9.7: Low Energy Limit

The generalization of Dirac's theory to the case of a (spin- $1/2$) particle with an electric charge q, moving in a classically-described electromagnetic field, may be obtained using the same replacement (90). As a result, Eq. (95) turns into

$$\left[c\hat{\boldsymbol{\alpha}}\cdot(-i\hbar\nabla-q\mathbf{A})+mc^2\hat{\beta}+(q\phi-\hat{H})\right]\Psi=0 \tag{9.7.1}$$

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

$$\left\{c^2[\hat{\boldsymbol{\alpha}}\cdot(-i\hbar\nabla-q\mathbf{A})]^2+\left(mc^2\right)^2-c[\hat{\boldsymbol{\alpha}}\cdot(-i\hbar\nabla-q\mathbf{A}),(q\phi-\hat{H})]-(q\phi-\hat{H})^2\right\}\Psi=0. \tag{9.7.2}$$

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

$$[\hat{\boldsymbol{\alpha}}\cdot(-i\hbar\nabla-q\mathbf{A})]^2\equiv(-i\hbar\nabla-q\mathbf{A})^2-2q\hat{\mathbf{S}}\cdot\nabla\times\mathbf{A} \tag{9.7.3}$$

But the last vector product on the right-hand side is just the magnetic field - see, e.g., Eqs. (3.21):

$$\mathscr{B}=\nabla\times\mathbf{A}. \tag{9.7.4}$$

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

$$\mathscr{E}=-\nabla\phi-\frac{\partial\mathbf{A}}{\partial t}, \tag{9.7.5}$$

to simplify the commutator participating in Eq. (9.113):

$$[\hat{\boldsymbol{\alpha}}\cdot(-i\hbar\nabla-q\mathbf{A}),(q\phi-\hat{H})]\equiv-q\hat{\boldsymbol{\alpha}}\cdot[\hat{H},\mathbf{A}]-i\hbar q\hat{\boldsymbol{\alpha}}\cdot[\nabla,\phi]\equiv-i\hbar q\frac{\partial\mathbf{A}}{\partial t}-i\hbar\hat{\boldsymbol{\alpha}}\cdot\nabla\phi\equiv i\hbar q\hat{\boldsymbol{\alpha}}\cdot\mathscr{E} \tag{9.7.6}$$

As a result, Eq. (113) becomes

$$\left\{c^2(-i\hbar\nabla-q\mathbf{A})^2+(q\phi-\hat{H})^2-\left(mc^2\right)^2-2qc^2\hat{\mathbf{S}}\cdot\mathscr{B}+i\hbar cq\hat{\boldsymbol{\alpha}}\cdot\mathscr{E}\right\}\Psi=0 \tag{9.7.7}$$

So far, this is an exact result, equivalent to Eq. (112), but it is more convenient for an analysis of the low-energy limit, in which not only the energy offset $E-mc^2$ (which is just the energy used in the non-relativistic 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

$$\hat{\tilde{H}}\equiv\hat{H}-mc^2\hat{I}. \tag{9.7.8}$$

we may approximate their difference, up to the first non-zero term, as

$$(q\phi\hat{I}-\hat{H})^2-\left(mc^2\right)^2\hat{I}\equiv\left(q\phi\hat{I}-mc^2\hat{I}-\hat{\tilde{H}}\right)^2-\left(mc^2\right)^2\hat{I}\approx 2mc^2(\hat{\tilde{H}}-q\phi\hat{I}). \tag{9.7.9}$$

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

$$\hat{\tilde{H}}\Psi=\left[\frac{1}{2m}(-i\hbar\nabla-q\mathbf{A})^2+q\phi-\frac{q}{m}\hat{\mathbf{S}}\cdot\mathscr{B}+\frac{i\hbar q}{2mc}\hat{\boldsymbol{\alpha}}\cdot\mathscr{E}\right]\Psi \tag{9.7.10}$$

Let us discuss this important result. The first two terms in the square brackets give the nonrelativistic Hamiltonian (3.26), which was extensively used in Chapter 3 for the discussion of charged particle motion. 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 $v<<c$, 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 because of being produced by relativistic effects - such as aligned spins of a permanent magnet.

