Chapter 9. Introduction to Relativistic Quantum Mechanics

This chapter gives a brief introduction to relativistic quantum mechanics. It starts with a discussion of the basic elements of the quantum theory of electromagnetic field (quantum electrodynamics, QED), including the quantization scheme, photon statistics, radiative atomic transitions, the spontaneous and stimulated radiation, and the so-called cavity QED. Then I will briefly review the relativistic quantum theory of particles with nonvanishing rest mass, notably Dirac’s theory of spin-½ particles, and mark the point of entry into the most complete relativistic quantum theory – the quantum field theory, QFT – which is beyond the scope of these notes.¹

9.1. Electromagnetic field quantization

Classical mechanics tells us² that the relativistic relation between momentum $p$ and energy $E$ of a free particle with rest mass $m$ may be simplified in two limits, non-relativistic and ultra-relativistic:

$$E = \left[(pc)^2 + (mc^2)^2\right]^{1/2} \rightarrow \begin{cases} me^2 + p^2 / 2m, & \text{for } p \ll mc, \\ pc, & \text{for } p \gg mc. \end{cases}$$ (9.1)

In both limits, the transfer from classical to quantum mechanics is easier than in the arbitrary case. Since all the previous part of this course was committed to the first, non-relativistic limit, I will now jump to a brief discussion of the ultra-relativistic limit $p \gg mc$, for a particular but very important system - the electromagnetic field. Since the excitations of this field, called photons, are currently believed to have zero rest mass $m$³, the ultra-relativistic limit is valid for any photon energy $E$, and the quantization scheme is rather straightforward.

As usual, the quantization has to be based on the classical theory of the system, in this case the Maxwell equations. As the simplest case, let us consider electromagnetic field in a free-space volume limited by ideal walls that reflect incident waves perfectly.⁴ Inside the volume, the Maxwell equations may be reduced to a simple wave equation⁵ for electric field

$$\nabla^2 \mathcal{E} - \frac{1}{c^2} \frac{\partial^2 \mathcal{E}}{\partial t^2} = 0,$$ (9.2)

and an absolutely similar equation for magnetic field $\mathcal{B}$. We may look for the general solution of Eq. (2) in the variable-separating form

¹ Note that some material of this chapter is frequently taught as a part of the QFT. I will focus on a few most important results that may be obtained without starting heavy QFT engines.
² See, e.g., EM Chapter 9.
³ By now this fact has been verified experimentally with an accuracy of at least $\sim 10^{-22} m_e$ – see S. Eidelman et al., Phys. Lett. B 592, 1 (2004).
⁴ In the case of finite energy absorption in the walls, or in the wave propagation media (say, described by complex constants $\varepsilon$ and $\mu$), the system would not be energy-conserving (Hamiltonian), i.e. would interact with the dissipative environment. Specific cases of such interaction will be considered in Sections 2 and 3 below.
⁵ See, e.g., EM Eq. (7.3), for the particular case $\varepsilon = \varepsilon_0$, $\mu = \mu_0$, $\nu^2 \equiv 1/\varepsilon\mu = 1/\varepsilon_0\mu_0 \equiv c^2$. 
\[ \mathbf{E}(r, t) = \sum_j p_j(t) \mathbf{e}_j(r). \] (9.3)

Physically, each term of this sum is a standing wave whose spatial distribution and polarization ("mode") is described by vector function \( \mathbf{e}_j(r) \), and the temporal dynamics, by function \( p_j(t) \). Plugging an arbitrary term of this sum into Eq. (2), and separating variables exactly as we did, e.g., for the Schrödinger equation in Sec. 1.4, we get

\[ \frac{\nabla^2 \mathbf{e}_j}{\mathbf{e}_j} = \frac{1}{c^2} \frac{\dot{p}_j}{p_j} = \text{const} \equiv -k_j^2, \] (9.4)

so that the spatial distribution of the mode satisfies the 3D Helmholtz equation:

\[ \nabla^2 \mathbf{e}_j + k_j^2 \mathbf{e}_j = 0. \] (9.5)

The set of solutions of this equation, with appropriate boundary conditions, determines the set of functions \( \mathbf{e}_j \) and simultaneously the spectrum of wave number moduli \( k_j \). The latter values determine mode eigenfrequencies, following from Eq. (4):

\[ \ddot{p}_j + \omega_j^2 p_j = 0, \quad \text{with} \quad \omega_j \equiv k_j c. \] (9.6)

There is a big philosophical difference between the approaches to equations (5) and (6), despite their single origin (4). The first (Helmholtz) equation may be rather difficult to solve in realistic geometries, but it remains intact in quantum theory, with the scalar components of vector functions \( \mathbf{e}_j(r) \) still treated (at each point \( r \)) as \( c \)-numbers. In contrast, Eq. (6) is readily solvable (giving sinusoidal oscillations with frequency \( \omega_j \)), but this is exactly where we can make a transfer to quantum mechanics, because we already know how to quantize a mechanical 1D harmonic oscillator that obeys, in classics, the same equation.

As usual, we need to start with the appropriate Hamiltonian corresponding to the classical Hamiltonian function \( H \) of the proper set of generalized coordinates and momenta. The electromagnetic field’s Hamiltonian function (that in this case coincides with field’s energy) is

\[ H = \int d^3 r \left( \frac{E_0 E^2}{2} + \frac{B^2}{2 \mu_0} \right). \] (9.7)

Let us represent the magnetic field in a form similar to Eq. (3),

\[ \mathbf{B}(r, t) = -\sum_j \omega_j q_j(t) \mathbf{b}_j(r). \] (9.8)

Since, according to the Maxwell equations, in our case the magnetic field satisfies the equation similar to Eq. (2), the time-dependent amplitude \( q_j \) of each of its modes obey the equation similar to Eq. (6), i.e. also changes in time sinusoidally, with the same frequency \( \omega_j \). Plugging Eqs. (3) and (8) into Eq. (7), we may recast it as

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6 See, e.g., various problems discussed in EM Chapter 7, especially in Sec. 7.9.

7 See, e.g., EM Sec. 9.8, in particular, Eq. (9.225). I am using use SI units, with \( \varepsilon_0 \mu_0 \equiv c^2 \); in the Gaussian units, coefficients \( \varepsilon_0 \) and \( \mu_0 \) disappear, but there is an additional common factor \( 1/4 \pi \) in the equation for energy. If we modify the normalization conditions accordingly, all the subsequent results look similar in any system of units.
\[ H = \sum_j \frac{p_j^2}{2} + \frac{\omega_j^2 q_j^2}{2} + \frac{1}{\mu_0} b_j^*(r) d^3 r, \quad (9.9) \]

Since the distribution of constant factors between two multiplication operands in each term of Eq. (3) is arbitrary, we may fix it by requiring the first integral in Eq. (9) to equal 1. It is straightforward to check that according to the Maxwell equations, which give a specific relation between vectors \( \mathbf{E} \) and \( \mathbf{B} \), this normalization makes the second integral in Eq. (9) equal 1 as well, and Eq. (9) becomes

\[ H = \sum_j H_j, \quad H_j = \frac{p_j^2}{2} + \frac{\omega_j^2 q_j^2}{2}. \quad (9.10) \]

Now we can carry out the standard quantization procedure, namely declare \( H_j, p_j, \) and \( q_j \) the quantum-mechanical operators related exactly as in Eq. (10),

\[ \hat{H}_j = \frac{\hat{p}_j^2}{2} + \frac{\omega_j^2 \hat{q}_j^2}{2}. \quad (9.11) \]

we see that this Hamiltonian coincides with that of a 1D harmonic oscillator with the mass \( m_j \) formally equal to 1, and the eigenfrequency equal to \( \omega_j \). Now, in order to plug Eq. (11) into Eq. (4.199) for the time evolution of Heisenberg-picture operators \( \hat{p}_j \) and \( \hat{q}_j \), we need to know the commutation relation between these operators. For that, returning to the classical case, let us calculate the Poisson bracket (4.204) for “functions” \( A = q_{j'} \) and \( B = p_{j''} \):

\[ \{ q_{j'}, p_{j''} \} = \sum_j \left( \frac{\partial q_{j'}}{\partial p_j} \frac{\partial p_{j''}}{\partial q_j} - \frac{\partial q_{j'}}{\partial q_j} \frac{\partial p_{j''}}{\partial p_j} \right). \quad (9.12a) \]

Since in the classical Hamiltonian mechanics, all generalized coordinates \( q_j \) and momenta \( p_j \) have to be considered independent arguments of \( H \), only one term (with \( j = j' = j'' \)) in only one sum (12) (with \( j' = j'' \)), gives a nonvanishing value (-1), so that

\[ \{ q_{j'}, p_{j''} \} = -\delta_{j'j''}. \quad (9.12b) \]

Hence, according to the general quantization rule (4.205), the commutation relation of the operators corresponding to \( q_{j'} \) and \( p_{j''} \) is

\[ [\hat{q}_{j'}, \hat{p}_{j''}] = i\hbar \delta_{j'j''}, \quad (9.13) \]

i.e. is exactly the same as for the usual Cartesian components of the radius-vector and momentum of a mechanical particle.

As the reader already knows, Eqs. (11) and (13) open for us several alternative ways to proceed:
(i) Use the Schrödinger-picture wave mechanics based on wavefunctions \( \Psi_j(q_j, t) \). As we know from Sec. 2.10, this way is inconvenient for most tasks, because eigenfunctions of the harmonic oscillator are rather clumsy.

(ii) A substantially better way is to write the equations of time evolution of the Heisenberg-picture operators \( \hat{q}_j(t) \) and \( \hat{p}_j(t) \).

(iii) An even more convenient approach is to use equations similar to Eqs. (5.99) to decompose operators \( \hat{q}_j(t) \) and \( \hat{p}_j(t) \) into the creation-annihilation operators \( \hat{a}_j^\dagger \) and \( \hat{a}_j \), and work with these operators using either the Schrödinger or the Heisenberg picture, depending on the problem.

I will mostly use the last route. Replacing \( m \) with \( m_j \equiv 1 \), and \( \omega_0 \) with \( \omega_j \), the last forms of Eqs. (5.98) become

\[
\hat{a}_j = \left( \frac{\omega_j}{2\hbar} \right)^{1/2} \left( \hat{q}_j + i \frac{\hat{p}_j}{\omega_j} \right), \quad \hat{a}_j^\dagger = \left( \frac{\omega_j}{2\hbar} \right)^{1/2} \left( \hat{q}_j - i \frac{\hat{p}_j}{\omega_j} \right), \quad (9.14)
\]

and due to Eq. (13), the creation-annihilation operators obey the commutation similar to Eq. (5.101),

\[
\left[ \hat{a}_j, \hat{a}_j^\dagger \right] = \hat{I} \delta_{jj'}, \quad (9.15)
\]

so that, according to Eqs. (3) and (8), the quantum-mechanical operators corresponding to the electric and magnetic fields are

\[
\hat{\mathbf{E}}(r, t) = i \sum_j \left( \frac{\hbar \omega_j}{2} \right)^{1/2} \mathbf{e}_j(r) \left( \hat{a}_j^\dagger - \hat{a}_j \right), \quad (9.16a)
\]

\[
\hat{\mathbf{B}}(r, t) = \sum_j \left( \frac{\hbar \omega_j}{2} \right)^{1/2} \mathbf{b}_j(r) \left( \hat{a}_j^\dagger + \hat{a}_j \right), \quad (9.16b)
\]

and Eq. (11) for \( j \)th mode’s Hamiltonian becomes

\[
\hat{H}_j = \hbar \omega_j \left( \hat{a}_j^\dagger \hat{a}_j + \frac{1}{2} I \right) = \hbar \omega_j \left( \hat{n}_j + \frac{1}{2} I \right), \quad \text{with } \hat{n}_j \equiv \hat{a}_j^\dagger \hat{a}_j, \quad (9.17)
\]

absolutely similar to Eq. (5.505) for a mechanical oscillator.

Now comes a very important conceptual step. From Sec. 5.4 we know that eigenstates (Fock states \( n_j \)) of Hamiltonian (17) have energies

\[
E_j = \hbar \omega_j \left( n_j + \frac{1}{2} \right), \quad n_j = 0, 1, 2, \ldots \quad (9.18)
\]

and, according to Eq. (5.115), operators \( \hat{a}_j^\dagger \) and \( \hat{a}_j \) act on the eigenkets of these states as

\[
\hat{a}_j \ket{n_j} = \sqrt{n_j} \ket{n_j - 1}, \quad \hat{a}_j^\dagger \ket{n_j} = \sqrt{n_j + 1} \ket{n_j + 1}, \quad (9.19)
\]
regardless of the quantum states of other modes (frequently called field oscillators). These rules coincide with definitions (8.56) and (8.60) of bosonic creation-annihilation operators, and hence their action may be considered as the creation/annihilation of certain bosons. Such a “particle” (actually, an excitation of an electromagnetic field oscillator) is exactly what is, strictly speaking, called a photon. Note immediately that according to Eq. (16), such an excitation does not change the spatial distribution of the $j$th mode of the field. So, such a “global” photon is an excitation created simultaneously at all points of the field confinement region.

If this picture is too contrary to the intuitive image of a particle, please recall that we had a similar situation in Chapter 2 with eigenstates of the non-relativistic Schrödinger equation: the represented a standing de Broglie wave existing simultaneously in all points of the particle confinement region. The (partial :-)) reconciliation with the classical picture of a moving particle might be obtained by using the linear superposition principle to assemble a quasi-localized wave packet of sinusoidal waves, with close wave numbers. Very similarly, we may form a quasi-localized wave packet using a linear superposition of the “global” photons with close values of $k_j$ (and hence $\omega_j$). An additional simplification here is that since the dispersion relation for electromagnetic waves is linear:

$$\frac{\partial \omega_j}{\partial k_j} = c = \text{const}, \quad \text{i.e.} \quad \frac{\partial^2 \omega_j}{\partial k_j^2} = 0,$$

so that, according to Eq. (2.39a), the electromagnetic wave packets (localized photons) do not spread out during their propagation.

The next important conceptual issue is that of the ground-state energy. Equation (18) implies that the total ground-state (i.e., the lowest) energy of the field is

$$E_g = \sum_j \langle E_g \rangle_j = \sum_j \frac{\hbar \omega_j}{2}.$$

This sum diverges at high frequencies for any realistic any realistic model of the field-confining volume – either infinite or not. Any attempt to dismiss this paradox by declaring the zero-point energy unobservable and hence non-existing fails due to several experimental facts.

First of all, the ground-state “fluctuations” (sometimes called “quantum noise”) can be directly observed – see Sec. 7.5 and in particular the literature cited therein. Second, there is the Casimir effect. The simplest manifestation of the effect involves two parallel plates separated by a vacuum gap of thickness $d \ll A^{1/2}$, where $A$ is the plate area (Fig. 1). Rather counter-intuitively, the plates attract each other with a force proportional to area $A$, and rapidly increasing at the decrease of gap $d$.

