x) = (\gamma^0 q_0 - \gamma \cdot q - m_e c) \phi_q, (x) = 0
\]

(C.12b) \( \text{MomNeg} \)
or, after changing \( q \) to \(-q\),

\[
(\gamma^0 \hat{p}_0 - \gamma \cdot \hat{p} - m_e c) \phi_{q,-} (x) = (\gamma^0 q_0 + \gamma \cdot q - m_e c) \phi_{q,-} (x) = 0,
\]

where

\[
\phi_{q,-} (x) \propto \frac{1}{\sqrt{V}} u_- (-q) e^{-iq \cdot x} = \frac{1}{\sqrt{V}} v(q) e^{-iq \cdot x}
\]

(C.13) \( \text{MomNeg2} \)
The vectors

\[
u(q) = u_+(q) \quad \text{and} \quad v(q) = u_- (-q) = N_- \begin{pmatrix}
\boldsymbol{\sigma} \cdot \boldsymbol{q} \\
q_0 + m_e c
\end{pmatrix}
\]

(C.14) \( u \)

then satisfy the eqns

\[
(\hat{q} - mc) u(q) = 0 \quad \text{and} \quad (\hat{q} + mc) v(q) = 0,
\]

(C.15) \( u \)veqns

where \( q_0 \) is given by (C.9). Note that the negative energy solution corresponds here to the momentum \(-q\) for the electron (or \(+q\) for the hole/positron).
C.2 Projection operators

It follows from (C.15) that
\[(\gamma + m_e c) u(q) = 2m_e c u(q),\]
which implies that
\[\Lambda_+(q) = (\gamma + m_e c)/2m_e c \quad (C.16a) \]  
has the property of a projection operator in momentum space, projecting out the two positive energy solutions of the four solutions corresponding to a given \(q\). Similarly,
\[\Lambda_- (q) = (-\gamma + m_e c)/2m_e c \quad (C.16b) \]
projects out the negative solutions,
\[\Lambda_+ (q) u(q) = u(q) \quad \text{and} \quad \Lambda_+ (q) v(q) = 0 \quad (C.17a) \]
and
\[\Lambda_- (q) u(q) = 0 \quad \text{and} \quad \Lambda_- (q) v(q) = v(q) \quad (C.17b) \]
\[\Lambda_+ (q) + \Lambda_- (q) = 1. \quad (C.18) \]

It should be noted that the corresponding momentum operators, operating in coordinate space,
\[\Lambda_\pm (\hat{p}) = (\pm \gamma \cdot \hat{p} + m_e c)/2m_e c \quad (C.19) \]
do not have the corresponding properties when operating on the eigenfunctions \(\phi_{q\pm}\). For instance, with \(\hat{p}_0 = \sqrt{\hat{p}^2 + m_e^2 c^2}\) and \(q_0 = \sqrt{q^2 + m_e^2 c^2}\)
\[\Lambda_+ \phi_{q-} (x) \propto (\gamma^0 \hat{p}_0 - \gamma \cdot \hat{p} + m_e c) \phi_{q-} (x) = (\gamma^0 q_0 - \gamma \cdot q + m_e c) \phi_{q-} (x) \neq 0 \]
and
\[\Lambda_+ \phi_{-q+} (x) \propto (\gamma^0 \hat{p}_0 - \gamma \cdot \hat{p} + m_e c) \phi_{-q+} (x) = (\gamma^0 q_0 + \gamma \cdot q + m_e c) \phi_{-q+} (x) \neq 0 \]
Instead, we can get the correct projection operators in coordinate space from (C.5),
\[(\pm \gamma^0 \hat{p}_0 - \gamma \cdot \hat{p} - m_e c) \phi_{q\pm} (x) = 0. \quad (C.20) \]
It then follows that the operators
\[\Lambda_\pm (\hat{p}) = (\hat{p}_0 \pm \gamma_0 (\gamma \cdot \hat{p} + m_e c))/2\hat{p}_0 = (\hat{p}_0 \pm (\alpha \cdot \hat{p} + \gamma_0 m_e c))/2\hat{p}_0 \quad (C.21) \]
have the following projection properties in coordinate space
\[\Lambda_\pm^+(\hat{p}) \phi_{q+} (x) = \phi_{q+} (x) \quad \text{and} \quad \Lambda_\pm^+(\hat{p}) \phi_{q-} (x) = 0 \quad (C.22) \]
etc.
C.3 Normalization