The next, third term in the square brackets of Eq. (121) should be also familiar to the reader: this is the Pauli Hamiltonian - see Eqs. (4.3), (4.5), and (4.163). When justifying this form of interaction in Chapter 4, I referred mostly to the 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 the Zeeman effect in Sec. 6.4, the magnetic field effects on the orbital motion of an electron (described by the orbital angular momentum $\mathbf{L}$) and its spin $\mathbf{S}$ are of the same order, though quantitatively different.

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 a classical, spherical-symmetric electric field $\mathscr{E}$ corresponding to the potential $\phi(r)=U(r)/q$, this term may be reduced to Eq. (6.56):

$$\hat{H}_{\mathrm{so}}=\frac{1}{2m^2c^2}\hat{\mathbf{S}}\cdot\hat{\mathbf{L}}\frac{1}{r}\frac{dU}{dr}\equiv-\frac{q}{2m^2c^2}\hat{\mathbf{S}}\cdot\hat{\mathbf{L}}\frac{1}{r}\mathscr{E} \tag{9.7.11}$$

The proof of this correspondence requires a bit of additional work. [57] Indeed, in Eq. (121), the term responsible for the spin-orbit interaction acts on 4-component wavefunctions, while the Hamiltonian (122) is supposed to act on non-relativistic state vectors with an account of spin, whose coordinate representation may be given by 2 -component spinors:[58]

$$\psi=\begin{pmatrix}\psi_{\uparrow}\\ \psi_{\downarrow}\end{pmatrix}. \tag{9.7.12}$$

The simplest way to prove the equivalence of these two expressions is not to use Eq. (121) directly, but to return to the Dirac equation (112), for the particular case of motion in a static electric field but no magnetic field, when Dirac's Hamiltonian is reduced to

$$\hat{H}=c\hat{\boldsymbol{\alpha}}\cdot\hat{\mathbf{p}}+\hat{\beta}mc^2+U(\mathbf{r}),\qquad \text{with } U=q\phi. \tag{9.7.13}$$

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

$$\Psi(\mathbf{r},t)=\begin{pmatrix}\psi_{+}(\mathbf{r})\\ \psi_{-}(\mathbf{r})\end{pmatrix}\exp\left(-i\frac{E}{\hbar}t\right), \tag{9.7.14}$$

where each of $\psi_{\pm}$is a 2-component column of the type (123), representing two spin states of the particle (index $+$) and its antiparticle (index -). Plugging Eq. (125) into Eq. (95) with the Hamiltonian (124), and using Eq. (98a), we get the following system of two linear equations:

$$\left[E-mc^2-U(\mathbf{r})\right]\psi_{+}-c\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}\psi_{-}=0,\quad \left[E+mc^2-U(\mathbf{r})\right]\psi_{-}-c\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}\psi_{+}=0. \tag{9.7.15}$$

Expressing $\psi.$ from the latter equation, and plugging the result into the former one, we get the following single equation for the particle's spinor:

$$\left[E-mc^2-U(\mathbf{r})-c^2\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}\frac{1}{E+mc^2-U(\mathbf{r})}\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}\right]\psi_{+}=0. \tag{9.7.16}$$

So far, this is an exact equation for eigenstates and eigenvalues of the Hamiltonian (124), but it may be substantially simplified in the low-energy limit when both the potential energy [59] and the nonrelativistic eigenenergy

$$\widetilde{E}\equiv E-mc^2 \tag{9.7.17}$$

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

$$\frac{1}{E+mc^2-U(\mathbf{r})}\equiv\frac{1}{2mc^2+\widetilde{E}-U(\mathbf{r})}\equiv\frac{1}{2mc^2}\left[1+\frac{\widetilde{E}-U(\mathbf{r})}{2mc^2}\right]^{-1}\approx\frac{1}{2mc^2}\left[1-\frac{\widetilde{E}-U(\mathbf{r})}{2mc^2}\right], \tag{9.7.18}$$

in which Eq. (127) is reduced to

$$\left[\widetilde{E}-U(\mathbf{r})-\frac{\hat{p}^2}{2m}+\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}\frac{\widetilde{E}-U(\mathbf{r})}{(2mc^2)^2}\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}\right]\psi_{+}=0 \tag{9.7.19}$$