![Fig. 9.1. Generic geometry of the Casimir effect manifestation.](image)

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The effect’s explanation is that the energy of each the electromagnetic field mode, including the ground-state energy, is intimately related with the average pressure,

\[ \langle P_j \rangle = -\frac{\partial E_j}{\partial V}, \]  

exerted by the field on the walls constraining it to volume \( V \). While its pressure on the external surfaces on the plates is due to sum (21) over all free-space modes, with arbitrary values of \( k_z \) (the \( z \)-component of the wave vector \( k_j \)), between the plates the spectrum of \( k_z \) is limited to multiples of \( \pi/d \), so that the pressure on the internal surfaces is lower. The net pressure may be found as the sum of contributions (22) from all “missing” low-frequency modes in the gap. The calculations are rather simple if the plates are made of an ideal conductor (which provides boundary conditions \( E_n = 0 \) and \( B_\tau = 0 \) on the plate surfaces), and the result is\(^\text{11}\)

\[ \langle P \rangle = \sum_j \langle P_j \rangle = -\frac{\pi^2 \hbar c}{240d^4}. \]  

Note that for this summation, the high-frequency divergence of Eq. (21) at high frequencies is not important, because it participates in the forces exerted on all surfaces of each plate, and hence cancels out from the net pressure. In this way, the Casimir effect not only gives a confirmation of Eq. (21), but also teaches us an important lesson how to deal with the divergence of this sum at \( \omega_j \to \infty \): just get accustomed to the idea that the divergence exists and ignore the fact while you can. However, for more complex tasks of quantum electrodynamics (and quantum theory of any other field) this approach becomes impossible, and then more complex, renormalization techniques become necessary. For their study, I have to refer the reader to a quantum field theory course – see the literature cited in the end of this chapter.

9.2. Photon statistics

As a matter of principle, the Casimir effect may be used to measure not only the free-space electromagnetic field, but also that arriving from local sources - lasers, etc. However, usually this is done by simpler detectors in which the absorption of a photon by a single atom leads to its ionization. This ionization, i.e. emission of a free electron, triggers a chain reaction (i.e., an electric discharge in a Geiger-type counter) that may readily be registered by appropriate electronic circuitry. In order to discuss the statistics of such photon counts, it is sufficient to consider the field interaction with just one,

\(^\text{11}\) For realistic metals, the reduction of \( d \) below \( \sim 1 \mu m \) causes significant deviations from this simple model, and hence from Eq. (23). The reason is that at the important frequencies \( \omega \sim c/d \), the depth of field penetration into the metal (see, e.g., EM Secs. 2.1 and 6.2) becomes comparable with \( d \), and a theory of the Casimir effect has to involve a certain model of field penetration. (It is curious that in-depth analyses of this problem, pioneered in 1956 by E. Lifshitz, have revealed a deep relation between the Casimir effect and the long-range London dispersion forces which were the subject of Problems 3.7, 5.10 and 6.8 – for a review see, e.g., either I. Dzyaloshinskii \textit{et al.}, \textit{Sov. Phys. Uspekhi} \textbf{4}, 153 (1961), or K. Milton, \textit{The Casimir Effect}, World Scientific, 2001.) Recent experiments in the 100 nm – \( 2 \mu m \) range of distances \( d \), with accuracy better than 1\%, allowed even to distinguish the difference between alternative approximate models of field penetration – see D. Garcia-Sanchez \textit{et al.}, \textit{Phys. Rev. Lett.} \textbf{109}, 027202 (2012).
“trigger” atom. The atom’s size $a$ is typically much smaller that the radiation wave length $\lambda_j = 2\pi k_j$, so that their interaction is adequately described in the electric dipole approximation,

$$\hat{H}_{\text{int}} = -\hat{\mathbf{d}} \cdot \hat{\mathbf{d}}, \quad (9.24)$$

where $\hat{\mathbf{d}}$ is the dipole moment’s operator.$^{12}$ In Sec. 6.5 we have already developed an approach suitable for the analysis of this problem, based on the Golden Rule – see Fig. 6.14 and Eq. (6.152).$^{13}$ In our current case, we may associate system $b$ with the “trigger atom” (whose ionized states form a continuum spectrum), and hence operator $\hat{\mathbf{d}}$ in Eq. (24) with operand $\hat{B}$ in Eq. (6.148), while the electromagnetic field is represented by system $a$, and its electric field operator $\hat{\mathbf{E}}$ is associated with operand $\hat{A}$ in that relation. Let us assume, for simplicity, that our field consists of only one mode $\mathbf{e}(\mathbf{r})$.$^{14}$ Then we can keep only one term in Eq. (16a), and drop index $j$, so that Eq. (6.152), for the transition from certain initial state $\text{ini}$ to a final state $\text{fin}$ may be rewritten as

$$\Gamma = \frac{2\pi}{\hbar} \left\langle \text{fin} | \hat{\mathbf{E}}(\mathbf{r}, t) | \text{ini} \right\rangle^2 \left\langle \text{fin} | \hat{\mathbf{d}} \cdot \mathbf{n} | \text{ini} \right\rangle^2 \rho_f,$$

$$= \frac{2\pi \hbar \omega}{\hbar} \left\langle \text{fin} \left| \hat{\mathbf{a}} - \hat{\mathbf{A}}(\mathbf{r}) \right| \text{ini} \right\rangle \left\langle \text{fin} \left| \mathbf{r} \cdot \mathbf{n} \right. | \text{ini} \right\rangle \rho_f, \quad (9.25)$$

where $e(\mathbf{r})$ is the local magnitude of vector $\mathbf{e}(\mathbf{r})$, and $\mathbf{n}_e \equiv \mathbf{e}(\mathbf{r})/e(\mathbf{r})$ is its local direction.$^{15}$ As a reminder, in the Heisenberg picture of quantum mechanics, the initial and final states are time-independent, while the creation-annihilation operators are functions of time. In this Golden Rule formula, as in any perturbation result, this time dependence has to be calculated ignoring the perturbation - in this case the field-atom interaction. For the field’s creation-annihilation operators, this dependence coincides with that of the usual 1D oscillator – see Eq. (5.171), in which $\omega_0$ should be now replaced with $\omega$.

$$\hat{a}(t) = \hat{a}(0)e^{-i\omega t}, \quad \hat{a}^\dagger(t) = \hat{a}^\dagger(0)e^{i\omega t}. \quad (9.26)$$

Hence Eq. (9.25) becomes

$$\Gamma = \pi \omega \left\langle \text{fin} \left| \hat{\mathbf{a}}^\dagger(0)e^{i\omega t} - \hat{\mathbf{a}}(0)e^{-i\omega t} \right| e(\mathbf{r}) \right\rangle \left\langle \text{fin} | \hat{\mathbf{d}}(t) \cdot \mathbf{n} | \text{ini} \right\rangle \rho_{\text{fin}}. \quad (9.27a)$$

Now let us multiply the first bra-ket by $\exp\{i\omega t\}$, and the second one by $\exp\{-i\omega t\}$:

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$^{12}$ As a reminder: this relation, with the single-particle expression $\mathbf{d} = q\mathbf{r}$, has already been used several times – see, e.g., Eqs. (6.32) and (6.149). In contrast to the former of those cases, now we have to account for the quantum nature of the electromagnetic field $\mathbf{E}$, so in Eq. (24) it is represented by the (vector) operator (16a).

$^{13}$ Please note that (as was promised) we have gradually slipped to the analysis of open, irreversible systems, with the detector(s) playing the role of a continuous-spectrum environment for the quantized electromagnetic field.

$^{14}$ In a multimode field, the modes are typically incoherent, so that the total transition rate may be calculated as the sum of the partial rates of each mode – as we will do for a certain case below.

$^{15}$ By the way, this expression shows that for the single-particle transitions from the ground state to $n$th Fock state, the absorption rate is indeed proportional to the oscillator strength $f_n \equiv (2m/\hbar^2)(E_n - E_0) |\langle n|x|0\rangle|^2$ of the transition, where $x$ is particle’s coordinate in the direction of the external field. As was discussed in Chapter 5, the strengths obey the Thomas-Reiche-Kuhn sum rule $\Sigma_n f_n = 1$.
\[ \Gamma = \pi \omega \left| \left\langle \text{fin} \left( \hat{a}^\dagger(0)e^{2i\omega t} - \hat{a}(0) \right)e(\mathbf{r}|\text{ini}) \right| \right|^2 \left| \left\langle \text{fin} \left| \mathbf{d}(t) \cdot \mathbf{n}_e e^{-i\omega t} \right| \text{ini} \right\rangle \right|^2 \rho_{\text{fin}}. \] (9.27b)

The physical sense of this, mathematically trivial, operation is that at resonant photon absorption, only the \textit{annihilation} operator gives a significant time-averaged contribution to the first bra-ket matrix element. (Similarly, according to Eq. (4.199), the Heisenberg operator of the dipole moment, corresponding to the \textit{increase} of atom’s energy, has only the Fourier components that differ from \( \omega \) only by \( -\Gamma \ll \omega \), so that its time dependence compensates the additional factor in the second bra-ket of Eq. (27b), so that this bra-ket is also frequency-independent and has a substantial time average.) Hence, we can neglect the fast-evolving term in the first bra-ket whose average over time interval \( \sim 1/\Gamma \) is very close to zero.\(^\text{16}\)

Now let us assume that we use the same detector, characterized by the same second bra-ket and the same state density \( \rho_{\text{fin}} \), for measurement of various electromagnetic fields - or just the same field at different points \( \mathbf{r} \). Then we are only interested in the behavior of the first, field-related factor, and may write

\[ \Gamma \propto \left| \left\langle \text{fin} \hat{a}(\mathbf{r}|\text{ini}) \right| \right|^2 = \left| \left\langle \text{fin} \hat{a}(\mathbf{r}|\text{ini}) \right| \right|^2 = \left| \left\langle \text{fin} \hat{a}^{\dagger}(\mathbf{r}^*|\text{ini}) \right| \left\langle \text{fin} \hat{a}(\mathbf{r}|\text{ini}) \right\rangle \right|^* = \left| \left\langle \text{fin} \hat{a}^{\dagger}(\mathbf{r}) \right| \left\langle \text{fin} \hat{a}(\mathbf{r}|\text{ini}) \right\rangle \right|^* = \left| \left\langle \text{fin} \hat{a}^{\dagger}(\mathbf{r}) \right| \left\langle \text{fin} \hat{a}(\mathbf{r}|\text{ini}) \right\rangle \right|^* = \Gamma_{\text{fin}}, \] (9.28)

where the creation-annihilation operators are assumed to be taken in the initial moment (i.e., in the Schrödinger picture), and the initial and final states are those of the field alone. As we know, any 1D harmonic oscillator (and hence the electromagnetic field oscillator) has many equidistant levels, so even if it initially was in a certain state, it may undergo several coherent transitions to different finite Fock states. If we want to calculate the total rate, we may sum the transition rates into all finite states. Then, since these states form a full and orthonormal set, we may use the closure condition (4.44) to get

\[ \Gamma \propto \sum_{\text{fin}} \left| \left\langle \text{fin} \hat{a}^{\dagger}(\mathbf{r}) \right| \left\langle \text{fin} \hat{a}(\mathbf{r}|\text{ini}) \right\rangle \right| = \sum_{\text{fin}} \left| \left\langle \text{fin} \hat{a}^{\dagger}(\mathbf{r}) \right| \left\langle \text{fin} \hat{a}(\mathbf{r}|\text{ini}) \right\rangle \right| = \sum_{\text{fin}} \left| \left\langle \text{fin} \hat{a}^{\dagger}(\mathbf{r}) \right| \left\langle \text{fin} \hat{a}(\mathbf{r}|\text{ini}) \right\rangle \right| = \sum_{\text{fin}} \left| \left\langle \text{fin} \hat{a}^{\dagger}(\mathbf{r}) \right| \left\langle \text{fin} \hat{a}(\mathbf{r}|\text{ini}) \right\rangle \right|^2. \] (9.29)

Let us apply this formula to several possible quantum states of the field mode.

(i) First, as a sanity check, the ground initial state \( n = 0 \) gives no photon counts at all. The interpretation is easy: the ground state cannot emit a photon that would trigger an atom in the counter. Again, this does not mean that the ground-state motion is not observable (if you still think so, please review the Casimir effect discussion in the last section), just that it cannot ionize an atom in the detector – because it does not have any \textit{spare} energy for doing that.

(ii) All other coherent states (Fock, Glauber, squeezed, etc.) of the field oscillator give the same counting rate, provided that their \( \langle n \rangle \) is the same. This result may be less evident if we apply Eq. (29) to an interference of two light beams from the same source (say, in the double-slit or the Bragg-scattering configurations). In this case we may present the spatial distribution of the field as a sum

\[ e(\mathbf{r}) = e_1(\mathbf{r}) + e_2(\mathbf{r}), \] (9.30)

Here each term describes one possible wave path, so that the field product in Eq. (29) may be a rapidly changing function of the detector position. For this configuration, our result (29) means that the

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\( ^{16} \) This is essentially the same rotating wave approximation (RWA) which was already used in Sec. 6.3 – see the transition from Eq. (6.90) to the first of Eqs. (6.94).
interference pattern (and its contrast) are independent of the particular state of the electromagnetic field’s mode.

(iii) Surprisingly, the last statement is also valid for a classical mixture of the different eigenstates of the same field mode, for example for its thermal-equilibrium state. Indeed, in this case we need to average Eq. (29) over the corresponding classical ensemble, but it would only result in a different meaning of averaging \( n \) in that equation; the field part describing the interference pattern is not affected.

The last result may look a bit counter-intuitive, because common sense tells us that the stochasticity associated with thermal equilibrium has to suppress the interference pattern contrast. These expectations are (partly :-) justified, because a typical thermal source of radiation produces many field modes \( j \), rather than one mode we have analyzed. These modes may have different wave numbers \( k_j \) and hence different field distribution functions \( \mathbf{e}_j(\mathbf{r}) \), resulting in shifted interference patterns. Their summation would indeed smear the interference, suppressing its contrast.

So the use of a single photon detector is not a suitable way to distinguish different quantum states of an electromagnetic field modes. This task, however, may be achieved using the photon counting correlation technique shown in Fig. 2.\textsuperscript{17}

In this experiment, the counter rate correlation may be characterized by the so-called second-order correlation function\textsuperscript{18} of the counting rates,

\[
g^{(2)}(\tau) \equiv \frac{\langle \Gamma_1(t)\Gamma_2(t-\tau) \rangle}{\langle \Gamma_1(t) \rangle \langle \Gamma_2(t) \rangle}, \tag{9.31}
\]

\textsuperscript{17} It was pioneered as early as in the mid-1950s (i.e. before the advent of lasers!), by R. Hanbury Brown and R. Twiss. Their first experiment was also remarkable for the rather unusual light source they used – star Sirius! (It was a part of an attempt to improve astrophysics interferometry techniques.)