The norm of the vectors \( u_+^\dagger(q) u_+(q) = |N_+|^2(q_0 + mc, \sigma \cdot q) \prod (q_0 + mc, \sigma \cdot q) \)
\[ = |N_+|^2(q_0^2 + m^2c^2 + (\sigma \cdot q)^2 + 2q_0 mc) I(2 \times 2) \]
\[ = |N_+|^22q_0(q_0 + mc) I(2 \times 2) = u_+^\dagger(q) u_-(q) \]
using \( (\sigma \cdot q)^2 = q_0^2 - m^2c^2 \). Two different normalization schemes are used in the literature

I. \[ u_{r,r}^\dagger(q) u_r(q) = \delta_{r,r'} \frac{q_0}{mc} \]
II. \[ u_{r,r}^\dagger(q) u_r(q) = \delta_{r,r'}. \]

The first scheme is used, for instance, in ref. [1], but we shall apply the second scheme.

Normalization I

This scheme gives
\[ N_+ = N_- = \frac{1}{\sqrt{2mc(q_0 + mc)}} \] (C.25)
and the normalized eigenfunctions \( \phi_{N0}^2 \)
\[ \phi_{q\pm}(q) = \sqrt{\frac{mc}{q_0 V}} u_{q\pm}(q) e^{iq \cdot x}. \] (C.26)

The adjoint vectors are defined
\[ \bar{u}(q) = \bar{u}_+(q) = u_+^\dagger(q)\gamma_0 = N_+(q_0 + mc, -\sigma \cdot q) \] (C.27a)
\[ \bar{v}(q) = \bar{u}_-(q) = u_-^\dagger(q)\gamma_0 = N_-(\sigma \cdot q, -q_0 - mc) \] (C.27b)
\[ \bar{u}(q) u(q) = |N_+|^2(q_0^2 + m^2c^2 - (\sigma \cdot q)^2 + 2q_0 mc) \]
\[ = |N_+|^22mc(q_0 + mc) I(2 \times 2) = -\bar{v}(q)v(q). \] (C.28)

It also follows that
\[ u(q) \bar{u}(q) = |N_+|^2 \prod (q_0 + mc, \sigma \cdot q) (q_0 + mc, -\sigma \cdot q) \]
\[ = \frac{1}{2mc(q_0 + mc)} \prod (q_0 + mc)^2 - (q_0 + mc) \sigma \cdot q \]
\[ = \frac{1}{2mc} \prod (q_0 + mc, -\sigma \cdot q) = \frac{\gamma + mc}{2mc} = \Lambda_+(q) \] (C.29a)

and similarly
\[ v(q) \bar{v}(q) = \frac{\gamma - mc}{2mc} = -\Lambda_-(q). \] (C.29b)

This gives
\[ u(q) \bar{u}(q) - v(q) \bar{v}(q) = I(4 \times 4). \] (C.30)
Normalization II

The normalization \( N_+ = N_- = \frac{1}{\sqrt{2q_0 (q_0 + m_e c)}} \) (C.31) gives

\[ N_+ + N_- = 1 \]

\[ \sqrt{2q_0 (q_0 + m_e c)} (q_0 + m_e c, \sigma \cdot q) \]

and the normalized eigenfunctions (MomFcn2)

\[ \phi_{q \pm} (x) = \frac{1}{\sqrt{V}} u_{q \pm} (q) e^{i q \cdot x}. \] (C.32) NormFcnII

