Einführung in die Quantenelektrodynamik
Introduction to Quantum Electrodynamics

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1   Fundamentals

Quantum electrodynamics is the unification of electrodynamics and quantum theory in conformity with the principles of special relativity.

Ordinary quantum mechanics is usually based on the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle \tag{1.1}$$

which appears to be noncovariant by the distinguished role of time, but is not actually in conflict with special relativity. Rather, the Schrödinger equation can be understood as merely expressing the requirement that the symmetry of time translation be representable as a unitary transformation $U = \exp(-iHt/\hbar)$.

What renders ordinary quantum mechanics nonrelativistic is a nonrelativistic choice of the Hamilton operator H and a restriction to a fixed number of particles. As we shall see, a relativistic interacting quantum theory cannot be found for a fixed number of particles, but we shall nevertheless begin by setting up a relativistic wave equation for a single particle.

1.1   Relativistic notation

Before doing so we fix our relativistic notation and conventions: The Euclidean 3-dimensional space (x, y, z) is generalised to a 4-dimensional space-time with coordinates

$$x^\mu = (x^0, x^1, x^2, x^3) = (ct, x, y, z) \tag{1.2}$$

with *Minkowski metric*

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{1.3}$$

Greek indices run over values $0, 1, \ldots, 3$; when we want to restrict to spatial components $1, \ldots, 3$ we shall use lower-case Latin letters.

The spatial components of the Minkowski metric are proportional to the Kronecker delta δ_{ij}. Just as the latter is invariant under 3-dimensional rotations and translations, the indefinite Minkowski metric is invariant under Lorentz transformations and 4-dimensional translations

$$x'^\mu = L^\mu{}_\nu x^\nu + a^\mu \tag{1.4}$$

where we used the Einstein convention of summing over repeated indices. This leaves the line element

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu \tag{1.5}$$

invariant, for $g_{\mu\nu}L^\mu{}_\sigma L^\nu{}_\rho = g_{\sigma\rho}$ (in matrix notation: $L^T g L = g$). In particular, a Lorentz *boost* with velocity v in x-direction is given by

$$L^\mu{}_\nu = \begin{pmatrix} \gamma & \gamma\beta & 0 & 0 \\ \gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{1.6}$$

with

$$\beta = \frac{v}{c}, \qquad \gamma = \frac{1}{\sqrt{1-\beta^2}}.$$

Vectors transforming under Lorentz transformations like dx^μ are called contravariant vectors and carry upper indices; those transforming like

$$\partial_\mu \equiv \frac{\partial}{\partial x^\mu} \tag{1.7}$$

are called covariant vectors.

Indices are lowered and raised by multiplication with the metric $g_{\mu\nu}$ and $g^{\mu\nu}$, where the latter is defined by

$$g_{\mu\nu}g^{\nu\lambda} = \delta^\lambda_\mu = \begin{cases} 1 & \text{for } \mu = \lambda \\ 0 & \text{for } \mu \neq \lambda \end{cases} \tag{1.8}$$

Numerically, $g_{\mu\nu} = g^{\mu\nu}$. Note that raising or lowering the indices of a Lorentz vector changes the sign of its spatial components.

A scalar product of a covariant and a contravariant vector gives a quantity invariant under Lorentz transformation (a scalar under Lorentz transformations). Examples are the d'Alembertian (or quabla)

$$\partial_\mu\partial^\mu = g^{\mu\nu}\partial_\mu\partial_\nu = \left(\frac{\partial}{c\,\partial t}\right)^2 - \nabla^2 \equiv \Box \tag{1.9}$$

and the square of the 4-momentum

$$p^\mu = (E/c, \vec{p}), \quad p_\mu = (E/c, -\vec{p}) \tag{1.10}$$

giving

$$p^2 = p^\mu p_\mu = E^2/c^2 - \vec{p}^2 = m^2 c^2 \tag{1.11}$$

where m is the invariant (rest) mass.

In quantum mechanics, the 4-momentum operator in configuration space is represented by $p^\mu = i\hbar\partial^\mu = (i\hbar\partial_t, -i\hbar\nabla)$.

1.2   Natural units

In relativistic quantum theory, a natural system of units is obtained by setting

$$\hbar = 1, \qquad c = 1. \tag{1.12}$$

$c = 1$ puts spatial lengths and time intervals on equal footing in that a unit for time implies a unit for length. (Which is also common practice in astronomy where distances are often given in light-years.)

$\hbar$ has the dimension of energy $\times$ time. $\hbar = 1$ therefore allows one to express time (and therefore space) intervals in terms of inverse energy. For instance, $1\,\mathrm{eV}^{-1} \approx 200\,\mathrm{nm}$ is an adequate unit for the physics of atomic transitions, whereas in nuclear physics $1\,\mathrm{fm} = 10^{-15}\mathrm{m} \approx 1/200\,\mathrm{MeV}$ is a typical length scale, and the GeV (10^9eV) $\approx (0.2\,\mathrm{fm})^{-1}$ is the most frequently used energy unit in elementary particle physics.

Instead of using a unit for electrical charge and expressing the charge of an electron in its terms, it is customary to use the *fine structure constant* $\alpha \equiv e^2/(4\pi\hbar c) \approx 1/137.036$

2   Relativistic wave equations

Simply replacing the nonrelativistic expression for (kinetic) energy, $E = \frac{\vec{p}^2}{2m}$, by its relativistic version, $E = \sqrt{\vec{p}^2 + m^2}$, would lead to a Schrödinger equation with a configuration space representation which is asymmetric in spatial and temporal derivatives and, even worse, nonlocal. However, a symmetric and local equation is obtained by iterating both sides of the Schrödinger equation and using $E^2 = \vec{p}^2 + m^2 \rightarrow H^2 = -\nabla^2 + m^2$:

$$-\partial_t^2 \psi(t, x) = (-\nabla^2 + m^2)\psi(t, x) \quad \Rightarrow \quad (\Box + m^2)\psi = 0 \tag{2.1}$$

This is the so-called *Klein-Gordon equation*.[1]

The fact that the nonrelativistic Schrödinger equation

$$i\partial_t \psi(t, x) = [-\frac{1}{2m}\nabla^2 + V]\psi(t, x) \tag{2.2}$$

---

[1]Found independently by Klein and Gordon in 1926 after Schrödinger had published his nonrelativistic wave equation, but actually discovered first by Schrödinger, who did not include it in his 1926 series of papers because it gave a wrong expression for the fine structure of the H atom — the spin-orbit coupling as the cause for this discrepancy was noted by Schrödinger only later.

is linear in the time derivative, is however crucial in interpreting $\rho = |\psi|^2$ as the density for the probability of finding the (single) particle it is describing at a given point. (2.2) implies that

$$
\begin{aligned}
\frac{\partial}{\partial t}(\psi^*\psi) &= \frac{i}{2m}\left(\psi^*\nabla^2\psi - (\nabla^2\psi^*)\psi\right) \\
&= \frac{i}{2m}\nabla\cdot(\psi^*\nabla\psi - \nabla\psi^*\cdot\psi)
\end{aligned}
\tag{2.3}
$$

and so ρ obeys a continuity equation and the total probability $\int dx|\psi|^2 = 1$ is a conserved quantity.

In the Klein-Gordon equation, this interpretation has to be abandoned. One instead finds

$$
\nabla\cdot(\psi^*\nabla\psi - \nabla\psi^*\cdot\psi) = \frac{\partial}{\partial t}\left(\psi^*\dot\psi - \dot\psi^*\psi\right)
\tag{2.4}
$$

This is again a continuity equation, but the corresponding $\rho \propto (\psi^*\dot\psi - \dot\psi^*\psi)$ is not positive definite.

A (many-)particle interpretation can be found in a quantum field theory based on the Klein-Gordon equation,[2] but historically this impasse was the motivation for Dirac to look for a different relativistic wave equation, linear in the time derivative so that the usual probabilistic interpretation applies.

2.1 Derivation of the Dirac equation

Dirac stuck to the Schrödinger equation (1.1) with its first-order time derivative, but generalized it to a multi-component wave-function ψ ("spinor") and H to a matrix. In order to have a chance for Lorentz-invariance, H, in x-space, must be linear in spatial derivatives as well,

$$
i\frac{\partial\psi}{\partial t} = H\psi = \left(\frac{1}{i}\alpha_i\partial_i + \beta m\right)\psi \,,
\tag{2.5}
$$

where α_i and β are matrices acting on the components of ψ.

When iterated, this must coincide with the Klein-Gordon equation, because the latter just expresses the relativistic relation between energy and momentum (1.11). This leads to

$$
\begin{aligned}
(-i\alpha_i\partial_i + \beta m)(-i\alpha_j\partial_j + \beta m) &= (-\partial_i\partial_j\delta_{ij} + m^2)\mathbf{1} \\
&= -\alpha_i\alpha_j\partial_i\partial_j - im(\beta\alpha_j + \alpha_j\beta)\partial_j + \beta^2 m^2
\end{aligned}
\tag{2.6}
$$

---

[2]The right-hand-side of Eq. (2.4) turns out to have then the interpretation of a charge density for the charged scalar particles described by the Klein-Gordon equation.

which requires that

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij} \qquad (2.7)$$

$$\{\alpha_i, \beta\} = 0 \qquad (2.8)$$

$$\beta^2 = \mathbf{1} \qquad (2.9)$$

Because of (2.9), multiplying (2.5) by β gives the Lorentz-covariant form of the *Dirac equation*

$$(i\gamma^\mu \partial_\mu - m)\psi(x) =: (i\,\slashed{\partial} - m)\psi(x) = 0 \qquad (2.10)$$

with the *Dirac γ-matrices*

$$\gamma^\mu = (\gamma^0, \gamma^m) = (\beta, \beta\alpha_m) \qquad (2.11)$$

which satisfy the *Clifford algebra* relation

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}\mathbf{1} \qquad (2.12)$$

2.2   Properties of the Dirac matrices

Before giving an explicit representation of the Dirac matrices, let us list their general, representation-independent properties.

i) Hermiticity of the Hamilton operator H requires Hermiticity of the matrices $\vec{\alpha}, \beta$. This implies that $\gamma^0 = \beta$ is hermitian, $(\gamma^0)^\dagger = \gamma^0$, and that γ^i is anti-hermitian:

$$(\gamma^i)^\dagger = (\beta\alpha_i)^\dagger = \alpha_i\beta = -\beta\alpha_i = -\gamma^i .$$

ii) Because $(\alpha_i)^2 = \beta^2 = \mathbf{1}$, the eigenvalues of the matrices $\alpha_i, \beta\,(=\gamma^0)$ are ± 1. On the other hand, $(\gamma^i)^2 = -\mathbf{1}$ and the eigenvalues of the γ^i are $\pm i$.

iii) The matrices $\alpha_i, \beta, \gamma^\mu$ are all traceless. This follows from taking the trace of both sides of

$$\alpha_i = -\beta\alpha_i\beta, \quad \beta = -\alpha_{(i)}\beta\alpha_{(i)}, \quad \gamma^i = -\gamma^0\gamma^i\gamma^0$$

(brackets around repeated indices denote exemption from the Einstein summation convention) and using cyclicity of the trace, i.e. $\text{tr}(ABC) = \text{tr}(BCA)$.

iv) From ii) and iii) follows that the dimension of the Dirac matrices must be even.

Among 2-dimensional matrices, one can find just 3 anticommuting, hermitean matrices with the required properties for α_i, β: the Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \qquad (2.13)$$

These can be used to write a Dirac equation in up to 2+1 space-time dimensions. In 4 dimensions, the Pauli matrices suffice for (2.5), if we omit the mass term, leading to the so-called *Weyl equation*, which however cannot be rewritten into (2.10) with (2.12), because that would require 4 matrices.

In 3+1 dimensional space-time, the matrix dimension of the γ's must be ≥ 4. Indeed, using the Pauli matrices as building blocks, one possibility is the following (Dirac representation)

$$\alpha_i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbf{1}_2 & 0 \\ 0 & -\mathbf{1}_2 \end{pmatrix} = \gamma^0, \quad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}. \tag{2.14}$$

However, this choice is not unique. $\gamma^\mu \to U\gamma^\mu U^{-1}$ with U unitary (to preserve the Hermiticity properties) gives an equivalent representation.

Another useful representation is the so-called Weyl or chiral representation

$$\gamma^0 = \begin{pmatrix} 0 & \mathbf{1}_2 \\ \mathbf{1}_2 & 0 \end{pmatrix}, \qquad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}. \tag{2.15}$$

Yet another one is the so-called Majorana representation

$$\gamma^0 = \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix}, \gamma^1 = \begin{pmatrix} i\sigma^3 & 0 \\ 0 & i\sigma^3 \end{pmatrix}, \gamma^2 = \begin{pmatrix} 0 & -\sigma^2 \\ \sigma^2 & 0 \end{pmatrix}, \gamma^3 = \begin{pmatrix} -i\sigma^1 & 0 \\ 0 & -i\sigma^1 \end{pmatrix}, \tag{2.16}$$

where all γ-matrices are purely imaginary. This implies that $(i\gamma^\mu \partial_\mu - m)\psi = 0$ becomes a purely real equation, and that the real and imaginary parts of ψ are decoupled. As we shall see, this nice feature is lost when ψ is coupled to electromagnetic fields. Neutral particles on the other hand may well be "Majorana", meaning that, in the Majorana representation[3], they can be described by a real field ψ, and thus by half as many degrees of freedom as those of a complex Dirac field. However, the standard model of elementary particle physics does not (yet) have Majorana particles.

2.3   Dirac adjoint and Dirac current

Because the Hermiticity properties of the γ-matrices can be summarized by

$$\gamma^{\mu\dagger} = \gamma^0 \gamma^\mu \gamma^0 \tag{2.17}$$

it is natural to define the Dirac adjoint spinor by

$$\bar{\psi} := \psi^\dagger \gamma^0 \tag{2.18}$$

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[3]In other representations, a reality condition on ψ is slightly more involved, but of course still possible to formulate.

Taking the adjoint of the Dirac equation $(i\gamma^\mu\partial_\mu - m)\psi = 0$ gives

$$\psi^\dagger(-i\gamma^{\mu\dagger}\overleftarrow{\partial}_\mu - m) = 0 \quad \Rightarrow \quad \bar\psi(i\overleftarrow{\partial\!\!\!/} + m) = 0. \tag{2.19}$$

(2.19) together with the original form of the Dirac equation establishes that there is a conserved current

$$\bar\psi(\overleftarrow{\partial\!\!\!/} + \overrightarrow{\partial\!\!\!/})\psi = \partial_\mu(\underbrace{\bar\psi\gamma^\mu\psi}_{j^\mu}) = 0 \tag{2.20}$$

with positive definite density

$$j^0 = \rho = \bar\psi\gamma^0\psi = \psi^\dagger\psi = \sum_{\alpha=1}^4 \psi_\alpha^\dagger\psi_\alpha \geq 0 \;. \tag{2.21}$$

This opens the possibility of interpreting ρ as a probability density in analogy with the nonrelativistic Schrödinger equation, or in other words to use the Dirac equation as a single-particle relativistic wave equation. The price to pay is that the Dirac wave function has 4 components (Dirac spinor), which we shall label by indices from the beginning of the Greek alphabet. As we shall see presently, a spinor transforms rather differently from a 4-vector. (That both involve the same number of components is an accident of 4-dimensional space-time; in n dimensions a Dirac spinor has $2^{[n/2]}$ components.)

2.4   Covariance of the Dirac equation

Although we have suggested covariance of the Dirac equation by using a relativistic notation for the γ-matrices, it remains to show that the Dirac equation is indeed co-variant under Lorentz transformations, or, more generally, under the Lorentz group plus translations (Poincaré group). This means that the Dirac equation should pre-serve its form after a transformation to a different frame of reference by an arbitrary Poincaré transformation

$$x'^\mu = L^\mu{}_\nu x^\nu + a^\mu, \quad L^T g L = g \tag{2.22}$$

with a well-defined local relation between $\psi'(x')$ and $\psi(x)$ so that

$$i\gamma^\mu\frac{\partial}{\partial x^\mu}\psi(x) - m\psi(x) = 0$$
$$\Rightarrow \quad i\gamma^\mu\frac{\partial}{\partial x'^\mu}\psi'(x') - m\psi'(x') = 0 \tag{2.23}$$

i) Translations: Because $\partial/\partial x^\mu = \partial/\partial(x+a)^\mu = \partial/\partial x'^\mu$, these are trivially realized by $\psi'(x') = \psi(x)$ or

$$\psi'(x) = \psi(x-a) \tag{2.24}$$

7

ii) Lorentz transformations: If we assume a linear relation

$$\psi'_\alpha(x') = S_{\alpha\beta}(L)\psi_\beta(x), \quad x'^\mu = L^\mu{}_\nu x^\nu, \tag{2.25}$$

form invariance of the Dirac equation, in which

$$\frac{\partial}{\partial x'^\mu} = \underbrace{\frac{\partial x^\nu}{\partial x'^\mu}}_{(L^{-1})^\nu{}_\mu} \frac{\partial}{\partial x^\nu}$$

requires that

$$S^{-1}\gamma^\mu (L^{-1})^\nu{}_\mu S = \gamma^\nu \quad \Rightarrow \quad S^{-1}(L)\gamma^\mu S(L) = L^\mu{}_\nu \gamma^\nu \tag{2.26}$$

This fits perfectly to the Clifford relation (2.12) which is left unchanged because of $L^\mu{}_\sigma L^\nu{}_\rho g^{\sigma\rho} = g^{\mu\nu}$.

The existence of a matrix $S(L)$ for all Lorentz transformations L is guaranteed by the following theorem from group theory:[4] The Clifford algebra relation $\{A_i, A_j\} = 2q_{ij}\mathbf{1}$ with q_{ij} a symmetric $n \times n$ matrix and n even has precisely one equivalence class of irreducible representations of dimension $2^{n/2}$.

This determines $S(L)$ uniquely up to a factor, which turns out to be ± 1; the $S(L)$ thus form a two-valued representation of the Lorentz group.

For infinitesimal Lorentz transformations, however, the relation $L \to S(L)$ is unique once we require that $S(\mathbf{1}) = \mathbf{1}$. Consider

$$L^\mu{}_\nu = \delta^\mu_\nu + \varepsilon\, \omega^\mu{}_\nu \tag{2.27}$$

with infinitesimal ε.

Requiring that (2.27) be a Lorentz transformation ($L^T g L = g$) is equivalent to $\omega_{\mu\nu} = -\omega_{\nu\mu}$. There are therefore 6 independent $\omega_{\mu\nu}$, matching the number of the generators of spatial rotations (3) plus those of Lorentz boosts (3).

An ansatz $S = \mathbf{1} + \varepsilon T$, $S^{-1} = \mathbf{1} - \varepsilon T$ in (2.26) leads to

$$[\gamma^\mu, T] = \omega^\mu{}_\nu \gamma^\nu \tag{2.28}$$

and this is solved by (exercise!)

$$T = \frac{1}{8}\omega_{\mu\nu}[\gamma^\mu, \gamma^\nu]. \tag{2.29}$$

---

[4]See e.g. Sexl/Urbantke: Relativität, Gruppen, Teilchen (Springer Verlag)

2.4.1   Example: Rotation about z-axis

An infinitesimal rotation about the z-axis is given by

$$x' = x + \varepsilon y, \quad y' = y - \varepsilon x, \quad z' = z \tag{2.30}$$

The corresponding $\omega^{\mu\nu}$ is given by $\omega^{12} = g^{2\nu}\omega^1{}_\nu = -1$, $\omega^{21} = +1$, and all other components zero. This gives

$$S = \mathbf{1} + \frac{\varepsilon}{8}\omega_{\mu\nu}[\gamma^\mu, \gamma^\nu] = \mathbf{1} - \frac{\varepsilon}{4}[\gamma^1, \gamma^2] = 1 + \varepsilon\frac{i}{2}\Sigma_3 \tag{2.31}$$

with $\Sigma_3 = \sigma_3 \oplus \sigma_3$ in the Dirac and in the chiral representation of the γ matrices.

Writing out $\psi'(x') = S\psi(x)$ gives

$$
\begin{aligned}
\psi'(\vec{x}) &= (1 + \varepsilon\frac{i}{2}\Sigma_3)\psi(x - \varepsilon y, y + \varepsilon x, z) \\
&= \psi(\vec{x}) + i\varepsilon\Big[\ \underbrace{\frac{1}{2}\Sigma_3}_{\text{Spin } s_z} + \underbrace{(x\frac{\partial}{i\partial y} - y\frac{\partial}{i\partial x})}_{\ell_z}\ \Big]\psi(\vec{x})
\end{aligned}
\underbrace{}_{J_z}
\tag{2.32}
$$

Because Σ_3 has eigenvalues ± 1, this shows[5] that ψ carries spin $\frac{1}{2}$.

Finite rotations with angle φ can be obtained as

$$\psi'(\vec{x}') = \lim_{N\to\infty}\left(\mathbf{1} + \frac{i}{2}\frac{\varphi}{N}\Sigma_3\right)^N\psi(\vec{x}) = \exp\{i\frac{\varphi}{2}\Sigma_3\}\psi(\vec{x}) \tag{2.33}$$

and we see that a rotation by $\varphi = 2\pi$, which corresponds to $L = \mathbf{1}$, is mapped to $S = e^{i\pi\Sigma_3} = -\mathbf{1}$. Only a rotation by $\varphi = 4\pi$ brings us back to $S = \mathbf{1}$.

This two-valuedness of the spinor representation of the rotation group is inherited by the full Lorentz group (with all complications coming solely from the rotations).[6]

---

[5]Strictly speaking, the identification of spin $s_z = \frac{1}{2}\Sigma_3$ or more generally $s_i = \frac{1}{2}\Sigma_i = \frac{i}{8}\varepsilon_{ijk}[\gamma^j, \gamma^k]$ does not make sense relativistically: $\vec{s}$ commutes with the Dirac operator $\not{P}$ only in the rest frame $P_\mu = m\delta_\mu^0$. The proper definition is through the Pauli-Lubanski vector $W_\mu = -\frac{1}{2}\varepsilon_{\mu\nu\rho\sigma}S^{\nu\rho}P^\sigma$, which for $P_\mu = m\delta_\mu^0$ reduces to $W_\mu = (0, m\vec{s})$. [$\varepsilon_{\mu\nu\rho\sigma}$ is the totally antisymmetric ε-tensor with $\varepsilon_{0123} = +1 = -\varepsilon^{0123}$.]

[6]In group theory language: the spinor representation is a one-valued representation of the group SU(2), which is the universal (2:1) covering group of SO(3). The covering group of the (component of unity) of the Lorentz group $SO_0(3,1) \supset SO(3)$ is the group $SL(2,C) \supset SU(2)$. For more details see Sexl/Urbantke: Relativität, Gruppen, Teilchen (Springer Verlag).

2.4.2   Example: Lorentz boost along x-axis

A Lorentz boost along x axis is generated by $\omega^0{}_1 = \omega^1{}_0 = 1$. Because $(\omega^\mu{}_\nu)^2 = \mathbf{1}_2 \oplus \mathbf{0}_2$, and therefore $(\omega^\mu{}_\nu)^3 = \omega^\mu{}_\nu$ we find for $L^\mu{}_\nu = \exp\left(\xi\omega^\mu{}_\nu\right)$

$$
\begin{aligned}
L &= \sum_{n=0}^\infty \omega^n \frac{\xi^n}{n!} = \sum_{n=0}^\infty \underbrace{\omega^{2n}}_{\substack{\omega^2 \\ \forall n > 0}} \frac{\xi^{2n}}{(2n)!} + \sum_{n=0}^\infty \underbrace{\omega^{2n+1}}_{\substack{\omega \\ \forall n}} \frac{\xi^{2n+1}}{(2n+1)!} \\
&= \mathbf{1} - \omega^2 + \omega^2 \cosh\xi + \omega \sinh\xi
\end{aligned}
\tag{2.34}
$$

Explicitly,

$$
L^\mu{}_\nu = \begin{pmatrix} \cosh\xi & \sinh\xi & 0 & 0 \\ \sinh\xi & \cosh\xi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}
\tag{2.35}
$$

which can be identified with (1.6) through $\beta = v = \tanh\xi$. Indeed, $\cosh\xi = 1/\sqrt{1-\beta^2} = \gamma$, and $\sinh\xi = \beta\gamma$. The parameter ξ is called *rapidity*; it is particularly useful because it is additive under successive boosts.

The corresponding spinor transformation $S(L)$ is given by

$$
S(L) = \exp\left(\frac{1}{8}\xi\omega_{\mu\nu}[\gamma^\mu,\gamma^\nu]\right) = \exp\left(\frac{1}{4}\xi[\gamma^0,\gamma^1]\right).
\tag{2.36}
$$

In the Dirac representation (2.14), $[\gamma^0,\gamma^1] = 2\begin{pmatrix} \mathbf{0} & \sigma^1 \\ \sigma^1 & \mathbf{0} \end{pmatrix} = 2\alpha_1$. Because $(\alpha_1)^2 = \mathbf{1}_4$, $(\alpha_1)^3 = \alpha_1$, etc., we obtain

$$
S(L) = \mathbf{1}\underbrace{\cosh\frac{\xi}{2}}_{=:C} + \alpha_1\underbrace{\sinh\frac{\xi}{2}}_{=:S} = \begin{pmatrix} C & 0 & 0 & S \\ 0 & C & S & 0 \\ 0 & S & C & 0 \\ S & 0 & 0 & C \end{pmatrix}
\tag{2.37}
$$

This expression is admittedly not too illuminating, but we shall use this result later. We shall also find it useful to express ξ in terms of E and p_x: With $v = \frac{p_x}{E} = \tanh\xi$ we get

$$
\tanh\frac{\xi}{2} = \frac{\tanh\xi}{1+\sqrt{1-\tanh^2\xi}} = \frac{v}{1+\sqrt{1-v^2}} = \frac{p}{E+m}
\tag{2.38}
$$

$$
\Rightarrow \cosh\frac{\xi}{2} = \sqrt{\frac{E+m}{2m}}, \qquad \sinh\frac{\xi}{2} = \tanh\frac{\xi}{2}\cosh\frac{\xi}{2}
\tag{2.39}
$$

2.4.3   Components of the Lorentz group

The finite Lorentz transformation (2.34) and generally any Lorentz transformation of the form $L^\mu{}_\nu = \exp\left(\xi\omega^\mu{}_\nu\right)$ is one that is continuously connected with the identity through the parameter ξ. This does not exhaust all elements of the Lorentz group, but only those with determinant $\det(L) = +1$ and $L^0{}_0 \geq 1$, for it is not possible by a continuous change of parameters to jump from these values to the other possibilities $\det(L) = -1$ and/or $L^0{}_0 \leq -1$. The subgroup of Lorentz transformations with $\det(L) = +1$ and $L^0{}_0 \geq 1$ is called the *proper orthochronous Lorentz group* $\mathcal{L}^\uparrow_+$.