\textsuperscript{18} The reader may be interested what is the first-order correlation function. It is usually defined as

\[
g^{(1)}(\tau) \equiv \left\langle \hat{\mathbf{e}}(\mathbf{r}_1,t)\hat{\mathbf{e}}^\dagger(\mathbf{r}_2,t-\tau) \right\rangle \left[ \left\langle \hat{\mathbf{e}}(\mathbf{r}_1,t)\hat{\mathbf{e}}^\dagger(\mathbf{r}_1,t) \right\rangle \right]^{1/2}. \]

In the single-mode case, and the rotating-wave approximation, the function is proportional to the c-number product \( \mathbf{e}(\mathbf{r}_1)\mathbf{e}^*(\mathbf{r}_2) \), with all creation-annihilation operators cancelled, i.e. is suitable for characterizing interference patterns (30), but not the quantum state of the electromagnetic field.
where the averaging may be carried out either over many similar experiments, or over time $t$, due to the ergodicity of the experiment (with a stationary light source). Using the normalized correlation function (31) is very convenient, because characteristics of the detectors and beam splitter drop out from this fraction.

Very unexpectedly for the mid-1950s, Hanbury Brown and Twiss discovered that the correlation function depends on time delay $\tau$ in the way shown schematically by the solid line in Fig. 3. It is evident from Eq. (31) that if the counting events are completely independent, \( g^{(2)}(\tau) \) should be equal 1 – which is always the case in the limit $\tau \to \infty$. Hence, the observed behavior at $\tau \to 0$ corresponds to the positive correlation of detector counts at small time delays, i.e. to a higher probability of the nearly-simultaneous arrival of photons to both counters. This effect is called the photon bunching.

\[
\text{Fig. 9.3. Photon bunching (solid line) and antibunching for various } n \text{ (dashed lines). The lines approach level } g^{(2)} = 1 \text{ at } \tau \to \infty \text{ (on the time scale depending on the light source).}
\]

Let us use our simple single-mode model to analyze this experiment. Now the elementary quantum process, characterized by the nominator of Eq. (31), is the correlated triggering of two counters, at two spatial-temporal points \( \{ r_1, t \} \) and \( \{ r_2, t - \tau \} \), by the same field mode, so that we need to make the following replacement, in the first of Eqs. (25):

\[
\hat{\mathcal{E}}(r,t) \to \text{const} \times \hat{\mathcal{E}}(r_1,t) \hat{\mathcal{E}}(r_2,t-\tau). \tag{9.32}
\]

Repeating all the manipulations done in the single-counter case, we get

\[
\langle \Gamma_1(t) \Gamma_2(t-\tau) \rangle \propto \langle ini | \hat{a}(t) \hat{a}(t-\tau) \hat{a}(t-\tau) \hat{a}(t) | ini \rangle e^* (r_1) e (r_2) e (r_1) e (r_2). \tag{9.33}
\]

Plugging this expression, as well as Eq. (29) for single-counter rates, into Eq. (31), we see that the field distribution factors (as well as the detector-specific bra-kets and the density of states $\rho_{\text{fin}}$) cancel, giving a very simple final expression

\[
g^{(2)}(\tau) = \frac{\langle \hat{a}^\dagger (t) \hat{a}^\dagger (t-\tau) \hat{a}(t-\tau) \hat{a}(t) \rangle}{\langle \hat{a}^\dagger (t) \hat{a}(t) \rangle^2}, \tag{9.34}
\]

where the averaging should be carried out, as before, over the initial state of the field. Still, the calculation of this expression for arbitrary $\tau$ may be quite complex, because the relaxation of the correlation function to the asymptotic value $g^{(2)}(\infty)$ in many cases is due to the interaction of the light source with environment, and hence requires the open-system techniques which were discussed in Chapter 7. However, the zero-delay value $g^{(2)}(0)$ may be calculated in a straightforward way, because the time arguments of all operators are equal, so that we may write
Let us evaluate this ratio for the simplest states of the field. (Remember, we are working in the Schrödinger picture now.)

(i) \( n \)th Fock state. In this case, it is convenient to act by the annihilation operators upon the ket-vectors, and by the creation operators, upon the bra-vectors, using Eq. (19):

\[
g^{(2)}(0) = \frac{\langle \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} | n \rangle}{\langle \hat{a}^\dagger \hat{a} | n \rangle^2} = \frac{n - 2 \left[ n(n - 1) \right]^{1/2} \left[ n(n - 1) \right]^{1/2} | n - 2 \rangle}{n^2} = 1 - \frac{1}{n}.
\]  

We see that the correlation function at small delays is suppressed rather than enhanced – see the dashed line in Fig. 3. This photon antibunching effect has a very simple explanation: a single photon emitted by the wave source may be absorbed by just one of the detectors. For the initial state \( n = 1 \), this is the only option, and it is very natural that Eq. (36) predicts no simultaneous counts at \( \tau = 0 \). Despite this theoretical simplicity, reliable observations of the antibunching have not been carried out until 1977, due to the experimental difficulty of creating Fock states of electromagnetic field oscillators – see Sec. 4 below.

(ii) The Glauber state \( \alpha \). A similar procedure, but now using Eq. (5.155) and its Hermitian conjugate, \( \langle \alpha | \hat{a}^\dagger = \langle \alpha | \alpha^\ast \), yields

\[
g^{(2)}(0) = \frac{\langle \alpha | \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} | \alpha \rangle}{\langle \alpha | \hat{a}^\dagger \hat{a} | \alpha \rangle^2} = \frac{\alpha^\ast \alpha^\ast \alpha \alpha}{(\alpha^\ast \alpha)^2} = 1,
\]

for any parameter \( \alpha \). We see that the result is very different result from the Fock states, unless in the latter case \( n \rightarrow \infty \). (We know that the Fock and Glauber properties should also coincide for the ground state, but at that state the correlation function’s value is uncertain, because there are no photon counts at all.)

(iii) Classical mixture. From Chapter 7, we know that such ensembles cannot be described by single state vectors, and require the density matrix \( \rho \) for their description. In particular, we can use the key Eq. (7.5) to write

\[
g^{(2)}(0) = \frac{\text{Tr} \left( \hat{\rho} \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \right)}{\left[ \text{Tr} (\hat{\rho} \hat{a}^\dagger \hat{a}) \right]^2}.
\]

The calculation is easy for an ensemble in thermodynamic equilibrium, because here the density matrix is diagonal in the basis of Fock states \( n \) - see Eqs. (7.23)-(7.25):

\[ w_{m_n} = W_n \delta_{m_n}, \quad W_n = \frac{1}{Z} \exp \left\{ - \frac{E_n}{k_B T} \right\} = \frac{\lambda^n}{\lambda_0^n}, \quad \text{where} \quad \lambda = \exp \left\{ - \frac{\hbar \omega}{k_B T} \right\}. \quad (9.39) \]

So, for the operators in the nominator and denominator of Eq. (38) we also need just the diagonal terms of the operator products that have already been calculated – see Eq. (36). As a result, we get

\[ g^{(2)}(0) = \frac{\sum_{n=0}^{\infty} W_n n(n-1)}{\left( \sum_{n=0}^{\infty} W_n n \right)^2} = \frac{\sum_{n=0}^{\infty} \lambda^n n(n-1) \times \sum_{n=0}^{\infty} \lambda^n}{\left( \sum_{n=0}^{\infty} \lambda^n n \right)^2}. \quad (9.40) \]

One of these sums is just the geometric progression,

\[ \sum_{n=0}^{\infty} \lambda^n = \frac{1}{1-\lambda}, \quad (9.41) \]

and the remaining two sums may be readily calculated by its differentiation over parameter \( \lambda \):

\begin{align*}
\sum_{n=0}^{\infty} \lambda^n n &= \lambda \sum_{n=0}^{\infty} \lambda^{n-1} n = \lambda \frac{d}{d\lambda} \sum_{n=0}^{\infty} \lambda^n = \lambda \frac{d}{d\lambda} \frac{1}{1-\lambda} = \frac{\lambda}{(1-\lambda)^2}, \\
\sum_{n=0}^{\infty} \lambda^n n(n-1) &= \lambda^2 \sum_{n=0}^{\infty} \lambda^{n-2} n(n-1) = \lambda^2 \frac{d^2}{d\lambda^2} \left( \sum_{n=0}^{\infty} \lambda^n \right) = \lambda^2 \frac{d^2}{d\lambda^2} \frac{1}{1-\lambda} = \frac{2\lambda^2}{(1-\lambda)^3},
\end{align*} \quad (9.42)

and for the correlation function we get an extremely simple result independent of parameter \( \lambda \) and hence of temperature:

\[ g^{(2)}(0) = \frac{\left[ 2\lambda^2 / (1-\lambda)^3 \right] \left[ 1/(1-\lambda) \right]}{\lambda/(1-\lambda)^2} = 2. \quad (9.43) \]

This is the exactly the photon bunching effect first observed by Hanbury Brown and Twiss (Fig. 3). We see that in contrast to antibunching, this is an essentially classical (statistical) effect. Indeed, Eq. (43) allows a purely classical proof. In the classical theory, the counting rate is proportional to the wave intensity \( I \), so that Eq. (31) is reduced to

\[ g^{(2)}(0) = \frac{\langle I^2 \rangle}{\langle I \rangle^2}, \quad \text{with} \quad I \propto E\times(t) \propto E_\alpha E_\alpha^\ast. \quad (9.44) \]

For a sinusoidal field, the intensity is constant, and \( g^{(2)}(0) = 1 \). (This is also evident from Eq. (37), because the classical state may be considered as the Glauber state with \( \alpha \to \infty \).) On the other hand, if intensity fluctuates (either in time, or from one experiment to another), the averages should be calculated as

\[ \langle I^N \rangle = \int_0^\infty w(I) I^N dI, \quad \text{with} \quad \int_0^\infty w(I) dI = 1, \quad (9.45) \]
where \( w(I) \) is the probability density. For the classical (Boltzmann) statistics, the probability is an exponential function of the electromagnetic field energy, and hence its intensity:

\[
 w(I) = Ce^{-\beta I}, \quad \text{where } \beta \approx 1/ k_B T, \tag{9.46}
\]

so that Eqs. (48) yield:

\[
 \int_0^\infty C \exp\{-\beta I\} dI = 1, \quad \text{so that } C = \beta,
\]

\[
 \langle I^N \rangle = \int_0^\infty w(I) I^N dI = C \int_0^\infty \exp\{-\beta I\} I^N dI = \frac{1}{\beta^N} \int_0^\infty \exp\{-\xi\} \xi^N d\xi = \begin{cases} 1/\beta^N, & \text{for } N=1, \\ 2/\beta^2, & \text{for } N=2. \end{cases} \tag{9.47}
\]

Plugging these results into Eq. (44), we get \( g(2)(0) = 2 \), in a complete agreement with Eq. (43).20

### 9.3. Spontaneous and stimulated emission

In our simple model for photon counting, considered in the last section, trigger atoms of the photon counter absorbed light. Now let us have a look at the opposite process of spontaneous emission of photons by an atom in an excited state, still using the same electric-dipole approximation for the atom-to-field interaction. We may still use the Golden Rule for the model depicted in Fig. 6.14, but now the roles have changed: we have to associate operator \( \hat{A} \) with the electric dipole moment of the atom, while operator \( \hat{B} \) with the electric field, and the continuous spectrum of system \( b \) represents the plurality of the electromagnetic field modes into which the spontaneous radiation may happen. Since now the transition increases the energy of the electromagnetic field, after the multiplication of the field bra-ket by \( \exp\{i\omega t\} \), we may keep only the photon creation operator whose time evolution compensates this fast “rotation”. As a result, the Golden Rule takes the following form:

\[
 \Gamma_s = \pi\omega \left| \left\langle \text{fin} | \hat{d} \cdot \mathbf{e}(\mathbf{r}) | \text{ini} \right\rangle \right|^2 \rho_{\text{fin}}, \tag{9.48}
\]

where all operators and states are time-independent, and \( \rho_{\text{fin}} \) is now the density of finite states of the electromagnetic field – which in this problem plays the role of atom’s environment. Here the electromagnetic field has been assumed to be initially in the ground state – the assumption that will be altered later in this section.

Relation (48), together with Eq. (19), shows that in order for field’s matrix element be different from zero, the finite state of the field has to be the first excited Fock state, \( n = 1 \). (By the way, \( this \) is exactly the most practicable way of generating an excited Fock state of a field oscillator field – whose existence was taken for granted in our discussion in Sec. 2.) With that, Eq. (48) yields

\[
 \Gamma_s = \pi\omega \left| \left\langle \text{fin} | \hat{d} \cdot \mathbf{e}(\mathbf{r}) | \text{ini} \right\rangle \right|^2 \rho_{\text{fin}} = \pi\omega \left| \left\langle \text{fin} | \hat{d} \mathbf{e}(\mathbf{r}) | \text{ini} \right\rangle \right|^2 \rho_{\text{fin}}, \tag{9.49}
\]

\[\text{20 For some field states, including the squeezed ground states } \xi \text{ discussed in the end of Sec. 5.5, values } g(2)(0) \text{ may be even higher than 2 – the so-called super-bunching. Analysis of one particular case of super-bunching is offered to the reader – see the exercise problem list.}\]
where the density $\rho_{\text{fin}}$ of excited electromagnetic field states should be calculated at energy $h\omega$, and $e_d$ is the component of the vector $e(r)$ along the electric dipole direction.\(^{21}\) For plane waves, the calculation of this density was our first step in this course – see Eq. (1.1).\(^{22}\) From it, we get

$$\rho_{\text{fin}} = \frac{dN}{dE} = V \frac{8\pi v^2}{c^3} \frac{dE}{dE} = V \frac{\omega^2}{\pi^2 \hbar^3}, \quad (9.50)$$

where the bounding volume $V$ should be large enough to ensure spectrum’s virtual continuity. Because of that, in the normalization condition used to simplify Eq. (9), we may consider $e^2(r)$ constant. Let us present the square of this vector as a sum of squares of its three perpendicular components (one of those, $e_d$, aligned with the dipole direction), due to space isotropy we may write

$$e^2 = e^2_d + e^2_{\perp 1} + e^2_{\perp 2} = 3e^2_d. \quad (9.51)$$

As a result, the normalization condition yields

$$e^2_d = \frac{1}{3\epsilon_0 V}. \quad (9.52)$$

and Eq. (49) gives the famous (and very important) formula\(^{23}\)

$$\Gamma_s = \frac{1}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \left| \langle \text{fin} | \hat{d} | \text{ini} \rangle \right|^2 = \frac{1}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \langle \text{fin} | \hat{d} | \text{ini} \rangle \cdot \langle \text{ini} | \hat{d} | \text{fin} \rangle^\ast. \quad (9.53)$$

Leaving a comparison of this formula with the classical theory of radiation,\(^{24}\) and the exact evaluation of $\Gamma_s$ for a particular transition in the hydrogen atom, for reader’s exercises, let me just estimate its order of magnitude. Assuming that $d \sim e\rho_B \equiv e\hbar^2/m_\alpha(e^2/4\pi\epsilon_0)$ and $h\omega \sim E_H \equiv m_\alpha(e^2/4\pi\epsilon_0)^2/\hbar^2$, and taking into account the definition (6.62) of the fine structure constant $\alpha \approx 1/137$, we get

$$\frac{\Gamma}{\omega} \sim \left( \frac{e^2}{4\pi\epsilon_0 \hbar c} \right)^3 \equiv \alpha^3 \sim 3 \times 10^{-7}. \quad (9.54)$$

This estimate says that the emission lines at atomic transitions are typically very sharp. With the present-day availability of high-speed electronics, it also makes sense to evaluate the time scale $\tau = 1/\Gamma$ of the typical quantum transition: for a typical optical frequency $\omega \sim 3 \times 10^{15}$ s\(^{-1}\), it is close to 1 ns. This is

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\(^{21}\) Here I have smuggled back the sum over all electromagnetic field modes $j$ – see Eq. (16). Since in the quasistationary approximation, $k_d << 1$, which is necessary for the interaction presentation by Eq. (24), matrix elements (49) are independent on $k_j$, the summation is reduced to the calculation of the total $\rho_{\text{fin}}$ for all modes.