In analogy with (baruuI C.28) we then get

\[ u_+ (q) u_+^\dagger (q) = \frac{1}{2q_0} \begin{pmatrix} q_0 + m_e c & \sigma \cdot q \\ \sigma \cdot q & q_0 + m_e c \end{pmatrix} = \frac{q_0 + \alpha \cdot q + \beta m_e c}{2q_0} = \Lambda_+ (q) \] (C.33a) uudag

and similarly

\[ u_- (q) u_-^\dagger (q) = \frac{1}{2q_0} \begin{pmatrix} q_0 - m_e c & -\sigma \cdot q \\ -\sigma \cdot q & q_0 + m_e c \end{pmatrix} = \frac{q_0 - \alpha \cdot q - \beta m_e c}{2q_0} = \Lambda_- (q) \] (C.33b) vvdag

This gives the analogue of (vvdagID)

\[ u_+ (q) u_+^\dagger (q) + u_- (q) u_-^\dagger (q) = I (4 \times 4). \] (C.34) uudagID

We also observe that the expressions (ubaruu I C.29a), (vbarv C.29b)) have the same form as the projection operators in coordinate space (ProjOp3 C.21), i.e.,

\[ \Lambda_\pm (\hat{p}) = u_\pm (\hat{p}) u_\pm^\dagger (\hat{p}). \] (C.35) ProjOpCoord

In the following we shall use the normalization II, where the basic formulas are

\[ \phi_{q \pm} (x) = \sqrt{\frac{1}{V}} u_{q \pm} (q) e^{i q \cdot x} \]

\[ u_{r \pm} (q) = \delta_{r, r'} \]

\[ \sum_{r} u_{r} (q) u_{r}^\dagger (q) = I (4 \times 4) \]
The coordinate representation of the free-electron propagator is, using the wave functions (C.32) in the normalization II, given by

\[ S^\text{Free}_F(x, x_1) = \sum_{q,r} \phi_{q,r}(x) \phi_{q,r}(x_1) = \frac{1}{V} \sum_{q,r} u_r(q) u_r^\dagger(q) \frac{e^{iq(x-x')}}{z - \varepsilon_{q,r}(1 - i\eta)} \]

\[ \rightarrow \int \frac{d^3q}{(2\pi)^3} \sum_r u_r(q) u_r^\dagger(q) \frac{e^{iq(x-x')}}{z - \varepsilon_{q,r}(1 - i\eta)} \]

\[ = \int \frac{d^3q}{(2\pi)^3} \left[ u_+(q) u_+^\dagger(q) \frac{1}{z - E_q(1 - i\eta)} + u_-(q) u_-^\dagger(q) \frac{1}{z + E_q(1 - i\eta)} \right] . \tag{C.36} \]

The expression in the square brackets is the Fourier transform of \( S^\text{Free}_F(x, x') \),

\[ S^\text{Free}_F(q, z) = u_+(q) u_+^\dagger(q) \frac{1}{z - E_q(1 - i\eta)} + u_-(q) u_-^\dagger(q) \frac{1}{z + E_q(1 - i\eta)} \]

\[ = \frac{1}{2} \left[ \frac{1}{z - E_q(1 - i\eta)} + \frac{1}{z + E_q(1 - i\eta)} \right] \]

\[ = \frac{\alpha \cdot q + \beta m_e c}{2q_0} \left[ \frac{1}{z - E_q(1 - i\eta)} - \frac{1}{z + E_q(1 - i\eta)} \right] . \tag{C.37} \]

using (C.35a). With \( q_0 = E_q/c = \sqrt{q^2 + m_e^2c^2} \) this becomes

\[ S^\text{Free}_F(q, z) = \frac{z + \alpha \cdot q + \beta m_e c^2}{z^2 - E_q^2 + i\eta} = \frac{z + \alpha \cdot q + \beta m_e c^2}{z^2 - c^2q^2 - m_e^2c^4 + i\eta} \]

\[ = \frac{1}{z - (\alpha \cdot q + \beta m_e c^2)(1 - i\eta)} . \tag{C.38} \]

or

\[ S^\text{Free}_F(q, z) = \frac{1}{z - \sqrt{q_0^2 - \alpha \cdot q - \beta m_e c^2}} . \tag{C.39} \]

where \( \sqrt{q_0^2 - \alpha \cdot q - \beta m_e c^2} \) is the momentum representation of the Dirac Hamiltonian (C.4).