As long as only elements from $\mathcal{L}^\uparrow_+$ are considered, the representation $S(L)$ of the Lorentz group[7] is reducible (i.e.: there are nontrivial invariant subspaces). This becomes manifest in the chiral representation of the Dirac matrices (2.15), in which the generators of

$$S(L) = \exp\left(-\frac{i}{2}\omega_{\mu\nu}S^{\mu\nu}\right), \qquad L \in \mathcal{L}^\uparrow_+ \tag{2.40}$$

(where the parameter ξ is now implicit in $\omega_{\mu\nu}$) read

$$S^{0i} = \frac{i}{4}[\gamma^0, \gamma^i] = -\frac{i}{2}\begin{pmatrix} \sigma^i & 0 \\ 0 & -\sigma^i \end{pmatrix}, \qquad S^{ij} = \frac{i}{4}[\gamma^i, \gamma^j] = \frac{1}{2}\varepsilon^{ijk}\begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix}. \tag{2.41}$$

The upper two and lower two components of a four-component spinor therefore transform without being mixed.

It is in fact possible to write a relativistic wave equation for a spinor which has only half of the components of a Dirac spinor: when the mass is put to zero, the Dirac equation (in the chiral representation) also does not mix the upper and lower half of a spinor. Putting to zero one half, $\psi = \binom{\phi}{0}$, or $\psi = \binom{0}{\chi}$ leads to the so-called *Weyl equation*

$$\left(p^0 + \vec{p} \cdot \vec{\sigma}\right)\phi = 0 \quad \text{or} \quad \left(p^0 - \vec{p} \cdot \vec{\sigma}\right)\chi = 0 \tag{2.42}$$

which is of great importance in the theory of weak interactions, where it describes massless neutrinos.

The full Lorentz group is obtained by composing elements of $\mathcal{L}^\uparrow_+$ with the discrete operations of space inversion P or time reversal T or both together.

Space inversion ("parity transformation") is effected by

$$L^\mu{}_\nu = \begin{pmatrix} 1 & \\ & -\mathbf{1}_3 \end{pmatrix}$$

and so this must be represented by a matrix $S(L) = P$ with the properties

$$\gamma^0 = P^{-1}\gamma^0 P, \qquad \vec{\gamma} = -P^{-1}\vec{\gamma}P. \tag{2.43}$$

---

[7]More precisely: the covering group of $\mathcal{L}^\uparrow_+$

This is solved by $P = \pm\gamma^0$. In the chiral representation (2.15), γ^0 is block-off-diagonal, so the upper and lower halves of a spinor no longer define invariant subspaces if parity is included. A Weyl spinor which involves only one half therefore breaks parity, and indeed parity has been found to be violated in weak interactions. The Dirac equation on the other hand is parity invariant and so is quantum electrodynamics.

Space inversion together with time reversal, PT, is effected by $L^\mu{}_\nu = -\delta^\mu_\nu$, and so

$$\gamma^\mu = -S(PT)^{-1}\gamma^\mu S(PT) \tag{2.44}$$

One easily verifies that a solution for $S(PT)$ is

$$\gamma^5 := i\gamma^0\gamma^1\gamma^2\gamma^3 \equiv \frac{i}{4!}\varepsilon_{\mu\nu\rho\sigma}\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma \tag{2.45}$$

γ^5 has the properties

$$\gamma^5 = (\gamma^5)^\dagger, \tag{2.46}$$

$$(\gamma^5)^2 = \mathbf{1}, \tag{2.47}$$

$$\{\gamma^5, \gamma^\mu\} = 0 \tag{2.48}$$

The last relation (2.48) implies that $[\gamma^5, S^{\mu\nu}] = 0$, which again proves, by Schur's lemma[8], that $S(L \in \mathcal{L}_+^\uparrow) = \exp(-\frac{i}{2}\omega_{\mu\nu}S^{\mu\nu})$ is reducible. The invariant subspaces under the latter transformations are given by the two projection operators

$$P_L = \frac{1}{2}(1 - \gamma^5), \qquad P_R = \frac{1}{2}(1 + \gamma^5) \tag{2.49}$$

which project onto left- and right-handed *chiralities*, respectively.

$\psi_L = P_L\psi$ and $\psi_R = P_R\psi$ are eigenstates of γ^5 with eigenvalues $+1$ and -1, respectively. Dirac spinors which are solutions of the Dirac equation can have definite chiralities only in the massless case. By acting with $\gamma^5\gamma^0$ on $\not{p}\psi = 0$ one can readily show that (exercise!)

$$\vec{\Sigma} \cdot \vec{p}\,\psi = \gamma^5 p^0 \psi \tag{2.50}$$

so that with $p^0 = E = |\vec{p}|$

$$\frac{1}{2}\gamma^5\psi = \frac{1}{2}\frac{\vec{\Sigma} \cdot \vec{p}}{|\vec{p}|}\psi = \frac{\vec{s} \cdot \vec{p}}{|\vec{p}|}\psi \tag{2.51}$$

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[8]If a matrix commutes with all elements of a matrix representation of a group, then either it is proportional to the unit matrix or this representation is reducible.

Chirality defined as $\frac{1}{2}$ times the eigenvalue of γ^5 thus equals the helicity (the projection of spin on the direction of $\vec{p}$) of massless particles. This is a boost-invariant quantity, because massless particles cannot be overtaken. It does however change under parity.

In the chiral representation (2.15)

$$\gamma^5_{\text{chiral rep.}} = \begin{pmatrix} -\mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix} \tag{2.52}$$

and so the upper (lower) half of a Dirac spinor is of left (right) chirality. As we saw in (2.41), they transform under different, namely complex conjugated, representations of $\mathcal{L}^\uparrow_+$, sometimes denoted as $(\frac{1}{2}, 0)$ and $(0, \frac{1}{2})$, respectively.

In other representations, notably in the Dirac representation (2.14) where

$$\gamma^5_{\text{Dirac rep.}} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix} \tag{2.53}$$

the above reducibility (when parity is excluded) is less conspicuous.

2.4.4   Dirac field bilinears

The advantage of the Dirac representation is instead in the diagonal form of γ^0, which (besides representing parity) is of singular importance because it effects Hermitian conjugation of the γ matrices as we have seen in (2.17) and so enters the definition of Dirac adjoints (2.18).

We still have to establish the transformation properties of the Dirac adjoint in order to verify covariance of the conserved current (2.20).

Under a Lorentz transformation $\psi \to S(L)\psi$, and so $\bar{\psi} \to \psi^\dagger S^\dagger \gamma^0 = \bar{\psi} \gamma^0 S^\dagger \gamma^0$. With (2.17) and the explicit form of the $S(L)$ in (2.40) as well as of the $S(L)$ associated with parity one can show that (exercise!)

$$\gamma^0 S^\dagger \gamma^0 = S^{-1}. \tag{2.54}$$

Therefore (under orthochronous Lorentz transformations[9]) $\bar{\psi}\psi \to \bar{\psi}S^{-1}S\psi = \bar{\psi}\psi$ is a scalar and $\bar{\psi}\gamma^\mu\psi \to \bar{\psi}S^{-1}\gamma^\mu S\psi = L^\mu{}_\nu \bar{\psi}\gamma^\nu\psi$ a vector, as is necessary for the conserved current (2.20) to make sense.

More generally, $\bar{\psi}\gamma^{\mu_1}\cdots\gamma^{\mu_k}\psi$ transforms as a tensor of rank k. Inserting additionally the matrix γ^5 does not change that as long as we consider Lorentz transformations $L \in \mathcal{L}^\uparrow_+$, because $[\gamma^5, S^{\mu\nu}] = 0$. But under the parity transformation we pick

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[9]We exclude time reversal here, which would lead to a change of sign of $\bar{\psi}\psi$. In the full quantum field theory, $\bar{\psi}\psi$ is made invariant by representing time reversal by an anti-linear transformation.

up an extra minus sign:

$$\bar{\psi}'(x')\gamma^5\psi'(x') = \bar{\psi}(x)\ \underbrace{P^{-1}\gamma^5 P}_{\gamma^0\gamma^5\gamma^0=-\gamma^5}\ \psi(x) = -\bar{\psi}(x)\gamma^5\psi(x). \tag{2.55}$$

$\bar{\psi}\gamma^5\psi$ is therefore called pseudo-scalar, and similarly $\bar{\psi}\gamma^{\mu_1}\cdots\gamma^{\mu_k}\gamma^5\psi$ pseudo-tensor.

In fact, any 4×4 spinor matrix Γ can be decomposed in a linear combination of the unit matrix or products of γ-matrices and thus into terms with well-defined Lorentz transformation properties when sandwiched by Dirac fields. Only antisymmetrized products of γ-matrices must be considered, because (2.12) reduces symmetric combinations. The resulting "Clifford algebra" is spanned by the basis

$$\Gamma_S = \mathbf{1},\ \Gamma_V^\mu = \gamma^\mu,\ \Gamma_T^{\mu\nu} = \frac{i}{2}[\gamma^\mu,\gamma^\nu] =: \sigma^{\mu\nu},\ \Gamma_A^\mu = \gamma^\mu\gamma^5,\ \Gamma_P = \gamma^5 \tag{2.56}$$

corresponding to scalar, vector, (antisymmetric) tensor, axial vector, and pseudo-scalar, respectively, with a total of $1 + 4 + 6 + 4 + 1 = 16 = 4^2$ matrices. (In n (even) dimensions, where the dimension of Dirac matrices is $2^{n/2}$, an analogous decomposition is possible because $1 + n + \binom{n}{2} + \ldots \binom{n}{n} = 2^n = (2^{n/2})^2$.)

2.5   Higher spin

Higher, non-integer spin fields can be obtained by replacing the spinor ψ by spinor fields with additional Lorentz indices, $\psi^{\mu\cdots}$. These can again be subjected to a Dirac equation which acts on the spinor components only. In general, such fields will be highly reducible.

For example, a vector-spinor ψ_μ contains spin $\frac{1}{2}$ and $\frac{3}{2}$. The quantity $\gamma^\mu\psi_\mu$ is a Dirac spinor, so this can be used to project out the spin $\frac{1}{2}$ content. The two equations

$$(i\,\partial\!\!\!/ - m)\psi_\mu(x) = 0, \qquad \gamma^\mu\psi_\mu(x) = 0 \tag{2.57}$$

(Rarita-Schwinger equations) therefore describe a spin-$\frac{3}{2}$ field.

However, it is rather difficult to find a consistent quantum theory of spin-$\frac{3}{2}$ field interacting with other quantum fields.[10]

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[10]Minimal coupling to electromagnetic fields for example leads to the so-called Velo-Zwanziger anomaly.

3 Solutions of the Dirac equation

3.1 Plane-wave solutions

The simplest solution of the Klein-Gordon equation are plane waves $e^{\mp ik_\mu x^\mu}$ with $k^2 = m^2$, where for $k^0 > 0$ the minus sign corresponds to positive energy ($E = i\partial_t$).

For plane-wave solutions of the Dirac equation we make the ansatz

$$\psi_\alpha^{(+)}(x) = e^{-ik\cdot x}u_\alpha(k), \qquad \psi_\alpha^{(-)}(x) = e^{+ik\cdot x}v_\alpha(k) \tag{3.1}$$

and obtain from $(i\slashed{\partial} - m)\psi^{(\pm)} = 0$ the algebraic equations

$$(\slashed{k} - m)u(k) = 0, \qquad (\slashed{k} + m)v(k) = 0 . \tag{3.2}$$

Hermitian conjugation and use of (2.17) shows that the corresponding Dirac adjoints obey similarly

$$\bar{u}(k)(\slashed{k} - m) = 0, \qquad \bar{v}(k)(\slashed{k} + m) = 0 . \tag{3.3}$$

In the rest frame $k^\mu = (m, \vec{0})$, and we have

$$(\gamma^0 - \mathbf{1})u(m, \vec{0}) = 0, \qquad (\gamma^0 + \mathbf{1})v(m, \vec{0}) = 0. \tag{3.4}$$

In the Dirac representation (2.14), $\gamma^0 = \begin{pmatrix} \mathbf{1}_2 & 0 \\ 0 & -\mathbf{1}_2 \end{pmatrix}$, so any spinor $\begin{pmatrix} \varphi \\ 0 \end{pmatrix}$ with only upper components is a solution for u; conversely, any spinor of the form $\begin{pmatrix} 0 \\ \chi \end{pmatrix}$ is a solution for the negative-energy case v. A basis is given by

$$u^{(1)}(m, \vec{0}) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \ u^{(2)}(m, \vec{0}) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \ v^{(1)}(m, \vec{0}) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \ v^{(2)}(m, \vec{0}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \tag{3.5}$$

which moreover gives the eigenvectors of the spin operator $\frac{1}{2}\Sigma_3 = \frac{1}{2}\sigma_3 \oplus \sigma_3$ with eigenvalues $+\frac{1}{2}, -\frac{1}{2}, +\frac{1}{2}, -\frac{1}{2}$, respectively.

Note that in other representations of the Dirac matrices, the above unit spinors would have a different interpretation. For example, in the chiral representation (2.15) the rest-frame spinors with positive and negative energy have the form $u = \begin{pmatrix} \varphi \\ \varphi \end{pmatrix}$, $v = \begin{pmatrix} \chi \\ -\chi \end{pmatrix}$.

Solutions for $\vec{k} \neq 0$ can be obtained by a Lorentz transformation which subjects u and v to a linear transformation with the matrix $S(L)$. For Lorentz boosts in x-direction we have calculated $S(L)$ in the Dirac representation in the previous section.

It is simpler, though, to construct the general solution by using

$$(\slashed{k} - m)(\slashed{k} + m) = k^2 - m^2 = 0 \tag{3.6}$$

and writing

$$u(k) = \frac{1}{N}(\slashed{k} + m)u(m, \vec{0}) = \frac{1}{N}\begin{pmatrix} (E + m)\varphi \\ \vec{\sigma} \cdot \vec{k}\,\varphi \end{pmatrix} \tag{3.7}$$

$$v(k) = \frac{1}{N}(-\slashed{k} + m)v(m, \vec{0}) = \frac{1}{N}\begin{pmatrix} \vec{\sigma} \cdot \vec{k}\,\chi \\ (E + m)\chi \end{pmatrix} \tag{3.8}$$

where $E \equiv k^0$ and $N = \sqrt{2m(m + E)}$ is fixed by

$$\bar{u}^{(a)}(k)u^{(b)}(k) = \delta^{ab}, \quad \bar{v}^{(a)}(k)v^{(b)}(k) = -\delta^{ab}, \quad \bar{u}^{(a)}(k)v^{(b)}(k) = 0 = \bar{v}^{(a)}(k)u^{(b)}(k) \tag{3.9}$$

In the Dirac representation, a positive-energy spinor is thus seen to be dominated by the upper components as long as the momentum does not get highly relativistic, i.e. $|\vec{k}| \ll m$.

3.2   Klein's paradox

For the time being, the only sensible solutions seem to be those with positive energy. It turns out, however, that it is inconsistent to restrict oneself to these only.

Let us consider the simple example of reflection of plane waves on a potential step

$$V(\vec{x}) = \begin{cases} 0 & \text{for} \quad x_1 < 0 \\ V & \text{for} \quad x_1 \geq 0 \end{cases} \tag{3.10}$$

For $x_1 < 0$ take an incident positive-energy plane wave travelling in positive x_1 direction with momentum $k = \sqrt{E^2 - m^2}$, $E > m$, and spin up (in x_3 direction). In the Dirac representation, the relevant spinor is given by (3.7) or by applying the matrix (2.37) onto $u^{(1)}(m, \vec{0})$,

$$\psi_{\text{in}} = a\,e^{ikx_1}\begin{pmatrix} 1 \\ 0 \\ 0 \\ \frac{k}{E+m} \end{pmatrix} \tag{3.11}$$

where a is a constant and the oscillatory factor e^{-iEt} has been dropped.

For the reflected wave we make the ansatz of plane waves travelling in negative x_1 direction with a superposition of spin up and spin down,

$$\psi_{\text{refl}} = b \, e^{-ikx_1} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \frac{-k}{E+m} \end{pmatrix} + b' \, e^{-ikx_1} \begin{pmatrix} 0 \\ 1 \\ \frac{-k}{E+m} \\ 0 \end{pmatrix}, \tag{3.12}$$

and similarly for the transmitted wave

$$\psi_{\text{trans}} = d \, e^{ik'x_1} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \frac{k'}{E-V+m} \end{pmatrix} + d' \, e^{ik'x_1} \begin{pmatrix} 0 \\ 1 \\ \frac{k'}{E-V+m} \\ 0 \end{pmatrix}, \tag{3.13}$$

but with $k' = \sqrt{(E-V)^2 - m^2}$.

Continuity requires that $\psi_{\text{in}} + \psi_{\text{refl}}\big|_{x_1=0} = \psi_{\text{trans}}\big|_{x_1=0}$. This gives $b' = d' = 0$ (i.e. no spin flips) and

$$\frac{b}{a} = \frac{1-\rho}{1+\rho}, \quad \frac{d}{a} = \frac{2}{1+\rho}, \quad \rho := \frac{k'}{k}\frac{E+m}{E-V+m}. \tag{3.14}$$

As long as $E - m > V$, there is partial reflection and partial transmission with reflection and transmission coefficients

$$R = \frac{j_{\text{refl}}}{j_{\text{in}}} = \left(\frac{b}{a}\right)^2 = \left(\frac{1-\rho}{1+\rho}\right)^2, \quad T = \frac{j_{\text{trans}}}{j_{\text{in}}} = 1 - \frac{j_{\text{refl}}}{j_{\text{in}}} = \frac{4\rho}{(1+\rho)^2} \tag{3.15}$$

with $R \to 1$ and $T \to 0$ as the barrier is increased to $V \to E - m$.

When $V > E - m$, k' becomes imaginary and there is exponential decay with a penetration length

$$d = 1/\sqrt{m^2 - (V - E)^2}. \tag{3.16}$$

However, something very strange happens when V is increased further and further. First, the penetration length decreases as one would expect. But obviously, there is a minimum at $d = 1/m$, the Compton wavelength ($\approx 4 \times 10^{-13} m$ for electrons), which is reached when $V - (E - m) = m$. Increasing V still further no longer restricts the penetration region but makes it larger again. Even weirder, when $V - (E - m) > 2m$, k' becomes real again, and ψ_{trans} oscillatory. In this case, $\rho < 0$, and therefore $j_{\text{trans}} < 0$ and $j_{\text{refl}} > j_{\text{in}}$.

This is Klein's paradox. It shows that the Dirac equation can be interpreted as a single-particle theory only as long as there are no external forces and energies which are comparable to the mass scale m.

Although the above example is rather artificial, it points to phenomena such as pair creation in strong fields. It also indicates that in a relativistic theory there is, besides the well-known uncertainty principle, a fundamental lower limit to the localizability of a single particle, which is given by its Compton wavelength.

Let us confirm this latter statement by an attempt to construct a localized wave packet. At time $t = 0$ we take

$$\psi(0, \vec{x}) = e^{-\vec{x}^2/(2D^2)} w \tag{3.17}$$

with a fixed spinor $w = \binom{\varphi}{0}$.

The general solution of the free Dirac equation is given by a superposition of the plane waves obtained in the preceding section,

$$\psi(t, \vec{x}) = \int \frac{d^3p}{(2\pi)^3} \frac{m}{E} \sum_{a=1}^{2} \left\{ b(p; a) \, u^{(a)}(p) e^{-ip \cdot x} + d^*(p; a) \, v^{(a)}(p) e^{ip \cdot x} \right\} \tag{3.18}$$

where b and d^* are the expansion coefficients of positive and negative-energy solutions (the factor m/E is introduced for convenience only). These are determined by the initial condition (3.17) through

$$\int d^3x e^{-i\vec{p}\vec{x}} \psi(0, \vec{x}) = (2\pi D^2)^{3/2} e^{-\vec{p}^2 D^2/2} w = \frac{m}{E} \sum_{a=1}^{2} \left\{ b(p; a) \, u^{(a)}(p) + d^*(\tilde{p}; a) \, v^{(a)}(\tilde{p}) \right\} \tag{3.19}$$

where $\tilde{p} := (p^0, -\vec{p})$.

As one easily verifies from the explicit expressions (3.7) and (3.8), the following orthogonality relations hold

$$u^{\dagger(a)}(k) u^{(b)}(k) = \frac{E}{m} \delta^{ab} = v^{\dagger(a)}(k) v^{(b)}(k),$$
$$v^{\dagger(a)}(\tilde{k}) u^{(b)}(k) = 0 = u^{\dagger(a)}(\tilde{k}) v^{(b)}(k). \tag{3.20}$$

These we can use to calculate

$$b(p; a) = (2\pi D^2)^{3/2} e^{-\vec{p}^2 D^2/2} \, u^{\dagger(a)}(p) w$$
$$d^*(p; a) = (2\pi D^2)^{3/2} e^{-\vec{p}^2 D^2/2} \, v^{\dagger(a)}(p) w. \tag{3.21}$$

From (3.7) and (3.8) we see that the ratio of the amplitudes of negative-energy solutions over positive-energy ones is of the order of $d^*/b \sim |\vec{p}|/(E + m)$. As long as D is much larger than the Compton wavelength, $D \gg 1/m$, there are essential contributions only from $|\vec{p}| \ll m$, and thus $d^*/b \ll 1$. However, if one tries to localise

the wavefunction to be comparable or smaller than the Compton wavelength, the negative-energy solutions become important and can no longer be neglected.

The presence of non-negligible negative-energy solutions has a curious consequence for the behaviour of the current density $\vec{j} = \bar{\psi}\vec{\gamma}\psi$. While this current equals $\langle \vec{p}/E \rangle$ (the group velocity of the wave packet) so long as there is only a positive-energy component, with both components there is also an interference term involving e^{2iEt}. Because $E \geq m$, this introduces an oscillatory contribution with extremely high frequencies $\geq 2m \approx 2 \times 10^{21}\mathrm{Hz}$ called "zitterbewegung".

Despite these limitations, the Dirac equation used as a generalization of the Schrödinger equation is of great importance and we shall elaborate on it further before setting up the full quantum field theory, bearing in mind however that a single (or fixed-number) particle theory makes sense only as long as all energies involved are well below the particles' rest mass and therefore all length scales are much larger than the Compton wavelength.

3.3   Electromagnetic coupling

We begin by recapitulating the relativistic form of Maxwell's equations, using units where $c = 1$ and the Coulomb force between charges is $Q_1 Q_2/4\pi r$ (Heaviside units).

The electric and magnetic fields are part of an antisymmetric tensor

$$F^{\mu\nu} = -F^{\nu\mu} = \begin{pmatrix} 0 & -E^1 & -E^2 & -E^3 \\ E^1 & 0 & -B^3 & B^2 \\ E^2 & B^3 & 0 & -B^1 \\ E^3 & -B^2 & B^1 & 0 \end{pmatrix}. \tag{3.22}$$

Combining the electric charge and current in

$$j^\mu = (\rho, \vec{j}) \tag{3.23}$$

one half of Maxwell's equation, namely,

$$\mathrm{div}\,\vec{E} = \rho, \quad \mathrm{rot}\,\vec{B} - \partial_t \vec{E} = \vec{j} \tag{3.24}$$

can be written covariantly as

$$\partial_\mu F^{\mu\nu} = j^\nu \tag{3.25}$$

and the other half

$$\mathrm{div}\,\vec{B} = 0, \quad \mathrm{rot}\,\vec{E} + \partial_t \vec{B} = 0 \tag{3.26}$$

in terms of the "dual" field strength tensor $\tilde{F}^{\mu\nu} := \frac{1}{2}\varepsilon^{\mu\nu\sigma\rho}F_{\sigma\rho}$ as

$$\partial_\mu \tilde{F}^{\mu\nu} = 0. \tag{3.27}$$

$\tilde{F}$ is obtained from (3.22) by substituting $\vec{E} \to -\vec{B}$ and $\vec{B} \to \vec{E}$, so (3.27) expresses the absence of magnetic sources. The totally antisymmetric tensor $\varepsilon_{\mu\nu\sigma\rho}$ equals $+1$ (-1) for (μ, ν, σ, ρ) an even (odd) permutation of (0,1,2,3). Note that $\varepsilon^{0123} = -\varepsilon_{0123}$.

The second set of Maxwell's equations (3.27) can be solved by writing

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu, \qquad A^\mu = (\phi, \vec{A}) \tag{3.28}$$

where the 4-potential A^μ is determined only up to local *gauge* transformations $\delta A^\mu = \partial^\mu \Lambda(x)$ which leave $F^{\mu\nu}$ invariant.

The source-containing set of Maxwell's equations (3.25) are compatible with the antisymmetry of $F^{\mu\nu}$ only if j is a conserved current: $\partial_\nu j^\nu = \partial_\nu \partial_\mu F^{\mu\nu} \equiv 0$.

In the Dirac theory, $j^\mu = e\bar{\psi}\gamma^\mu\psi$ is a suitable candidate for the electromagnetic current. Conversely, the Dirac field can be coupled to the electromagnetic field by the "minimal" substitution $\partial_\mu \to \partial_\mu + ieA_\mu$, leading to

$$(i\slashed{\partial} - e\slashed{A}(x) - m)\psi(x) = 0. \tag{3.29}$$

The arbitrariness of the gauge potential A due to gauge transformations $A_\mu(x) \to A_\mu(x) + \partial_\mu \Lambda(x)$ can be compensated by a local phase rotation $\psi(x) \to e^{-ie\Lambda(x)}\psi(x)$. The latter shows that electrodynamics is associated with the (Abelian) *gauge group* U(1) — unitary matrices with dimension 1. It is the simplest example of the more general class of Yang-Mills theories, where Λ becomes a nontrivial matrix built from the generators of some generally nonabelian group.

Writing (3.29) in terms of the $\vec{\alpha}$ and β matrices we have

$$i\frac{\partial\psi}{\partial t} = \underbrace{(\vec{\alpha} \cdot \vec{p} + \beta m)}_{H_0}\psi + \underbrace{\left(-e\vec{\alpha} \cdot \vec{A} + e\phi\right)}_{H_{\text{int}}}\psi. \tag{3.30}$$

This resembles the interaction of a classical particle in an external field with $\vec{\alpha}$ playing the role of velocity. Indeed, we have $\dot{\vec{x}} = i[H, \vec{x}] = \vec{\alpha}$.