\(^{22}\) Note the essential dependence of Eq. (50), and hence of Eq. (53) on the field geometry; all following formulas of this section are valid for free 3D space only. If the same atom is placed into a high-$Q$ resonant cavity (see, e.g., EM 7.9), the rate of its photon emission is strongly suppressed at frequencies between the cavity resonances (where $\rho_{\text{fin}} \to 0$) – see, e.g., the review of first experiments by S. Haroche and D. Klepner, Phys. Today 42, 24 (Jan. 1989). On the other hand, the emission is strongly (by a factor $\sim (\lambda/V)Q$, where $V$ is cavity’s volume) enhanced at resonance frequencies – the so-called Purcell effect, discovered by E. Purcell already in the 1940s. For a brief discussion of these and other quantum effects in cavities, see the next section.

\(^{23}\) An equivalent expression was first obtained in 1930 by V. Weisskopf and E. Wigner, so that the whole calculation is sometimes referred to as the Weisskopf-Wigner theory.

\(^{24}\) See, e.g., EM Sec. 8.2, in particular Eq. (8.28).
exactly the time constant that determines the photon counting statistics of the emitted radiation – see Fig. 3. Colloquially, this is the temporal scale of the photon spontaneously emitted by an atom.²⁵

Note, however, that the above estimate of $\tau$ is only valid for a transition with a non-vanishing dipole matrix element. If it equals zero - say, due to the initial and final state symmetry - the dipole transitions are “forbidden”. (Another commonly used term is the transition selection rules.²⁶) The “forbidden” transition may still take place due to a different, smaller interaction (say, via a magnetic dipole field of the atom, or its quadrupole electric field²⁷), but would take much longer. In some cases the increase of $\tau$ is rather dramatic - sometimes to hours! Such long-lasting radiation is called luminescence – or fluorescence if the initial atom’s excitation was due to an external radiation of higher frequency, followed first by non-radiative transitions down the energy level ladder.

Now let us consider a more general case when the electromagnetic field is initially in an arbitrary Fock state $n$, and from it may either get energy from the atomic system (photon emission) or, vice versa, give it back to the atom (photon absorption). For the photon emission rate, an evident generalization of Eq. (48) gives

$$\frac{\Gamma_e}{\Gamma_s} = \frac{\Gamma_{n\to fin}}{\Gamma_{0\to 1}} = \frac{\langle fin|\hat{a}^\dagger|n\rangle^2}{\langle 1|\hat{a}^\dagger|0\rangle^2},$$  \hspace{1cm} (9.55)

where both bra-kets may be taken in the Schrödinger picture, and $\Gamma_s$ is the spontaneous emission rate (53) of the same atomic system. This relation, with the account of Eq. (19), shows that at photon emission, the final field state $fin$ has to be the Fock state with $n' = n + 1$, and that

$$\Gamma_e = (n + 1)\Gamma_s.$$  \hspace{1cm} (9.56)

Thus the initial field increases the photon emission rate; this effect is called the stimulated emission of radiation. Note that the spontaneous emission may be considered as a particular case of stimulated emission for $n = 0$, and interpreted as the emission stimulated by zero-point fluctuations of the electromagnetic field.

On the other hand, in accordance with the arguments of Sec. 2, for the description of radiation absorption the photon creation operator has to be replaced with the annihilation one, to get

$$\frac{\Gamma_a}{\Gamma_s} = \frac{\langle fin|\hat{a}|n\rangle^2}{\langle 1|\hat{a}^\dagger|0\rangle^2}. \hspace{1cm} (9.57)$$

²⁵ The scale $c\tau$ of the spatial extension of the corresponding wave packet is surprisingly macroscopic – in the range of a few millimeters. Such “human” size of the emitted photons makes the optical table the key component of many optical experiments.

²⁶ As was already mentioned in Sec. 5.6, for a single particle moving in a spherically-symmetric potential (e.g., a hydrogen-like atom), the selection rules are simple: the only allowed electric-dipole transitions are those with $\Delta l = l_{fin} - l_{ini} = \pm 1$ and $\Delta m = m_{fin} - m_{ini} = 0$. The simplest example of the transition that does not satisfy this rule is that between states with $n = 2$ and $n = 1$, both with $l = 0$; because of that, the lifetime of the lowest excited s-state in hydrogen is as long as ~0.15 s.

²⁷ See, e.g., EM Sec. 8.9.
According to this equation, the final state of the field at absorption is the Fock state with \( n' = n - 1 \), and Eq. (57) yields

\[
\Gamma_a = n\Gamma_s. \tag{9.58}
\]

Results (56) and (58) are usually be formulated in terms of between the Einstein coefficients \( A \) and \( B \) defined in the way shown in Fig. 4, where the two energy levels are those of the atom, \( \Gamma_a \) is the rate of energy absorption from the electromagnetic field, and \( \Gamma_e \) is that of the energy emission into the field. In this notation, Eqs. (56) and (58) say

\[
A_{21} = B_{21} = B_{12}, \tag{9.59}
\]

because each of these coefficients equals the spontaneous emission rate \( \Gamma_s \).

It is curious that from this point, there is just one step to an alternative derivation of the Bose-Einstein statistics for photons. Indeed, in the thermodynamic equilibrium, the average probability flows between levels 1 and 2 should be equal:

\[
W_2 \langle \Gamma_e \rangle = W_1 \langle \Gamma_a \rangle, \tag{9.60}
\]

where \( W_1 \) and \( W_2 \) are the probabilities for the atomic system to be on the corresponding levels, so that Eqs. (56) and (58) yield

\[
W_2 \Gamma_s \langle 1 + n \rangle = W_1 \Gamma_s \langle n \rangle, \quad \text{i.e.} \quad \frac{W_2}{W_1} = \frac{\langle n \rangle}{\langle n \rangle + 1}. \tag{9.61}
\]

But, on the other hand, for the atomic subsystem, only weakly coupled to its electromagnetic environment, we ought to have the Gibbs distribution of probabilities:

\[
\frac{W_2}{W_1} = \frac{\exp\{-E_2/k_BT\}}{\exp\{-E_1/k_BT\}} = \exp\left\{-\frac{\Delta E}{k_BT}\right\} = \exp\left\{-\frac{\hbar \omega}{k_BT}\right\}. \tag{9.62}
\]

Requiring Eqs. (61) and (62) to give the same result for the probability ratio, we get the Bose-Einstein distribution for the electromagnetic field in equilibrium:

\[
\langle n \rangle = \frac{1}{\exp[\hbar \omega/k_BT] - 1}, \tag{9.63}
\]

the same as obtained in Sec. 7.1 by other means – see Eqs. (7.26).

---

28 Relations (56) and (58) were conjectured, from very general arguments, by A. Einstein as early as in 1916.
Another, very important implication of Eqs. (56) and (58) is the possibility to achieve the stimulated emission coherence by level occupancy (or “population”) inversion. Indeed, if \( W_2 > W_1 \), then the net power flow from the atomic system into the electromagnetic field,

\[
\text{power} = h\omega \times \Gamma_s \left[ W_2 \langle n \rangle + 1 \right] - W_1 \langle n \rangle, \tag{9.64}
\]

may be positive. The necessary inversion may be produced using several ways, notably by a intensive quantum transitions to level 2 from an even higher level (which, in turn, is populated, e.g., by absorption of an external radiation, called pumping, at a higher frequency.)

A less obvious feature of the stimulated emission is spelled out by Eq. (55): again, it shows that the final state of the field after the absorption of energy \( h\omega \) from the atom is a pure (coherent) Fock state \((n + 1)\). Colloquially, one may say that the new, \((n + 1)\)th photon emitted from the atom is automatically in phase with the \(n\) photons that had been in the field mode initially.\(^{29}\) The idea of stimulated emission of coherent radiation using population inversion\(^{30}\) was implemented in the early 1950s in the microwave range (masers) and in 1960 in the optical range (lasers). Nowadays, lasers are ubiquitous and constitute one of cornerstones of our technological civilization.

A quantitative discussion of laser operation is beyond the framework of this course, and I have to refer the reader to special literature,\(^ {31}\) and would only like to mention only two key points:

(i) In a typical laser, each generated electromagnetic field mode is in the Glauber (rather than the Fock) state, so that Eqs. (56) and (58) are applicable only for \( n \) is averaged over the Fock-state decomposition of the Glauber state – see Eq. (5.165).

(ii) Since in a typical laser \( \langle n \rangle \gg 1 \), its operation may be well described using quasi-classical theories that use Eq. (64) to describe the electromagnetic energy balance (with the addition of a term describing the energy loss due to field absorption in external components of the laser, including the useful load), plus the equation describing the balance of occupancies \( W_{1,2} \) due to all inter-level transitions – similar to Eq. (60), but including also the contribution(s) from the particular population inversion mechanism used in the laser. At this approach, the role of quantum mechanics is essentially reduced to the calculation of parameter \( \Gamma_s \).

The role becomes more prominent if one needs to describe fluctuations of the laser field. Here two approaches are possible, following the two options discussed in Chapter 7. If the fluctuations are relatively small, one can linearize the Heisenberg equations of motion of the field oscillator operators near their stationary-lasing “values”, with the Langevin “forces” (also time-dependent operators) to describe the fluctuation sources, and use these Heisenberg-Langevin equations to the radiation fluctuations, just as was described in Sec. 7.5. On the other hand, near the lasing threshold the field fluctuations are relatively strong, smearing the phase transition between the no-lasing and lasing states. Here the linearization is not an option, but one can use the density-matrix approach described in Sec. 7.6, for the fluctuation analysis.\(^ {32}\)

\(^{29}\) It is straightforward to show that this fact is also true if the field is initially in the Glauber state – which is more typical for lasers.

\(^{30}\) This idea has been traced back at least to an obscure 1939 publication by V. Fabrikant.


\(^{32}\) This path has been developed (also in the mid-1960s), by several researchers, notably including M. Sully and W. Lamb – see, e.g., M. Sargent III, M. Scully, and W. Lamb, Jr., Laser Physics, Westview, 1977. Note that
9.4. Cavity QED

Now I have to mention, at least in passing, the cavity quantum electrodynamics (usually called cavity QED for short) – an art and science of creating and using entanglement between quantum states of a single atomic system (either an atom, or an ion, or a molecule, etc.) and the electromagnetic field in a macroscopic volume called the resonant cavity (or just “resonator”, or just “cavity”). This field is very popular nowadays, especially in the context of the quantum computation and communication research discussed in Sec. 8.5.33

Let me start its discussion by noting that the narrative of two last sections was based on an implicit assumption that the energy spectrum of the electromagnetic field interacting with an atomic system is essentially continuous. This assumption has justified the use of Golden Rule, implying that the emitted radiation is spread among many field modes, effectively loosing their coherence with the initial quantum state of the atom. However, this assumption becomes invalid if the electromagnetic field is contained inside a relatively small volume, with a linear size comparable with the radiation wavelength. Classical electrodynamics shows34 that if the walls of such a cavity mostly reflect, rather than absorb, radiation, so that in the crude approximation the power dissipation may be disregarded, then particular solutions $e^j(r)$ of the Helmholtz equation (5) correspond to discrete, well separated mode wavenumbers $k_j$ and hence well separated eigenfrequencies $\omega_j$. Due to the energy conservation, an atomic transition corresponding to energy $\Delta E = |E_{\text{ini}} - E_{\text{fin}}|$ may be effective only if the corresponding quantum oscillation frequency $\Omega \equiv \Delta E/h$ is close to one of $\omega_j$ and hence relatively far from other eigenfrequencies.35 As a result, the quantum states of a single atomic system and the resonant electromagnetic mode may become entangled.

A very popular approximation for the qualitative description of this effect is the so-called Rabi model,36 in which the atom is treated as a two-level system37 interacting with a single electromagnetic field mode of the resonant cavity. As the reader knows well from Chapters 4-6, any two-level (“spin-½”) system may be described by Hamiltonian $\sigma \cdot \hat{\sigma}$, and we may always select the state basis in that the Hamiltonian is diagonal:

$$\hat{H}_{\text{atom}} = c \hat{\sigma}_z \equiv \frac{\hbar \Omega}{2} \hat{\sigma}_z,$$

where $\hbar \Omega = 2c$ is the energy difference between the eigenenergies in the absence of interaction with the field. Next, according to Eq. (17), ignoring the constant ground-state energy $\hbar \omega/2$ (that may be added to while the laser radiation fluctuations may look like a peripheral issue, pioneering research in that field has led to the development of the general theory of open quantum systems (which was discussed in Chapter 7), that has much broader applications.