Formally, (C.38) can be written in four-component form with \( z = q_0 \), where \( q_0 \) is now disconnected from \( E_q = \sqrt{c^2q^2 + m_e^2c^4} \), and using the relations (C.2)

\[ S^\text{Free}_F(q, z) = \frac{1}{c} \frac{q_0 + \alpha \cdot q + \beta m_e c}{q_0^2 - \alpha \cdot q - \beta m_e c^2 + i\eta} = \frac{1}{c} \frac{q_0 + \alpha \cdot q + \beta m_e c}{q_0^2 - \alpha \cdot q - \beta m_e c^2 + i\eta} \]

\[ = \frac{1}{c} \frac{1}{\gamma^0} = \frac{1}{c} S^\text{Free}_F(q) . \tag{C.40} \]

with

\[ S^\text{Free}_F(q) = \frac{1}{\gamma^0} . \tag{C.41} \]

The coordinate representation of the free-electron propagator (C.36) can also be expressed

\[ S^\text{Free}_F(x, x'; z) = \frac{\langle x | q, r \rangle \langle q, r | x' \rangle}{z - \varepsilon_{q,r}(1 - i\eta)} = \langle x | S^\text{Free}_F(z) | x' \rangle \]

39
where
\[
\hat{S}_F^{\text{Free}}(z) = \frac{|q, r\rangle\langle q, r|}{z - \varepsilon_{q,r}(1 - i\eta)} = \frac{1}{z - h_D^{\text{Free}}(1 - i\eta)}
\] (C.42) \(SF\text{freeOp}\)

where is the Dirac operator (C.4).

The momentum representation of the operator (C.42), which is obviously diagonal, is given by the matrix representation with momentum eigenfunctions as basis functions
\[
\langle q, r | \hat{S}_F^{\text{Free}}(z) | q, r \rangle = \langle q, r | \frac{1}{z - h_D^{\text{Free}}(1 - i\eta)} | q, r \rangle = \frac{1}{z - \varepsilon_{q,r}(1 - i\eta)},
\] (C.43) \(SF\text{matrix}\)

which is distinct from (C.38). The corresponding *fourier transform* is according to (B.38) and (C.34)
\[
\langle q | \hat{S}_F^{\text{Free}}(z) | q \rangle = \sum_r u_r(q) \langle q | \frac{1}{z - h_D^{\text{Free}}(1 - i\eta)} | q \rangle u_r^\dagger(q),
\] (C.44) \(SF\text{FT}\)

which is identical to (C.37) and (C.38).
Appendix D

The free-electron self energy

The wave function for the free electron is in normalization II given by (A5.32) $\psi_{q+}(x) = u_{q+}(q) e^{i q \cdot x}$ The Feynman amplitude for the first-order free-electron self energy is $M = e^{2c(x^2)} \alpha_{nm} \psi_{q+}(x_1) DF_{nm}(x_2 - x_1, z)$ (A6.1) where the free-electron propagator is from (A5.36) $SF(x_2, x_1, Eq - z) = e^{i q \cdot (x_2 - x_1)}$ (A6.2) and the photon propagator in the Feynman gauge (A3.13) $DF_{nm}(x_2 - x_1, z) = - g_{nm}$ (A6.3) Integration over $d^3x_1$ and $d^3x_2$ gives $M = \alpha_{nm} u_{q+}(q) = u_{q+}(q)$ (A6.4) where is the free-electron self energy in the momentum representation. Using the relations $\alpha_{nm} = -2 \alpha_{nm}$, $\alpha_{nm} \alpha_{nm} = -2 \alpha_{nm}$, $\alpha_{nm} \alpha_{nm} = -2 \alpha_{nm}$, we then get $\alpha_{nm} = (A6.5)$ With $Eq = cq_0$ and $z = cko$ this can be expressed $\alpha_{nm} = g_{nm}$ (A6.6) which agrees with (MS 9.20).