To study the physical content of the Dirac equation coupled to electromagnetic fields we shall first consider its nonrelativistic limit.

3.3.1   Nonrelativistic limit

In the limit of $E - m \ll m$, it is appropriate to separate off the large energy associated with the particle's rest mass and to write

$$\psi(t, \vec{x}) = e^{-imt}\begin{pmatrix} \varphi(t, \vec{x}) \\ \chi(t, \vec{x}) \end{pmatrix}. \tag{3.31}$$

In the standard Dirac representation (2.14), this gives

$$i\frac{\partial\varphi}{\partial t} = \vec{\sigma}\cdot(\vec{p}-e\vec{A})\,\chi + eA^0\,\varphi \tag{3.32}$$

$$i\frac{\partial\chi}{\partial t} = \vec{\sigma}\cdot(\vec{p}-e\vec{A})\,\varphi + eA^0\,\chi - 2m\,\chi \tag{3.33}$$

The latter equation is dominated by the mass term, against which $i\dot{\chi}$ can be neglected in the nonrelativistic limit, so this equation can be solved algebraically. Assuming further that $eA^0 \ll m$, we have

$$\chi \approx \frac{1}{2m}\vec{\sigma}\cdot(\vec{p}-e\vec{A})\varphi \ll \varphi. \tag{3.34}$$

The Dirac spinor is thus seen to be separated in large and small components φ and χ, with φ being determined by the so-called Pauli equation obtained by inserting (3.34) into (3.32),

$$i\frac{\partial\varphi}{\partial t} = \left[\frac{1}{2m}(\vec{\sigma}\cdot\vec{\pi})^2 + eA^0\right]\varphi, \qquad \vec{\pi} := \vec{p} - e\vec{A}(x). \tag{3.35}$$

Because $\sigma_i\sigma_j = \frac{1}{2}\{\sigma_i,\sigma_j\} + \frac{1}{2}[\sigma_i,\sigma_j] = \delta_{ij} + i\varepsilon_{ijk}\sigma_k$ we can rewrite this according to

$$(\vec{\sigma}\cdot\vec{\pi})^2 = \vec{\pi}^2 + \frac{i}{2}\varepsilon_{ijk}\sigma_k[\pi_i,\pi_j] = \vec{\pi}^2 - e\,\underbrace{\varepsilon_{ijk}\partial_i A_j}_{B_k}\,\sigma_k \tag{3.36}$$

yielding the alternative version

$$i\frac{\partial\varphi}{\partial t} = \left[\frac{1}{2m}\left(\vec{p}-e\vec{A}\right)^2 + eA^0 - \frac{e}{2m}\,\vec{\sigma}\cdot\vec{B}\right]\varphi. \tag{3.37}$$

In the special case of a weak constant magnetic field, $\vec{A} = \frac{1}{2}\vec{B}\times\vec{x}$, one has $(\vec{p}-e\vec{A})^2 \approx \vec{p}^2 - e\,(\vec{x}\times\vec{p})\cdot\vec{B}$ and the operator on the right-hand-side of the Pauli equation becomes

$$H_{\text{Pauli}} \approx \frac{\vec{p}^2}{2m} + eA^0 - \underbrace{\frac{e}{2m}}_{\mu_{\text{B}}}\left(\vec{L}+2\vec{S}\right)\cdot\vec{B}, \qquad \vec{S} \equiv \frac{1}{2}\vec{\sigma}. \tag{3.38}$$

The magnetic moment associated with spin is thus seen to have an anomalous factor of 2. This gyromagnetic ratio $g = (|\text{magnetic moment}| \times |\text{spin}|)/(\text{Bohr magneton } \mu_{\text{B}}) = 2$ is our first nontrivial prediction of the Dirac theory, and it is indeed in good agreement with the actual magnetic moment of electrons and muons[11]; the small deviations from $g = 2$ that are observed experimentally will find their explanation in the full quantum electrodynamics.

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[11]The gyromagnetic ratio for protons and neutrons is however substantially different from 2, pointing to their important internal structure.

In the relativistic Dirac equation, the spin-dependent interactions can be isolated by acting on (3.29) with $(i\not\partial - e\not A + m)$. In analogy to the steps leading from (3.35) to (3.37) one obtains

$$\left[(i\not\partial - e\not A)^2 - m^2\right]\psi = \left[(i\partial - eA)^2 - m^2 - \frac{e}{2}\sigma^{\mu\nu}F_{\mu\nu}\right]\psi = 0, \quad \sigma^{\mu\nu} := \frac{i}{2}[\gamma^\mu, \gamma^\nu]$$

(3.39)

with $\frac{1}{2}\vec{\sigma}^{\mu\nu}F_{\mu\nu} = (i\vec{\alpha}\cdot\vec{E} + \vec{\Sigma}\cdot\vec{B})$.

3.4   Foldy-Wouthuysen transformation

By decoupling large and small components of a Dirac spinor in the nonrelativistic approximation we have been able to highlight some of its physical content. Such a procedure can be carried out systematically in a series expansion in powers of E_{kin}/m and has been worked out by Foldy and Wouthuysen (1950).

The goal is to find a unitary transformation

$$\psi' = e^{iS}\psi$$

(3.40)

for ψ of (3.30) such that in

$$i\partial_t\psi' = e^{iS}\left(He^{-iS} - i(\partial_t e^{-iS})\right)\psi' =: H'\psi'$$

(3.41)

H' takes a block-diagonal form, at least up to some order of a nonrelativistic expansion.

A familiar similar problem is the diagonalization of a Hamilton operator $H = \sigma_x B_x + \sigma_z B_z$. This is achieved by a rotation about the y-axis by $e^{\frac{i}{2}\sigma_y\theta} = e^{\frac{1}{2}\sigma_z\sigma_x\theta}$ with $\tan\theta = B_x/B_z$.

3.4.1   Free Dirac equation

In the case of the free Dirac equation where $H = \vec{\alpha}\cdot\vec{p} + \beta m$ with α and β as given in the Dirac representation (2.14), we have a similar structure with $\sigma_x \leftrightarrow \vec{\alpha}\cdot\vec{p}$ and $\beta \leftrightarrow \sigma_z$. This motivates an ansatz of the form

$$e^{iS} = \exp\left(\beta\vec{\alpha}\cdot\vec{p}\,\theta(p)/|\vec{p}|\right) = \exp\left(\frac{1}{|\vec{p}|}\vec{\gamma}\cdot\vec{p}\,\theta(p)\right).$$

(3.42)

Because $\left(\frac{\vec{\gamma}\cdot\vec{p}}{|\vec{p}|}\right)^2 = -\mathbf{1}$, we can easily calculate

$$e^{iS} = \cos\theta + \frac{\vec{\gamma}\cdot\vec{p}}{|\vec{p}|}\sin\theta$$

(3.43)

and

$$
\begin{aligned}
H' &= e^{iS}He^{-iS} = \left(\cos\theta + \beta\frac{\vec{\alpha}\cdot\vec{p}}{|\vec{p}|}\sin\theta\right)(\vec{\alpha}\cdot\vec{p} + \beta m)\left(\cos\theta - \beta\frac{\vec{\alpha}\cdot\vec{p}}{|\vec{p}|}\sin\theta\right) \\
&= (\vec{\alpha}\cdot\vec{p} + \beta m)\underbrace{\left(\cos\theta - \beta\frac{\vec{\alpha}\cdot\vec{p}}{|\vec{p}|}\sin\theta\right)^2}_{\exp(-2\beta\frac{\vec{\alpha}\cdot\vec{p}}{|\vec{p}|}\theta)} = (\vec{\alpha}\cdot\vec{p} + \beta m)\left(\cos 2\theta - \beta\frac{\vec{\alpha}\cdot\vec{p}}{|\vec{p}|}\sin 2\theta\right) \\
&= \vec{\alpha}\cdot\vec{p}\left[\cos 2\theta - \frac{m}{|\vec{p}|}\sin 2\theta\right] + \beta\left[m\cos 2\theta + \frac{\vec{p}^2}{|\vec{p}|}\sin 2\theta\right] \tag{3.44}
\end{aligned}
$$

In order that H' becomes diagonal, the first of the square brackets has to vanish. This leads to $\tan 2\theta = \frac{|\vec{p}|}{m}$, which entails $\sin 2\theta = \frac{|\vec{p}|}{E}$, $\cos 2\theta = \frac{m}{E}$, for $E \equiv \sqrt{\vec{p}^2 + m^2}$, and so

$$
H' = \beta\sqrt{\vec{p}^2 + m^2} = \begin{pmatrix} \sqrt{\vec{p}^2 + m^2}\mathbf{1}_2 & \mathbf{0} \\ \mathbf{0} & -\sqrt{\vec{p}^2 + m^2}\mathbf{1}_2 \end{pmatrix} \tag{3.45}
$$

We have therefore managed to diagonalize the Dirac Hamitonian, which clearly displays the solutions corresponding to positive and negative energies.

Note however that the transformation leading to (3.45) is nonlocal. In configuration space, the FW-transformed spinor (3.40) would have to be written as a nontrivial integral $\int dx' \langle x|e^{iS}|x'\rangle \psi(x')$ over all of 3-space, where the main contribution comes from a neighbourhood of x with radius $1/m$. Also, the usual $\vec{x}$-operator changes its meaning when applied directly to ψ'. As such it is referred to as "mean location". Transformed back into the standard formulation it corresponds to the nonlocal operator $\vec{x}_{\text{mean}} = e^{-iS}\vec{x}e^{iS}$. If one defines similarly a mean angular momentum and a mean spin operator, these are found to commute with the free Hamilton operator, in constrast to the usual local quantities.

3.4.2   Interacting Dirac equation

When external fields are present, e^{iS} will have to depend explicitly on space and time[12] as well. This makes a solution in closed form impossible in general and one has to be content with an approximate solution. We shall consider a nonrelativistic expansion, where $|\vec{p}|/m$, $|\vec{A}|/m$, and $|A_0|/m$ are supposed to be small parameters.

The interaction Hamiltonian

$$
H = \beta m + \mathcal{O} + \mathcal{E} \equiv \beta m + (\vec{\alpha}\cdot(\vec{p} - e\vec{A})) + eA^0\mathbf{1} \tag{3.46}
$$

is dominated by the block-diagonal mass term. The aim is to get rid of the off-diagonal ("odd") term $\mathcal{O}$.

---

[12]A time dependence moreover leads to a shift of the energy eigenvalues.

In the free case, this was achieved by $iS = \beta \mathcal{O}_{\text{free}} \theta(p)/|\vec{p}|$ with $\theta = \frac{1}{2} \arctan(|\vec{p}|/m)$. For $|\vec{p}|/m \ll 1$ we can approximate $\theta \approx |\vec{p}|/2m$.

As a first step, we can try $e^{iS} = e^{\frac{1}{2m}\beta\mathcal{O}}$. This gives $H' = \beta m + \mathcal{O}' + \mathcal{E}'$ where $\mathcal{O}' = O(\frac{1}{m})$. This procedure can now be repeated with $e^{iS'} = e^{\frac{1}{2m}\beta\mathcal{O}'}$ and so forth, successively increasing the order of the odd terms.

After 3 iterations, one finds[13] in terms of "mean" operators

$$
\begin{aligned}
H''' &= \beta m + \mathcal{E}''' + O(\frac{1}{m^3}) \\
&= \beta \left[m + \frac{(\vec{p} - e\vec{A})^2}{2m} - \frac{\vec{p}^4}{8m^3} \right] + e\phi - \frac{e}{2m}\beta\vec{\sigma}\cdot\vec{B} \qquad (3.47) \\
&\quad + \left(-i\frac{e}{8m^2}\vec{\sigma}\cdot\text{rot}\,\vec{E} - \frac{e}{4m^2}\vec{\sigma}\cdot(\vec{E}\times\vec{p}) \right) \qquad (3.48) \\
&\quad - \frac{e}{8m^2}\vec{\nabla}\cdot\vec{E} \qquad (3.49)
\end{aligned}
$$

The first terms (3.47) are what we have found in the Pauli equation (3.37) except that there is now a relativistic correction term to the kinetic energy.

The terms (3.48) contain spin-orbit interactions. With $\vec{p} \approx m\vec{v}$, the latter of the two reads

$$
-\frac{1}{2}\frac{e}{2m}\vec{\sigma}\cdot(\vec{E}\times\vec{v}).
$$

$(\vec{E}\times\vec{v})$ is the magnetic field as seen from a particle moving with velocity $\vec{v}$ through the electric field $\vec{E}$, $\frac{-e}{2m}$ is the usual coefficient of the magnetic dipol energy as in (3.47), and the extra factor $\frac{1}{2}$ can be understood as the effect of Thomas precession, which happens to reduce the gyromagnetic factor $g = 2$ to the standard value 1.

In a static, spherically symmetric potential, rot $\vec{E} = 0$ and the spin-orbit terms (3.48) reduce to

$$
\frac{e}{4m^2 r}\frac{d\phi}{dr}\vec{L}\cdot\vec{\sigma}.
$$

The last term (3.49) is called Darwin term. It can be interpreted as arising from fluctuations of the position of an electron $\vec{x}$ with $\langle\delta\vec{x}\rangle = 0$ but $\langle(\delta\vec{x})^2\rangle > 0$, which entails a shift of the electrostatic energy according to

$$
e\langle\phi(\vec{x} + \delta\vec{x})\rangle = e\phi(\vec{x}) + \frac{e}{2}\frac{\partial^2\phi}{\partial x^i \partial x^j}\underbrace{\langle\delta x^i \delta x^j\rangle}_{\frac{1}{3}\delta_{ij}\langle(\delta\vec{x})^2\rangle} = e\phi(\vec{x}) + \frac{e}{6}\underbrace{\triangle\phi}_{-\text{div}\,\vec{E}}\langle(\delta\vec{x})^2\rangle \qquad (3.50)
$$

The fundamental uncertainty of position that we have observed before (zitterbewegung) was of the order of the Compton wavelength, so we expect $\langle(\delta\vec{x})^2\rangle \sim 1/m^2$. So (3.50) is consistent in sign and order of magnitude with the Darwin term (3.49).

---

[13]See e.g. Bjorken/Drell: Relativistic quantum mechanics, ch. 4.

3.5   Hydrogen-like atoms

3.5.1   Spinor harmonics

The free Hamilton operator $H_0 = \vec{\alpha} \cdot \vec{p} + \beta m$ commutes with the total angular momentum $\vec{J} = \vec{L} + \vec{S}$, $\vec{S} = \frac{1}{2}\vec{\Sigma}$, but not separately with $\vec{L}$ or $\vec{S}$. The same holds true in a spherical symmetric electrostatic potential, because $[\vec{L}, f(r)] = 0 = [\vec{\Sigma}, f(r)]$,

$$H = \vec{\alpha} \cdot \vec{p} + \beta m + eA^0(r), \qquad [H, \vec{J}] = 0. \tag{3.51}$$

Intuitively, one might expect that if not all of $\vec{S}$ then at least $\vec{S} \cdot \vec{J}$ should be conserved, which would be the case for a spin in precession around the conserved total angular momentum. However, one finds

$$[H, \vec{\Sigma} \cdot \vec{J}] = [H, \vec{\Sigma}] \cdot \vec{J} = 2i(\vec{\alpha} \times \vec{p}) \cdot \vec{J}. \tag{3.52}$$

As a second guess, let us try $\beta \vec{\Sigma} \cdot \vec{J}$

$$[H, \beta\vec{\Sigma} \cdot \vec{J}] = \underbrace{[H, \beta]}_{-2\beta\vec{\alpha}\cdot\vec{p}} \vec{\Sigma} \cdot \vec{J} + \beta\, [H, \vec{\Sigma}] \cdot \vec{J} \tag{3.53}$$

This can be streamlined by using that $\vec{\alpha} = \gamma^5 \vec{\Sigma}$ and rewriting

$$\vec{\alpha} \cdot \vec{p}\, \vec{\Sigma} \cdot \vec{J} = \gamma^5\, \vec{\Sigma} \cdot \vec{p}\, \vec{\Sigma} \cdot \vec{J} = \gamma^5 \vec{p} \cdot \vec{J} + i(\vec{\alpha} \times \vec{p}) \cdot \vec{J} \tag{3.54}$$

which shows that

$$[H, \beta\vec{\Sigma} \cdot \vec{J}] = -2\beta\gamma^5\vec{p} \cdot \vec{J} = -\beta\gamma^5\vec{p} \cdot \vec{\Sigma} = -\beta\vec{p} \cdot \vec{\alpha} = \frac{1}{2}[H, \beta]. \tag{3.55}$$

Hence,

$$[H, \beta(\vec{\Sigma} \cdot \vec{J} - \frac{1}{2})] =: [H, K] = 0, \tag{3.56}$$

so the "spin-orbit" operator K defines a further conserved quantity. Using that $(\vec{\Sigma})^2 = 3$, it can be alternatively expressed as

$$K = \beta(\vec{\Sigma} \cdot \vec{J} - \frac{1}{2}) = \beta(\vec{\Sigma} \cdot \vec{L} + 1) = \beta(\vec{J}^2 - \vec{L}^2 + \frac{1}{4}). \tag{3.57}$$

In the standard Dirac representation where $\vec{\Sigma} = \vec{\sigma} \oplus \vec{\sigma}$, this is a block-diagonal operator with just a different sign in the upper and lower blocks. We can therefore construct eigenstates of $\vec{J}^2$, J_z, and K out of 2-component spinors φ which are eigenstates of $\vec{J}^2$, J_z, and $(\vec{\sigma} \cdot \vec{L} + 1)$. The eigenvalues of the latter are

$$k = j(j + 1) - l(l + 1) + \frac{1}{4}.$$

Because $j = l \pm \frac{1}{2}$, there are only two possibilities

$$k = \begin{cases} j + \frac{1}{2} & \text{for} \quad j = l + \frac{1}{2} \\ -(j + \frac{1}{2}) & \text{for} \quad j = l - \frac{1}{2} \end{cases} \tag{3.58}$$

The eigenspinors φ are thus characterised by the values of j, m, and $\text{sign}(k)$, where the latter is also the sign in $j = l \pm \frac{1}{2}$. They are called spinor harmonics and are linear combination of products of the eigenvectors of σ_z,

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

and the spherical harmonics $Y_{l,l_z}(\theta, \varphi)$. With the relevant Clebsch-Gordan coefficients they are given explicitly by

$$\varphi_{jm}^{(+)}(\theta, \varphi) = \frac{1}{\sqrt{2l+1}} \begin{pmatrix} \sqrt{l+m+\frac{1}{2}}\, Y_{l,m-\frac{1}{2}}(\theta, \varphi) \\ \sqrt{l-m+\frac{1}{2}}\, Y_{l,m+\frac{1}{2}}(\theta, \varphi) \end{pmatrix}, \tag{3.59}$$

$$\varphi_{jm}^{(-)}(\theta, \varphi) = \frac{1}{\sqrt{2l+1}} \begin{pmatrix} \sqrt{l-m+\frac{1}{2}}\, Y_{l,m-\frac{1}{2}}(\theta, \varphi) \\ -\sqrt{l+m+\frac{1}{2}}\, Y_{l,m+\frac{1}{2}}(\theta, \varphi) \end{pmatrix}. \tag{3.60}$$

For a given value of j, the spinor harmonics with different sign of k have opposite parity (l differs by one). They are transformed into each other by

$$\frac{\vec{\sigma} \cdot \vec{x}}{|\vec{x}|} \varphi_{jm}^{(\pm)} = \varphi_{jm}^{(\mp)}. \tag{3.61}$$

This can be inferred from the following properties of $\vec{\sigma} \cdot \hat{\vec{x}} := \vec{\sigma} \cdot \vec{x}/|\vec{x}|$ (exercises!):

$[\vec{\sigma} \cdot \hat{\vec{x}}, \vec{J}] = 0$, from which it follows that j, m are unchanged;

$\{\vec{\sigma} \cdot \hat{\vec{x}}, \vec{\sigma} \cdot \vec{L} + 1\} = 0$, which implies that the sign of k is changed;

$(\vec{\sigma} \cdot \hat{\vec{x}})^2 = \mathbf{1}_2$, which requires that $\vec{\sigma} \cdot \hat{\vec{x}} \varphi_{jm}^{(\pm)} = \eta \varphi_{jm}^{(\mp)}$ with $\eta^2 = 1$. $\eta = 1$ is secured by the particular choice of phase in (3.59), (3.60).

3.5.2 Separation of variables

In the spherically symmetric case (3.51) one can separate the dependence of the Dirac spinor in $H\psi = E\psi$ on angular variables by the ansatz

$$\psi = \frac{1}{r} \begin{pmatrix} ig(r)\varphi_{jm}^{\kappa}(\theta, \varphi) \\ f(r)\varphi_{jm}^{-\kappa}(\theta, \varphi) \end{pmatrix} \tag{3.62}$$

where $\kappa = \text{sign}(k)$, which introduces two functions $f(g)$ and $g(r)$ for a given set of j, m, κ.

This gives

$$(E - m - eA^0)\frac{ig}{r}\varphi^\kappa_{jm} = \vec{\sigma}\cdot\vec{p}\,\frac{f}{r}\varphi^{-\kappa}_{jm} \qquad (3.63)$$

$$(E + m - eA^0)\frac{f}{r}\varphi^{-\kappa}_{jm} = \vec{\sigma}\cdot\vec{p}\,\frac{ig}{r}\varphi^\kappa_{jm}. \qquad (3.64)$$

The parity of the spinor harmonics on the right-hand side can be reversed by inserting $\left(\vec{\sigma}\cdot\hat{\vec{x}}\right)^2 = \mathbf{1}_2$ and rewriting

$$\vec{\sigma}\cdot\vec{p} = \left(\vec{\sigma}\cdot\hat{\vec{x}}\right)^2\vec{\sigma}\cdot\vec{p} = \vec{\sigma}\cdot\hat{\vec{x}}\,\frac{1}{r}\left(\vec{x}\cdot\vec{p} + i\vec{\sigma}\cdot\vec{L}\right) = \vec{\sigma}\cdot\hat{\vec{x}}\,\frac{1}{ir}\left(\frac{\partial}{\partial r}r - \underbrace{(1 + \vec{\sigma}\cdot\vec{L})}_{\mp k \text{ for } \varphi^\mp}\right).$$

The spinor harmonics therefore drop out, yielding the radial equations

$$(E - m - eA^0)\,g(r) + (\frac{d}{dr} + \frac{k}{r})\,f(r) = 0, \qquad (3.65)$$

$$(E + m - eA^0)\,f(r) - (\frac{d}{dr} - \frac{k}{r})\,g(r) = 0. \qquad (3.66)$$

3.5.3   Exact solutions for the Coulomb potential

We shall now consider the motion of an electron in the Coulomb potential $A^0 = -\frac{Ze}{4\pi r}$, assuming that the central charge is sufficiently heavy to neglect its dynamics.

The asymptotic behaviour of the radial functions is determined by the $r \to \infty$ limit of (3.65), (3.66), leading to $f, g \sim \exp(\pm\sqrt{m^2 - E^2}\,r)$. A bound state has $E < m$, and the negative sign has to be chosen for normalizability.

Separating off this asymptotic behaviour, we make the ansatz

$$f(r) = \sqrt{1 - \frac{E}{m}}\,e^{-\lambda r}\,(F_1 - F_2)(\rho), \qquad g(r) = \sqrt{1 + \frac{E}{m}}\,e^{-\lambda r}\,(F_1 + F_2)(\rho) \qquad (3.67)$$

with $\lambda := \sqrt{m^2 - E^2}$, $\rho := 2\lambda r$. A generalized power series ansatz

$$F_{1,2} = \rho^\gamma(a_{1,2} + b_{1,2}\rho + \ldots)$$

gives (exercise!)

$$\gamma = \sqrt{k^2 - Z^2\alpha^2} \qquad (3.68)$$

and a power series for $\rho^{-\gamma}F_{1,2}$ corresponding to a degenerate hypergeometric function $F(a, b; \rho)$, namely

$$\rho^{-\gamma}F_1(\rho) = A\,F\left(\gamma + 1 - \tfrac{Z\alpha E}{\lambda}, 2\gamma + 1; \rho\right), \qquad (3.69)$$

$$\rho^{-\gamma}F_2(\rho) = B\,F\left(\gamma - \tfrac{Z\alpha E}{\lambda}, 2\gamma + 1; \rho\right), \qquad (3.70)$$

where $A/B = (\gamma\lambda - Z\alpha E)/(k\lambda + Z\alpha m)$. The degenerate hypergeometric function grows exponentially like e^ρ for $\rho \to \infty$ unless its first argument vanishes or equals a negative integer, in which case it reduces to a polynomial. So (3.70) gives a quantization condition for the energy in terms of a nonnegative *radial quantum number* n_r,

$$\gamma - \frac{Z\alpha E}{\lambda} = -n_r, \quad n_r = 0, 1, 2, \ldots \tag{3.71}$$

with n_r giving the degree of the polynomial in (3.70). $n_r = 0$ is excluded for (3.69) unless $A = 0$. Now $A/B \propto n_r$ and thus vanishes for $n_r = 0$, provided however that $k > 0$ — when $n_r = 0$ one finds that $|k| = Z\alpha m/\lambda$, so that for $k < 0$ the denominator in A/B also vanishes, leading to $A/B = -m/E \neq 0$ instead. So for $n_r = 0$ only $\kappa = +1$ leads to a normalizable solution; for each other value of n_r, there are two different solutions corresponding to the two different signs κ.

Solving (3.71) for E gives

$$E = E_{nj} = m\left[1 + \frac{Z^2\alpha^2}{(\gamma + n_r)^2}\right]^{-\frac{1}{2}} = m\left[1 + \frac{Z^2\alpha^2}{\left(n - (j + \frac{1}{2}) + \sqrt{(j + \frac{1}{2})^2 - Z^2\alpha^2}\right)^2}\right]^{-\frac{1}{2}} \tag{3.72}$$

where in view of $\gamma = |k| + O(\alpha^2)$ we have introduced the *main quantum number*

$$n := n_r + |k| = n_r + j + \frac{1}{2}, \quad n = 1, 2, \ldots \tag{3.73}$$

Expanding (3.72) in powers of $Z^2\alpha^2$ we find

$$E_{nj} = m\left\{1 - \frac{Z^2\alpha^2}{2n^2} - \frac{Z^4\alpha^4}{n^3(2j+1)} + \frac{3Z^4\alpha^4}{8n^4} + O(\alpha^6)\right\}. \tag{3.74}$$

The term proportional to α^2 corresponds to the nonrelativistic Balmer spectrum. It is independent of j thanks to an accidental dynamical O(4) symmetry of the non-relativistic Coulomb problem. The degeneracy in j is lifted by the subsequent terms ("fine structure") resulting from relativistic effects and the spin-orbit coupling.[14] The remaining degeneracy is twofold in terms of $l = j \pm \frac{1}{2}$, except for $n_r = 0$, i.e. $j = n - \frac{1}{2}$, where the maximal value of $l = n - 1$ for a given n is reached.