33 This popularity was demonstrated, for example, by the 2012 Nobel Prize in Physics award to cavity QED experimentalists S. Haroche and D. Wineland.
34 See, e.g., EM Sec. 7.9.
35 On the contrary, if $\Omega$ is far from any $\omega_j$, the interaction is much suppressed; in particular, the spontaneous emission rate may be much lower than that given by Eq. (53) – so that this result is not as fundamental as it may look.
36 After the pioneering work by I. Rabi in 1936-37.
37 As was shown in Sec. 6.5, this model is justified, e.g., if transitions between all other energy level pairs have considerably different frequencies.
the final energy in the very end – if necessary), the contribution of a single mode of eigenfrequency $\omega$ to the Hamiltonian is

$$\hat{H}_{\text{cavity}} = \hbar \omega \hat{\alpha}^\dagger \hat{\alpha}. \quad (9.66)$$

Finally, according to Eq. (16a), in quantum electrodynamics the electric field of the mode may be presented as

$$\hat{\mathcal{E}}(\mathbf{r}, t) = \frac{1}{i} \left( \frac{\hbar \omega}{2} \right)^{1/2} \mathbf{e}(\mathbf{r}) \left( \hat{a} - \hat{a}^\dagger \right), \quad (9.67)$$

so that in the electric-dipole approximation (24), the cavity-atom interaction may be presented as a product of the field by one of Cartesian components (say, $\sigma_y$) of the “spin” operator:\[38\]

$$\hat{H}_\text{int} = \text{const} \times \hat{\sigma}_y \times \hat{\mathcal{E}} = \text{const} \times \hat{\sigma}_y \times \left( \frac{\hbar \omega}{2} \right)^{1/2} \left( \frac{i}{i} \left( \hat{a} - \hat{a}^\dagger \right) = i\hbar \kappa \sigma_y \left( \hat{a} - \hat{a}^\dagger \right), \quad (9.68)$$

where $\kappa$ is a coupling constant (with the dimension of frequency). The sum of these terms is called the Rabi Hamiltonian,

$$\hat{H} \equiv \hat{H}_\text{atom} + \hat{H}_{\text{cavity}} + \hat{H}_\text{int} = \frac{\hbar \Omega}{2} \hat{\sigma}_z + \hbar \omega \hat{\alpha}^\dagger \hat{\alpha} + \hbar \kappa \sigma_y \left( \hat{a} - \hat{a}^\dagger \right). \quad (9.69)$$

Despite its apparent simplicity, using this Hamiltonian for calculations is not that simple. For example, an exact quasi-analytical expression for its eigenenergies (as zeros of a Taylor series in parameter $\kappa$, with coefficients determined by a recurrence relation) was found only recently.\[39\] Only in the case when the electromagnetic field is very intensive and hence may be treated as the classical one, the results following from Eq. (69) are reduced to the Rabi oscillations discussed in Sec. 6.3.

In the opposite case when the field oscillator is in an essentially quantum state, $\langle \hat{a}^\dagger \hat{a} \rangle \sim 1$, Eq. (69) may be simplified in a different way, assuming that frequencies $\Omega$ and $\omega$ are very close, and the atom-to-cavity interaction is relatively weak, so that magnitudes of the coupling constant $\kappa$ and the detuning parameter (similar to parameter $\Delta$ used in Sec. 6.5),

$$\xi \equiv \Omega - \omega, \quad (9.70)$$

are both much smaller than $\Omega \approx \omega$. To discuss this limit, it is convenient to use the spin ladder operators defined absolutely similarly for those of the orbital angular momentum – see Eqs. (5.182):

$$\hat{\sigma}_z \equiv \hat{\sigma}_x \pm i \hat{\sigma}_y, \quad \text{so that} \quad \hat{\sigma}_z = \frac{\hat{\sigma}_+ - \hat{\sigma}_-}{2i}. \quad (9.71)$$

From Eq. (4.105), it is easy to find matrices of these operators (in the standard $z$-basis),

$$\sigma_+ = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}, \quad \sigma_- = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}. \quad (9.72)$$

---

\[38\] The exact choice of this component is not important, while the formulas simplify if it is proportional to either pure $\sigma_x$ or pure $\sigma_y$.

and their commutation rules – that are naturally similar to Eqs. (5.183):
\[
[\hat{\sigma}_+, \hat{\sigma}_-] = 4\hat{\sigma}_z, \quad [\hat{\sigma}_z, \hat{\sigma}_\pm] = \pm 2\hat{\sigma}_\pm.
\] (9.73)

In this notation, the Rabi Hamiltonian looks like
\[
\hat{H} = \frac{\hbar \Omega}{2} \hat{\sigma}_z + \hbar \omega \hat{a} + \frac{\hbar \kappa}{2} (\hat{\sigma}_+ - \hat{\sigma}_-) (\hat{a} - \hat{a}^\dagger),
\] (9.74)

and it is straightforward to use Eq. (4.199) and (73) to derive the Heisenberg-picture equations of motion for the involved operators. (Doing this, we have to remember that operators of the “spin” subsystem, on one hand, and of the field mode, on the other hand, are defined in different Hilbert spaces and hence commute – at least at coinciding time moments.) The result (so far, exact!) is
\[
\begin{align*}
\dot{\hat{a}} &= -i\omega \hat{a} - \frac{i\kappa}{2} (\hat{\sigma}_+ - \hat{\sigma}_-), \\
\dot{\hat{a}}^\dagger &= i\omega \hat{a}^\dagger = \frac{i\kappa}{2} (\hat{\sigma}_+ - \hat{\sigma}_-), \\
\dot{\hat{\sigma}}_z &= \pm i\Omega \hat{\sigma}_z + 2\kappa (\hat{a} - \hat{a}^\dagger) \hat{\sigma}_z, \\
\dot{\hat{\sigma}}_z &= i\kappa (\hat{a}^\dagger - \hat{a}) (\hat{\sigma}_+ + \hat{\sigma}_-).
\end{align*}
\] (9.75)

Now note that at negligible coupling, \(\kappa \rightarrow 0\), equations (75) have very simple solutions,
\[
\begin{align*}
\hat{a}(t) \propto e^{-i\omega t}, \quad \hat{a}^\dagger(t) \propto e^{i\omega t}, \quad \hat{\sigma}_z(t) \propto e^{\pm i\Omega t}, \quad \hat{\sigma}_z(t) \approx \text{const},
\end{align*}
\] (9.76)

and small terms proportional to \(\kappa\) in the right-hand parts of Eqs. (75) cannot affect these time evolution laws dramatically even if \(\kappa\) is not exactly zero (but small). Of those terms, ones with frequencies close to the “basic” frequency of each variable would act in resonance and hence may have a substantial impact on system dynamics, while non-resonant terms may be ignored. In this rotating-wave approximation (RWA), used several times before in this course, Eqs. (*) are reduced to a much simpler system of equations:
\[
\begin{align*}
\dot{\hat{a}} &= -i\omega \hat{a} - \frac{i\kappa}{2} \hat{\sigma}_-, \\
\dot{\hat{a}}^\dagger &= i\omega \hat{a}^\dagger + \frac{i\kappa}{2} \hat{\sigma}_+, \\
\dot{\hat{\sigma}}_+ &= i\Omega \hat{\sigma}_+ + 2\kappa \hat{a}^\dagger \hat{\sigma}_z, \\
\dot{\hat{\sigma}}_- &= -i\Omega \hat{\sigma}_- - 2\kappa \hat{a} \hat{\sigma}_z, \\
\dot{\hat{\sigma}}_z &= i\kappa (\hat{a}^\dagger \hat{\sigma}_- - \hat{a} \hat{\sigma}_+).
\end{align*}
\] (9.77)

Alternatively, these equations of motion may be obtained from the Rabi Hamiltonian after it has been cleared of the terms proportional to \(\hat{\sigma}_+ \hat{a}^\dagger\) and \(\hat{\sigma}_- \hat{a}\), that oscillate fast and hence self-average to virtually zero:
\[
\hat{H} = \frac{\hbar \Omega}{2} \hat{\sigma}_z + \hbar \omega \hat{a} + \frac{\hbar \kappa}{2} (\hat{\sigma}_+ \hat{a} + \hat{\sigma}_- \hat{a}^\dagger), \quad \text{at } \kappa |\xi| \ll \omega, \Omega.
\] (9.78)

This is the famous Janes-Cummings Hamiltonian,\(^{40}\) which is central to the cavity QED and its applications.\(^{41}\) In order to find its eigenstates and eigenenergies, let us note that at negligible interaction

\(^{40}\) It was first proposed and analyzed in 1963 by two electronic engineers, E. Janes and F. Cummings, and it took the physics community a while to recognize and acknowledge the fundamental importance of that work.

\(^{41}\) In most applications, Hamiltonian (78) is augmented by additional term(s) describing, for example, incoming radiation and/or coupling to environment, say due to the electromagnetic energy loss in the cavity walls – see Eq. (7.68).
(κ → 0), the spectrum of the total energy \( E \) of the system, that in this limit is the sum of two independent contributions from the atomic (“spin”) and resonant-cavity subsystems,

\[
E|_{\kappa=0} = \pm \frac{\hbar \Omega}{2} + \hbar \omega n \equiv E_n \pm \frac{\hbar \xi}{2},
\]  

(9.79)

consists\(^{42}\) of close level pairs (Fig. 5) centered to values

\[
E_n = \hbar \omega \left( n - \frac{1}{2} \right), \quad \text{with} \quad n = 1, 2, \ldots
\]

(9.80)

(At the exact resonance \( \omega = \Omega \), i.e. at \( \xi = 0 \), each pair merges into one double-degenerate level \( E_n \).)

\[
\begin{array}{c}
... \\
E = 0 \\
\hbar \Omega \\
\hbar \omega \\
\hbar \omega
\end{array}
\]

\[
\text{"spin-1/2" cavity} \quad \text{total system}
\]

\[
E_\gamma = -\hbar \Omega/2
\]

Fig. 9.5. Energy spectrum of the Janes-Cummings Hamiltonian at \( \kappa \ll |\xi| \).

Since at \( \kappa \rightarrow 0 \) the two subsystems do not interact, the eigenstates corresponding to the sublevels of \( n \)-th pair may be represented by products of their independent ket-vectors:

\[
| + \rangle \equiv | \uparrow \rangle \otimes | n - 1 \rangle \quad \text{and} \quad | - \rangle \equiv | \downarrow \rangle \otimes | n \rangle.
\]  

(9.81)

As we know from Chapter 6, weak interaction leads to strong hybridization of quantum states with close energies (in this case, two states (81) with each pair with the same \( n \)) and their negligible mixing with other states. Hence, at \( 0 < \kappa \ll \omega \approx \Omega \), a good approximation of an eigenstate with \( E \approx E_n \) is given by a linear superposition of states (81):

\[
| \alpha \rangle = c_+ | \uparrow \rangle \otimes | n - 1 \rangle + c_- | \downarrow \rangle \otimes | n \rangle,
\]  

(9.82)

with certain \( c \)-number coefficients \( c_\pm \). This relation describes the entanglement of atomic eigenstates \( \uparrow \) and \( \downarrow \) with Fock states \( n \) and \( n - 1 \) of the field mode.

Let me leave the (straightforward) calculation of coefficients \( c_\pm \) and eigenenergies of the two entangled state pairs for reader’s exercise. This calculation shows, in particular, that at the exact resonance (\( \omega = \Omega \)), \( |c_+| = |c_-| = 1/\sqrt{2} \) for both states of each pair. This fact may be interpreted as a (coherent!) equal sharing of an energy quantum \( \hbar \omega = \hbar \Omega \) by the atom and the cavity.

A by-product of the calculation of \( c_\pm \) is the fact that the dynamics of state \( \alpha \) described by Eq. (82) is similar to that of the generic two-level system that was repeatedly discussed in this course - first

\(^{42}\) Besides the non-degenerate ground state level \( E_\gamma = -\hbar \Omega/2 \).
time in Sec. 2.6 and then in Chapters 4-6. In particular, if the composite system had been initially prepared to be in one component state, for example $|\uparrow\rangle \otimes |0\rangle$ (i.e. the atom excited, while the cavity in its ground state) and allowed to evolve on its own, after some time interval it may be found in the counterpart state $|\downarrow\rangle \otimes |1\rangle$, including the first excited Fock state $n = 1$ of the field mode. This is one more (resonant) version of the same method for generation of Fock states of electromagnetic field which was discussed in Sec. 3.43

Unfortunately, my time devoted to cavity QED is over, and for further reading I have to refer the reader to special literature.44

9.5. The Klein-Gordon and relativistic Schrödinger equations

Now let us discuss the basics of relativistic quantum mechanics of particles with a nonvanishing rest mass $m$ - i.e., in terms of Eq. (1), the intermediate range of energies: $E \sim mc^2$, i.e. for $p \sim mc$. Historically, the first attempt45 to extend the non-relativistic wave mechanics into the relativistic energy range was based on performing the same transitions from classical observables to their quantum-mechanical operators as in the non-relativistic limit:

$$\mathbf{p} \rightarrow \hat{\mathbf{p}} = -i\hbar \nabla, \quad E \rightarrow \hat{H} = i\hbar \frac{\partial}{\partial t}. \quad (9.83)$$

Substitution of these operators, acting on the Schrödinger-picture wavefunction $\Psi(r,t)$, into the classical relation between the energy $E$ and momentum $p$ (for of a free particle) leads to the following equations:

Table 9.1. Deriving the Klein-Gordon equation for a free relativistic particle.46

<table>
<thead>
<tr>
<th>Classical mechanics</th>
<th>Non-relativistic limit $E = \frac{1}{2m} p^2$</th>
<th>Relativistic case $E^2 = c^2 p^2 + (mc^2)^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wave mechanics</td>
<td>$i\hbar \frac{\partial}{\partial t} \Psi = \frac{1}{2m}(-i\hbar \nabla)^2 \Psi$</td>
<td>$(i\hbar \frac{\partial}{\partial t})^2 \Psi = c^2 (-i\hbar \nabla)^2 \Psi + (mc^2)^2 \Psi$</td>
</tr>
</tbody>
</table>

43 Another important corollary of the level structure shown in Fig. 5 is the Purcell effect already mentioned in Sec. 3. As we already know from Chapter 7, if the system is coupled to environment, the coupling suppresses its quantum coherence, in our case the coherence between components of each pair (82). As a result, if the atom is initially in state $\uparrow$ with higher energy (79), it may perform incoherent (dissipative) transition to the lower-energy state $\downarrow$, giving energy $\hbar \omega$ to the cavity ($n - 1 \rightarrow n$), which rapidly drains it into the environment. Since the total energies of these initial and finite states are close (Fig. 5), the rate of such transitions may be much higher than in free space. The quantitative analysis of such enhancement is left for reader’s exercise.


45 This approach was suggested almost simultaneously in 1926-1927 by (at least) V. Fock, E. Schrödinger, O. Klein and W. Gordon, J. Kudar, T. de Donder and F.-H. van der Dungen, and L. de Broglie.

46 Note that in the sense of Eq. (1), in the non-relativistic column of this table, the energy is referred to the rest energy $mc^2$, while in the relativistic column, to zero.
The resulting equation for the non-relativistic limit is just the usual Schrödinger equation (1.28) for a free particle. Its relativistic generalization, usually rewritten as

\[
\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2\right)\Psi + \mu^2\Psi = 0, \quad \text{with} \quad \mu \equiv \frac{mc}{\hbar},
\]

(9.84)

is called the *Klein-Gordon* (or sometimes “Klein-Gordon-Fock”) *equation*. The most fundamental solutions of this equation are the same plane, monochromatic waves

\[
\Psi(r, t) \propto \exp\left[i(k \cdot r - \omega t)\right].
\]

(9.85)
as in the non-relativistic case. Indeed, such waves are eigenstates of operators (83), with eigenvalues

\[
p = \hbar k, \quad E = \hbar \omega,
\]

(9.86)

so that their substitution into Eq. (84) immediately returns us to Eq. (1) with replacements (86):

\[
E_{\pm} = \hbar \omega_{\pm} = \pm \left[\hbar ck + \left(mc^2\right)^{1/2}\right].
\]

(9.87)

Though one may say that this dispersion relation is just a simple combination of the classical relation (1) and the same basic quantum-mechanical relations (86) as in non-relativistic limit, it attracts our attention to the fact that energy \(\hbar \omega\) as a function of momentum \(\hbar k\) has two rather than one branches, with \(E(p) = -E_+(p)\) – see Fig. 6a.