As Eqs. (5.34) shows, the operators of the momentum and of a function of coordinates commute as

$$[\hat{\mathbf{p}}, U(\mathbf{r})] = -i\hbar\nabla U, \tag{9.7.20}$$

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

$$\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}\frac{\widetilde{E}-U(\mathbf{r})}{(2mc)^2}\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}} \equiv \frac{\widetilde{E}-U(\mathbf{r})}{(2mc)^2}\hat{p}^2 - \frac{i\hbar}{(2mc)^2}(\hat{\boldsymbol{\sigma}}\cdot\nabla U)(\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}). \tag{9.7.21}$$

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

$$(\hat{\boldsymbol{\sigma}}\cdot\nabla U)(\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}) \equiv (\nabla U)\cdot\hat{\mathbf{p}} + i\hat{\boldsymbol{\sigma}}\cdot[(\nabla U)\times\hat{\mathbf{p}}]. \tag{9.7.22}$$

Of the two terms on the right-hand side of this relation, only the second one depends on spin, [60] giving the following spin-orbital interaction contribution to the Hamiltonian,

$$\hat{H}_{\mathrm{so}} = \frac{\hbar}{(2mc)^2}\hat{\boldsymbol{\sigma}}\cdot[(\nabla U)\times\hat{\mathbf{p}}] \equiv \frac{q}{2m^2c^2}\hat{\mathbf{S}}\cdot[(\nabla\phi)\times\hat{\mathbf{p}}]. \tag{9.7.23}$$

For a central potential $\phi(r)$, its gradient has only the radial component: $\nabla\phi = (d\phi/dr)\mathbf{r}/\mathrm{r} = -\delta\mathbf{r}/r$, and with the angular momentum definition (5.147), Eq. (134) is (finally!) reduced to Eq. (122).

As was shown in Sec. 6.3, the perturbative treatment of Eq. (122), together with the kineticrelativistic correction (6.47), in the hydrogen-like atom/ion problem, leads to the fine structure of each Bohr level E_n, given by Eq. (6.60):

$$\Delta E_{\text{fine}} = -\frac{2E_n}{mc^2}\left(3 - \frac{4n}{j+1/2}\right). \tag{9.7.24}$$

This result receives a confirmation from the surprising fact that for the hydrogen-like atom/ion problem, the Dirac equation may be solved exactly - without any assumptions. I would not have time/space to reproduce the solution, [61] and will only list the final result for the energy spectrum:

$$\frac{E}{mc^2} = \left\{1 + \frac{Z^2\alpha^2}{\left[n + \{(j+1/2)^2 - Z^2\alpha^2\}^{1/2} - (j+1/2)\right]^2}\right\}^{-1/2} \tag{9.7.25}$$

Here $n = 1, 2, \ldots$ is the same principal quantum number as in Bohr's theory, while j is the quantum number specifying the eigenvalues (5.175) of J^2, in our case of a spin- $1/2$ particle taking half-integer values: $j = l \pm 1/2 = 1/2, 3/2, 5/2, \ldots -$ see Eq. (5.189). This is natural, because due to the spin-orbit interaction, the orbital momentum and spin are not conserved, while their vector sum, $\mathbf{J} = \mathbf{L} + \mathbf{S}$, is $-$ at least in the absence of an external field. Each energy level (136) is doubly-degenerate, with two eigenstates representing two directions of the spin. (In the low-energy limit, we may say: corresponding to two values of $l = j \mp 1/2$, at fixed j.)