Alternatively, we can start from (A6.1) with the electron propagator in operator form (A5.41), $M = e^{2c(x^2)} \alpha_{nm} \psi_{q+}(x_1) DF_{nm}(x_2 - x_1, z)$ (A6.7) which gives $\alpha_{nm} \alpha_{nm} \psi_{q+}(q) = i g_{nm} \psi_{q+}(q)$ (A6.8) and this leads to the same result as before. By evaluating the integral in (A6.6), which is logarithmically divergent (A7.10), the expression (A6.4) becomes $M = u_{q+}(q) = i g_{nm} \psi_{q+}(q) = i A u_{q+}(q)$ (A6.9) where $A$ is a number which depends logarithmically on the cut-off momentum $L$ (see Appendix; Mandl- Shaw p 191; Jauch - Rohrlich p 181) $A = -$ atomic units (A6.10) With the expressions (A5.11) and the normalization II (A5.32,24), we get $M = i u_{q+}(q) = A g_{nm} \psi_{q+}(q) = A (q_0 + mc) = A (1 - ) = A (1 - + . . )$ (A6.10) This is the expectation value of $g_{nm}$ in the free-electron state $q_+, q_+ = g_{nm}$ (A6.11)
Appendix E

Evaluation of the free-electron self-energy integral

(See Mandl- Shaw sect 10.2) The free-electron self energy is according to \( (A6.6) = g \) \( (A7.1) \) In \( (A6.4) \) this operates on the \( u+(q) \) vector and in view of the eqn \( (A5.16) \), \( (-mc) u+(q) = 0 \), we can then replace by \( mc \), \( u+(q) = -go u+(q) = igo A u+(q) \) \( (A7.2) \) Regularizing the photon propagator by the substitution \( = - (A7.3) \) and using the identity \( = 2 \) \( (A7.4) \) with \( a = k^2 - t \) and \( b = k^2 - 2qk \) gives \( A = - i \) \( (A7.5) \) With the identities \( = \) \( (A7.6) \) this gives \( A = - = (2 - x) \) \( (A7.7) \) This expression is logarithmically divergent when \( L(r) \) but convergent when \( l(r) \) 0. The leading term then becomes \( A - (2 - x) \) \( (A7.8) \) and \( (2 - x) = - 3x \ln x \) \( (A7.9) \) gives \( A - (A7.10) \)
Appendix F

Some fourier transforms

F.1 Evaluation of the integral $\int \frac{d^3k}{(2\pi)^3} \frac{e^{ik\cdot r_{12}}}{q^2 - k^2 + i\eta}$

Using spherical coordinates $k = (k, \theta, \phi), (k = |k|)$, we have with $d^3k = k^2 dk \sin \Theta d\Theta d\Phi$ and $r_{12} = |x_1 - x_2|$,

$$\int \frac{d^3k}{(2\pi)^3} \frac{e^{ik\cdot (x_1 - x_2)}}{q^2 - k^2 + i\eta} = (2\pi)^{-2} \int_0^\infty \frac{k^2 dk}{q^2 - k^2 + i\eta} \int_0^\pi d\Theta \sin \Theta e^{ikr_{12} \cos \Theta} = \frac{i}{8 \pi^2 r_{12}} \int_{-\infty}^\infty dk \frac{e^{ikr_{12}} - e^{-ikr_{12}}}{k^2 - q^2 - i\eta}. \quad (F.1)$$

where we have in the last step utilized the fact that the integrand is an even function of $k$. The poles appear at $k = \pm q(1 + i\eta/2q)$. $e^{ikr_{12}}$ is integrated over the positive half-plane, which yields $-e^{\pm iqr_{12}}/(4\pi r_{12})$ with the upper sign for $q > 0$. The same result is obtained if we change the sign of the exponent in the numerator of the original integrand. Thus, we have the result

$$\int \frac{d^3k}{(2\pi)^3} \frac{e^{\pm ik\cdot (x_1 - x_2)}}{q^2 - k^2 + i\eta} = -\frac{e^{iqr_{12}}}{4\pi r_{12}}. \quad (F.2)$$

The imaginary part of the integrand, which is an odd function, does not contribute to the integral.