Historically, this fact has played a very important role for spurring the fundamental idea of *particle-antiparticle pairs*. In this idea (very similar to the concept of electrons and holes in semiconductors, which was discussed in Sec. 2.8), what we call the vacuum actually corresponds to all states of the lower branch, with energies \(E_-(p) < 0\), being filled, while the states on the upper branch, with energies \(E_+(p) > 0\), being empty. Then an externally supplied energy

\[
\Delta E = E_+ - E_- = E_+ + (-E_-) \geq 2mc^2 > 0
\]

(9.88)

may bring the system from the lower branch to the upper one (Fig. 6b). The resulting excited state is interpreted as a combination of a particle (formally, of the infinite spatial extension) with energy \(E_+\) and momentum \(p\), and a “hole” (antiparticle) of positive energy \((-E_-)\) and momentum \(-p\). This idea\(^\text{47}\) has led

\(^{47}\) Due to the same P. A. M. Dirac!
to a search for, and discovery of the positron: electron’s antiparticle with charge \( q = +e \), in 1932, and later of the antiproton and other antiparticles.

Free particles of a finite spatial extension may be described, in this approach, just in the non-relativistic Schrödinger equation, by wave packets: linear superpositions of de-Broglie waves (85) with close wave vectors \( \mathbf{k} \), and \( \omega \) given by Eq. (87), with the positive sign for the “usual” particles, and negative sign for antiparticles – see Fig. 6a above. Note that in order to form, from a particle’s wave packet, a similar wave packet for the antiparticle, with the same phase and group velocities (2.33) in each direction, we need to change the sign not only before \( \omega \), but also before \( \mathbf{k} \), i.e. to replace all component wavefunctions (85), and hence the full wavefunction, with their complex conjugates.

Of more formal properties of the equation, it is easy to prove that its solutions satisfy the same continuity equation (1.52) with the probability current density \( j \) still given by Eq. (1.47), but a different expression for the probability density \( \rho \) – which becomes very similar to that for \( j \):

\[
\rho = \langle \Psi^* \nabla \Psi - \text{c.c.} \rangle.
\]

(In the non-relativistic limit \( \nu/c \to 0 \), Eq. (84) allows a reduction of the first relation to Eq. (1.22): \( \rho \to \Psi \Psi^* \).

The Klein-Gordon equation may be readily generalized to describe a single particle moving in external fields; for example, the electromagnetic field effects on a particle with charge \( q \) may be described by the same replacement as in the non-relativistic limit (see Sec. 3.1):\(^{48}\)

\[
\hat{p} \to \hat{p} - q \mathbf{A}(r,t), \quad \hat{H} \to \hat{H} - q \phi(r,t),
\]

where \( \hat{p} = -i\hbar \nabla \) is the canonical momentum operator (3.25), and the vector- and scalar potentials, \( \mathbf{A} \) and \( \phi \), should be treated appropriately – either as \( c \)-number functions if the electromagnetic field quantization is unimportant, or as operators (see Secs. 1-4 above) if it is.

However, the practical value of the relativistic Schrödinger equation is rather limited, because of two main reasons. First of all, it does not give the correct description of particles with spin. For example, for the hydrogen-like atom, i.e. the motion of an electron with electric charge \(-e\) in the Coulomb central field (3.182) of an immobile nucleus with charge \(+Ze\), the equation may be readily solved exactly\(^{49}\) and yields the following spectrum of (doubly-degenerate) energy levels:

\[
E = mc^2 \left( 1 + \frac{Z^2 \alpha^2}{\lambda^2} \right)^{-1/2}, \quad \text{with} \quad \lambda \equiv n + \left[ \left( l + \frac{1}{2} \right)^2 - Z^2 \alpha^2 \right]^{1/2} - \left( l + \frac{1}{2} \right),
\]

where \( n = 1, 2, \ldots \) and \( l = 0, 1, \ldots, n - 1 \) are the same quantum numbers as in the non-relativistic theory (see Sec. 3.6), and \( \alpha \equiv e^2/4\pi\varepsilon_0 \hbar c \approx 1/137 \) is the fine structure constant – see Eq. (6.62). The three leading terms of the Taylor expansion of this result in small parameter \( Z\alpha \) are as follows:

\[
E \approx mc^2 \left[ 1 - \frac{Z^2 \alpha^2}{2n^2} - \frac{Z^4 \alpha^4}{2n^4} \left( \frac{n}{l+1/2} - \frac{3}{4} \right) \right].
\]

\(^{48}\) After such generalization, Eq. (84) is usually called the relativistic Schrödinger equation.

\(^{49}\) The task left for the reader.
The first of these terms is just the rest energy of the particle. The second term,

$$E_n = -mc^2 \frac{Z^2 \alpha^2}{2n^2} = - \frac{mZ^2 e^4}{(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{2n^2} = - \frac{E_0}{2n^2},$$

with $E_0 = Z^2 E_{11},$ (9.93)

reproduces the non-relativistic Bohr’s formula (3.191). Finally, the third term,

$$-mc^2 \frac{Z^4 \alpha^4}{2n^4} \left( \frac{n}{l+1/2} - \frac{3}{4} \right) = - \frac{2E_n^2}{mc^2} \left( \frac{n}{l+1/2} - \frac{3}{4} \right),$$

(9.94)

is just the kinetic-relativistic contribution (6.52) to the fine structure of the Bohr levels (93). However, as we already know from Sec. 6.3, for a spin-$\frac{1}{2}$ particle such as the electron, the spin-orbit interaction (6.56) gives an additional contribution of the same order to the fine structure, so that the net result, confirmed by experiment, is given by Eq. (6.60), i.e. different from Eq. (94). This is very natural, because the relativistic Schrödinger equation does not have the very notion of spin.

Second, even for massive spinless particles (such as $Z_0$ bosons), for which this equation is believed to be valid, the most important problems are related to particle interactions at high energies of the order of $\Delta E \sim 2mc^2$ (88) and beyond. Due to possibility of creation and annihilation of particle-antiparticle pairs at such energies, the number of particles participating in such interactions is typically considerable (and variable), and its adequate description of the system is given not by the relativistic Schrödinger equation (which is formulated in single-particle terms), but by the quantum field theory - to which I will devote just a few sentences in the very end of this chapter.

### 9.6. Dirac’s theory

The real breakthrough toward the quantum relativistic theory of electrons (and any spin-$\frac{1}{2}$ fermions) was achieved in 1928 by P. A. M. Dirac. For that time, the structure of his theory was highly nontrivial. Namely, while formally preserving, in the coordinate representation, the same Schrödinger-picture equation of quantum dynamics as in the non-relativistic quantum mechanics,\(^{50}\)

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi,$$

(9.95)

it postulates that wavefunction $\Psi$ is not a scalar complex function of time and coordinates, but a four-component column-vector (sometimes called the bispinor) of such functions, its Hermitian-conjugate bispinor $\Psi^\dagger$ being a 4-component row-vector of their complex conjugates:

$$\Psi = \begin{pmatrix} \Psi_1(r,t) \\ \Psi_2(r,t) \\ \Psi_3(r,t) \\ \Psi_4(r,t) \end{pmatrix}, \quad \Psi^\dagger = \begin{pmatrix} \Psi_1^*(r,t) & \Psi_2^*(r,t) & \Psi_3^*(r,t) & \Psi_4^*(r,t) \end{pmatrix},$$

(9.96)

\(^{50}\) After the “naturally-relativistic” form of the Klein-Gordon equation (84), this apparent return to the non-relativistic Schrödinger equation may look very counter-intuitive. However, it becomes a bit less surprising taking into account the fact (whose proof is left for the reader) that Eq. (84) may also be recast into form (95) for a two-component column-vector (spinor) $\Psi$, with a Hamiltonian which may be represented by a $2\times2$ matrix - and hence expressed via the Pauli matrices (4).
and that the Hamiltonian participating in Eq. (95) is a $4\times4$ matrix in the Hilbert space of bispinors $\Psi$. For a free particle, the postulated Hamiltonian looks amazingly simple: \(^{51}\)

$$
\hat{H} = c\mathbf{\hat{a}} \cdot \mathbf{\hat{p}} + \hat{\beta} mc^2. \tag{9.97}
$$

where $\mathbf{\hat{p}} = -i\hbar \nabla$ is the same 3D vector of momentum component operators as in the non-relativistic case, while operators $\mathbf{\hat{a}}$ and $\hat{\beta}$ may be presented in the following shorthand $2\times2$ form:

$$
\mathbf{\hat{a}} \equiv \begin{pmatrix} 0 & \hat{\sigma} \\ \hat{\sigma} & 0 \end{pmatrix}, \quad \hat{\beta} \equiv \begin{pmatrix} \hat{I} & 0 \\ 0 & -\hat{I} \end{pmatrix}. \tag{9.98a}
$$

Operator $\mathbf{\hat{a}}$, composed of the Pauli vector operators $\hat{\sigma}$, is also a vector in the usual 3D space, so that each of its 3 Cartesian components is a $4\times4$ matrix. The particular form of the $2\times2$ matrices corresponding to operators $\hat{\sigma}$ and $\hat{I}$ in Eq. (98a) depends on the basis selected for representation of the spin states of the particle; for example, in the standard $z$-basis, in which the Cartesian components $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ of $\hat{\sigma}$ are represented by the Pauli matrices (4.105), the full matrix form of Eq. (98a) is

$$
\alpha_x = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \alpha_y = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \alpha_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{9.98b}
$$

(According to the second of Eq. (98a), $\beta$ has this form in any spin basis.) It is straightforward to use Eqs. (98) to verify that matrices $\alpha_x$, $\alpha_y$, $\alpha_z$ and $\beta$ satisfy the following relations:

$$
\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1, \quad \alpha_x\alpha_y + \alpha_y\alpha_x = \alpha_y\alpha_z + \alpha_z\alpha_y = \alpha_z\alpha_x + \alpha_x\alpha_z = \alpha_x\beta + \beta\alpha_x = \alpha_y\beta + \beta\alpha_y = \alpha_z\beta + \beta\alpha_z = 0, \tag{9.100}
$$

i.e. anticommute.

Acting essentially as in Sec. 4.1, but using commutation relations (99)-(100), it is straightforward to show that any solution to the Dirac equation obeys the probability conservation law, i.e. the continuity equation (1.52), with the probability density,

\(^{51}\) Moreover, if the time derivative participating in Eq. (95) and the three coordinate derivatives participating (via the momentum operator) in Eq. (97), are merged into one 4-vector operator $\partial / \partial \xi_k \equiv \{ \nabla, \partial / \partial (ct) \}$, the Dirac equation (95) may be rewritten in an even simpler, manifestly Lorentz-invariant 4-vector form (with the implicit summation over the repeated index $k = 1, ..., 4$ – see, e.g., EM Sec. 9.4):

$$
\left( \gamma_k \frac{\partial}{\partial \xi_k} + \mu \right) \Psi = 0, \quad \text{where} \quad \gamma \equiv \left\{ \gamma_1, \gamma_2, \gamma_3 \right\} = \begin{pmatrix} 0 & -i\hat{\sigma} \\ i\hat{\sigma} & 0 \end{pmatrix}, \quad \gamma_4 = \hat{\beta},
$$

where $\mu \equiv mc / \hbar$ - just as in Eq. (84). Note also that, very counter-intuitively, the Dirac Hamiltonian (97) is linear in momentum, while the non-relativistic Hamiltonian of a particle, as well as the relativistic Schrödinger equation, are quadratic in $\mathbf{p}$. In my humble opinion, the Dirac theory (including the concept of antiparticles) may compete for the title of the most revolutionary theoretical idea in physics, despite such heavy contenders as the Newton laws, the Maxwell equations, the Einstein’s relativity, the Bohr atom, and the Gibbs’ statistical distributions.
\[ w = \Psi^\dagger \Psi, \quad (9.101) \]

and the probability current,

\[ j = c \Psi^\dagger \hat{a} \Psi, \quad (9.102) \]

looking almost as in the non-relativistic theory – cf. Eqs. (1.22) and (1.47). Note, however, the Hermitian conjugation used in these formulas instead of the complex conjugation, in order to form scalars \( w, j_x, j_y, \) and \( j_z \) from 4-component vectors (96).

This qualified similarity is extended to the fundamental, plane-wave solutions of the Dirac equations in free space. Indeed, plugging such solution, in the form

\[
\Psi = u e^{i(k \cdot r - \omega t)} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix},
\]

(9.103)

into Eqs. (95) and (97), we get a system of 4 coupled, linear algebraic equations for 4 complex \( c \)-number amplitudes \( u_{1,2,3,4} \). The condition of their consistency yields the same dispersion relation (87), i.e. the same two-branch diagram shown in Fig. 6, as follows from the Klein-Gordon equation. The difference is that plugging each value of \( \omega \), given by Eq. (87), back into the system of equations for amplitudes \( u \), we get two solutions for vector \( u \) for each of the energy branches. In the standard spin \( z \)-basis they may be presented as:

\[
\begin{align*}
\text{for } E = E_+ > 0: & \quad u_{\uparrow} = c_{\uparrow} \begin{pmatrix} 1 \\ 0 \\ \frac{c p_z}{E_+ + mc^2} \\ \frac{c(p_x + ip_y)}{E_+ + mc^2} \end{pmatrix}, & u_{\downarrow} = c_{\downarrow} \begin{pmatrix} 0 \\ 1 \\ \frac{c(p_x - ip_y)}{E_+ + mc^2} \\ \frac{-c p_z}{E_+ + mc^2} \end{pmatrix}, \\
\text{for } E = E_- < 0: & \quad u_{\uparrow} = c_{\uparrow} \begin{pmatrix} \frac{c p_z}{E_- - mc^2} \\ \frac{c(p_x + ip_y)}{E_- - mc^2} \\ 1 \\ 0 \end{pmatrix}, & u_{\downarrow} = c_{\downarrow} \begin{pmatrix} \frac{c(p_x - ip_y)}{E_- - mc^2} \\ \frac{-c p_z}{E_- - mc^2} \\ 0 \\ 1 \end{pmatrix},
\end{align*}
\]

(9.104a, 9.104b)

where \( c \) are normalization coefficients.