Speaking of that limit (when $E - mc^2 \sim E_{\mathrm{H}} < mc^2$): since according to Eq. (1.13) for E_{H}, the square of the fine-structure constant $\alpha \equiv e^2/4\pi\varepsilon_0\hbar c$ may be represented as the ratio E_{H}/mc^2, we may follow this limit expanding Eq. (136) into the Taylor series in $(Z\alpha)^2 << 1$. The result,

$$E \approx mc^2\left[1 - \frac{Z^2\alpha^2}{2n^2} - \frac{Z^4\alpha^4}{2n^4}\left(\frac{n}{|j+1/2|} - \frac{3}{4}\right)\right], \tag{9.7.26}$$

has the same structure, and allows the same interpretation as Eq. (92), but with the last term coinciding with Eq. (6.60) - and with experimental results. Historically, this correct description of the fine structure of the atomic levels provided the 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 annihilation of particle-antiparticle pairs by an energy influx higher than $2mc^2$, the number of particles participating in high-energy interactions is not fixed. An adequate general description of such situations is given by the quantum field theory, in which the particle's wavefunction is treated as a field to be quantized, using so-called field operators $\hat{\Psi}(\mathbf{r}, t) -$ very much similar to the electromagnetic field operators (16). The Dirac equation follows from such theory in the single-particle approximation.

As was mentioned above on several occasions, the quantum field theory is well beyond the time/space limits of this course, and I have to stop here, referring the interested reader to one of several excellent textbooks on this discipline. [62] However, I would strongly encourage the students going in this direction to start by playing with the field operators on their own, taking clues from Eqs. (16), but replacing the creation/annihilations operators $\hat{a}_j^\dagger$ and $\hat{a}_j$ of the electromagnetic field oscillators with those of the general second quantization formalism outlined in $\mathrm{Sec}. 8.3$.

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[55] This difference may be traced by classical means - see, e.g., EM Sec. 5.1.

[56] Note that in this result, the g-factor of the particle is still equal to exactly 2 - see Eq. (4.115) and its discussion in Sec. 4.4. In order to describe the small deviation of g_{e} from 2 , the electromagnetic field should be quantized (just as this was discussed in Secs. 1-4 of this chapter), and its potentials $\mathbf{A}$ and ϕ, participating in Eq. (121), should be treated as operators - rather than as c-number functions as was assumed above.

[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{\boldsymbol{\alpha plays the role of the velocity operator, so that the expectation values of the term } } are of the order of $\hbar q v \varepsilon / 2 m c^2$. Since the expectation values of the operators participating in the Hamiltonian (122) scale as $S \sim \hbar / 2$ and $L \sim m v r$, the spin-orbit interaction energy has the same order of magnitude.

[58] In this course, the notion of spinor (popular in some textbooks) was not used much; it was introduced earlier only for two-particle states - see Eq. (8.13). For a single particle, such definition is reduced to $\psi(\mathbf{r})|s\rangle$, whose representation in a particular spin-1/2 basis is the column (123). Note that such spinors may be used as a basis for an expansion of the spin-orbitals $\psi_j(\mathbf{r})$ defined by Eq. (8.125), where the index j is used for numbering both the spin's orientation (i.e. the particular component of the spinor's column) and the orbital eigenfunction.

[59] Strictly speaking, this requirement is imposed on the expectation values of $U(\mathbf{r})$ in the eigenstates to be found.

[60] The first term gives a small spin-independent energy shift, which is very difficult to verify experimentally.

[61] Good descriptions of the solution are available in many textbooks (the older the better :-) - see, e.g., Sec. 53 in L. Schiff, Quantum Mechanics, 3[rd] ed., McGraw-Hill (1968).

[62] For a gradual introduction see, e.g., either L. Brown, Quantum Field Theory, Cambridge U. Press (1994) or R. Klauber, Student Friendly Quantum Field Theory, Sandtrove (2013). On the other hand, M. Srednicki, Quantum Field Theory, Cambridge U. Press (2007) and A. Zee, Quantum Field Theory in a Nutshell, 2[nd] ed., Princeton (2010), among others, offer steeper learning curves.