---

[14]For spinless particles, the Klein-Gordon equation leads to a similar fine structure formula but with $j + \frac{1}{2} = 1, 2, \ldots$ replaced by $l + \frac{1}{2} = \frac{1}{2}, \frac{3}{2}, \ldots$. This differs from Sommerfeld's fine structure formula which had $l + 1$ instead and accidentally produced the correct result without taking into account spin. The failure to reproduce Sommerfeld's result was the reason that Schrödinger gave up on the relativistic (Klein-Gordon) equation in favour of his nonrelativistic one.

States with higher values of j but equal n are shifted to higher energies by about $4.5Z^4 \times 10^{-5}$eV (for $n = 2$), which is to be compared with the Rydberg energy ≈ 13.6 eV.

The lowest energy eigenstates in increasing order
in standard spectroscopic notation $n(l)_j$:

n	j	$l = 0$	$l = 1$	$l = 2$	$\dots$	n_r
1	$\frac{1}{2}$	$1s_{1/2}$				0
2	$\frac{1}{2}$	$2s_{1/2}$	$2p_{1/2}$			1
2	$\frac{3}{2}$		$2p_{3/2}$			0
3	$\frac{1}{2}$	$3s_{1/2}$	$3p_{1/2}$			2
3	$\frac{3}{2}$		$3p_{3/2}$	$3d_{3/2}$		1
3	$\frac{5}{2}$			$3d_{5/2}$		0

Clearly, for too large values of Z, the above results cease to hold: when $Z^2\alpha^2 > k^2 \geq 1$, that is when $Z \gtrsim 137$, γ in (3.72) turns imaginary and the energy eigenvalues of the lowest-lying states become complex. Then also the wave function develops an essential singularity at $r = 0$: $\psi \rightarrow r^{\gamma-1} \sim \frac{1}{r}\cos(|\gamma|\ln r)$. However, for such extreme field strength the binding energy becomes comparable to the rest mass of the electron and therefore we should expect a breakdown of the single-particle theory.

Actually, the Dirac solution of the Coulomb problem is also singular for $Z \ll 137$ for all solutions with $|k| = 1$, i.e. $j = \frac{1}{2}$. Then $\gamma \approx |k|(1 - \frac{Z^2\alpha^2}{2|k|}) < 1$ for $|k| = 1$, so $\psi \sim r^{\gamma-1}$ is singular at the origin, although square integrable. For small Z this behaviour is however noticable only for extremely small values of r, because $\psi \sim r^{-Z^2\alpha^2/2} \approx r^{-Z^2/16300}$.

The exact solutions for the Dirac equation in a Coulomb potential are still only an approximate solution for the real hydrogen and hydrogen-like atoms. There are a number of other effects that need to be taken into account:

Hyperfine structure: The nucleus of an atom has a magnetic moment which couples to the total angular momentum of the electron. In the hydrogen atom, every level is split into narrow doublets. Treated nonrelativistically, the energy corrections are approximately

$$\langle H_{\text{hf}} \rangle \propto \vec{\sigma}_e \cdot \vec{\sigma}_p |\psi(0)|$$

with $\psi_{n,l=0}(0) = \sqrt{\frac{1}{\pi}(\frac{mZ\alpha}{n})^3}$, $\psi_{n,l>0}(0) = 0$, and $\vec{\sigma}_e \cdot \vec{\sigma}_p$ equals $+1$ and -3 in the triplett and singlett states, respectively. So the main effect is a splitting of the s states, with the splitting of the $1s_{1/2}$ state being responsible for the 21cm line that

is famous for its role in radio astronomy. Compared to the fine-structure splitting, the hyperfine splitting is suppressed by an extra factor of $m_e/m_p \approx 1/1800$.

Nuclear effects: The finite size of the nucleus and its charge distribution modifies the electrostatic potential close to the origin. This again affects mainly the s states. The slightly different energy levels that result for different isotopes can even be used for isotopic separation.

Two-body corrections: As a first approximation, the dynamics of the nucleus with mass m_N can be taken into account by using the reduced mass $m^{-1} = m_e^{-1} + m_N^{-1}$ in all the terms of (3.74) other than the rest mass. However, ultimately the recoil of the nucleus has to be taken into account in a relativistic manner. This gives further corrections that are of the order of magnitude of the hyperfine splitting.

Radiative corrections: An obvious shortcoming of the above results is that the excited states are in reality unstable and should not correspond to stationary solutions. The excited states instead have a finite width arising from the possibility of emission of photons.

There are however more effects resulting from interactions with the quantized electromagnetic field, whose systematic treatment requires quantum field theoretical methods which we shall develop later on.

The most important of these effects in the hydrogen atom is the so-called Lamb-shift (Lamb and Retherford, 1947) of the $ns_{1/2}$ states against $np_{1/2}$. In particular, the $2s_{1/2}$ state is shifted towards higher energies by an amount of about one-tenth of the fine structure split between $2p_{1/2}$ and $2p_{3/2}$.

Qualitatively, this effect can be described by the same kind of argument as in the discussion of the Darwin term in the previous section. If we consider fluctuations in the position caused by a quantized electromagnetic field, the effect is like that of the relativistic zitterbewegung, but it is in addition to the latter which is already taken into account by the Dirac equation.

Analogously to (3.50), we may expect

$$\Delta H_{\text{Lamb}} = \frac{e}{6} \underbrace{\triangle A^0}_{4\pi Z\alpha\delta^3(\vec{x})} \langle(\delta\vec{x})^2\rangle. \tag{3.75}$$

The main effect will therefore occur for s states, because $\psi_{n,l>0}(0) = 0$ for the Schrödinger wave functions of the hydrogen atom,

$$\Delta E_{\text{Lamb}}(n) = \frac{2\pi Z\alpha}{3}|\psi_{n,0}(0)|^2\langle(\delta\vec{x})^2\rangle \propto \frac{Z^4\alpha^5 m}{n^3} \tag{3.76}$$

when we assume that $\langle(\delta\vec{x})^2\rangle \propto \alpha/m^2$ on dimensional grounds and because the induced fluctuations involve electromagnetic interactions.

Evaluated for $Z = 1$ and $n = 2$, (3.76) gives a frequency of ~ 500 MHz for the order of magnitude of the Lamb shift, which indeed fits roughly to the experimental value $\Delta E_{\text{Lamb}}^{\text{exp}}(2) \approx 1058$ MHz.

4 Towards a many-body theory

4.1 Hole theory

So far we have interpreted the Dirac equation as a one-particle wave theory by simply ignoring the solutions of negative energy. We have however seen that negative-energy solutions necessarily appear when one tries to construct a localized wave packet. Moreover, despite its success to explain the magnetic moment of the electron and the fine structure of the hydrogen atom, Klein's paradox and also the instability of the lowest energy eigenstates for the Coulomb problem with $Z \gtrsim 1/\alpha$ indicate that the one-particle theory has serious theoretical limitations. These can no longer be ignored when, in attempts to further refinements, interactions with radiation fields are to be included. One inevitably would find transitions of any positive-energy state to the negative-energy ones, releasing infinite energy at an infinite rate.

A solution was proposed in 1930 by Dirac in which it is postulated that, in the vacuum, all negative energy levels are filled by electrons. Because of the Pauli exclusion principle, no positive-energy state can then decay into a negative-energy one. However, it should be possible to excite one of the electrons of the "Dirac sea" such that there appears both a positive-energy electron and a hole in the Dirac sea. Compared to the vacuum state which is defined as a completely filled Dirac sea, the absence of a negative charge with negative energy appears as a state with positive electric charge, positive energy, and flipped spin. Dirac's hole theory therefore predicts the existence of particles with the properties of electrons except for a positive charge: positrons, which were discovered 1932 by Anderson (without knowing of Dirac's prediction). These can annihilate with electrons by the emission of radiation with energy $> 2mc^2 \approx 1$MeV or can be produced if such energy is available.

Besides the prediction of antiparticles, Dirac's hole theory anticipates qualitatively certain physical effects such as vacuum polarization which indeed occur. Vacuum polarization means that an electron with positive energy repels electrostatically the electrons in the Dirac sea, leading to a positive charge density of the vacuum around an electron such that at large distances the apparent charge should be weaker than at smaller ones. Indeed, at typical current collider energies $\sim m_W \approx 80$ GeV,

which corresponds to distances $\sim 10^{-3}$ fm, the fine-structure constant has increased from its low-energy (large-distance) value $1/137$ to $1/128$.

On the other hand, the assumption of an infinitely charged unobservable sea of electrons seems unsatisfactory for various reasons. Because it relies on the Pauli principle, it cannot be used for making sense of the negative-energy solutions of the Klein-Gordon equation. However, charged scalar particles and antiparticles thereof exist in nature. Also, it seems arbitrary to fill the Dirac sea with electrons rather than positrons.

Indeed, in quantum field theory to be introduced below, antiparticles do not require an interpretation as in Dirac's hole theory. Despite its original heuristic value, hole theory should therefore, according to J. Schwinger, be best regarded as a historic curiosity and forgotten.

4.2   Charge conjugation

The existence of antiparticles with the same mass and spin but opposite charges that obey the same equation corresponds to a new symmetry called charge conjugation symmetry.

To each solution ψ of the Dirac equation for electrons $(i\slashed{\partial} - e\slashed{A} - m)\psi = 0$ one can relate a solution ψ^c of the Dirac equation for positrons, $(i\slashed{\partial} + e\slashed{A} - m)\psi^c = 0$.

The relative sign between $\slashed{\partial}$ and $\slashed{A}$ is easily reversed by complex conjugation. Consider therefore the Dirac adjoint spinor to ψ, but transposed, $\bar{\psi}^T = \gamma^{0T}\psi^*$. This obeys

$$\left[\gamma^{\mu T}(-i\partial_\mu - eA_\mu) - m\right]\bar{\psi}^T = 0. \tag{4.1}$$

This differs from a Dirac equation for positrons by a replacement of $\gamma^\mu \leftrightarrow -\gamma^{\mu T}$. Now $-\gamma^{\mu T}$ is also a solution of the Clifford relation (2.12). Just as in the discussion following (2.26), we can infer that in any representation of the γ algebra there must exist a unitary matrix C satisfying

$$C(-\gamma^{\mu T})C^{-1} = \gamma^\mu. \tag{4.2}$$

Up to an unobservable overall phase, we can therefore identify

$$\psi^c = C\bar{\psi}^T. \tag{4.3}$$

One can show (exercise!) that C must be either symmetric or antisymmetric. Which of the two possibilities holds depends on the number of space-time dimensions.

In 4 dimensions, C is antisymmetric. In the Dirac representation, it reads

$$C_{\text{Dirac rep.}} = i\gamma^2\gamma^0 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{4.4}$$

For example, in the Dirac representation a spin-down negative-energy spinor with momentum $\vec{k} = -k\vec{e}_x$ is mapped to a positive-energy one with spin up and momentum $+k\vec{e}_x$ according to

$$\psi = e^{iEt-ikx} \begin{pmatrix} \frac{k}{E+m} \\ 0 \\ 0 \\ 1 \end{pmatrix} \rightarrow \psi^c = C\bar{\psi}^T = e^{-iEt+ikx} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \frac{k}{E+m} \end{pmatrix}.$$

Charge conjugation can be viewed as a symmetry of the Dirac equation itself by combining the transformations[15]

$$\psi \rightarrow \psi^c = C\bar{\psi}^T, \quad A_\mu \rightarrow A_\mu^c = -A_\mu. \tag{4.5}$$

In the chiral representation we have

$$C_{\text{chiral rep.}} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \tag{4.6}$$

Together with the off-diagonal γ^0 from (2.15), a Weyl spinor $\binom{\varphi}{0}$ is transformed to $\binom{0}{\varphi^c}$ with $\varphi^c = -i\sigma^2\varphi^*$.

The antiparticles of Weyl particles with a definite chirality are therefore of opposite chirality. Because this is described by the other of the pair of Weyl equations (2.42), C is not a symmetry if there are only particles with one chirality (and antiparticles with the other). However, the combination of C and parity P,

$$\psi \rightarrow \psi^{CP}(t, \vec{x}) = C \underbrace{(\gamma^0)^2}_{\mathbf{1}} \psi^*(t, -\vec{x}), \tag{4.7}$$

is a symmetry transformation, as one easily checks (exercise!).

[15]In order that also the Maxwell equations are invariant, we should have $j_\mu^c = -j_\mu$. But with $\psi^c = C\gamma^{0T}\psi^* = -\gamma^0 C\psi^*$ and $\bar{\psi}^c = -\psi^T C^\dagger$ we have $j_\mu^c = \bar{\psi}^c\gamma_\mu\psi^c = -\psi^T C^\dagger\gamma_\mu C\bar{\psi}^T = +\psi^T\gamma_\mu^T\bar{\psi}^T$, which is identical to $\bar{\psi}\gamma_\mu\psi$ for $\psi_\sigma(x) \in \mathbb{C}$. C invariance thus requires that the spinor ψ be treated as an anticommuting object. This can be done formally through Grassmann numbers, which is indeed usual practice in path integral formulations. In the quantum field theory to be introduced below, ψ will be turned into an anticommuting operator, which resolves this problem.

5 Quantum field theory

A genuine many-body quantum theory requires a vastly larger Hilbert space than the one we have used up to now. Because in a relativistic theory we have to allow for the possibility of particle creation and annihilation, there must be operators connecting the various subspaces of given particle and antiparticle numbers. An operator corresponding to the addition of a particle or antiparticle with certain quantum numbers and at a certain point in space-time clearly depends on these quantum numbers and a space-time coordinate. We therefore have to consider operator-valued fields. Relativistic covariance and irreducibility again require relativistic wave equations, but now for operators instead of wave functions.[16]

5.1 Canonical quantization reviewed

Given a Lagrangian formulation, the transition from ordinary mechanics to quantum mechanics is performed after identifying the canonical variables and momenta.

With an action

$$I = \int_{t_1}^{t_2} dt \, L(q(t), \dot{q}(t)) \tag{5.1}$$

the equations of motion follow from the requirement of stationarity of I under variations $q^i(t) \to q^i(t) + \delta q^i(t)$ which leave the end-points fixed. This gives the Euler-Lagrange equations

$$\frac{\delta I}{\delta q^i(t)} \equiv \frac{\partial L}{\partial q^i(t)} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i(t)} = 0. \tag{5.2}$$

In the Hamiltonian formulation one introduces the conjugate momentum

$$p_i = \frac{\partial L}{\partial \dot{q}^i}(q, \dot{q}) \tag{5.3}$$

Assuming that this can be inverted to express the velocities in terms of the coordinates and the momenta, the Hamiltonian is given by a Legendre transformation

$$H(p, q) = p_i \dot{q}^i(p, q) - L(q, \dot{q}(p, q)). \tag{5.4}$$

Canonical quantization replaces the functions $p_i(t)$ and $q^i(t)$ by operators in a Hilbert space with (equal-time) commutation relations

$$[q^i(t), p_j(t)] = i\hbar \, \delta^i_j. \tag{5.5}$$

---

[16]This is sometimes called "second quantization", but this term is rather misleading and is better avoided. What really takes place is the introduction of a formalism that unifies the infinitely many Hilbert spaces of one, two, three etc. particles that one would have to deal with separately otherwise.

5.2   Quantization of a free scalar field

The transition to fields as dynamical variables that are to be quantized is best understood as a generalization of the index i on $q^i(t)$ to one which collectively denotes all discrete and continuous labels that characterize a field: $\vec{x}, \mu, \sigma, \ldots$. The Kronecker symbol δ^i_j then generalizes to products of ordinary Kronecker delta's and Dirac delta functions, since the latter is needed to pick a given "component" from the continuously infinite sum that makes up an integration.

A complex scalar field $\varphi(x)$ can thus be viewed as a coordinate with index $i = (\vec{x}, \mathrm{Re}, \mathrm{Im})$. The Klein-Gordon equation $(\Box + m^2)\varphi = 0$ can be obtained as the Euler-Lagrange equation of an action of the form

$$
\begin{align}
I &= \int dt\, L = \int dt \int d^3x\, \mathcal{L}(\varphi, \partial\varphi) \tag{5.6}\\
\mathcal{L} &= (\partial_\mu \varphi^*)(\partial^\mu \varphi) - m^2 \varphi^* \varphi \tag{5.7}
\end{align}
$$

where instead of considering independent variations of $\mathrm{Re}\varphi$ and $\mathrm{Im}\varphi$ one may equivalently view φ and φ^* as independent variables.

The conjugate momentum is now a field, too,

$$
\pi(t, \vec{x}) := \frac{\partial \mathcal{L}}{\partial[\partial_0 \varphi(t, \vec{x})]} \tag{5.8}
$$

and the Hamiltonian is defined as

$$
H = \int d^3x\, \mathcal{H}(\pi, \varphi) = \int d^3x\, [\pi \partial_0 \varphi + \pi^* \partial_0 \varphi^* - \mathcal{L}(\varphi, \partial\varphi)]. \tag{5.9}
$$

With the specific Lagrangian (5.7) we have

$$
\pi = \dot{\varphi}^*, \quad \pi^* = \dot{\varphi}, \quad H = \int d^3x\, [\pi^* \pi + \nabla\varphi^* \cdot \nabla\varphi + m^2 \varphi^* \varphi]. \tag{5.10}
$$

Canonical quantization promotes the fields $\varphi, \varphi^*, \pi, \pi^*$ to operators $\varphi, \varphi^\dagger, \pi, \pi^\dagger$ with the nonvanishing equal-time commutators

$$
[\varphi(t, \vec{x}), \pi(t, \vec{y})] = [\varphi^\dagger(t, \vec{x}), \pi^\dagger(t, \vec{y})] = i\delta^3(\vec{x} - \vec{y}). \tag{5.11}
$$

The physical content becomes more evident by rewriting (5.10) in momentum space:

$$
H = \int \frac{d^3k}{(2\pi)^3} \left[|\tilde{\pi}(t, \vec{k})|^2 + \omega_k^2 |\tilde{\varphi}(t, \vec{k})|^2 \right], \qquad \omega_k^2 = \vec{k}^2 + m^2. \tag{5.12}
$$

This is just a continuously infinite sum of independent harmonic oscillators, one for each value of $\vec{k}$.

$\tilde{\varphi}(t, \vec{k})$ and $\tilde{\pi}(t, \vec{k})$ can therefore be written as linear combinations of creation and annihilation operators for an harmonic oscillator with frequency ω_k. In configuration space we can therefore write for a given time t, say $t = 0$,

$$
\begin{aligned}
\varphi(0, \vec{x}) &= \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_k} \left[a(k)e^{i\vec{k}\cdot\vec{x}} + b^\dagger(k)e^{-i\vec{k}\cdot\vec{x}} \right] \\
\varphi^\dagger(0, \vec{x}) &= \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_k} \left[b(k)e^{i\vec{k}\cdot\vec{x}} + a^\dagger(k)e^{-i\vec{k}\cdot\vec{x}} \right] \\
\pi(0, \vec{x}) &= \frac{-i}{2} \int \frac{d^3k}{(2\pi)^3} \left[b(k)e^{i\vec{k}\cdot\vec{x}} - a^\dagger(k)e^{-i\vec{k}\cdot\vec{x}} \right] \\
\pi^\dagger(0, \vec{x}) &= \frac{-i}{2} \int \frac{d^3k}{(2\pi)^3} \left[a(k)e^{i\vec{k}\cdot\vec{x}} - b^\dagger(k)e^{-i\vec{k}\cdot\vec{x}} \right]
\end{aligned}
$$

(5.13)

(5.14)

and (5.11) implies

$$
[a(k), a^\dagger(k')] = [b(k), b^\dagger(k')] = (2\pi)^3 2\omega_k \delta^3(\vec{k} - \vec{k}') \tag{5.15}
$$

and vanishing commutators for the other combinations. (For a real field we would have had to introduce only one pair $a, a^\dagger$.)

The normalization of the creation and annihilation operators is conveniently chosen in such a way that the integration measure is manifestly Lorentz-invariant:

$$
\int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_k} = \int \frac{d^4k}{(2\pi)^4} 2\pi \delta(k^2 - m^2)\theta(k^0) =: \int d\tilde{k} \tag{5.16}
$$

The quantum theory of a simple harmonic oscillator now makes it clear that we can define the vacuum (ground) state by

$$
a(k)|0\rangle = 0 = b(k)|0\rangle \quad \forall \vec{k}, \quad \langle 0|0\rangle = 1. \tag{5.17}
$$

The Hamilton operator reads

$$
H = \frac{1}{2} \int d\tilde{k} \, \omega_k \left[a^\dagger(k)a(k) + a(k)a^\dagger(k) + (a \leftrightarrow b) \right]. \tag{5.18}
$$

This leads to the problem that $\langle 0|H|0\rangle = \infty$ because of an accumulation of infinitely many zero-point energies. Declaring that only differences of energy to the vacuum be observable (this requires a neglect of gravity, though), we can simply replace

$$
H \to \; :H: \; = H - \langle 0|H|0\rangle = \int d\tilde{k} \, \omega_k \left[a^\dagger(k)a(k) + (a \leftrightarrow b) \right], \tag{5.19}
$$

where $: \ldots :$ denotes the prescription of *normal ordering* which places all annihilation operators to the right of all creation operators.

The vacuum state is thus defined to have zero energy. The action of a creation operator $a^\dagger(k)$ or $b^\dagger(k)$ produces a state which carries energy ω_k and momentum $\vec{k}$. Many-particle states are obtained by repeated action of these operators. They obey Bose statistics because $[a^\dagger(k), a^\dagger(k')] = 0$. The resulting Hilbert space is called *Fock space*. It is the union of all subspaces with a given number of quanta n_a and n_b (eigenspaces of the number operators $N_a = \int d\tilde{k}\, a^\dagger(k)a(k)$ and $N_b = \int d\tilde{k}\, b^\dagger(k)b(k)$.)

In the free theory that we are considering now, it is trivial to solve for the time evolution: In the Heisenberg picture we obtain $a(k,t) = e^{iHt}a(k)e^{-iHt} = e^{-i\omega_k t}a(k)$, etc., and therefore

$$\varphi(t, \vec{x}) = \int d\tilde{k} \left[a(k)e^{-ik\cdot x} + b^\dagger(k)e^{ik\cdot x} \right]. \tag{5.20}$$

Because of the δ-function in $d\tilde{k}$, this solves automatically the Klein-Gordon equation and clearly contains all the positive and negative energy solutions. However, in the quantum field theory they do not appear as negative-energy *states*. Instead, we have found two species of quanta with the same spectrum, particles and antiparticles, without the need for hole theory, which would anyway make no sense for bosons. (In the case of a real (hermitian) field where $b^\dagger \to a^\dagger$ one would say that "the particle is its own antiparticle".)

5.2.1   Causality

At fixed time, field operators referring to different positions in space commute, that is, they define independent observables. This is no longer true for different time variables:

$$[\varphi(t, \vec{x}), \varphi^\dagger(t', \vec{x}')] = \int d\tilde{k} \left[e^{-ik\cdot(x-x')} - e^{ik\cdot(x-x')} \right] = i\Delta(x - x'). \tag{5.21}$$

$\Delta(z)$ is a homogeneous Green function for the Klein-Gordon equation because of the δ-function contained in $d\tilde{k}$. It is manifestly invariant under proper Lorentz transformations, so the fact that it vanishes for $z^0 = 0$ and $\vec{z} \neq 0$ by virtue of the equal-time commutation relations implies that it vanishes for all $z^2 < 0$. This is explicitly seen from (5.21) because the second term cancels the first for $x^0 = x^{0\prime}$ upon $\vec{k} \to -\vec{k}$. On the other hand, for $\vec{x} = \vec{x}'$ but $x^0 \neq x^{0\prime}$, this is no longer true.

The vanishing of (5.21) can also be understood immediately by noting that for spacelike (and only for spacelike) z a proper Lorentz transformation permits to transform $z \to -z$, so that the two terms in (5.21) cancel each other. Since these terms correspond to the propagation of particles and antiparticles respectively, causality is

seen to be realized not by forbidding spacelike propagation at all, but by a destructive interference of the particles' and the antiparticles' amplitudes for propagation over spacelike separations. Without antiparticles (negative energy solutions in the wave equations) causality could never have been achieved!

5.2.2   Internal symmetry

The Lagrangian (5.7) is invariant under global U(1) transformations

$$\varphi \to \varphi' = e^{i\alpha}\varphi, \quad \varphi^\dagger \to \varphi^{\dagger\prime} = e^{-i\alpha}\varphi^\dagger. \tag{5.22}$$

This could be turned into a local gauge transformation by minimal electromagnetic coupling.

Global invariance transformations are generated by

$$Q = \int d^3x \; \pi(t,\vec{x}) \frac{\delta\varphi'(t,\vec{x})}{\delta\alpha}\Big|_{\alpha=0} \tag{5.23}$$

through commutators:

$$[iQ\delta\alpha, \varphi] = \frac{\delta\varphi'(t,\vec{x})}{\delta\alpha}\Big|_{\alpha=0} \delta\alpha. \tag{5.24}$$

This automatically gives a conserved (Noether) charge from the invariance of the Hamiltonian: $\dot{Q} = i[H,Q] = 0$.

In our case, $\frac{\delta\varphi'(t,\vec{x})}{\delta\alpha}\Big|_{\alpha=0} = i\varphi$, $\frac{\delta\varphi^{\dagger\prime}(t,\vec{x})}{\delta\alpha}\Big|_{\alpha=0} = -i\varphi^\dagger$, so

$$Q = i\int d^3x \left[\varphi^\dagger\dot{\varphi} - \dot{\varphi}^\dagger\varphi\right]. \tag{5.25}$$

Again, we should go over to the normal ordered operator $:Q:$ in order to assign a vanishing expectation value to the vacuum. Then

$$:Q: = \int d\tilde{k} \left[a^\dagger a - b^\dagger b\right] = N_a - N_b \tag{5.26}$$

which shows that a-quanta carry charge $+1$, and b-quanta charge -1. This fits to their interpretation as particles and antiparticles. Which is which is pure convention, so the arbitrariness that was present in Dirac's hole theory, where one species was singled out for occupying the negative energy states does not occur any longer.