F.2 Evaluation of the integral $\int \frac{d^3k}{(2\pi)^3} (\alpha_1 \cdot \hat{k})(\alpha_2 \cdot \hat{k}) \frac{e^{ik\cdot r_{12}}}{q^2 - k^2 + i\eta}$

The integral appearing in the derivation of the Breit interaction (1.40) is

$$I_2 = \int \frac{d^3k}{(2\pi)^3} (\alpha_1 \cdot \hat{k})(\alpha_2 \cdot \hat{k}) \frac{e^{ik\cdot r_{12}}}{q^2 - k^2 + i\eta} = (\alpha_1 \cdot \nabla_1)(\alpha_2 \cdot \nabla_2) \int \frac{d^3k}{(2\pi)^3} \frac{1}{k^2 q^2 - k^2 + i\eta}. \quad (F.3)$$

Using (F.1), we then have

$$I_2 = \frac{i}{8 \pi^2 r_{12}} (\alpha_1 \cdot \nabla_1)(\alpha_2 \cdot \nabla_2) \int_{-\infty}^\infty dk \frac{e^{ikr_{12}} - e^{-ikr_{12}}}{k(k^2 - q^2 - i\eta)}. \quad (F.4)$$
The poles appear at \( k = 0 \) and \( k = \pm (q + i\eta/2q) \). The pole at \( k = 0 \) can be treated with half the pole value in each half plane. For \( q > 0 \) the result becomes

\[
- \frac{1}{4\pi r_{12}} \frac{e^{iqr_{12}}}{q^2}
\]

and for \( q > 0 \) the same result with \(-q\) in the exponent. The final result then becomes

\[
\int \frac{d^3k}{(2\pi)^3} (\alpha_1 \cdot \hat{k})(\alpha_2 \cdot \hat{k}) \frac{e^{i|q| r_{12}}}{q^2 - k^2 + i\eta} = - \frac{1}{4\pi r_{12}} (\alpha_1 \cdot \nabla_1)(\alpha_2 \cdot \nabla_2) \frac{e^{i|q| r_{12}}}{q^2}
\]

Assuming that our basis functions are eigenfunctions of the Dirac hamiltonian \( \hat{h}_D \) (Eq. 2.20), we can process this integral further. Then the commutator with an arbitrary function of the space coordinates is

\[
[\hat{h}_D, f(x)] = c \alpha \cdot \hat{p} f(x) + [U, f(x)].
\]

The last term vanishes, if the potential \( U \) is a local function, yielding

\[
[\hat{h}_D, f(x)] = c \alpha \cdot \hat{p} f(x) = -ic \alpha \cdot \nabla f(x).
\]

In particular

\[
[\hat{h}_D, e^{i|k| \cdot x}] = -ic \alpha \cdot \nabla e^{i|k| \cdot x} = c \alpha \cdot \hat{k} e^{i|k| \cdot x}.
\]

We then find that

\[
(\alpha \cdot \nabla)_1(\alpha \cdot \nabla)_2 e^{i|k| \cdot x} = \frac{1}{c^2} [\hat{h}_D, e^{i|k| \cdot x}]_1 [\hat{h}_D, e^{i|k| \cdot x}]_2
\]

with the matrix element

\[
\langle rs | (\alpha \cdot \nabla)_1(\alpha \cdot \nabla)_2 e^{i|k| \cdot x} | ab \rangle = q^2 e^{i|k| \cdot x},
\]

using the notation in (Eq. 2.35). The integral (IntH2) then becomes

\[
I_2 = \int \frac{d^3k}{(2\pi)^3} (\alpha_1 \cdot \hat{k})(\alpha_2 \cdot \hat{k}) \frac{e^{i|k| r_{12}}}{q^2 - k^2 + i\eta} = \int \frac{d^3k}{(2\pi)^3} \frac{q^2}{k^2} \frac{e^{i|k| r_{12}}}{q^2 - k^2 + i\eta}
\]

provided that the orbitals are generated by a hamiltonian with a local potential.
Appendix G