The simplest interpretation of these solutions is that Eq. (103) with vectors \( u_{\uparrow} \), given by Eq. (104a), represents a spin-\( \frac{1}{2} \) particle (say, an electron), while that with vectors \( u_{\downarrow} \) given by Eq. (104b) represents an antiparticle (a positron), and two solutions for each particle correspond to two opposite directions of spin, \( \sigma_z = \pm 1, S_z = \pm \hbar/2 \). This interpretation is indeed solid in the non-relativistic limit, when two last components of vector (104a) and two first components of vector (104b) are negligibly small.
\[
\begin{pmatrix}
1 \\
0 \\
0 \\
0
\end{pmatrix}, \quad
\begin{pmatrix}
0 \\
1 \\
0 \\
0
\end{pmatrix}, \quad
\begin{pmatrix}
0 \\
0 \\
1 \\
0
\end{pmatrix}, \quad
\begin{pmatrix}
0 \\
0 \\
0 \\
1
\end{pmatrix}, \quad \text{at } \frac{p_k}{mc} \to 0. \quad (9.105)
\]

In order to show this, let us use the Dirac equation to calculate the Heisenberg-picture law of time evolution of operators of the Cartesian components of the orbital angular momentum \( L = r \times p \), for example of \( L_x = yp_z - zp_y \), taking into account that operators (98a) commute with those of \( r \) and \( p \), and also the Heisenberg commutation relations (2.14):
\[
\begin{align*}
\hbar \frac{\partial \hat{L}_x}{\partial t} &= \left[ \hat{L}_x, \hat{H} \right] = c \hat{\alpha} \cdot \left[ (\hat{y} \hat{p}_z - \hat{z} \hat{p}_y) \hat{\hat{p}} \right] = -i \hbar c (\hat{\alpha}_z \hat{\hat{p}}_y - \hat{\alpha}_y \hat{\hat{p}}_z), \\
\end{align*}
\]
with similar relations for two other Cartesian components of the operator. Since the right-hand part of these equations is different from zero, the orbital momentum is generally not conserved - even for a free particle! Let us, however, consider the following vector operator,
\[
\hat{S} \equiv \frac{\hbar}{2} \begin{pmatrix}
\hat{\sigma} & 0 \\
0 & \hat{\sigma}
\end{pmatrix}, \quad (9.107a)
\]
whose Cartesian components, in the \( z \)-basis, are represented by 4×4 matrices
\[
\begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0
\end{pmatrix}, \quad S_y = \frac{\hbar}{2} \begin{pmatrix}
0 & 0 & 0 & i \\
0 & 0 & i & 0 \\
0 & i & 0 & 0 \\
i & 0 & 0 & 0
\end{pmatrix}, \quad S_z = \frac{\hbar}{2} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & -1
\end{pmatrix}, \quad (9.107b)
\]
and calculate the Heisenberg-picture law of time evolution of these components, for example
\[
\begin{align*}
\hbar \frac{\partial \hat{S}_x}{\partial t} &= \left[ \hat{S}_x, \hat{H} \right] = c \hat{\alpha} \cdot \left[ (\hat{\alpha}_x \hat{\hat{p}}_x + \hat{\alpha}_y \hat{\hat{p}}_y + \hat{\alpha}_z \hat{\hat{p}}_z) \right] = i \hbar c (\hat{\alpha}_z \hat{\hat{p}}_y - \hat{\alpha}_y \hat{\hat{p}}_z). \\
\end{align*}
\]
A direct calculation of the commutators of matrices (98) and (107) yields
\[
\begin{align*}
\left[ \hat{S}_x, \hat{\alpha}_x \right] &= 0, \quad \left[ \hat{S}_x, \hat{\alpha}_y \right] = -i \hbar \hat{\alpha}_z, \quad \left[ \hat{S}_z, \hat{\alpha}_z \right] = -i \hbar \hat{\alpha}_y, \\
\end{align*}
\]
so that we finally get
\[
\hbar \frac{\partial \hat{S}_x}{\partial t} = i \hbar c (\hat{\alpha}_z \hat{\hat{p}}_y - \hat{\alpha}_y \hat{\hat{p}}_z), \quad (9.110)
\]
with similar expressions for other two components of the operator. Comparing this result with Eq. (106), we see that any Cartesian component of operator (5.198),
\[
\hat{J} \equiv \hat{L} + \hat{S}, \quad (9.111)
\]
is an integral of motion,\textsuperscript{52} so that this operator may be interpreted as the one presenting the total angular momentum. Hence, operator (104) \textit{may} be interpreted as the spin operator of a spin-$\frac{1}{2}$ particle (e.g., electron). As it follows from the last of Eq. (107b), columns (105) represent the eigenkets of the $z$-component of that operator, with eigenstates $S_z = \pm h/2$, depending on the arrow index. So, the Dirac theory provides a justification for spin-$\frac{1}{2}$ – or, somewhat more humbly, replaces the spin hypothesis by an assumption of a simpler (and hence more plausible), Lorentz-invariant Hamiltonian (97).

Note, however, that this fact is not true for the exact solutions (103)-(104), so that generally the eigenstates of the Dirac Hamiltonian are certain linear (coherent) superpositions of component wavefunctions describing the particle and its antiparticle - each with both directions of spin. This fact leads to several interesting effects, including the so-called \textit{Klien paradox} at reflection of a particle from a tunnel barrier.\textsuperscript{53} It is curious that some of these effects may be reproduced in such non-relativistic systems as electron moving in a 2D honeycomb lattice (e.g., in graphene), since they also feature a (locally) linear dispersion relation – see Eq. (3.122).\textsuperscript{54}

9.7. Low-energy limit

The generalization of the Dirac’s theory to the case of a particle with electric charge $q$, moving in a classically-described electromagnetic field may be obtained using the same Eqs. (90). As a result, Eq. (95) becomes

\[
\left[ c\hat{\mathbf{a}} \cdot (-i\hbar\nabla - q\mathbf{A}) + mc^2\hat{\beta} + (q\phi - \hat{H}) \right] \Psi = 0, \tag{9.112}
\]

where the Hamiltonian operator $\hat{H}$ is understood in the sense of Eq. (95), i.e. as the partial time derivative with multiplier $i\hbar$. Let us prepare this equation for a low-energy approximation by acting on its left-hand part by a similar square bracket (also an operator!), but with the opposite sign before the last parentheses. Using relations (99) and (100), and the fact that space- and time-independent operators $\hat{\alpha}$ and $\hat{\beta}$ commute with the spin-independent functions $\mathbf{A}(\mathbf{r},t)$ and $\phi(\mathbf{r},t)$, as well as with the Hamiltonian operator $i\hbar\partial/\partial t$, the result is

\[
\left\{ c^2\left[ \hat{\mathbf{a}} \cdot (-i\hbar\nabla - q\mathbf{A}) \right]^2 + \left( mc^2 \right)^2 - c\left[ \hat{\mathbf{a}} \cdot (-i\hbar\nabla - q\mathbf{A}) \right] \left( q\phi - \hat{H} \right) - \left( q\phi - \hat{H} \right)^2 \right\} \Psi = 0. \tag{9.113}
\]

A direct calculation of the first square bracket, using Eqs. (98) and (107), yields

\[
\left[ \hat{\mathbf{a}} \cdot (-i\hbar\nabla - q\mathbf{A}) \right]^2 = \left( -i\hbar\nabla - q\mathbf{A} \right)^2 - 2q\hat{\mathbf{S}} \cdot \nabla \times \mathbf{A}. \tag{9.114}
\]

But according to the last of Eqs. (3.21), the last vector product in the right-hand part is just the magnetic field

\[
\mathbf{B} = \nabla \times \mathbf{A}. \tag{9.115}
\]

Similarly, we may use the first of Eqs. (3.21), for the electric field,

\[
\mathbf{E} = -\nabla \phi - \frac{\partial \mathbf{A}}{\partial t}, \tag{9.116}
\]

\textsuperscript{52} It is straightforward to show that this result remains valid for a particle in the field of central potential $U(\mathbf{r})$.


\textsuperscript{54} For a review see, e.g., T. Robinson, \textit{Am. J. Phys.} \textbf{80}, 141 (2012).
to simplify the commutator participating in Eq. (9.113):

\[
\left[ \hat{\mathbf{a}} \cdot \left( -i \hbar \nabla - q \mathbf{A} \right), \left( q \phi - \hat{H} \right) \right] = -q \hat{\mathbf{a}} \cdot \left[ \hat{H}, \mathbf{A} \right] - i \hbar q \hat{\mathbf{a}} \cdot \left[ \nabla, \phi \right] = -i \hbar q \frac{\partial \mathbf{A}}{\partial t} - i \hbar \hat{\mathbf{a}} \cdot \nabla \phi = i \hbar q \hat{\mathbf{a}} \cdot \mathbf{E}.
\]  

(9.117)

As a result, Eq. (110) becomes

\[
\left\{ \mathcal{E}^2 \left( -i \hbar \nabla - q \mathbf{A} \right)^2 + \left( q \phi - \hat{H} \right)^2 + (mc^2)^2 - 2q \mathbf{c} \cdot \hat{\mathbf{S}} + i \hbar \mathbf{c} q \hat{\mathbf{a}} \cdot \mathbf{E} \right\} \Psi = 0.
\]  

(9.118)

So far, this is an exact result, equivalent to Eq. (112), but more convenient for an analysis of the low-energy limit in that not only the offset energy \(E - mc^2\) (which is the energy used in non-relativistic quantum mechanics), but also the electrostatic energy of the particle, \(|q\langle \phi \rangle|\), are much smaller than the rest energy \(mc^2\). In this limit, the second and third terms of Eq. (118) almost cancel, and introducing the offset Hamiltonian

\[
\hat{\mathcal{H}} \equiv \hat{H} - mc^2 \hat{I}.
\]  

(9.119)

we may approximate their difference, up to the first nonvanishing term, as

\[
\left( q \phi \hat{\mathbf{I}} - \hat{\mathcal{H}} \right)^2 - \left( mc^2 \right)^2 \hat{I} \equiv \left( q \phi \hat{\mathbf{I}} - mc^2 \hat{I} - \hat{\mathcal{H}} \right)^2 - \left( mc^2 \right)^2 \hat{I} \approx 2mc^2 \left( \hat{\mathcal{H}} - q \phi \hat{\mathbf{I}} \right).
\]  

(9.120)

As a result, after division of all terms by \(2mc^2\), Eq. (118) may be approximated as

\[
\hat{\mathcal{H}} \Psi = \left[ \frac{1}{2m} \left( -i \hbar \nabla - q \mathbf{A} \right)^2 + q \phi - \frac{q}{m} \hat{\mathbf{S}} \cdot \mathbf{B} + \frac{i \hbar q}{2mc} \hat{\mathbf{a}} \cdot \mathbf{E} \right] \Psi.
\]  

(9.121)

Let us discuss this important result. The first two terms in the square brackets give the Hamiltonian (3.26) that was extensively used in Chapter 3 for the discussion of non-relativistic motion of charged particles. Note again that the contribution of the vector-potential \(\mathbf{A}\) into that Hamiltonian is essentially relativistic, in the following sense: when used for the description of magnetic interaction of two charged particles, due to their orbital motion with speed \(v \ll c\), the magnetic interaction is a factor of \((v/c)^2\) smaller than the electrostatic interaction of the particles.\(^55\) The reason why we did discuss the effects of \(\mathbf{A}\) in Chapter 3 was that is was used there to describe external magnetic fields, keeping our analysis valid even for the cases when that field is strong by being produced by relativistic effects – such as aligned spins in a permanent magnet.

The next, third term in the square brackets is also familiar to the reader: it was introduced informally in Sec. 4.1, and then formally in Sec. 4.4 to describe the effect of magnetic field on particle’s spin – see Eqs. (4.3), (4.5), and (4.163). When justifying this form of interaction, I referred mostly to results of Stern-Gerlach-type experiments, but it is extremely pleasing that this result\(^56\) follows from such a fundamental relativistic treatment as Dirac’s theory. As we already know from the discussion of

\(^{55}\) This difference may be traced even by classical means – see, e.g., EM Sec. 5.1.

\(^{56}\) With the \(g\)-factor still equal to exactly 2 - see Eq. (4.116) and its discussion. In order to describe the small deviation of \(g_e\) from 2, the electromagnetic field should be quantized (just as this was done in Secs. 1-4), and its potentials \(\mathbf{A}\) and \(\phi\), participating in Eq. (112) should be treated as operators – rather than as \(c\)-number functions as was assumed above. The calculation of this deviation is one of the basic problems of quantum field theory. Other small but important effects of electromagnetic interactions, described by the theory, include the so-called Lamb shift of atomic levels – see the end of this chapter for references.
the Zeeman effect in Sec. 6.4, the effects of magnetic field on the orbital motion of an electron (described by orbital angular momentum $L$) and its spin $S$ are of the same order, i.e. present an essentially relativistic effect.

Finally, the last term in the square brackets of Eq. (121) is also not quite new for us: in particular it describes the spin-orbit interaction. Indeed, in the case of classical, spherical-symmetric electric field $E$ with potential $\phi(r) = U(r)/q$, the term may be reduced to Eq. (6.56b):

$$
\hat{H}_{so} = \frac{1}{2m^2c^2} \hat{S} \cdot \hat{L} \frac{1}{r} \frac{dU}{dr} = -\frac{q}{2m^2c^2} \hat{S} \cdot \hat{L} \frac{1}{r} .
$$

The proof of this correspondence requires a bit of additional work, because in Eq. (121), the term responsible for the spin-orbit interaction acts on 4-component wavefunctions, while Hamiltonian (122) is supposed to act on non-relativistic wavefunctions with account of spin, whose coordinate representation is given by 2-component columns – spinors:

$$
\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} .
$$

The simplest way to prove the identity of the two formulas is not to use Eq. (121) directly, but to return to the Dirac equation (112), for the particular case of motion in a stationary electric field with no magnetic field, when Dirac’s Hamiltonian is reduced to

$$
\hat{H} = c \hat{\alpha} \cdot \hat{p} + \hat{\beta} mc^2 + U(r) .
$$

Since this Hamiltonian is time-independent, we may look for its 4-component eigenfunctions in the form

$$
\Psi(r, t) = \begin{pmatrix} \psi_+(r) \\ \psi_-(r) \end{pmatrix} \exp\left(-i \frac{E}{\hbar} t\right) ,
$$

where each of $\psi_\pm$ is a 2-component column of the type (123), representing two spin states of the particle (index +) and antiparticle (index -). Plugging Eq. (125) into Eq. (124), and using Eq. (98a), we get the following system of two linear equations:

\[
\begin{align*}
[E - mc^2 - U(r)] \psi_+ - c \hat{\sigma} \cdot \hat{p} \psi_- &= 0 , \\
[E + mc^2 - U(r)] \psi_- - c \hat{\sigma} \cdot \hat{p} \psi_+ &= 0 .
\end{align*}
\]

\[57\] The only facts immediately evident from Eq. (121) are that the term we are discussing is proportional to the electric field, as required by Eq. (122), and that it is of the proper order of magnitude. Indeed, Eqs. (101)-(102) imply that in the Dirac theory, $c \hat{\alpha}$ plays the role of the velocity operator, so that the expectation values of the term are of the order of $\hbar qvE/2mc^2$. Since the expectation values of the operators participating in Hamiltonian (122) scale as $S \sim \hbar/2$ and $L \sim mv$, the spin-orbit interaction energy has the same order of magnitude.