5.2.3   Time-ordered product and Feynman propagator

The field operator φ is built from annhihilation operators a and creation operators $b^\dagger$. It therefore carries charge -1. Conversely, $\varphi^\dagger$ carries charge $+1$. The amplitude

for a positive charge transport from a space-time point x' to x is described by the expectation value of the charge-neutral products $\varphi^\dagger(x)\varphi(x')$ or $\varphi(x')\varphi^\dagger(x)$, depending on whether the time $x^{0\prime}$ or x^0 is the earlier one. It is therefore natural to define the *time-ordered product*

$$\mathsf{T}\varphi(x')\varphi^\dagger(x) := \theta(t'-t)\varphi(x')\varphi^\dagger(x) + \theta(t-t')\varphi^\dagger(x)\varphi(x'). \qquad (5.27)$$

Using that $\varphi(x')$ is a homogeneous solution of the Klein-Gordon equation and the equal-time commutation relations one can readily show that the time-ordered product satisfies the operator equation

$$\left(\Box_{x'} + m^2\right)\mathsf{T}\varphi(x')\varphi^\dagger(x) = -i\delta^4(x'-x). \qquad (5.28)$$

(Note that the time derivatives contained in $\Box$ prevent it from commuting with T.)

It follows that its vacuum expectation value is one of the inhomogeneous Green functions of the Klein-Gordon wave operator.

Using that $\langle 0|\varphi(x')\varphi^\dagger(x)|0\rangle = \int d\tilde{k}e^{-ik(x'-x)}$, $\langle 0|\varphi^\dagger(x)\varphi(x')|0\rangle = \int d\tilde{k}e^{+ik(x'-x)}$ and

$$\theta(t'-t) = \int \frac{d\omega}{2\pi i}\frac{e^{i\omega(t'-t)}}{\omega - i\varepsilon}$$

one finds that

$$i\langle 0|\mathsf{T}\varphi(x')\varphi^\dagger(x)|0\rangle = G_F(x'-x) = -\int \frac{d^4k}{(2\pi)^4}\frac{1}{k^2 - m^2 + i\varepsilon}e^{-ik\cdot(x'-x)}. \qquad (5.29)$$

G_F is called Feynman or causal propagator. It will play a central role in the development of perturbation theory later on, for which we record the following important relation (exercise!)

$$\mathsf{T}\varphi(x')\varphi^\dagger(x) = \langle 0|\mathsf{T}\varphi(x')\varphi^\dagger(x)|0\rangle + :\varphi(x')\varphi^\dagger(x): \qquad (5.30)$$

The explicit form (5.29) shows that G_F is a manifestly Lorentz-covariant quantity. In Fock space, it has the interpretation of the amplitude for propagation of a particle from x' to x if $t > t'$ and of an antiparticle from x to x' if $t' > t$. Note that for spacelike momenta it depends on the choice of frame of reference which event is at a later time. For timelike and lightlike separation however there is no ambiguity when we restrict ourselves to proper Lorentz transformations.

The $i\varepsilon$-prescription in (5.29) is often referred to as Feynman boundary condition. In terms of the positive and negative energy plane waves it amounts to requiring that only positive frequencies propagate forward in time, which by symmetry implies that negative frequencies must propagate backward in time.

5.3   Quantization of the free Dirac field

The free Dirac equation (2.10) as well as its adjoint verion (2.19) can be obtained as (Euler-Lagrange) field equations of the Lagrangian density

$$\mathcal{L} = \bar{\psi}(i\!\not{\partial} - m)\psi \tag{5.31}$$

by independent functional variation of $\psi(x)$ and $\psi^\dagger(x)$, which is equivalent to varying the real and imaginary part of $\psi(x)$. Because γ^0 is invertible, one may equally well consider independent variations of ψ and $\bar{\psi}$.

However, the canonical quantization procedure is hampered by the fact that the canonical momenta are algebraically determined by the coordinates,

$$\pi_\psi(x) = \frac{\partial \mathcal{L}}{\partial \partial_0 \psi(x)} = i\bar{\psi}\gamma^0 = i\psi^\dagger \tag{5.32}$$

i.e. without involving time derivatives of the latter as usual. So on the one hand we expect $[\psi, \psi^\dagger] = 0$ for the independent coordinates, and on the other hand we should have $[\psi, \pi_\psi] = i[\psi, \psi^\dagger] = i\mathbf{1}$. Because of the "constraint" (5.32), one has to modify the canonical formalism. However, we shall not embark on the general formalism of quantization with constraints which has been developed by Dirac, but shall proceed heuristically.

Consider the expansion of the Dirac field in plane-wave solutions (3.7), (3.8):

$$\psi_\alpha(x) = \int \underbrace{\frac{d^3k}{(2\pi)^3}\frac{m}{\omega_k}}_{\tilde{d}k}\sum_{a=1,2}\left\{b_a(k)u_\alpha^{(a)}(k)e^{-ik\cdot x} + d_a^\dagger(k)v_\alpha^{(a)}(k)e^{ik\cdot x}\right\}, \tag{5.33}$$

$$\bar{\psi}_\alpha(x) = \int \tilde{d}k \sum_{a=1,2}\left\{b_a^\dagger(k)\bar{u}_\alpha^{(a)}(k)e^{ik\cdot x} + d_a(k)\bar{v}_\alpha^{(a)}(k)e^{-ik\cdot x}\right\}, \quad k^0 = \omega_k, \tag{5.34}$$

where we have chosen a slightly different normalization of the Lorentz invariant integration measure than in the case of scalar fields (cp. to (5.16)).

In analogy to the scalar case we may expect that the expansion coefficients $b(k)$, $d(k)$, and their conjugates become annihilation and creation operators of particles (b) and antiparticles (d). Imposing commutation relations like $[b, b^\dagger] \propto \mathbf{1}$ would lead to the Bose-Einstein statistics in conflict with Pauli's exclusion principle. The latter can be realized by adopting anticommutation relations instead,

$$\{b_a(k), b_b^\dagger(k')\} = (2\pi)^3\frac{k^0}{m}\delta^3(\vec{k} - \vec{k}')\delta_{ab} \tag{5.35}$$

$$\{d_a(k), d_b^\dagger(k')\} = (2\pi)^3\frac{k^0}{m}\delta^3(\vec{k} - \vec{k}')\delta_{ab} \tag{5.36}$$

and zero anticommutators for all other combinations. This is equivalent to the equal-time anticommutation relation for field operators

$$\{\psi_\alpha(t,\vec{x}), \psi_\beta^\dagger(t,\vec{y})\} = \delta^3(\vec{x} - \vec{y})\delta_{\alpha\beta}. \tag{5.37}$$

The use of anticommutators in place of commutators achieves the desired anti-symmetrization of multi-particle states $a^\dagger(1)\cdots a^\dagger(n)|0\rangle$ in $1\ldots n$, where the integer labels represent particular choices of b or d-type, spin index, and momentum variable.

The free time evolution is effected by the operator (exercise!)

$$H = \int \tilde{d}k\, \omega_k \sum_{a=1,2} \left[b_a^\dagger(k)b_a(k) + d_a^\dagger(k)d_a(k)\right] \tag{5.38}$$

which is positive definite, and thus a suitable Hamilton operator.

Had we used commutation relations in (5.35) instead, the Hamilton operator would have turned out to be unbounded from below. Conversely, had we used anti-commutators in the quantization rules for the scalar fields, we would have found a violation of causality. This is in essence the spin-statistics theorem proved by Pauli – a consistent quantization of relativistic fields depends on Bose-Einstein statistics for integer-spin fields and Pauli-Dirac statistics for half-integer spin. Hence, the Pauli exclusion principle, which in nonrelativistic quantum mechanics cannot be deduced but is so important to the structure of atoms and the stability of ordinary matter, can be understood as a manifestation of the principles of relativistic quantum mechanics!

Using the anticommutation relations (5.35) one finds that for unequal times

$$\{\psi_\alpha(x), \psi_\beta^\dagger(x')\} = (i\,\slashed{\partial}_x + m)_{\alpha\beta}\, i\Delta(x - x') \tag{5.39}$$

with Δ as given by (5.21). Causality is now realized by vanishing anticommutators for spacelike separation. Observables such as the Dirac current are bilinear in the Dirac field operators and commute outside the light-cone.

The time-ordered product of Dirac field operators is defined with an extra minus sign according to

$$\mathsf{T}\psi(x')\bar{\psi}(x) := \theta(t' - t)\psi(x')\bar{\psi}(x) - \theta(t - t')\bar{\psi}(x)\psi(x'). \tag{5.40}$$

Its vacuum expectation value again gives a Green function, now for the Dirac wave operator. This is the Feynman propagator for fermions

$$\begin{aligned}
\langle 0|\mathsf{T}\psi_\alpha(x)\bar{\psi}_\beta(y)|0\rangle &=: \ iS_F(x - y)_{\alpha\beta} \\
S_F(x - y) &= \ \int \frac{d^4k}{(2\pi)^4} e^{-ik\cdot(x-y)} \frac{\slashed{k} + m}{k^2 - m^2 + i\varepsilon}.
\end{aligned} \tag{5.41}$$

5.4   Quantization of the free electromagnetic field

The source-free Maxwell's equations can be obtained from the Lagrangian density

$$\mathcal{L}(A, \partial A) = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu}, \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \qquad (5.42)$$

The canonical momenta associated to the 4-vector potential A_μ are found to be the electric field strength components

$$\pi^\mu = \frac{\partial \mathcal{L}}{\partial(\partial_0 A_\mu)} = -F^{0\mu}. \qquad (5.43)$$

This is fine except for $\pi^0 = F^{00} \equiv 0$, so A^0 does not have a conjugate momentum, and the usual canonical quantization rules fail.

The reason for this trouble is gauge invariance. The photon field does not have 4 times as many degrees of freedom as a neutral scalar field, but only twice as many (corresponding to the two polarizations of a plane wave).

This suggests to eliminate the unphysical degrees of freedom by putting also $A^0 = 0$. In the Lagrangian, A^0 acts not so much as a dynamical field, but as a Lagrange multiplier field for the Gauss law constraint $\nabla \cdot \vec{E} = \nabla \cdot \vec{\pi} = 0$. Since for $A^0 = 0$ we have $\vec{E} = -\partial_t \vec{A}$, this can be implemented through div $\vec{A} = 0$. Then everything unphysical is eliminated, however at the price of a loss of manifest Lorentz covariance and locality.

A Lorentz-covariant alternative is to introduce "gauge-breaking terms" into $\mathcal{L}$ and to work temporarily with a larger Fock space than the physical one. The modern way of doing this has been introduced by Faddeev and Popov; in the case of electromagnetism we can however follow the equivalent but simpler method of Gupta and Bleuler.

By adding the gauge-breaking term

$$\mathcal{L} \to \mathcal{L} - \frac{\lambda}{2}(\partial \cdot A)^2 \qquad (5.44)$$

we change the theory such that there are nontrivial conjugate momenta for all four components of A_μ:

$$\pi^\mu = F^{\mu 0} - \lambda g^{\mu 0}(\partial \cdot A). \qquad (5.45)$$

This allows us to introduce the standard equal-time commutation relations

$$[A_\mu(t, \vec{x}), \pi^\nu(t, \vec{y})] = i\delta_\mu^\nu \delta^3(\vec{x} - \vec{y}). \qquad (5.46)$$

From (5.44) follow the (operator) field equations

$$\Box A_\mu - (1 - \lambda)\partial_\mu \partial \cdot A = 0 \qquad (5.47)$$

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which are simplest for $\lambda = 1$ ("Feynman gauge"). With this latter choice, the four components of A_μ are very much like four real massless Klein-Gordon field operators. The field equations are automatically satisfied by an expansion in plane waves with $k_0 = \omega_k = |\vec{k}|$,

$$A_\mu(x) = \int d\tilde{k} \sum_{\lambda=0}^{3} \left\{ a^{(\lambda)}(k)\varepsilon_\mu^{(\lambda)}(k)e^{-ik\cdot x} + a^{(\lambda)\dagger}(k)\varepsilon_\mu^{(\lambda)}(k)e^{ik\cdot x} \right\} \tag{5.48}$$

where for any given momentum k on the forward light-cone the $\varepsilon_\mu^{(\lambda)}(k)$ are a set of linearly independent vectors.

As a special choice we may pick the polarization vectors $\varepsilon_\mu^{(\lambda)}(k)$ such that in a Lorentz frame where $k_\mu = (k, 0, 0, k)$

$$\varepsilon_\mu^{(0)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \varepsilon_\mu^{(1)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \varepsilon_\mu^{(2)} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \varepsilon_\mu^{(3)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{5.49}$$

$\varepsilon^{(1)}$ and $\varepsilon^{(2)}$ are then transverse polarizations, $\varepsilon^{(3)}$ is longitudinal with respect to k, and $\varepsilon^{(0)}$ will be referred to as scalar polarization. For arbitrary k they satisfy

$$\sum_\lambda \frac{\varepsilon_\mu^{(\lambda)}(k)\varepsilon_\nu^{(\lambda)}(k)}{\varepsilon^{(\lambda)}(k) \cdot \varepsilon^{(\lambda)}(k)} = g_{\mu\nu}, \quad \varepsilon^{(\lambda)}(k) \cdot \varepsilon^{(\lambda')}(k) = g^{\lambda\lambda'}. \tag{5.50}$$

In the Feynman gauge, $\pi^\mu = -\partial^0 A^\mu +$ spatial derivatives, so that (5.46) implies

$$[\dot{A}_\mu(t,\vec{x}), A_\nu(t,\vec{y})] = ig_{\mu\nu}\delta^3(\vec{x} - \vec{y}) \tag{5.51}$$

while all the commutators of A and $\dot{A}$ among themselves vanish. The equal-time commutation rules therefore translate into

$$[a^{(\lambda)}(k), a^{(\lambda')\dagger}(k')] = -g^{\lambda\lambda'}2|\vec{k}|(2\pi)^3\delta^3(\vec{k} - \vec{k}') \tag{5.52}$$

which is what one would expect for massless Klein-Gordon fields except for a reversed sign on the right-hand side for the scalar polarization $\lambda = 0$.

Checking causality, we find $[A_\mu(x), A_\nu(y)] = -ig_{\mu\nu}\Delta(x - y)$ which vanishes for spacelike distances, as before.

However, the construction of the usual Fock space through

$$a^{(\lambda)}(k)|0\rangle = 0, \quad \langle 0|0\rangle = 1 \tag{5.53}$$

encounters a severe difficulty:

Because of the wrong sign of $[a^{(0)}, a^{(0)\dagger}]$, states generated by $a^{(0)\dagger}(k)$ can have negative norm! Consider $|1\rangle = \int d\tilde{k}\, f(k) a^{(0)\dagger}(k)|0\rangle$. Its norm is

$$\langle 1|1\rangle = \int\int d\tilde{k}\, d\tilde{k}'\, f^*(k) f(k') \langle 0| a^{(0)}(k) a^{(0)\dagger}(k')|0\rangle = -\langle 0|0\rangle \int d\tilde{k}\, |f(k)|^2. \quad (5.54)$$

However, we cannot simply interchange the roles of $a^{(0)}$ and $a^{(0)\dagger}$ as this would spoil Lorentz covariance.

But we anyway need to get rid of the unphysical polarizations that were made dynamical only through the introduction of a gauge-breaking term in (5.44).

The (Lorentz) gauge choice $\partial \cdot A = 0$ would eliminate the gauge-breaking term, but it cannot be imposed on the level of operators, for it would be inconsistent with the commutation relations (5.51).

We may however require that the Lorentz gauge holds in the mean

$$\langle \psi | \partial \cdot A | \psi \rangle = 0 \quad (5.55)$$

for physical states. But this is not a linear relation. A linear condition to define a physical Hilbert space as a subspace of the unphysical Fock space based on (5.53) which implies (5.55) is

$$\partial \cdot A^{(+)} |\psi\rangle = 0 \quad \Longleftrightarrow \quad |\psi\rangle \in \mathcal{H}_1 \quad (5.56)$$

where the subscript $(+)$ means that only the annihilation operator part (i.e. the positive frequency part) of A is to be taken:

$$\partial \cdot A^{(+)} = -i \int d\tilde{k}\, e^{-ik\cdot x} \sum_{\lambda=0,3} a^{(\lambda)}(k) \varepsilon^{(\lambda)}(k) \cdot k. \quad (5.57)$$

We may consider basis states $|\psi\rangle \in \mathcal{H}_1$ that are factored as $|\psi\rangle = |\psi_T\rangle |\phi\rangle$, where $|\psi_T\rangle$ is generated by transverse creation operators and $|\phi\rangle$ by scalar and longitudinal ones. The condition (5.56) means that

$$\left[a^{(0)}(k) - a^{(3)}(k) \right] |\phi\rangle = 0. \quad (5.58)$$

This implies that there are no longer any negative-norm states, however there exist still states with zero norm: If a state $|\phi_n\rangle$ has n scalar or longitudinal excitations and satisfies (5.58), then it is eigenstate to the number operator

$$N' = \int d\tilde{k}\, \left[a^{(3)\dagger}(k) a^{(3)}(k) - a^{(0)\dagger}(k) a^{(0)}(k) \right]$$

which counts the sum of scalar and longitudinal quanta (notice the sign!) then one easily shows that $0 = \langle\phi_n|N'|\phi_n\rangle = n\langle\phi_n|\phi_n\rangle$. Only $|\phi_0\rangle$, the vacuum state with respect to scalar and longitudinal quanta, is a positive-norm state; all other $|\phi_n\rangle$ have zero norm.

However, in expectation values of physical observables, the factors $|\phi\rangle$ in $|\psi\rangle$ drop out. For example,

$$: H := \int d\tilde{k}\,\omega_k \left[\sum_{\lambda=1}^{3} a^{(\lambda)\dagger}(k)a^{(\lambda)}(k) - a^{(0)\dagger}(k)a^{(0)}(k)\right] \tag{5.59}$$

and

$$
\begin{aligned}
\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} &= \frac{\langle\psi_T|\int d\tilde{k}\,\omega_k \sum_{\lambda=1,2} a^{(\lambda)\dagger}(k)a^{(\lambda)}(k)|\psi_T\rangle}{\langle\psi_T|\psi_T\rangle} \times \frac{\langle\phi|\phi\rangle}{\langle\phi|\phi\rangle} \\[2mm]
&+ \frac{\langle\psi_T|\psi_T\rangle}{\langle\psi_T|\psi_T\rangle} \times \overbrace{\frac{\langle\phi|\int d\tilde{k}\,\omega_k[a^{(3)\dagger}(k)a^{(3)}(k) - a^{(0)\dagger}(k)a^{(0)}(k)]|\phi\rangle}{\langle\phi|\phi\rangle}}^{0}
\end{aligned} \tag{5.60}
$$

This means that only equivalence classes of $|\psi\rangle$ have a physical interpretation, and we may choose as a representative those states where $|\phi\rangle = |\phi_0\rangle$.[17]

However, although only the states corresponding to transverse photons are given physical meaning, in intermediate steps the full indefinite-norm Fock space is required, e.g. when inserting unity as a sum over all states. The projection to transverse polarizations is possible only in the very end, for example for the external vectors of matrix elements.

5.5   Casimir effect

An important consequence of the quantization of fields is the existence of vacuum fluctuations. As noted by Casimir in 1948, these vacuum fluctuations have rather directly observable consequences. If macroscopic conducting bodies are present, they will introduce boundary conditions for electromagnetic fields: a perfect conductor forces the magnetic field perpendicular and the electric field parallel to its surface to vanish. As a consequence, the vacuum fluctuations will be different for different arrangements of conductors and so will the zero-point energies. While unmeasurable as such, differences in zero-point energies are measurable.

---

[17]Mathematically, the physical Hilbert space is the quotient of $\mathcal{H}_1$ with respect to the space of zero-norm states: $\mathcal{H}_{\text{phys}} = \mathcal{H}_1/\mathcal{H}_0$.

Let us consider the simplest case of two perfectly conducting parallel plates separated by a distance a in the z-direction, located at $z = 0$ and $z = a$. Let the extent of these plates in x- and y-directions be $L \gg a$.

In the previous section we have seen that only transverse modes ($\vec{E} \perp \vec{B} \perp \vec{k}$) contribute to the energy. Modes where $\vec{k}$ points in the z-direction have to have vanishing amplitude at $z = 0, a$. This constrains k_z to discrete values $k_z = n\pi/a$. The components k_x and k_y remain continuous and there are two transverse polarizations unless k_z vanishes – for $k_z = 0$ only the mode where $\vec{B}$ is parallel to the plates and $\vec{E}$ orthogonal is allowed.

Consider now the zero-point energy contribution $E = \sum \frac{1}{2}\hbar\omega = \frac{1}{2}\hbar c \sum |\vec{k}|$ from the allowed modes in the volume $L^2 a$ between the plates. With $|\vec{k}| = \sqrt{\vec{k}_\parallel^2 + (n\pi/a)^2}$, $\vec{k}_\parallel^2 = k_x^2 + k_y^2$,

$$E = \frac{\hbar c}{2} \int \frac{L^2 d^2 k_\parallel}{(2\pi)^2} \left\{ |\vec{k}_\parallel| + 2\sum_{n=1}^{\infty} \sqrt{\vec{k}_\parallel^2 + (n\pi/a)^2} \right\} \qquad (5.61)$$

while without boundary conditions from conducting plates we would have had

$$E_0 = \frac{\hbar c}{2} \int \frac{L^2 d^2 k_\parallel}{(2\pi)^2} \int \frac{a\, dk_z}{2\pi} 2\sqrt{\vec{k}_\parallel^2 + k_z^2} = \frac{\hbar c}{2} \int \frac{L^2 d^2 k_\parallel}{(2\pi)^2} \int_0^\infty dn\, 2\sqrt{\vec{k}_\parallel^2 + (n\pi/a)^2} \qquad (5.62)$$

where in the last expression we made the substitution $k_z = n\pi/a$ with a continuous variable n.

Both, (5.61) and (5.62) are divergent because the integrand grows at large $|\vec{k}|$ ("ultraviolet" divergence), and even their difference turns out to be ill-defined. However, when considering the difference $E - E_0$, we may assume that the boundary conditions of a perfect conductor apply only as long as the wavelength is larger than a typical atomic size R. Let us therefore regulate the integrands by multiplication with a cutoff function $f(|\vec{k}|)$ which is identically 1 as long as $|\vec{k}| \ll 1/R$ and identically 0 for $|\vec{k}| \gg 1/R$, and smoothly interpolating in between. Then

$$\frac{E - E_0}{L^2} = \frac{\hbar c}{2\pi} \int_0^\infty k_\parallel\, dk_\parallel \left\{ \frac{k_\parallel}{2} f(k_\parallel) + \left[\sum_{n=1}^{\infty} - \int_0^\infty dn \right] \sqrt{k_\parallel^2 + (n\pi/a)^2} f(\sqrt{\ldots}) \right\} \qquad (5.63)$$

Because of absolute convergence thanks to the cutoff function f, we can interchange sum and integration and rewrite (5.63) as

$$\frac{E - E_0}{L^2} = \hbar c \frac{\pi^2}{4a^3} \left\{ \tfrac{1}{2} F(0) + F(1) + F(2) + \ldots - \int_0^\infty dn\, F(n) \right\} \qquad (5.64)$$

with

$$F(n) := \int_0^\infty du \sqrt{u + n^2} f(\tfrac{\pi}{a}\sqrt{u + n^2}) = \int_{n^2}^\infty du' \sqrt{u'} f(\tfrac{\pi}{a}\sqrt{u'}) \qquad (5.65)$$

where $u = a^2 k_\parallel^2/\pi^2$.

This can be evaluated through the Euler-MacLaurin formula (A.11) as

$$\frac{E - E_0}{L^2} = \hbar c \frac{\pi^2}{4a^3} \left\{ -\frac{1}{2!} B_2 F'(0) - \frac{1}{4!} B_4 F'''(0) + \dots \right\} \qquad (5.66)$$

where the Bernoulli numbers are given in (A.2). We have $F'(n) = -2n^2 f(\tfrac{\pi}{a} n)$. Assuming that $f(0) = 1$, $f'(0) = f''(0) = \dots = 0$, we obtain $F'(0) = 0$, $F''(0) = 0$, $F'''(0) = -4$, and all higher derivatives zero. We thus find

$$\mathcal{E} := \frac{E - E_0}{L^2} = \frac{\hbar c \pi^2 B_4}{4! a^3} = -\frac{\pi^2 \hbar c}{720 a^3}. \qquad (5.67)$$

The force per unit area is

$$\mathcal{F} = -\frac{\partial \mathcal{E}}{\partial a} = -\frac{\pi^2 \hbar c}{240 a^4} = -\frac{0.013}{(a[\mu m])^4} \underbrace{\mathrm{dyn/cm^2}}_{0.1\,\mathrm{Pa}} \qquad (5.68)$$

and turns out to be attractive. It can be measured in practice only when $a \lesssim \mu$m. Its magnitude and dependence on a (which distinguishes it from other effects like residual electrostatic forces and the van der Waals force) has been confirmed experimentally in 1958 by Sparnaay, albeit with large ($\sim 100\%$) systematic errors. Higher precision tests have been performed only recently by Lamoreaux in 1997 ($\sim 5\%$ accuracy) and by Mohideen & Roy in 1998 ($\sim 1\%$), in perfect agreement with the theoretical prediction (which at this accuracy requires the inclusion of corrections due to surface roughness, finite conductivity, and temperature).

6 Perturbation theory

6.1 Interaction picture

In quantum mechanics, time evolution is usually studied in one of two "pictures". In the Schrödinger picture, the states are considered as time dependent and evolve according to

$$|\psi(t)\rangle_S = \exp\{-iH(\underbrace{t - t_0}_{=:\bar{t}})\}|\psi(t_0)\rangle, \tag{6.1}$$

the infinitesimal version of which is the Schrödinger equation. In the Heisenberg picture, which we have used above in the canonical quantization of fields, the states are left untouched and the evolution is entirely in the observables, $\mathcal{O}_H(t) = e^{iH\bar{t}}\mathcal{O}_S e^{-iH\bar{t}}$, $\mathcal{O}_H(t_0) \equiv \mathcal{O}_S$. This is completely equivalent as

$$_S\langle\chi(t)|\mathcal{O}_S|\psi(t)\rangle_S \equiv \langle\chi(t_0)|\mathcal{O}_H(t)|\psi(t_0)\rangle. \tag{6.2}$$

At t_0, the two pictures coincide, which is why we can omit any labels there.