Feynman diagrams for bound states

The scattering matrix can in the bound-interaction picture be expressed in terms of a Feynman amplitude, $\mathcal{M}$, as

$$S = 2\pi \delta \left( \sum (\varepsilon_{\text{in}} - \varepsilon_{\text{out}}) \right) \mathcal{M}$$

related to the matrix element of the corresponding effective potential by

$$i\mathcal{M} = \langle |V_{\text{eff}}| \rangle .$$

The Feynman amplitude, $\mathcal{M}$, is given by the following rules:

1. Incoming electron line: $\phi_a(x)$
2. Outgoing electron line: $\phi_a^\dagger(x)$
3. Vertex: $ieca^\mu$
4. Internal photon line – Photon propagator:

$$\frac{i}{c\varepsilon_0} D_{\mathcal{F}\nu\mu}(x_2 - x_1; z)$$
4. Internal electron line – Electron propagator:
\[ iS_F(x_2, x_1; z) \]

6. Closed electron loop: Factor of (-1) and trace symbol

7. Energy conservation at each vertex (z energy parameter)

8. Integration over all \( x \)'s and \( z \)'s. Factor of \( (2\pi)^{-1} \) for each non-trivial \( z \)-integration.
Appendix H

Dimensional analysis

The formulas given here are valid in any consistent unit system, like the SI system. The formulas can be checked by a dimensional analysis. The dimensions in the SI systems for some of the quantities are

\[
\text{[force]} = N = \frac{kg \, m}{s^2}
\]

\[
\text{[energy]} = J = N \cdot m = \frac{kg \, m^2}{s^2}
\]

\[
\text{[action, } \hbar] = Js = \frac{kg \, m_e^2}{s}
\]

\[
\text{[electric potential]} = V = \frac{J}{As} = \frac{kg \, m_e^2}{As^3}
\]

\[
\text{[electric field, } E] = V/m = \frac{kg \, m}{As^3}
\]

\[
\text{[magnetic field, } B] = V \cdot s/m_e^2 = \frac{kg}{As^2}
\]

\[
\text{[vector potential, } A] = V \cdot s/m = \frac{kg \, m}{As^2}
\]

\[
\text{[charge density, } \rho] = \frac{As}{m^3}
\]
\[
\text{[current density, } \mathbf{j}] = \frac{A}{m_e^2}
\]

\[
[\mu_0] = \frac{N/A^2}{kg m} = \frac{kg m}{A^2 s^2}
\]

\[
[\varepsilon_0] = \frac{1}{\mu_0 c^2} = \frac{A^2 s^4}{kg m^3}
\]

\[
[\rho/\varepsilon_0] = \frac{kg}{As^3} = [\nabla \cdot \mathbf{E}] \quad \text{Eq. (\text{Maxw. a})}
\]

\[
[\mu_0 \mathbf{j}] = \frac{kg}{Am s^2} = [\nabla \times \mathbf{B}] \quad \text{Eq. (\text{Maxw. b})}
\]

\[
\left[ \frac{\hbar}{\varepsilon_0 \omega V} \right] = \frac{kg m_e^2}{A^2 s^4} = [A^2] \quad \text{Eq. (\text{2.1})}
\]

\[
[D_{\text{D}F_{\nu \mu}}(x_2 - x_1)] = m^{-2} \quad [D_{\text{D}F_{\nu \mu}}(x - x')] = s/m^2
\]

\[
\left[ \frac{\hbar D_{\text{D}F_{\nu \mu}}(x_2 - x_1)}{\varepsilon_0 c} \right] = \frac{kg m_e^2}{A^2 s^4} = [A^2] \quad \text{Eq. (\text{PhotPropDef 2.6})}
\]

\[
[ecA] = \frac{kg m_e^2}{s^2} = [\text{energy}] \quad \text{Eq. (\text{Hint 2.37})}
\]

\[
\left[ \frac{e^2 c^2}{\hbar^2} \right] = \frac{A^2 s^2}{kg^2 m_e^2} = [A^{-2} s^{-2}] \quad \text{Eq. (\text{E22 2.38})}
\]