\[58\] As a reminder, in this course the notion of spinor was introduced earlier for two-particle states - see Eq. (8.14). For a single particle, that definition is reduced to $\psi(r)|\psi\rangle$, whose representation in a particular spin-$1/2$ basis is a column similar to Eq. (123). Also note that spinors (123) may be expanded into a series over the spin-orbitals (8.117) discussed in Sec. 8.3, with index $j$ used for numbering both the two directions of spin (i.e. two components of spinor's column) and orbital eigenfunctions.
Expressing $\psi$ from the latter equation, and plugging the result into the former one, we get the following single equation for particle’s spinor:

$$
\left[ E - mc^2 - U(r) - c^2 \mathbf{\sigma} \cdot \hat{p} \frac{1}{E + mc^2 - U(r)} \mathbf{\sigma} \cdot \hat{p} \right] \psi_+ = 0.
$$

(9.127)

So far, this is an exact equation for eigenstates and eigenvalues of Hamiltonian (124). It may be substantially simplified in the low-energy limit when both the potential energy $59$ and the non-relativistic eigenenergy

$$
\tilde{E} \equiv E - mc^2
$$

are much less than $mc^2$. Indeed, in this case the expression in denominator of the last term in the brackets of Eq. (127) is close to $2mc^2$. Since $\mathbf{\sigma}^2 = 1$, with that replacement, Eq. (127) is reduced to the non-relativistic Schrödinger equation, similar for both spin components of $\psi_+$, and hence giving spin-degenerate energy levels. In order to recover small relativistic and spin-orbit effects, we need a slightly more accurate approximation:

$$
\frac{1}{E + mc^2 - U(r)} = \frac{1}{2mc^2 + \tilde{E} - U(r)} = \frac{1}{2mc^2} \left[ 1 + \frac{\tilde{E} - U(r)}{2mc^2} \right]^{-1} \approx \frac{1}{2mc^2} \left[ 1 - \frac{\tilde{E} - U(r)}{2mc^2} \right],
$$

(9.129)

in which Eq. (127) is reduced to

$$
\left[ \tilde{E} - U(r) - \frac{\hat{p}^2}{2m} + \mathbf{\sigma} \cdot \hat{p} \frac{\tilde{E} - U(r)}{2mc^2} \mathbf{\sigma} \cdot \hat{p} \right] \psi_+ = 0.
$$

(9.130)

As follows from Eqs. (5.46)-(5.47), the operators of momentum and of a function of coordinates commute as

$$
[\hat{p}, U(r)] = -i\hbar \nabla U,
$$

(9.131)

so that the last term in square brackets of Eq. (130) may be rewritten as

$$
\mathbf{\sigma} \cdot \hat{p} \frac{\tilde{E} - U(r)}{2mc^2} \mathbf{\sigma} \cdot \hat{p} = \frac{\tilde{E} - U(r)}{2mc^2} \hat{p}^2 - \frac{i\hbar}{2mc^2}(\mathbf{\sigma} \cdot \nabla U)(\mathbf{\sigma} \cdot \hat{p}).
$$

(9.132)

Since in the low-energy limit both terms in the right-hand part of this relation are much smaller than the three leading terms of Eq. (130), in the first of them we may replace the nominator with its non-relativistic value $\hat{p}^2 / 2m$. With this replacement, the term coincides with the first relativistic correction to the kinetic energy operator – see Eqs. (6.47) and (6.49a). The second term, proportional to the electric field $E = -\nabla \phi = -\nabla U/q$, may be transformed further on, using a readily verifiable relation

$$
(\mathbf{\sigma} \cdot \nabla U)(\mathbf{\sigma} \cdot \hat{p}) = (\nabla U) \cdot \hat{p} + i\mathbf{\sigma} \cdot \left[ (\nabla U) \times \hat{p} \right].
$$

(9.133)

Of the two terms in the right-hand part, only the second one depends on spin, giving the following spin-orbital interaction contribution to the Hamiltonian,

$59$ Strictly speaking, this requirement is imposed on the expectation values of $U(r)$ in the eigenstates to be found.
\[ \hat{H}_{so} = \frac{\hbar}{(2mc^2)^2} \vec{\sigma} \cdot [\nabla U] \times \hat{p} = \frac{q}{2m^2c^2} \hat{S} \cdot [\nabla \phi] \times \hat{p}. \]  
(9.134)

For a central electric field with \( \phi(r) = \phi(r) \), the potential gradient has only one, radial component: \( \nabla \phi = (d\phi/dr)r/r = -E r/r \), and with the angular momentum definition \( \hat{L} = r \times \hat{p} \), Eq. (134) is reduced to Eq. (122).

As was shown in Sec. 6.3, the perturbative treatment of Eq. (122), together with the kinetic-relativistic correction (6.49), in the hydrogen-like atom problem, leads to the fine structure of each Bohr level \( E_n \), given by Eq. (6.60):

\[ \Delta E_{so} = -\frac{2E_n}{mc^2}\left(3 - \frac{4n}{j + 1/2}\right). \]  
(9.135)

This result gets a confirmation from the surprising fact that for the hydrogen-like atom problem, the Dirac equation may be solved exactly – without any assumptions. I do not have time/space to reproduce the solution,\(^61\) and will list just the final result for the energy spectrum:

\[ \frac{E}{mc^2} = \left\{1 + \frac{Z^2\alpha^2}{n + \frac{(j + 1/2)^2 - Z^2\alpha^2}{2} - (j + 1/2)^2}\right\}^{-1/2}. \]  
(9.136)

Here \( n = 1, 2, \ldots \) is the same main quantum number as in Bohr’s theory, while \( j \) is the quantum number specifying eigenvalues (5.203) of the total angular momentum’s square \( J^2 \) in the units of \( \hbar^2 \), taking half-integer values: \( j = l \pm \frac{1}{2} = 1/2, 3/2, 5/2, \ldots \) - see Eq. (5.215). Such set of quantum numbers is rather natural, because due to the spin-orbit interaction, the orbital and spin angular momenta are not conserved, while their vector sum, \( \mathbf{J} = \mathbf{L} + \mathbf{S} \), is - in the absence of external magnetic field. Each energy level (136) is doubly-degenerate, with two eigenstates representing two directions of spin – i.e. two values of \( l = j \mp \frac{1}{2} \) at fixed \( j \).

Since according to Eq. (1.9), the square of the fine-structure constant \( \alpha \equiv e^2/4\pi\varepsilon_0\hbar c \) may be presented as the ratio \( E_H/mc^2 \), the low-energy limit \( (E - mc^2 \sim E_H \ll mc^2) \) may be pursued by expanding Eq. (136) into the Taylor series in \((Z\alpha)^2 << 1\). The result,

\[ E \approx mc^2 \left[1 - \frac{Z^2\alpha^2}{2n^2} - \frac{Z^4\alpha^4}{2n^4}\left\{\frac{n}{(j + 1/2)}\right\}^2\right], \]  
(9.137)

has the same structure, and allows the same interpretation as Eq. (92), but with the last term coinciding with Eq. (6.52) - and with experimental results. Historically, this correct description of the fine structure of atomic levels provided a decisive proof of Dirac’s theory.

However, even such an impressive theory does not have too many direct applications. The main reason for that was already discussed in brief in the end of Sec. 5: due to the possibility of creation and

\(^{60}\) The first term gives a small, spin-independent shift of the energy spectrum, which is very difficult to verify experimentally.

\(^{61}\) Good descriptions of the solution are available in many textbooks (the older the better :-), for example see Sec. 53 in L. Schiff, *Quantum Mechanics*, 3rd ed., McGraw-Hill (1968).
annihilation of particle-antiparticle pairs at energies higher than $2mc^2$, the number of particles participating in high-energy interactions is not fixed. An adequate general description of such situation is given by the quantum field theory, in which the particle wavefunction is treated as a field to be quantized, using so-called field operators $\hat{\Psi}(\mathbf{r}, t)$—very much as the electromagnetic field was treated in Secs. 1-4 above. (The Dirac equation follows from the quantum field theory in the single-particle approximation.)

As was mentioned above on several occasions, the quantum field theory is beyond the scope of this course, and I have to stop here, referring the interested reader to one of several excellent available textbooks on this discipline.\(^{62}\) (I would strongly encourage the student going in this direction to start with playing with the field operators on this or her own, taking clues from Eqs. (16), but replacing the creation / annihilation operators $\hat{a}_j^\dagger$ and $\hat{a}_j$ of the harmonic oscillator with those of the general second quantization formalism outlined in Sec. 8.3.)

### 9.8. Exercise problems

9.1. Prove the Casimir formula (23) for the attraction force $F = -PA$ between two perfectly conducting parallel plates of area $A$, separated by a narrow vacuum gap $d \ll A^{1/2}$.

*Hint:* You may like to use the *Euler-Maclaurin formula*.\(^{63}\)

9.2. Radiation of some single-mode quantum sources may have such a high degree of coherence that it is possible to observe interference from two independent sources with virtually the same frequency, incident on one detector.

(i) Generalize Eq. (29) to this case.

(ii) Use the generalized expression to show that incident waves in different Fock states do not create an interference pattern.

9.3. Calculate the zero-delay value $g^{(2)}(0)$ of the second-order correlation function of a single-mode electromagnetic field in the so-called *Schrödinger-cat state*: a coherent superposition of two Glauber states, with equal amplitudes, equal but sign-opposite parameters $\alpha$, and a certain phase shift between them.

9.4. Calculate the zero-delay value $g^{(2)}(0)$ of the second-order correlation function of single-mode electromagnetic field in the squeezed ground state $\xi$ defined by Eq. (5.172).

9.5. Calculate the rate of spontaneous photon emission (into the unrestricted free space) by a hydrogen atom, initially in the $2p$ state ($n = 2$, $l = 1$) with $m = 0$. Would the result be different for $m = \pm$ $1$?

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\(^{63}\) See, e.g., MA Eq. (2.12).
1? for the 2s state \((n = 2, l = 0, m = 0)\)? Discuss the relation between these quantum-mechanical results and those given by the classical theory of radiation, using the simplest classical model of the atom.

9.6. An electron has been placed at the lowest excited level of a spherically-symmetric, quadratic potential well \(U(r) = \frac{m_e \omega^2}{2} r^2/2\). Calculate the rate of its relaxation to the ground state, with emission of a photon (to the free space). Compare the rate with that for a similar transition of the hydrogen atom, for the case when the radiation frequencies of these two systems are equal.

9.7. Derive an analog of Eq. (53) for the spontaneous photon emission into the free space, due to a change of its magnetic dipole moment \(m\) of a small-size system.

9.8. A spin-\(\frac{1}{2}\) particle, with the gyromagnetic ratio \(\gamma\), is in its orbital ground state in a dc magnetic field \(B_0\). Calculate the rate of its spontaneous transition from the higher to the lower energy level, with the emission of a photon into the free space. Evaluate the rate for in an electron in a field of \(10\) T, and discuss the implications of this result for experiments with electron spins.

9.9. Calculate the rate of spontaneous transitions between the two sublevels of the ground state of a hydrogen atom, formed as a result of its hyperfine splitting. Discuss the implications of the result for the width of the 21-cm spectral line.

9.10. Find the eigenstates and eigenvalues of the Janes-Cummings Hamiltonian \((78)\), and discuss their behavior near the resonance point \(\omega = \Omega\).

9.11. Analyze the Purcell effect, mentioned in Secs. 3 and 4, qualitatively; in particular, calculate the so-called Purcell factor \(F_P\), defined as the ratio of the spontaneous emission rates \(\Gamma_s\) of an atom in a resonant cavity (tuned exactly to the quantum transition frequency) and that in the free space.

9.12. Prove that the Klein-Gordon equation (9.84) may be rewritten in the form similar to the non-relativistic Schrödinger equation,

\[
i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi,
\]

for a two-component wavefunction \(\psi\), with the Hamiltonian represented (in the usual \(z\)-basis) by the following 2\(\times\)2-matrix:

\[
\hat{H} = -\frac{1}{2m} \left( \sigma_z + i \sigma_y \right) \frac{\hbar^2}{2m} \nabla^2 + mc^2 \sigma_z.
\]

Use your solution to discuss the physical meaning of the wavefunction’s components.

9.13. Calculate and discuss the energy spectrum of a relativistic, spinless, charged particle placed into an external uniform, time-independent magnetic field \(B\). Use the result to formulate the condition of validity of the non-relativistic theory.

\[64\] Here \(\psi\) is a function of both \(r\) and \(t\), and the lower-case letter is used only to distinguish this two-component spinor from the scalar function \(\Psi(r, t)\) obeying the Klein-Gordon equation.
Hint: Reduce the relativistic Schrödinger equation, describing the problem, to the non-relativistic one describing the same problem, with some effective parameter(s).

9.14. Prove Eq. (91) for the energy spectrum of a hydrogen-line atom, calculated from the relativistic Schrödinger equation.

Hint: Use the fact that, as a mathematical analysis of Eq. (3.184) shows, its eigenvalues are given by Eq. (3.191), \( \varepsilon_n = -1/2n^2 \), with \( n = l + 1 + n_r \), where \( n_r = 0, 1, 2, \ldots \), even if \( l \) is not integer.\(^{65}\)

9.15. Derive the general expression for the differential cross-section of the elastic scattering of a spinless relativistic particle by a static potential \( U(r) \), in the Born approximation, and formulate the conditions of its validity. Use these results to calculate the differential cross-section of scattering of a particle with electric charge \(-e\) by the Coulomb electrostatic potential \( \phi(r) = Z\varepsilon/4\pi\varepsilon_0 r \).

9.16. Calculate the commutator of operator \( \hat{L}^2 \) and the Dirac Hamiltonian of a free particle. Compare the result with that for the non-relativistic Hamiltonian of a free particle, and interpret the difference.

9.17.\(^*\) In the Heisenberg picture of quantum dynamics, derive an equation describing time evolution of free electron’s velocity in the Dirac theory. Solve the equation for the simplest state, with constant energy and momentum, and discuss the solution.

9.18.\(^*\) Calculate the eigenstates and eigenenergies of a spin-\(\frac{1}{2} \) particle with charge \( q \), placed into a uniform, time-independent external magnetic field \( \mathcal{B} \). Compare the calculated energy spectrum with those following from the non-relativistic theory and the relativistic Schrödinger equation.

9.19.\(^*\) Following the recommendation in the end of Chapter 9 of the lecture notes, introduce the quantum field operators \( \hat{\psi} \), which would be related to the usual wavefunctions \( \psi \) just as the EM field operators (9.16) are related to the classical electromagnetic fields, and explore the basic properties of these operators. (For this preliminary study, consider just the fixed-time situation.)

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\(^{65}\) Actually, the key relation (3.192), \( n \geq l + 1 \), mathematically stems from the fact that the “genuine” quantum number of the radial problem, \( n_r \), can only take non-negative integer values.