In perturbation theory it turns out to be extremely useful to separate off the known time evolution of the free theory such that all operators evolve like free Heisenberg operators. Let $H \equiv H_H \equiv H_S$ be the full, interacting Hamilton operator and $H = H_{0S} + H_{1S}$ a separation into free and interaction part in the Schrödinger picture. Operators and states in the interaction picture (subscript I) are then defined as

$$\mathcal{O}_I(t) \equiv e^{iH_{0S}\bar{t}}\mathcal{O}_S e^{-iH_{0S}\bar{t}} \equiv U(t)\mathcal{O}_H(t)U^{-1}(t), \quad U(t) = e^{iH_{0S}\bar{t}}e^{-iH\bar{t}} \tag{6.3}$$

$$|\psi(t)\rangle_I \equiv e^{iH_{0S}\bar{t}}|\psi(t)\rangle_S \equiv U(t)|\psi(t_0)\rangle . \tag{6.4}$$

Interaction-picture operators satisfy free Heisenberg equations

$$\frac{d\mathcal{O}_I(t)}{dt} = e^{iH_{0S}\bar{t}}iH_{0S}\,\mathcal{O}_S e^{-iH_{0S}\bar{t}} - e^{iH_{0S}\bar{t}}\mathcal{O}_S\,iH_{0S}e^{-iH_{0S}\bar{t}} = i[H_{0S}, \mathcal{O}_I(t)], \tag{6.5}$$

the states a Schrödinger-like equation

$$\begin{aligned}
i\frac{d}{dt}|t\rangle_I &= i\frac{d}{dt}\left[e^{iH_{0S}\bar{t}}|t\rangle_S\right] = \\
&\quad -H_{0S}|t\rangle_I + e^{iH_{0S}\bar{t}}(H_{0S} + H_{1S})e^{-iH_{0S}\bar{t}}\underbrace{e^{iH_{0S}\bar{t}}|t\rangle_S}_{|t\rangle_I} = H_{1I}(t)|t\rangle_I
\end{aligned} \tag{6.6}$$

which is governed by the interaction part of the Hamilton operator in the interaction picture.[18]

---

[18]Notice that $H \equiv H_S \equiv H_H \not\equiv H_I$, $H_{0S} \equiv H_{0I} \not\equiv H_{0H}$, $H_{1S} \not\equiv H_{1H} \not\equiv H_{1I}$.

Defining $U(t, t') \equiv U(t)U^{-1}(t')$, the general time evolution between two times in the interaction picture is

$$|t\rangle_I = U(t, t')|t'\rangle_I \tag{6.7}$$

and $U(t, t')$ satisfies $i\frac{d}{dt}U(t, t') = H_{1I}(t)U(t, t')$ with initial condition $U(t', t') = \mathbf{1}$, which can be cast into the integral equation

$$U(t, t') = \mathbf{1} - i \int_{t'}^{t} dt'' H_{1I}(t'')U(t'', t'). \tag{6.8}$$

The operator $U(t)$ which intertwines the Heisenberg and the interaction picture is given as the special case $U(t) \equiv U(t, t_0)$.

The interaction Hamiltonian consists of terms proportional to (generally powers of) coupling constants. If these are small in some sense, one can attempt to solve the integral equation (6.8) iteratively. This leads to

$$
\begin{aligned}
U(t, t_0) &= \mathbf{1} + (-i)\int_{t_0}^{t} dt_1\, H_{1I}(t_1) + (-i)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, H_{1I}(t_1)H_{1I}(t_2) \\
&+ (-i)^3 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3\, H_{1I}(t_1)H_{1I}(t_2)H_{1I}(t_3) + \dots
\end{aligned} \tag{6.9}
$$

All the operators on the right turn out to be time ordered. We can therefore simplify by using the time-ordering symbol T, letting all integrations run from t_0 to t and correcting for the overcounting according to

$$
\begin{aligned}
&\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\, H_{1I}(t_1)H_{1I}(t_2)\cdots H_{1I}(t_n) \\
&= \frac{1}{n!}\int_{t_0}^{t} dt_1 \cdots dt_n\, \mathsf{T}H_{1I}(t_1)H_{1I}(t_2)\cdots H_{1I}(t_n) =: \frac{1}{n!}\mathsf{T}\left(\int_{t_0}^{t} dt'\, H_{1I}(t')\right)^n
\end{aligned} \tag{6.10}
$$

since there are $n!$ possibilities of ordering $t_{i_1} \geq t_{i_2} \geq \dots \geq t_{i_n}$.

Formally we write (6.9) with (6.10) as

$$U(t, t_0) = \mathsf{T}\exp\left\{-i\int_{t_0}^{t} dt'\, H_{1I}(t')\right\} \tag{6.11}$$

where time ordering of the exponential is defined through its Taylor series with each term time-ordered.

6.2 S-matrix

An interacting field theory may in principle be wildly different from the corresponding free theory. An important example is quantum chromodynamics, where the elementary quanta of quarks and gluons do not appear as observable particles.

In quantum electrodynamics, we know that individual photons and electrons can be observed and that their interactions are characterized by a small parameter, the fine-structure constant. It is therefore natural to consider states which correspond to well separated particles at some early time, "in-states", and whose wavefunctions overlap and interact only for some finite span of time. The results of the interaction can be measured by considering the overlap with states that correspond to a particular configuration of well separated states at late times, "out-states".

This is the content of the *S-matrix*, which in the Heisenberg picture is defined by

$$S_{\beta\alpha} = {}_H\langle\beta \text{ out}|\alpha \text{ in}\rangle_H. \tag{6.12}$$

Note that in the Heisenberg picture, the entire history of an in-state is determined by a time-independent Hilbert-space vector and that only the operators evolve in time. A given state $|\alpha \text{ in}\rangle$ therefore corresponds, by construction, to well-separated wave packets for $t \to -\infty$, and to something arbitrarily complicated at later times; for out-states this situation is reversed.

In situations which can be treated by perturbation theory, one can assume that all interactions are switched off "adiabatically" before some very large time $-T$. For times earlier than this, there is no difference between Heisenberg and interaction picture, if $t_0 < -T$. Let us take $t_0 = -\infty$. Then

$$|\alpha(-\infty) \text{ in}\rangle_I = |\alpha \text{ in}\rangle_H \tag{6.13}$$

$$|\psi(t)\rangle_I = U(t, -\infty)|\psi\rangle_H \tag{6.14}$$

$$\varphi_H(t) = U^{-1}(t, -\infty)\varphi_I(t)U(t, -\infty) \tag{6.15}$$

The field operators in the interaction picture follow a free time evolution; all the nontrivial time evolution is in the states.

If we choose the basis of out-states such that

$$|\alpha \text{ out}(+\infty)\rangle_I = |\alpha \text{ in}(-\infty)\rangle_I \equiv |\alpha\rangle, \quad \langle\beta|\alpha\rangle = \delta_{\alpha\beta} \tag{6.16}$$

then we can express (6.12) as

$$\begin{aligned}
S_{\beta\alpha} &= {}_I\langle\beta \text{ out}(-\infty)|\alpha \text{ in}(-\infty)\rangle_I = {}_I\langle\beta \text{ out}(+\infty)|U(+\infty, -\infty)|\alpha \text{ in}(-\infty)\rangle_I \\
&= \langle\beta|U(+\infty, -\infty)|\alpha\rangle \equiv \langle\beta|S|\alpha\rangle.
\end{aligned} \tag{6.17}$$

S is the scattering operator, which in the absence of interactions reduces to the unit operator. Occasionally the S-matrix elements are written as $\langle\beta|S|\alpha\rangle =$

$\delta_{\alpha\beta} + i\langle\beta|\mathcal{T}|\alpha\rangle$, where forward-scattering is separated off and the latter terms form the so-called transition matrix.

When there are no derivatives in the interaction Hamiltonian as is the case in quantum electrodynamics,[19] we have $\mathcal{H}_{1I} = -\mathcal{L}_{1I} =: -\mathcal{L}_I$ and we can write

$$S \equiv U(+\infty, -\infty) = \mathsf{T}\exp\left\{i\int d^4x \mathcal{L}_I\right\}. \tag{6.18}$$

6.3   LSZ reduction technique

In the interaction picture, the evaluation of S-matrix elements (6.17) involves the calculation of commutators of the annihilation and creation operators which produce the initial and final states out of the in-vacuum with the operator (6.18). A systematic procedure for doing this can be based on the reduction formulae developed by Lehmann, Symanzik, and Zimmermann (1950).

For simplicity we shall derive them for neutral scalar fields ($b^{(\dagger)} \equiv a^{(\dagger)}$), where the quantum numbers α of an initial state be given simply by a set of initial momenta $\vec{p}_1, \vec{p}_2, \ldots, \vec{p}_n$, and $\beta = \{\vec{q}_1, \ldots, \vec{q}_m\}$. Pulling out one momentum $\vec{p} \equiv \vec{p}_1$ from the set α and writing $\alpha = \{\vec{p}, \alpha'\}$ we have

$$\begin{aligned} S_{\beta\alpha} &= \langle\beta|S|\alpha\rangle = \langle\beta|Sa^\dagger(p)|\alpha'\rangle \\ &= \langle\beta|a^\dagger(p)S|\alpha'\rangle + \langle\beta|Sa^\dagger(p) - a^\dagger(p)S|\alpha'\rangle. \end{aligned} \tag{6.19}$$

If $\vec{p} \notin \beta$, the first term vanishes; otherwise we fall back to the task of computing $S_{\beta'\alpha'}$ with $\beta' = \beta\backslash\vec{p}$. Such contributions are called disconnected and we shall simply assume that β and α are disjoint.

Since S is a functional of the fields φ_I, let us express $a^\dagger$ in terms of φ_I as well. Since φ_I obeys free-field evolution equations and thus an equation like (5.20), we may write for arbitrary t

$$a^\dagger(p) = \int d^3x e^{-ip\cdot x}\frac{1}{i}\underbrace{(\overrightarrow{\partial}_0 - \overleftarrow{\partial}_0)}_{\overleftrightarrow{\partial}_0}\varphi_I(x) \tag{6.20}$$

S is a time-ordered operator. In order that $Sa^\dagger(p)$ and $a^\dagger(p)S$ in (6.19) be time-ordered, too, choose $t = -T'$ and $t = +T'$ for these two terms with $T' > T$ and

---

[19]When there are derivative couplings, a similar formula holds where T has to be replaced by a "covariantized" time ordering prescription $\hat{\mathsf{T}}$ defined by $\hat{\mathsf{T}}\partial_\mu \cdots \partial_{\mu'} := \partial_\mu \cdots \partial_{\mu'}\mathsf{T}$ (Matthew's theorem).

interactions switched off adiabatically outside the interval $(-T, T)$. Then we can write

$$
\begin{aligned}
\langle\beta|Sa^\dagger(p) - a^\dagger(p)S|\alpha'\rangle &= \underbrace{\Big[\int_{t=-T'} d^3x - \int_{t=T'} d^3x\Big]}_{-\int_{-T'}^{T'} d^4x \frac{\partial}{\partial x^0}} e^{-ip\cdot x}\frac{1}{i}\overleftrightarrow{\partial}_0\langle\beta|\mathsf{T}\varphi_I(x)S|\alpha'\rangle \\
&= i\int_{-T'}^{T'} d^4x\Big(e^{-ip\cdot x}\partial_0^2 - [\underbrace{\partial_0^2 e^{-ip\cdot x}}_{(\triangle - m^2)e^{-ip\cdot x}}]\Big)\langle\beta|\mathsf{T}\varphi_I(x)S|\alpha'\rangle \\
&= i\int_{-T'}^{T'} d^4x\, e^{-ip\cdot x}(\Box_x + m^2)\,\langle\beta|\mathsf{T}\varphi_I(x)S|\alpha'\rangle \qquad (6.21)
\end{aligned}
$$

Repeating this for all annihilation and creation operators needed to relate $\langle\beta|$ and $|\alpha\rangle$ to the vacuum, choosing larger $T'' > T'$, $T''' > T''$, etc., and sending all $T^{(n)} \to \infty$ in the end, one obtains (up to disconnected terms, or by demanding that $q_i \neq p_j$ for all i, j)

$$
\begin{aligned}
\langle q_1 \cdots q_m|S|p_1 \cdots p_n\rangle &= i^{m+n}\int d^4y_1 \cdots d^4x_n\, e^{iq_1\cdot y_1}\cdots e^{-ip_n\cdot x_n}(\Box_{y_1} + m^2)\cdots \\
&\quad \cdots (\Box_{x_n} + m^2)\langle 0|\mathsf{T}\varphi_I(y_1)\cdots\varphi_I(x_n)e^{i\int d^4x\mathcal{L}_I}|0\rangle \quad (6.22)
\end{aligned}
$$

An analogous formula can be derived for other fields than scalar ones. For instance, for fermions we have

$$
b^\dagger(k, s) = \int d^3x\bar{\psi}_I(x)\gamma^0 e^{-ik\cdot x}u(k, s). \qquad (6.23)
$$

Proceeding as above, one partial integration of ∂_0 leads to the Dirac operator acting on the interaction-picture fields in place of the Klein-Gordon wave operator.

6.4 Wick's theorem and Feynman rules

The usefulness of (6.22) is rooted in Wick's theorem, which can be proved by induction starting from the relation between time- and normal-ordered products of two free field operators

$$
\mathsf{T}\varphi_1\varphi_2 = :\varphi_1\varphi_2: + \underbrace{\langle 0|T\varphi_1\varphi_2|0\rangle}_{-iG_F(x_1-x_2)} \qquad (6.24)
$$

where $\varphi_i := \varphi(x_i)$.

It reads

$$
\begin{aligned}
\mathsf{T}\varphi_1\cdots\varphi_n \;=\;& :\!\varphi_1\cdots\varphi_n\!: \\
&+\sum_{k<l} :\!\varphi_1\cdots\widehat{\varphi_k}\cdots\widehat{\varphi_l}\cdots\varphi_n\!:\,\langle 0|T\varphi_k\varphi_l|0\rangle + \ldots \\
&+\sum_{k_1<k_2<\cdots<k_{2p}} :\!\varphi_1\cdots\widehat{\varphi_{k_1}}\cdots\widehat{\varphi_{k_{2p}}}\cdots\varphi_n\!: \\
&\times\sum_P \langle 0|\mathsf{T}\varphi_{k_{P_1}}\varphi_{k_{P_2}}|0\rangle\cdots\langle 0|\mathsf{T}\varphi_{k_{P_{2p-1}}}\varphi_{k_{P_{2p}}}|0\rangle + \ldots
\end{aligned} \tag{6.25}
$$

where a caret over an operator indicates its omission and the last sum is over all permutations P. Stated in words, Wick's theorem expresses a time-ordered product as the sum of all possible normal products where pairs of field operators have been omitted and replaced by Feynman Green's functions. This substitution is often called "contraction".

(6.25) is easily generalized to time-ordered products of the form

$$
\mathsf{T}\varphi_1\cdots\varphi_n :\!\varphi_{n+1}\cdots\varphi_m\!: :\!\varphi_{m+1}\cdots\varphi_p\!:\cdots
$$

The only difference turns out to be that contractions within one group of normal-ordered operators do not occur.

In order to evaluate (6.22) in perturbation theory, one first expands S up to some power in the coupling constants. This reduces the problem to the evaluation of the vacuum expectation values of products of free (interaction-picture) fields. Wick's theorem then provides the building blocks as

$$
\begin{aligned}
\langle 0|\mathsf{T}\varphi_1\cdots\varphi_{2p-1}|0\rangle \;&=\; 0, &&(6.26)\\
\langle 0|\mathsf{T}\varphi_1\cdots\varphi_{2p}|0\rangle \;&=\; \sum_P \langle 0|\mathsf{T}\varphi_{k_{P_1}}\varphi_{k_{P_2}}|0\rangle\cdots\langle 0|\mathsf{T}\varphi_{k_{P_{2p-1}}}\varphi_{k_{P_{2p}}}|0\rangle. &&(6.27)
\end{aligned}
$$

In quantum electrodynamics, the relevant fields operators are ψ and A_μ. Their contractions are the Feynman propagators (5.41) and (in Feynman gauge)

$$
\langle 0|\mathsf{T}A_\mu(x)A_\nu(y)|0\rangle = -g_{\mu\nu}(-i)G_F(x-y). \tag{6.28}
$$

and the S-operator is built from

$$
\mathcal{L}_I(x) = -e :\!\bar\psi(x)\gamma^\mu A_\mu(x)\psi(x)\!: \tag{6.29}
$$

The latter provides "vertices" to which Feynman propagators connect. Representing the latter by lines, this gives a graphical representation in "Feynman diagrams".

The entire procedure can be cast into a few rules, "Feynman rules", which are conveniently given in momentum space. Basically, they consist of drawing all possible topologically distinct diagrams contributing to the process under consideration which contain at most as many vertices as the maximal power of the electric coupling e one wants to keep. In QED, a vertex connects a photon line with an incoming and an outgoing fermion line, and represents a factor $-ie\gamma_\mu$. At each vertex there is momentum conservation. Fermion lines correspond to the momentum-space propagator $i(\not{p} + m)/(p^2 - m^2 + i\varepsilon) \equiv i/(\not{p} - m + i\varepsilon)$, photon lines to $-ig_{\mu\nu}/(p^2 + i\varepsilon)$. Momenta running through closed loops are to be integrated over with $\int d^4k/(2\pi)^4$. Closed fermion loops are assigned an additional factor of (-1).

Diagrams without external lines (vacuum diagrams) can be drawn to each diagram with external lines. They factorize, i.e., they contribute an overall factor $\langle 0|S|0\rangle$, which by energy conservation is but an unobservable phase, $|\langle 0|S|0\rangle|^2 = 1$, so vacuum diagrams can be left out from the start.

As an example consider the propagation of an electron in an external potential $A_\mu^{ext}(x)$. This can be included into the S-operator by replacing the interaction-picture operator $A_\mu(x) \rightarrow A_\mu(x) + A_\mu^{ext}(x)\mathbf{1}$, where $A_\mu^{ext}(x)$ is a classical 4-vector potential.

Neglecting forward scattering, the lowest order contribution is given by

$$-ie\langle 0|\mathsf{T}\bar{\psi}_1\psi_2 \int_x : \bar{\psi}_x(\not{A} + \not{A}^{ext})_x \psi_x : |0\rangle. \tag{6.30}$$

Since the operator A cannot be paired up with another one, it drops from this expression.

At order e^2 there is a correction term which only contributes to forward scattering, and one involving $(A^{ext})^2$. For sufficiently weak external fields this is a negligible contribution.

The first important correction to Coulomb scattering thus comes from

$$(-ie)^3\langle 0|\mathsf{T}\bar{\psi}_1\psi_2 \int_x : \bar{\psi}_x \not{A}_x \psi_x : \int_y : \bar{\psi}_y \not{A}_y \psi_y : \int_z : \bar{\psi}_z \not{A}_z^{ext}\psi_z : |0\rangle \tag{6.31}$$

Representing fermion and photon propagators by straight and wiggly lines, resp., this gives rise to the following Feynman diagrams

$$\tag{6.32}$$

The corresponding S-matrix element is obtained after truncation ("amputation") of the external (fermion) lines.

7 One-loop corrections

7.1 Electron self-energy

The diagrams in (6.32) where a photon is emitted and absorbed by the same electron line contain a "loop" built from one electron propagator and one photon propagator. The latter is called the one-loop electron self-energy. In momentum space it is given by the integral

$$(-ie)^2 \int \frac{d^4k}{(2\pi)^4} \gamma_\mu \frac{i}{\not{p} - \not{k} - m + i\varepsilon} \gamma^\mu \frac{-i}{k^2 + i\varepsilon} =: -i\Sigma(p) \tag{7.1}$$

This integral is ill-defined, for the integrand does not fall off sufficiently for large values of k. In fact, it appears to be linearly divergent,

$$\Sigma \sim \int^\Lambda k^3 dk \frac{1}{k} \frac{1}{k^2} \sim \int^\Lambda dk \sim \Lambda, \tag{7.2}$$

when one introduces a cut-off at large momentum scale $\Lambda \gg m$.

The divergent part of Σ can be separated by expanding it on the "mass shell" $p^2 = m^2$ of physical electrons. Using that $\Sigma(p)$ is a Dirac matrix that can be a combination of $\mathbf{1}_4$ and $\not{p}$ only, we can write

$$\begin{aligned} \Sigma(p) &= \Sigma(p)\Big|_{\not{p}=m} + \Sigma'(p)\Big|_{\not{p}=m} (\not{p} - m) + \dots \\ &= A\mathbf{1}_4 + B(\not{p} - m) + C(\not{p} - m)^2 + \dots \end{aligned} \tag{7.3}$$

A is linearly divergent, but, on dimensional grounds, the coefficient B can at most be logarithmically divergent, whereas C and the following ones have finite integral representations.

In (6.32), the electron self-energy is needed only on the electron's mass shell. Its effect is to add a correction to the lowest-order propagation of electrons according to

$$\begin{aligned} & \frac{i}{\not{p} - m} + \frac{i}{\not{p} - m}(-i\Sigma)\frac{i}{\not{p} - m} = \frac{i}{\not{p} - m - \Sigma} + O(e^4) \\ &= \frac{i}{(1 - B)(\not{p} - m) - A + O(\not{p} - m)^2} + O(e^4) \\ &= \frac{i(1 + B)}{\not{p} - m - A + O(\not{p} - m)^2} + O(e^4) \end{aligned} \tag{7.4}$$

The divergent coefficients A and B are seen to correspond to an infinite "renormalization" of the mass parameter of the electron and of wave functions: The mass

that is physically relevant is the pole of the effective electron propagator, so it is sensible to define $m_{ren.} = m + A$ as the physical mass of electrons. Since A is a divergent constant (in the limit of removing any artificial cutoff Λ), m, the bare mass, must be likewise divergent to give a finite mass $m_{ren.}$. Similarly, one can absorb the divergent constant $(1 + B) =: Z_2^{-1}$ into a renormalization of the spinor fields $\psi_{ren.} = \psi / \sqrt{Z_2}$.

7.2   Vacuum polarization

The closed fermion loop appearing in (6.32) is called photon self-energy or vacuum-polarization diagram. In momentum space, it is given by the integral

$$-(-ie)^2 \int \frac{d^4k}{(2\pi)^4} \, \mathrm{tr} \, \gamma_\mu \frac{i}{\slashed{k} - m + i\varepsilon} \gamma_\nu \frac{i}{\slashed{k} - \slashed{q} - m + i\varepsilon} =: -i\Pi_{\mu\nu}(q) \qquad (7.5)$$

where tr refers to trace with respect to the spinor indices.

In contrast to the electron self-energy, we need the full functions $\Pi_{\mu\nu}(q)$ in (6.32), where q is the momentum transfer from the external field to the scattered electron.

However, by naive power-counting, $\Pi_{\mu\nu}(q)$ looks even more divergent than Σ. In order to separate divergent coefficients and hopefully be able to put them into the as yet unrenormalized coupling e and photon wave-function, we need a careful *regularization* of the ill-defined integral (7.5).

There are numerous possibilities for introducing a regulator. The most common ones are:

1. Cutting off the modulus of the integration momentum after analytic continuation to Euclidean momentum space $k_0 \to ik_4$ by

$$-k^2 = \vec{k}^2 + k_4^2 < \Lambda^2. \qquad (7.6)$$

   While perfectly possible, this has the drawback of spoiling gauge invariance in intermediary steps.

2. Lattice cut-off: Discretizing (Euclidean) space-time by replacing it with a lattice of finite lattice spacing a implies $|k_\mu| < \pi/a \; \forall \mu$. This regularization is much used in numerical approaches to strongly coupled theories like quantum chromodynamics. Its main drawback for us is that it produces expressions which are difficult to evaluate by analytic means and that it violates Lorentz invariance.

3. Pauli-Villars(-Rayski) regularization is a Lorentz-covariant alternative to cutoff-regularization by introduction of extra fields with a wrong-sign kinetic term

and mass Λ^2 for each of the fields in the theory. The extra fields are decoupled by sending $\Lambda \to \infty$ in the end, but for finite Λ this improves the ultraviolet behaviour of propagators because

$$\frac{1}{k^2 - m^2} \to \frac{1}{k^2 - m^2} - \frac{1}{k^2 - \Lambda^2} = \frac{m^2 - \Lambda^2}{(k^2 - m^2)(k^2 - \Lambda^2)}. \tag{7.7}$$

This is not well suited for the photon propagator, however, because a simple mass term violates gauge invariance.

4. A more modern way of regularization which is symmetry-preserving to a large extent is *dimensional regularization* which is due to 't Hooft & Veltman (1972). We shall use this method in what follows. The idea is to alter the number of space-time dimensions to $n < 4$, derive formulae for the loop integrals as functions of n, and to analyticly continue to a continuous variable $n \in \mathbb{C}$, keeping a small regulator ε, $n = 4 - \varepsilon$ to separate divergences.[20] In this scheme one has to use that $g^{\mu\nu} g_{\nu\mu} = \delta^\mu_\mu = n$. The dimension of spinor space, which actually goes like $2^{[n/2]}$, is usually kept as 4. Renormalized physical quantities do not depend on prescriptions like this (if they can be implemented consistently).

In dimensional regularization, we have to calculate

$$\Pi_{\mu\nu}(q) = -ie^2 \int \frac{d^n k}{(2\pi)^n} \frac{\mathrm{tr}(\gamma_\mu(\slashed{k} + m)\gamma_\nu(\slashed{k} - \slashed{q} + m))}{(k^2 - m^2 + i\varepsilon)((k - q)^2 - m^2 + i\varepsilon)} \tag{7.8}$$

For dimensions $n < 4$, e acquires the dimension of $(\mathrm{mass})^{(4-n)/2}$, so if we want to keep the fine-structure constant $e^2/(4\pi)$ a pure number free of mass dimension, we need to introduce a referential mass scale μ and replace $e^2 \to \tilde{e}^2 = e^2 \mu^{4-n}$.

Using that $\mathrm{tr}(\gamma_\mu \gamma_\nu) = 4g_{\mu\nu}$ and $\mathrm{tr}(\gamma_\mu \gamma_\sigma \gamma_\nu \gamma_\rho) = 4(g_{\mu\sigma} g_{\nu\rho} + g_{\mu\rho} g_{\sigma\nu} - g_{\mu\nu} g_{\sigma\rho})$ the numerator in the above integrand is found to be

$$\mathrm{tr}(\ldots) = 4[2k_\mu k_\nu - k_\mu q_\nu - k_\nu q_\mu + g_{\mu\nu}(m^2 + k \cdot q - k^2)].$$

The denominators can be combined by using the trick of *Feynman parametrization* according to

$$\frac{1}{a_1 a_2 \cdots a_n} = (n-1)! \int_0^1 dx_1 \int_0^{1-x_1} dx_2 \cdots \int_0^{1-x_1-\ldots-x_{n-2}} dx_{n-1}$$
$$\times \frac{1}{[a_n + x_1(a_1 - a_n) + \ldots + x_{n-1}(a_{n-1} - a_n)]^n}. \tag{7.9}$$

---

[20]This ε is of course different from the one appearing as $i\varepsilon$ in the propagators.

In our special case we need

$$\frac{1}{ab} = \int_0^1 \frac{dx}{[ax + b(1-x)]^2} \tag{7.10}$$

with $[ax + b(1-x)] = [(k - xq)^2 + q^2 x(1-x) - m^2 + i\varepsilon]$.

   The advantage of doing so is that after a linear shift of the integration variable $k - qx \to k$, the denominator no longer depends on two 4-vectors and their inner product, but only on their moduli k^2 and q^2.

   Using the formulae of dimensional regularization derived in Appendix B one then finds

$$
\begin{aligned}
\Pi_{\mu\nu}(q) &= -4i\tilde{e}^2 \int_0^1 dx \int \frac{d^n k}{(2\pi)^n} \frac{2k_\mu k_\nu + 2(x^2 - x)q_\mu q_\nu + g_{\mu\nu}(m^2 + (x - x^2)q^2 - k^2)}{[k^2 + q^2 x(1-x) - m^2 + i\varepsilon]^2} \\
&= \frac{4\tilde{e}^2}{(4\pi)^{n/2}} \int_0^1 dx [m^2 - q^2 x(1-x)]^{\frac{n}{2} - 2} \\
&\qquad \times \Bigg\{ \Gamma(2 - \frac{n}{2})[-2x(1-x)q_\mu q_\nu + x(1-x)g_{\mu\nu}q^2 + g_{\mu\nu}m^2] \\
&\qquad\quad + \underbrace{\Gamma(1 - \frac{n}{2})(1 - \frac{n}{2})}_{\Gamma(2 - \frac{n}{2})} \left(q^2 x(1-x) - m^2\right) g_{\mu\nu} \Bigg\} \\
&= \frac{8\tilde{e}^2}{(4\pi)^{n/2}} [g_{\mu\nu}q^2 - q_\mu q_\nu] \,\Gamma(2 - \frac{n}{2}) \int_0^1 dx\, x(1-x)[m^2 - q^2 x(1-x)]^{\frac{n}{2} - 2} \\
&=: [g_{\mu\nu}q^2 - q_\mu q_\nu]\Pi(q^2). \tag{7.11}
\end{aligned}
$$

   This expression is divergent as $n \to 4$, where $\Gamma(2 - \frac{n}{2})$ develops a pole. Naive power-counting suggested a quadratic divergence. This would have corresponded to a pole already for $n \to 2$ as $\Gamma(1 - \frac{n}{2})$ does have it. However, this pole got cancelled, so that $\Pi_{\mu\nu}(q)$ is actually only logarithmically divergent. The reason for this is gauge symmetry, which is reflected by $\Pi_{\mu\nu}$ turning out to be proportional to the transverse tensor $g_{\mu\nu}q^2 - q_\mu q_\nu$. Gauge invariance implies certain identities among Feynman diagrams, the so-called *Ward identities*, of which $\Pi_{\mu\nu}(q)q^\mu \equiv 0$ is one.

   We can isolate the ultraviolet divergence in (7.11) by expanding $n = 4 - \varepsilon$. Because of the pole in $\Gamma(2 - \frac{n}{2}) = \Gamma(\frac{\varepsilon}{2}) = \frac{2}{\varepsilon} - \gamma_E + O(\varepsilon)$, the other factors in (7.11) need to be expanded up to and including terms linear in ε:

$$
\begin{aligned}
\int_0^1 \cdots &= \int_0^1 dx\, x(1-x) - \frac{\varepsilon}{2} \int_0^1 dx\, x(1-x) \ln[m^2 - q^2 x(1-x)] + O(\varepsilon^2) \\
\frac{1}{(4\pi)^{n/2}} &= \frac{1}{16\pi^2} \left(1 + \frac{\varepsilon}{2} \ln(4\pi)\right) + O(\varepsilon^2) \\
\tilde{e}^2 &= e^2 \left(1 + \frac{\varepsilon}{2} \ln \mu^2\right) + O(\varepsilon^2) \tag{7.12}
\end{aligned}
$$

Putting everything together we obtain

$$\Pi(q^2) = \frac{e^2}{2\pi^2}\left\{\frac{1}{6}\left[\frac{2}{\varepsilon} - \gamma_E - \ln\frac{m^2}{4\pi\mu^2}\right] - \int_0^1 dx\, x(1-x)\ln\frac{m^2 - q^2 x(1-x)}{m^2}\right\} \quad (7.13)$$

The divergent piece in $\Pi(q^2)$ can be absorbed in an infinite wave-function renormalization of the photon field.

Technically this is done by replacing $A^\mu = Z_3^{1/2} A^\mu_{ren.}$. In the Lagrangian

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} = \frac{1}{2}A^\mu(g_{\mu\nu}\Box - \partial_\mu\partial_\nu)A^\nu = -\frac{1}{4}F^{ren.}_{\mu\nu}F^{\mu\nu}_{ren.} - (Z_3-1)\frac{1}{4}F^{ren.}_{\mu\nu}F^{\mu\nu}_{ren.} \quad (7.14)$$

this substitution generates terms which explicitly depend on e and thus enter the interaction part of $\mathcal{L}$. With the choice of

$$Z_3 = 1 - \frac{e^2}{2\pi^2}\frac{1}{6}\left(\frac{2}{\varepsilon} + c\right) \quad (7.15)$$

where c is an arbitrary finite constant, this produces an extra contribution, a *counterterm*, to $\Pi_{\mu\nu}$ which has precisely the required tensor structure to subtract out the infinities.

Different choices of the arbitrary constant c correspond to different *renormalization schemes*. They are all physically equivalent, but it is of course important to stick to one particular scheme until final results are obtained.

Popular schemes are:

1. Minimal subtraction (MS): Only the pole term of dimensional regularization is subtracted, i.e. $c = 0$.

2. Modified minimal subtraction ($\overline{\text{MS}}$): $c = -\gamma_E + \ln(4\pi)$. These constants invariably appear together with the pole term of dimensional regularization, so formulae can be simplified by removing them together with $\frac{2}{\varepsilon}$.

3. Momentum subtraction (MOM): c is determined by the requirement that the effective photon propagator equals the classical one at some fixed scale of momentum transfer, that is $\Pi^{\text{MOM}}(q^2 = -\mathcal{M}^2) = 0$.

4. On-shell renormalization (OS): This is a natural scheme for QED. It requires that on the mass-shell of the photons (the light-cone $q^2 = 0$) there be no corrections: $\Pi^{\text{OS}}(q^2 = 0) = 0$.
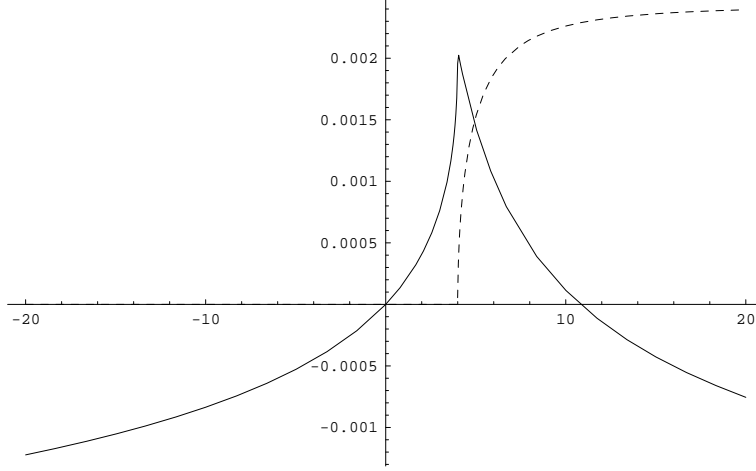
Figure 7.1: The real part (solid line) and the imaginary part (dashed line) of $\Pi^{\mathrm{OS}}(q^2)$.

In the OS-renormalization scheme all of the terms in the square bracket in (7.13) get subtracted. The remaining integral can be evaluated in terms of elementary functions. For $q^2 < 4m^2$ it reads

$$\Pi^{\mathrm{OS}}(q^2) = \frac{e^2}{6\pi^2}\left\{\frac{5}{6} + 2\frac{m^2}{q^2} - (1 + 2\frac{m^2}{q^2})\sqrt{\frac{4m^2 - q^2}{q^2}}\arctan\sqrt{\frac{q^2}{4m^2 - q^2}}\right\}. \quad (7.16)$$

For $q^2 > 4m^2$ the argument of the logarithm in (7.13) turns negative, because $x(1-x)$ varies between 0 and $\frac{1}{4}$ in the integration domain of x. $\Pi(q^2)$ therefore has a branch cut on the real axis for $q^2 > 4m^2$ with[21]

$$\mathrm{Im}\,\Pi(q^2 \pm i\varepsilon) = \pm\theta(q^2 - 4m^2)\frac{e^2}{12\pi}(1 + 2\frac{m^2}{q^2})\sqrt{\frac{q^2 - 4m^2}{q^2}}. \quad (7.17)$$

The appearance of this imaginary part is related to the physical process of the decay of a virtual (off-shell) photon with $q^2 > (2m)^2$ into real electron-positron pair.

7.2.1   Uehling potential

From (6.32) we see that an external potential $\tilde{A}_\mu^{ext}(q)$ receives a correction from the vacuum polarization diagram according to

$$\tilde{A}_\mu^{ext}(q) \rightarrow \left(\delta_\mu^\rho + \frac{-ig_{\mu\sigma}}{q^2}(-i)\Pi^{\sigma\rho}(q)\right)\tilde{A}_\rho^{ext}(q) \quad (7.18)$$

---

[21]The imaginary part of Π does not depend on the chosen renormalization scheme because the counter-terms have to be real.

In the S-matrix element containing (6.32) the contributions proportional to $q^\sigma q^\rho$ in $\Pi^{\sigma\rho}(q)$ do not contribute, because after spinor wave functions are attached to the amputated fermion lines, they give terms of the form $\bar{u}(p+q)\gamma^\mu u(p) \cdot q_\mu = 0$, since $\slashed{q} = (\slashed{p} + \slashed{q} - m) - (\slashed{p} - m)$. Only the term $g^{\sigma\rho}q^2\Pi(q^2)$ enters, so the effect of (7.18) is a multiplication of $A_\mu^{ext}(q) \to A_\mu^{ext}(q)(1 - \Pi(q^2))$.

In particular, a static ($q^0 = 0$) Coulomb potential, which in momentum space is $\propto 1/\vec{q}^2$, gets modified according to

$$\frac{1}{\vec{q}^2} \to \frac{1}{\vec{q}^2}\left(1 - \Pi(-\vec{q}^2)\right) \tag{7.19}$$

In the limit of nonrelativistic magnitude of $|\vec{q}|$, that is $\vec{q}^2/m^2 \to 0$,

$$\Pi^{\text{OS}}(-\vec{q}^2) \to -\frac{e^2}{2\pi^2}\frac{\vec{q}^2}{m^2}\int_0^1 dx[x(1-x)]^2 = -\frac{e^2\vec{q}^2}{60\pi^2 m^2} \tag{7.20}$$

and

$$\frac{1}{\vec{q}^2}\left(1 - \Pi(-\vec{q}^2)\right) \to \frac{1}{\vec{q}^2} + \frac{e^2}{60\pi^2 m^2}. \tag{7.21}$$

Fourier transformed to configuration space this gives a potential of the form

$$V(|\vec{x}|) \propto \frac{1}{4\pi|\vec{x}|} + \frac{e^2}{60\pi^2 m^2}\delta^3(\vec{x}). \tag{7.22}$$

In the nonrelativistic limit, the effect of vacuum polarization is seen to be approximated by a positive δ-function contribution at the origin.

In hydrogen-like atoms, this has an effect only for s-states, since

$$|\psi_{n,l}(0)|^2 = \frac{Z^3 m^3 \alpha^3}{\pi n^3}\delta_{l,0}. \tag{7.23}$$

First-order perturbation theory leads to an energy shift

$$\delta E_{n,l} = -\frac{Z\alpha e^2}{15\pi m^2}\delta_{l,0}|\psi_{n,0}(0)|^2 = -\frac{4Z^4\alpha^5 m}{15\pi n^3}\delta_{l,0}. \tag{7.24}$$

For the hydrogen atom ($Z = 1$), this result corresponds to a downward shift of the $2s_{1/2}$ level compared to the $2p_{1/2}$ level by an amount of ≈ 27 MHz. This prediction by Uehling and Serber in 1935 was the motivation for the experiment by Lamb and Retherford in 1947 which instead gave ≈ 1000 MHz, but in the opposite direction. The missing main contributions, which are partly associated with the vertex diagram in (6.32), were found soon thereafter by Bethe and others. By now, the theoretical and the experimental values for the Lamb shift have been determined at an accuracy

of $\sim 0.001\%$ with perfect agreement. The vacuum polarization contribution, which is part of the final result, is therefore equally well confirmed.

The nonrelativistic approximation to the corrected Coulomb potential (7.22) is a very good approximation as concerns wave functions of the hydrogen atom, which are nearly constant on the scale of the Compton wavelength $1/m$.

The full form of the corrected Coulomb potential has already been found in 1937 by Uehler and Serber on the basis of Dirac's hole theory. It is obtained from the complete expression for (7.19) by a Fourier transformation which yields

$$V(|\vec{x}|) \propto \frac{1}{|\vec{x}|} Q(|\vec{x}|) \tag{7.25}$$

with[22]

$$Q(r) = 1 + \frac{e^2}{6\pi^2} \int_1^\infty du\, e^{-2mru} \left(1 + \frac{1}{2u^2}\right) \frac{\sqrt{u^2 - 1}}{u^2}. \tag{7.26}$$

In the limits of large and small distances, this can be evaluated as

$$Q(r) = \begin{cases} 1 + \frac{e^2}{6\pi^2}[\ln \frac{1}{mr} - \gamma_E - \frac{5}{6}] & \text{for } mr \ll 1 \\ 1 + \frac{e^2}{16\pi^2} \frac{1}{\sqrt{\pi(mr)^3}} e^{-2mr} & \text{for } mr \gg 1 \end{cases} \tag{7.27}$$

The correction to the Coulomb potential is seen to be concentrated within about one Compton wavelength of the electron (Fig. 7.2). For small distances as one approaches the bare charge, leaving the cloud of vacuum polarization behind, it diverges logarithmically.

In the on-shell renormalization scheme, a static charge is effectively normalized at $\vec{q}^2 = 0$, which corresponds to infinite distance. In high-energy physics it turns out to be useful to define a running effective coupling constant which depends on the typical momentum scale under consideration. From the high-momentum limit of $\Pi^{\text{OS}}(q^2)$

$$\Pi^{\text{OS}}(q^2) \to \frac{\alpha}{3\pi} \left[\ln \frac{-q^2}{m^2} - \frac{5}{3}\right] \tag{7.28}$$

one can define

$$\alpha_{\text{eff.}}(q^2) = \frac{\alpha}{1 - \frac{\alpha}{3\pi} \ln \frac{-q^2}{e^{5/3} m^2}} \tag{7.29}$$

with $|q^2| \gg m^2$. Including also the vacuum polarization effects of heavier leptons and quarks, which also carry electric charge, one is lead to an effective fine-structure

---

[22]The Fourier integral can be evaluated by extending the integration over $|\vec{q}|$ to the entire real axis and then deforming the contour in the complex plane so that the only nontrivial contribution comes from a branch cut that runs from $|\vec{q}| = 2im$ to $i\infty$.
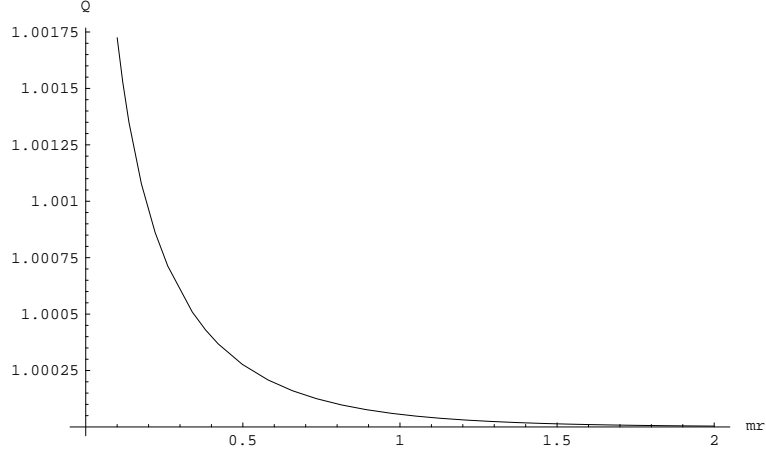
Figure 7.2: The effective charge $Q(r)$ in the Uehling potential as a function of $mr = r/(\lambda_{\text{Compton}}/2\pi)$.

constant that at current accelerator energies is significantly higher than the low-energy value of $\alpha \approx 1/137$, for instance $\alpha_{\text{eff}}(-M_W^2) \approx 1/128$.[23]

7.3   Vertex diagram

For the complete order-e^3 contribution to Coulomb scattering (6.32) we finally need the one-loop diagram built from two electron propagators and one photon propagator. It depends on the external momenta p, p' of the in- and out-going electrons and thus is a nonlocal correction to the local "classical" vertex $-ie\gamma_\mu$. Let us denote the sum by

$$-ie\Gamma_\mu(p', p) := -ie\gamma_\mu - ie\Lambda_\mu(p', p) \tag{7.30}$$

The Feynman rules in Feynman gauge give, in dimensional regularization,

$$-ie\Lambda_\mu(p', p) = (-i\tilde{e})^3 \int \frac{d^n k}{(2\pi)^n} \frac{-ig^{\nu\lambda}}{k^2 + i\varepsilon} \gamma_\nu \frac{i}{\not{p}' - \not{k} - m + i\varepsilon} \gamma_\mu \frac{i}{\not{p} - \not{k} - m + i\varepsilon} \gamma_\lambda \tag{7.31}$$

where k is the momentum of the internal photon line.

---

[23]One might worry about the fact that this effective coupling becomes infinite for a finite, albeit more than astronomical value of $-q^2 = m^2 \exp(\frac{3\pi}{\alpha} - \frac{5}{3}) \sim 10^{560} m^2$. This is sometimes referred to as Landau ghost. Perturbation theory cannot decide whether QED contains a Landau ghost and thus an inconsistency. At any rate, this problem occurs at such extreme energy/momentum scales that one even enters the regime of quantum gravity long before one would have to face it.

For the purposes of Coulomb scattering, we need $\Lambda_\mu(p, p')$ only for on-mass-shell momenta $p^2 = m^2 = p'^2$, and sandwiched between Dirac spinors in the form

$$
\begin{aligned}
\bar{u}(p')\Lambda_\mu(p', p)u(p) &= -i\tilde{e}^3 \int \frac{d^n k}{(2\pi)^n} \frac{1}{k^2 - \lambda^2 + i\varepsilon} \frac{1}{k^2 - 2kp' + i\varepsilon} \frac{1}{k^2 - 2kp + i\varepsilon} \\
&\times \bar{u}(p')\gamma^\nu (\not{p}' - \not{k} + m)\gamma_\mu(\not{p} - \not{k} + m)\gamma_\nu u(p) \qquad (7.32)
\end{aligned}
$$

where we have introduced a mass term λ^2 into the photon propagator because otherwise this expression is infrared-divergent. The mass-shell condition $p^2 = m^2 = p'^2$ makes the internal fermion propagators behave as $\sim \frac{1}{k}$ for $k \to 0$ so that the integral is logarithmically divergent at the origin for $n = 4$. Unfortunately, dimensional regularization requires $n < 4$ which seems to make the problem only worse.

These on-shell infrared divergences cannot be absorbed by the standard renormalization which removes the ultraviolet divergences. Instead, the solution turns out to be that the process of Coulomb scattering as considered in (6.32) is not really measurable as such. We need detectors that measure the scattered electrons and also detectors that can measure photons to distinguish it from a process that instead of only elastically scattering electrons produced bremsstrahlung photons in addition. However, any physical photon detector will be able to detect only the photons above some minimum limiting energy. But photons can be emitted with arbitrarily low energy ("soft bremsstrahlung"). A physical experiment measuring elastic scattering therefore always measures the combination of elastic scattering and unseen soft bremsstrahlung. It turns out that the bremsstrahlung process likewise has infrared singularities, which cancel in the sum. The measured cross section then only depends (logarithmically) on the value of the minimal photon energy that can still be detected, but no longer on the photon mass λ that one introduces to make the Feynman integrals finite in the infrared. This solution of the problem was found by Bloch & Nordsieck in 1937 already before relativistic perturbation theory was developed. A complete treatment of infrared divergences in QED to all orders of perturbation theory was achieved in 1961 by Yennie et al.

We shall be content here to evaluate Λ_μ in the limit $\lambda \to 0$, which will give terms involving a logarithm of λ and terms independent of λ.

Before doing the calculation, we can anticipate the structure of $\Lambda_\mu(p', p)$ in any order of perturbation theory as follows. Λ_μ (as well as Γ_μ) is a Lorentz vector and a matrix in spinor space. The only Lorentz vectors available are the momenta p_μ, p'_μ, and $g_{\mu\nu}$. (The external photon's momentum is given by the difference $(p' - p)_\mu =: q_\mu$ because of momentum conservation.) Λ_μ must therefore be of the form

$$
\Lambda_\mu(p', p) = \gamma_\mu A + (p' + p)_\mu B + (p' - p)_\mu C \qquad (7.33)
$$

where the coefficients A, B, and C may involve quantities like $\not{p}$ and $\not{p}'$ in addition to Lorentz scalars times $\mathbf{1}_4$. On-shell and sandwiched by Dirac spinors, however, one can bring $\not{p}'$ and $\not{p}$ to the left and right, respectively, which in the first term may give extra contributions proportional to p'_μ or p_μ, and replace $\not{p}'$, $\not{p} \to m$. We can therefore take the coefficients A, B, and C to be simple Lorentz scalars. Because $p^2 = m^2 = p'^2$, the only nontrivial scalar is $q^2 = -2p' \cdot p + 2m^2$.

It can be proved generally that as a consequence of gauge invariance Λ_μ as well as Γ_μ satisfy $q^\mu \bar{u}(p')\Lambda_\mu(p',p)u(p) = 0$ on mass-shell. At one-loop order, this may be verified directly on the explicit expression (7.32). The first two terms in (7.33) vanish when contracted with q^μ and sandwiched by on-shell spinors, but the last one does not. Hence, $C = 0$.

The general on-shell vertex function Γ_μ of QED therefore contains two independent "structure functions" A and B. An equivalent decomposition can be written down by using the so-called *Gordon identity*:

From the fact that

$$
\begin{aligned}
0 &= \bar{u}(p') \left[\not{d}(\not{p} - m) + (\not{p}' - m) \not{d} \right] u(p) \\
&= -2m\bar{u} \not{d} u + \bar{u} \left(\frac{1}{2} \{ \not{p}' + \not{p}, \not{d} \} + \frac{1}{2} [\not{p}' - \not{p}, \not{d}] \right) u
\end{aligned}
\tag{7.34}
$$

for arbitrary $\not{d}$ one immediately derives that

$$
\bar{u}(p') \left[-2m\gamma^\mu + (p + p')^\mu + i\sigma^{\mu\nu}q_\nu \right] u(p) = 0
\tag{7.35}
$$

with $\sigma^{\mu\nu} = \frac{i}{2}[\gamma^\mu, \gamma^\nu]$ and $q \equiv p' - p$.

The general form of the on-shell vertex correction $\Lambda_\mu(p',p)$ can therefore be written as

$$
\Lambda_\mu(p',p) = \gamma_\mu F_1(q^2) + \frac{i\sigma_{\mu\nu}q^\nu}{2m} F_2(q^2).
\tag{7.36}
$$

Since the first term is proportional to the lowest-order vertex between photons and electrons, it can be changed by renormalization. Indeed, this is again necessary to remove an ultraviolet divergence.

It turns out that gauge invariance relates the divergent piece in Λ_μ to the divergent electron self-energy $\Sigma(p)$ by the Ward identity

$$
\lim_{p' \to p} \Lambda_\mu(p,p') = -\frac{\partial}{\partial p^\mu} \Sigma(p)
\tag{7.37}
$$

which at one-loop order can be verified directly by comparing the Feynman integrals (7.31) and (7.1). On-shell renormalization of the electron propagator therefore

implies the renormalization condition

$$\bar{u}(p')\Lambda^{\text{OS}}_{\mu}(p',p)u(p)\Big|_{p^2=m^2=p'^2,p=p'} = 0 \quad \Rightarrow F_1^{ren.}(0) = 0 \qquad (7.38)$$

The other structure function F_2, called the magnetic structure function, cannot be renormalized this way, and indeed it turns out to be finite.

The explicit calculation of F_1 and F_2 from the Feynman integral (7.32) is carried out in Appendix C in order to make this chapter more readable. The final result is

$$
\begin{aligned}
F_1^{\text{ren.}}(q^2) &= \frac{e^2}{16\pi^2}\Bigg\{ -\int_0^1 dy\frac{2m^2-q^2}{m^2-q^2y(1-y)}\ln\frac{m^2-q^2y(1-y)}{\lambda^2} + 2\ln\frac{m^2}{\lambda^2} \\
&\quad -\int_0^1 dy\ln\frac{m^2-q^2y(1-y)}{m^2} + \int_0^1 dy\frac{6m^2-2q^2}{m^2-q^2y(1-y)} - 6 \Bigg\} \quad (7.39) \\
F_2(q^2) &= \frac{e^2}{16\pi^2}2\int_0^1 dy\frac{m^2}{m^2-q^2y(1-y)} \qquad\qquad\qquad\qquad\qquad (7.40)
\end{aligned}
$$

The magnetic structure function F_2 turns out to be not only ultraviolet finite, but infrared finite, too.

In the limit of small momentum transfer (7.39) and (7.40) are easily evaluated as

$$F_1^{\text{ren.}}(q^2) = \frac{\alpha}{3\pi}\frac{q^2}{m^2}\left(\ln\frac{m}{\lambda} - \frac{3}{8}\right) + O(q^4/m^4) \qquad (7.41)$$

$$F_2(q^2) = \frac{\alpha}{2\pi}\left(1 + \frac{1}{6}\frac{q^2}{m^2} + O(q^4/m^4)\right). \qquad (7.42)$$

7.4   Effective interaction with a weak external field

We finally have all pieces of the one-loop contributions (6.32) to the interaction of physical (on-shell) electrons with a weak external electromagnetic field. They can be summarized as follows: Because the electrons are on mass shell, the self-energy insertions in external lines can be absorbed in the physical definition of the electron mass and a proper normalization of the spinor wave functions, if the on-shell renormalization scheme is used. The vacuum polarization diagram is rendered finite by a renormalization of the electromagnetic fields and introduces a momentum-dependent modification of the external field according to (7.18). The vertex diagram has to be renormalized in a way consistent with renormalization of the electron self-energy. It contributes two different corrections to the interaction of an electron with the external field of the form (7.36). All together the interaction vertex of on-shell electrons gets replaced by an effective interaction according to

$$-ie\gamma_{\mu}\tilde{A}^{\text{ext}\mu}(q) \rightarrow -ie\left\{\gamma_{\mu}\left(1-\Pi^{\text{OS}}(q^2)\right) + \Lambda^{\text{OS}}_{\mu}(p,p')\right\}\tilde{A}^{\text{ext}\mu}(q). \qquad (7.43)$$

At low momentum transfer q, this effective interaction reads

$$-ie\left\{\gamma_\mu\left[1+\frac{\alpha q^2}{3\pi m^2}\left(\ln\frac{m}{\lambda}-\frac{3}{8}-\frac{1}{5}\right)\right]+\frac{i}{2m}\frac{\alpha}{2\pi}\sigma_{\mu\nu}q^\nu\right\}\tilde{A}^{\text{ext}\mu}(q). \qquad (7.44)$$

By replacing q by the derivative operator $i\partial$, this can be written in configuration space as

$$-ie\left\{\gamma_\mu\left[1-\frac{\alpha}{3\pi m^2}\left(\ln\frac{m}{\lambda}-\frac{3}{8}-\frac{1}{5}\right)\Box_x\right]-\frac{1}{2m}\frac{\alpha}{2\pi}\sigma_{\mu\nu}\partial^\nu\right\}A^{\text{ext}\mu}(x). \qquad (7.45)$$

7.4.1   Anomalous magnetic moment

Using the Gordon identity (7.35) to rewrite the lowest order vertex in (7.44) as

$$\gamma_\mu=\frac{1}{2m}(p+p')+\frac{i}{2m}\sigma_{\mu\nu}q^\nu$$

the effective interaction can be written as sum of a spin-independent convective term and one that involves spin nontrivially. From (7.45) we see that the latter has the form

$$ie\left(1+\frac{\alpha}{2\pi}\right)\frac{1}{2m}\sigma_{\mu\nu}\partial^\nu A^{\text{ext}\mu}(x)=-ie\left(1+\frac{\alpha}{2\pi}\right)\frac{1}{2m}\frac{1}{2}\sigma_{\mu\nu}F^{\mu\nu}. \qquad (7.46)$$

In a constant magnetic field this is just the magnetic dipole interaction energy

$$\left.\frac{1}{2}\sigma_{\mu\nu}F^{\mu\nu}\right|_{\vec{E}=0}=\vec{\Sigma}\cdot\vec{B}. \qquad (7.47)$$

Since we already know that the lowest-order term in (7.46) corresponds to the gyromagnetic ratio $g=2$, we see that the low-momentum limit of the vertex structure function F_2 gives rise to a modified value

$$g=2(1+a)\equiv 2\left(1+\frac{\alpha}{2\pi}+O(\alpha^2)\right) \qquad (7.48)$$

called the anomalous magnetic moment of the electron, derived first by Schwinger in 1948.

The current experimental value (Van Dyck, Schwinberg & Dehmelt 1987) reads

$$a=1\ 159\ 652\ 188.4(4.3)\times 10^{-12} \qquad (7.49)$$

The one-loop result (7.48) is numerically $a^{(1)}=\frac{\alpha}{2\pi}=0.0011614\ldots$. It agrees with the experimental value for a in 3 significant digits; for g it's even 6 digits!

At two-loop order (α^2), 7 vertex diagrams have to be evaluated. The first calculation was done in 1950 by Karplus & Kroll and found to disagree with experiment in

1957. Sommerfield & Petermann then found the error in the theoretical calculation, after which there was agreement in 8 digits of g.

At three-loop order there are 72 Feynman diagrams which have been calculated by Kinoshita and others during 1976-1995. All but 5 of these have been calculated analytically, the remaining numerically. The 891 Feynman diagrams at four-loop order (α^8) have been calculated since 1978 by Monte-Carlo numerical integration. Using α as given by quantum Hall effect measurements, the theoretical prediction is (Kinoshita 1995)

$$a^{(1-4)} = 1\ 159\ 652\ 201(2)(27) \times 10^{-12} \tag{7.50}$$

where the first error given is due to the theoretical uncertainty from the numerical integrations and the second error from the fine-structure constant. Evidently, there is perfect agreement of theory and experiment.

The theoretical result can even be turned around to give a value for the fine-structure constant α from the experimental value of a that is more accurate than the best direct measurements of α. This gives

$$\alpha^{-1}(a) = 137.035\ 999\ 44(57). \tag{7.51}$$

7.4.2   Main contribution to the Lamb shift

In (7.22) we have considered the contribution of vacuum polarization to a Coulomb potential. The additional $\delta^3(\vec{x})$ term that we obtained corresponds only to the term $\propto \frac{1}{5}\Box_x A^{\text{ext}\mu}$ in (7.45). Obviously, this is not the only term that will contribute to the Lamb shift. Unfortunately, the other terms contain a logarithmic infrared divergence which we have cut off by introducing an unphysical photon mass.

In the Coulomb scattering problem, this infrared divergence has to be combined with one that would appear in the soft bremsstrahlung process.

On the other hand, in the case of the hydrogen atom, the electrons are not really on the mass shell $p^2 = m^2$ of free electrons — they are bound! Now the infrared divergence appears only in the limit $p^2 \to m^2$. In order to calculate the Lamb shift, the on-shell vertex diagram is not sufficient.

However, one can obtain a crude estimate for the main contribution to the Lamb shift from the logarithmically divergent term. According to (3.74), an electron bound in a hydrogen-like atom has energy $p^0 \approx m(1 - \frac{Z^2\alpha^2}{2n^2}) =: m - V$. The kinetic energy of the electron is in good approximation nonrelativistic and thus related to V by $\vec{p}^2/2m = -\frac{1}{2}V$ as a consequence of the virial theorem. Taken together, the electron

is off-mass-shell by an amount

$$p^2 - m^2 = -3m^2 Z^2 \alpha^2 / 2n^2.$$

The denominators in (7.32) coming from the electron propagators are therefore not really $1/(k^2 - 2kp)$ but

$$\frac{1}{k^2 - 2kp + p^2 - m^2} = \frac{1}{k^2 - 2kp - O(m^2\alpha^2)}.$$

The k integration is therefore not infrared divergent, but effectively cut off at photon momenta $k \sim m\alpha^2$. Taking this as infrared cutoff λ in (7.45) gives a large contribution from the logarithm. Instead of (7.24) we arrive at the estimate

$$\delta E_{n,l} \sim +\frac{4Z^4 \alpha^5 m}{3\pi n^3} \underbrace{\ln(137)^2}_{\approx 10} \delta_{l,0}, \tag{7.52}$$

which dominates over the other contributions from (7.45). In the hydrogen atom, this corresponds to a Lamb shift of ≈ 1300 MHz which has both the correct sign and the correct order of magnitude.

More careful (and more complicated) calculations at one-loop order have been performed in 1947 by Bethe and subsequently by Kroll & Lamb and French & Weisskopf. These give 1052.19 MHz (s. Weinberg 1995).

Two current experimental values are 1057.845(9) MHz (Lundeen and Pipkin 1986) or 1057.857(2) MHz (Sokolov and Yakolev 1982). Accurate theoretical calculations involve more uncertainties than in the case of the anomalous magnetic moment of the electron (coming from the finite size of the proton and from nuclear recoil effects). Recent calculations vary between 1057.85 and 1057.88 MHz, in excellent agreement with experiment, although not as phantastic as is the case with $g - 2$.

A   Bernoulli and Euler-MacLaurin

Bernoulli numbers are defined through

$$\frac{t}{e^t - 1} =: \sum_{n=0}^{\infty} \frac{t^n}{n!} B_n \tag{A.1}$$

and the first few read

$$B_0 = 1, \ B_1 = -\frac{1}{2}, \ B_2 = \frac{1}{6}, \ B_3 = 0, \ B_4 = -\frac{1}{30}, \ B_{2n+1} = 0 \ \forall \, n \in \mathbb{N}. \tag{A.2}$$

Bernoulli polynomials are defined by

$$B_n(x) = \sum_{k=0}^{n} \binom{n}{k} B_{n-k} x^k \tag{A.3}$$

or through their generating function

$$e^{xt} \frac{t}{e^t - 1} =: \sum_{n=0}^{\infty} \frac{t^n}{n!} B_n(x). \tag{A.4}$$

Their most important properties are

$$B'_n(x) = n B_{n-1}(x) \tag{A.5}$$

$$B_n(1) = B_n(0) \quad \forall \, n \neq 1 \tag{A.6}$$

$$\Rightarrow \quad \int_0^1 B_n(x) dx = \frac{1}{n+1} B_{n+1} \Big|_0^1 = 0 \quad \forall \, n \geq 1 \tag{A.7}$$

With the help of the Bernoulli polynomials one can derive the Euler-MacLaurin formula as follows.

In a first step use $B'_1(x) = B_0(x) \equiv 1$ and $B_1(1) = -B_1(0) = \frac{1}{2}$ to write for the integral of a sufficiently differentiable function

$$\int_0^1 f(x) dx = \int_0^1 f(x) B'_1(x) dx = \tfrac{1}{2} \left(f(0) + f(1) \right) - \int_0^1 f'(x) B_1(x) dx \tag{A.8}$$

Continue by using (A.5) and (A.6) to rewrite

$$\begin{aligned} -\int_0^1 f'(x) B_1(x) dx &= -\tfrac{1}{2} \int_0^1 f'(x) B'_2(x) dx \\ &= -\tfrac{1}{2} B_2 \left(f'(1) - f'(0) \right) + \tfrac{1}{2} \int_0^1 f''(x) B_2(x) dx \end{aligned} \tag{A.9}$$

and so forth until one has

$$\int_0^1 f(x)dx = \tfrac{1}{2}\left(f(0) + f(1)\right) - \sum_{j=1}^{k} \frac{B_{2j}}{(2j)!}\left[f^{(2j-1)}(1) - f^{(2j-1)}(0)\right] + R_k \qquad \text{(A.10)}$$

with

$$R_k = -\frac{1}{(2k+1)!}\int_0^1 f^{(2k+1)}(x)B_{2k+1}(x)dx.$$

Continuing this formula to integrals $\int_1^2$, $\int_2^3$, ... $\int_{n-1}^n$ and summing gives the *Euler-MacLaurin formula* for the difference between sums and integrals

$$\sum_{i=0}^{n} f(i) = \int_0^n f(x)dx + \tfrac{1}{2}\left[f(0) + f(n)\right] + \sum_{j=1}^{k} \frac{B_{2j}}{(2j)!}\left[f^{(2j-1)}(n) - f^{(2j-1)}(0)\right] + R_{n,k},$$

$$\text{(A.11)}$$

where

$$R_{n,k} = -\frac{1}{(2k+1)!}\int_0^n f^{(2k+1)}(x)\hat{B}_{2k+1}(x)dx$$

and $\hat{B}_n(x) = B_n(x - [x])$. When convergent, this may be extended to $n \to \infty$.

B   Dimensional regularization

Using Feynman parametrization (7.9), the momentum integration of one-loop Feynman diagrams can be reduced to integrals of the form

$$J = \int d^n k \, \frac{1}{(k^2 + 2p \cdot k - M + i\varepsilon)^\alpha} = \int d^n k \, \frac{1}{(k^2 - L + i\varepsilon)^\alpha} \tag{B.1}$$

with $L = p^2 + M$. Integrals which have 4-vectors k_μ in the numerator can be obtained from J by differentiation with respect to p_μ.

In dimensional regularization, n is assumed to be sufficiently small so as to ensure convergence. Ultraviolet divergences are isolated as singularities in the complex n-plane after an analytic continuation of $n \in \mathbb{N}$ to $n \in \mathbb{C}$. For this we have to evaluate J for arbitrary integer values of n first.

The integrand in J has poles at $k_0 = \pm[\sqrt{\vec{k}^2 + L} - i\varepsilon]$. The pole prescription is such that one can deform the integration path for k_0 to run from $-i\infty$ to $i\infty$ with negligible arcs at infinity if $\alpha > \frac{1}{2}$. This "Wick rotation" turns the Minkowskian (momentum) space into an Euclidean one: $k^2 \to -k_E^2 = -(k_1^2 + \ldots + k_n^2)$ with $k_0 = i k_n$ and $\int d^n k \to i \int d^n k_E$.

Denoting $r = \sqrt{k_E^2}$, the integral (B.1) thus becomes

$$J = i(-1)^\alpha \int d\Omega_n \int_0^\infty \frac{r^{n-1} dr}{(r^2 + L)^\alpha}. \tag{B.2}$$

For general n, the latter integral is elementary and reads

$$\int_0^\infty \frac{r^{n-1} dr}{(r^2 + L)^\alpha} = \frac{\Gamma(\frac{n}{2})\Gamma(\alpha - \frac{n}{2})}{2\Gamma(\alpha)} L^{\frac{n}{2} - \alpha}. \tag{B.3}$$

$\int d\Omega_n$ is the area of a unit sphere in n dimensions. It can be most easily calculated by the following trick:

$$
\begin{aligned}
(\sqrt{\pi})^n &= \left(\int dx \, e^{-x^2} \right)^n = \int d^n x \, \exp\left(-\sum_{i=1}^n x_i^2 \right) \\
&= \int d\Omega_n \int_0^\infty dx \, x^{n-1} e^{-x^2} = \int d\Omega_n \frac{1}{2} \int_0^\infty d(x^2) \, (x^2)^{\frac{n}{2} - 1} e^{-(x^2)} \\
&= \frac{1}{2}\Gamma(\frac{n}{2}) \int d\Omega_n \quad \Rightarrow \quad \int d\Omega_n = \frac{2\pi^{n/2}}{\Gamma(\frac{n}{2})}.
\end{aligned}
\tag{B.4}
$$

This gives

$$J = i(-1)^\alpha \pi^{n/2} \frac{\Gamma(\alpha - \frac{n}{2})}{\Gamma(\alpha)} L^{\frac{n}{2} - \alpha}, \tag{B.5}$$

which is already in a form which can be taken as the analytic continuation to $n, \alpha \in \mathbb{C}$.

By differentiating the first version of J in (B.1) with respect to p_μ at $p_\mu = 0$ and the result (B.5) with $L = p^2 + M$, one can now easily derive the following more complicated formulae

$$\int d^n k \frac{k_\mu k_\nu}{(k^2 - L + i\varepsilon)^\alpha} = -C\Gamma(\alpha - \frac{n}{2} - 1)\frac{1}{2}L^{\frac{n}{2}-\alpha+1}g_{\mu\nu} \tag{B.6}$$

$$\int d^n k \frac{k_\mu k_\nu k_\lambda k_\rho}{(k^2 - L + i\varepsilon)^\alpha} = -C\Gamma(\alpha - \frac{n}{2} - 2)\frac{1}{4}L^{\frac{n}{2}-\alpha+2}$$
$$\times \{g_{\lambda\mu}g_{\rho\nu} + g_{\lambda\nu}g_{\rho\mu} + g_{\mu\nu}g_{\rho\lambda}\} \tag{B.7}$$

with $C := i(-1)^\alpha \pi^{n/2}/\Gamma(\alpha)$. Integrals with an odd number of vectors k in the numerator vanish by symmetry.

Recall that Euler's Gamma function $\Gamma(z)$, which is defined as the analytic continuation of the integral

$$\Gamma(z) = \int_0^\infty e^{-t}t^{z-1}dt, \quad \text{Re } z > 0, \tag{B.8}$$

has simple poles at $z = 0, -1, -2, \dots$. In the vicinity of the pole at $z = 0$ it has the expansion

$$\Gamma(\varepsilon) = \frac{1}{\varepsilon} - \gamma_E + O(\varepsilon) \tag{B.9}$$

with γ_E defined by

$$\gamma_E = -\int_0^\infty dt\, e^{-t}\ln t = 0.5772\dots \tag{B.10}$$

(Euler-Mascheroni constant).

Further,

$$\Gamma(z + 1) = z\Gamma(z) \tag{B.11}$$

$$\Gamma(n + 1) = n! \text{ for } n \in \mathbb{N}, \quad \Gamma(\tfrac{1}{2}) = \sqrt{\pi}. \tag{B.12}$$

C On-shell one-loop vertex diagram

This appendix gives some of the details of the evaluation of the on-shell vertex diagram (7.32) in dimensional regularization.

Numerator:

In a first step, the numerator of the integrand in (7.32) can be simplified by

$$\bar{u}(p')\gamma^\nu(\slashed{p}' - \slashed{k} + m)\gamma_\mu(\slashed{p} - \slashed{k} + m)\gamma_\nu u(p)$$
$$= \bar{u}(p')\{\gamma^\nu, \slashed{p}' - \slashed{k} + m\}\gamma_\mu\{\slashed{p} - \slashed{k} + m, \gamma_\nu\}u(p)$$
$$= \bar{u}(p')(2p'_\nu - \gamma_\nu\slashed{k})\gamma_\mu(2p^\nu - \slashed{k}\gamma^\nu)u(p). \tag{C.1}$$

The number of γ-matrices can be further reduced according to

$$(2p'_\nu - \gamma_\nu\slashed{k})\gamma_\mu(2p^\nu - \slashed{k}\gamma^n) \tag{C.2}$$
$$= \gamma_\mu[4m^2 - 2q^2 - 4(p+p')\cdot k + (n-2)k^2] + \slashed{k}[2(2-n)k_\mu + 4(p+p')_\mu] - 4mk_\mu$$

where $\gamma_\nu\gamma^\nu = n\mathbf{1}_4$ has been used as well as $q^2 \equiv (p'-p)^2 = 2m^2 - 2p\cdot p'$.

Denominators:

a) In the terms where there is a k^2 in the numerator, we do not encounter infrared divergences and do not need a regulating photon mass. In these, we cancel against the denominator from the photon propagator, and combine the denominators from the two electron propagtors by (7.10)

$$[k^2 - 2p'\cdot k]^{-1}[k^2 - 2p\cdot k]^{-1} = \int_0^1 dy[k^2 - 2k\cdot(py + p'(1-y)]^{-2} \tag{C.3}$$

With $(p_\mu y + p'_\mu(1-y))^2 = m^2 - q^2 y(1-y)$ formula (B.5) gives

$$\int d^n k[k^2 - 2k\cdot(py + p'(1-y)]^{-2} = i\pi^{n/2}\Gamma(2 - \frac{n}{2})\Big[\underbrace{m^2 - q^2 y(1-y)}_{=:M(y)}\Big]^{\frac{n}{2}-2} \tag{C.4}$$

b) In all other terms we have three denominators to combine by (7.9)

$$[k^2 - \lambda^2]^{-1}[k^2 - 2p'\cdot k]^{-1}[k^2 - 2p\cdot k]^{-1}$$
$$= 2\int_0^1 dz_1 \int_0^{1-z_1} dz_2[k^2 - 2k\cdot(p'z_1 + pz_2) - \lambda^2(1 - z_1 - z_2)]^{-3} \tag{C.5}$$

Abbreviating $r_\mu := p'_\mu z_1 + p_\mu z_2$ the momentum integrals that we need can be derived from (B.5) and (B.6) as

$$\int d^n k [k^2 - 2k \cdot r - \lambda^2 (1 - z_1 - z_2)]^{-3} \left\{ 1; k_\mu; \not{k} k_\mu \right\}$$

$$= -i \frac{\pi^{n/2}}{2} L^{\frac{n}{2} - 2} \left\{ \Gamma(3 - \frac{n}{2}); \right. \tag{C.6}$$

$$\Gamma(3 - \frac{n}{2}) r_\mu; \tag{C.7}$$

$$\left. \Gamma(3 - \frac{n}{2}) \not{r} r_\mu - \frac{1}{2} \Gamma(2 - \frac{n}{2}) L \gamma_\mu \right\} \tag{C.8}$$

with

$$L = r^2 + \lambda^2 (1 - z_1 - z_2) = m^2 (z_1 + z_2)^2 + \lambda^2 (1 - z_1 - z_2) - z_1 z_2 q^2 \tag{C.9}$$

Sandwiched between on-shell spinors we have $\not{r} = m(z_1 + z_2)$. Except for one vector r_μ, the integral and the integration domain is invariant under replacing $z_1 \leftrightarrow z_2$. This can be used to replace $r_\mu \to \frac{1}{2}(z_1 + z_2)(p + p')_\mu$.

Next, change variables by $z_1 = xy$, $z_2 = x(1 - y)$ and

$$\int_0^1 dz_1 \int_0^{1 - z_1} dz_2 \to \int_0^1 dx \, dy \, x \tag{C.10}$$

Altogether we now have

$$\begin{aligned} \Lambda_\mu(p', p) &= \frac{e^2}{(4\pi)^{n/2}} (n - 2) \Gamma(2 - \tfrac{n}{2}) \gamma_\mu \int_0^1 dy \, M^{\frac{n}{2} - 2}(y) \\ &\quad - \frac{e^2}{(4\pi)^{n/2}} \int_0^1 dx \, dy \, x L^{\frac{n}{2} - 3}(x, y) \left\{ \Gamma(3 - \tfrac{n}{2}) \left[4m^2 - 2q^2 - (p + p')^2 \frac{x}{2} \right] \gamma_\mu \right. \\ &\qquad + (2 - n) \Gamma(3 - \tfrac{n}{2}) m x^2 (p + p')_\mu - (2 - n) \Gamma(2 - \tfrac{n}{2}) L(x, y) \gamma_\mu \\ &\qquad \left. + 2 \Gamma(3 - \tfrac{n}{2}) m x (p + p')_\mu \right\} \end{aligned} \tag{C.11}$$

with $L(x, y) := x^2 M(y) + \lambda^2 (1 - x)$ and $M(y)$ as introduced in (C.4).

Using the Gordon identity (7.35) we can now collect the terms contributing to the structure functions F_1 and F_2 introduced in (7.36). In terms without singularities as $n \to 4$, we can put $n = 4$. The only singular piece is $\Gamma(2 - \frac{n}{2})$. Expanding in analogy to (7.12) and subtracting the divergent term by $F_1^{\text{ren.}}(q^2) = F_1(q^2) - F_1(0)$ gives the results (7.39) and (7.40), where terms that vanish for $\lambda \to 0$ have been discarded.

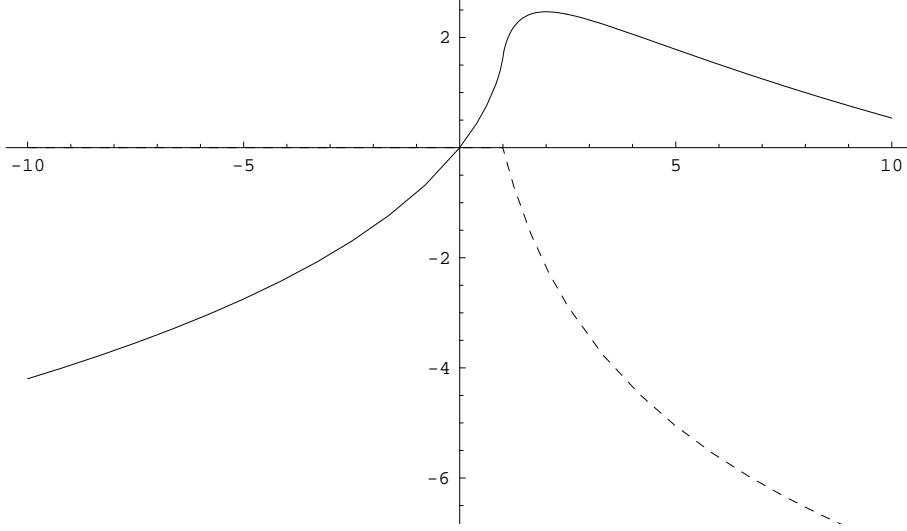Figure C.1: Real part (solid line) and imaginary part (dashed line) of $\mathrm{Li}_2(x)$.

Analytical results (for completeness only)

The magnetic structure function F_2 can be evaluated in terms of elementary functions as

$$F_2(q^2) = \frac{\alpha}{\pi} \frac{\xi \ln \xi}{\xi^2 - 1} \qquad \text{with} \quad \frac{q^2}{m^2} =: -\frac{(1-\xi)^2}{\xi}. \tag{C.12}$$

ξ runs from 0 to 1 as q^2 runs from $-\infty$ to 0. Beyond that one needs to continue analyticly.

The integrals in (7.39) can be written in closed form in terms of the so-called Spence function, or dilogarithm, Li_2:

$$\mathrm{Li}_2(x) = -\int_0^x \frac{\ln(1-t)}{t} dt = \sum_{n=1}^{\infty} \frac{x^n}{n^2}. \tag{C.13}$$

(This is a special member of the family of so-called polylogarithmic functions $\mathrm{Li}_m(x) := \sum_{n=1}^{\infty} \frac{x^n}{n^m}$, of which only $\mathrm{Li}_0(x) = x/(1-x)$ and $\mathrm{Li}_1(x) = -\ln(1-x)$ are elementary functions.) Special values are $\mathrm{Li}_2(-1) = -\pi^2/12$, $\mathrm{Li}_2(0) = 0$, $\mathrm{Li}_2(+1) = +\pi^2/6$.

With (C.13), $F_1^{\text{ren.}}$ can be written as

$$\begin{aligned}
F_1^{\text{ren.}} &= \frac{\alpha}{2\pi} \left\{ 2 \left(1 + \frac{1+\xi^2}{1-\xi^2} \ln \xi \right) \ln \frac{m}{\lambda} - \frac{3(1+\xi^2) + 2\xi}{2(1-\xi^2)} \ln \xi \right. \\
&\quad \left. + \frac{1+\xi^2}{1-\xi^2} \left[\frac{\pi^2}{6} - \frac{1}{2} \ln^2 \xi + 2\mathrm{Li}_2(-\xi) + 2 \ln \xi \ln(1+\xi) \right] \right\}. \quad \text{(C.14)}
\end{aligned}$$

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