Abstract  In this chapter, the tools to be used in the theoretical derivations provided later in this book are summarized. These include relativistic kinematics, perturbation, and quantum scattering theories and Dirac’s equation.

Contents

2.1 Introduction ................................................. 9
2.2 Physical Units ............................................. 11
2.3 Mathematical Notations .................................. 11
  2.3.1 Vector Notation ........................................ 11
  2.3.2 Complex Conjugation ................................. 12
  2.3.3 Hermitian Conjugation ............................... 12
  2.3.4 Adjoint Operator ...................................... 12
2.4 Relativistic Kinematics of a Two-Body  
  Elastic Collision .......................................... 12
  2.4.1 Introduction .......................................... 12
  2.4.2 Kinetic Energy of the Recoil Particle ............ 13
  2.4.3 Kinetic Energy of the Scattered Projectile ....... 14
2.5 Time-Dependent Perturbation Theory ................. 15
  2.5.1 Introduction .......................................... 15
  2.5.2 Transition Rate ...................................... 16
2.6 Quantum Scattering Theory ............................. 19
  2.6.1 Introduction .......................................... 19
  2.6.2 Scattering Amplitude ............................... 20
  2.6.3 Scattering Cross Sections ......................... 23
  2.6.4 Phase-Shift Analysis ............................... 24
  2.6.5 Optical Theorem ..................................... 27
2.7 Dirac’s Equation ......................................... 28
  2.7.1 Introduction .......................................... 28
  2.7.2 Derivation of Dirac’s Equation .................... 29

2.1 Introduction

The absorbed doses received by the tissues and organs of the nuclear medicine patient are the culmination of a series of physical phenomena\(^1\) as shown diagrammatically in Fig. 2.1. The three theoretical tools which to be used in the description of such processes are categorized as:

- Kinematics
- Theory of quantum transitions (perturbation and scattering)
- Dirac relativistic theory

These phenomena are taken to be the simplified culmination of four steps:

Step 1: This is the production of the radioactive substance itself through, for example, the fission of uranium within a reactor following the absorption of a neutron (e.g., to produce \(^{99}\text{Mo}\) which subsequently undergoes decays to produce the isomer \(^{99m}\text{Tc}\)) or the charged-particle bombardment of a nucleus to produce a radioactive daughter (such as in the charge exchange reaction of \(^{18}\text{O}(p,n)^{18}\text{F}\) to form the \(^{18}\text{F}\) used in PET imaging). Clearly, a complete understanding of radioisotope production requires knowledge of both the kinematics of the nuclear reaction and the quantum-mechanically derived probability of the reaction occurring.

\(^1\)Following the absorbed dose, biological effects occur which lead to the risk associated with the magnitude and type of radiation dose and the intrinsic radiosensitivity of the tissue irradiated.
Step 2: This series is the in vivo physical decay of the radioactive nucleus. For diagnostic nuclear medicine, the expectation is that the decay produces either a single photon (as with $^{99m}$Tc) or a positron, the anti-particle of the electron, which travels a short distance in tissue before annihilating with an atomic electron to produce two (sometimes, one or three) photons. The photons resulting from radioactive decay are detected externally and then used to form the diagnostic nuclear medicine image. On the other hand, therapeutic nuclear medicine seeks to deliver a high radiation dose to neoplasia and this is most easily achieved by the decay producing a short-ranged charged particle such as an $\alpha$ particle or an Auger/Coster–Krönig electron, either as a direct result of the decay or following atomic relaxation processes induced by the decay. Here, one needs to understand the requirements of an unsteady balance between nuclear mass and charge or the mechanisms through which internal degrees of freedom, such as angular momentum in a spinning nucleus, can couple to external emissions of energy, such as photons, and the relativistic theory of Dirac in explaining the production and existence of the positron. Again, the probability of a quantum event must be evaluated.

Step 3: The third step is a consequence of the interaction of a produced photon with matter and can be divided into two categories in terms of whether or not the photon transfers energy to the medium within which it is traveling. In classical Thomson scatter, for example, the photon does not transfer energy to an atomic electron, but its direction of travel is altered which, while not leading to energy deposition in tissue, can be important to calculating the transport of radiation in the body. A category of interactions in which energy is transferred to the medium can be further subdivided into subcategories of whether or not the photon is conserved. The process of Compton scatter, in which a fraction of the incident photon’s energy is transferred to an electron which recoils and the photon is scattered with a reduced energy, retains the photon. On the other hand, a photon can be absorbed by an atomic electron, thus transferring its energy to the electron which is then ejected if the photon energy exceeds the binding energy. Should the photon have an energy exceeding twice the electron rest-mass (plus a little more to allow for nuclear recoil – refer to the Appendices), it can interact with the nuclear electromagnetic field to produce an electron–positron pair. In both of these cases, the abilities to calculate the probabilities of the interaction occurring, their physical observables (differential cross sections) and the kinematics of the process are necessary in order to solve the dosimetry problem.

Step 4: The final step, is the transfer of the secondary charged particle’s kinetic energy to the medium as it slows down to be eventually thermalized. This transferred energy, per unit mass of medium, is the absorbed dose that we seek to eventually calculate. The probability and kinematics of energy transfer as a function of charged particle can, depending upon the particular scenario, be calculated classically or through quantum theory.
2.2 Physical Units

The question of units is inevitably contentious as consensus within the community appears to be perpetually unattainable! However, over the past 30 years, the Système International d’Unités (SI) system\(^2\) has become dominant in the practice of medical radiation dosimetry. Correspondingly, this book will use the SI system in order to maintain as much consistency as possible with the definitions of physical constants provided in the literature.\(^3\) Unfortunately, this exclusivity may have the potential to cause some difficulty and confusion for the reader who is more familiar with Gaussian/“natural” units favored by some (e.g., \(\hbar = c = 1\)) which provide time and distance with units of length and momentum in units of inverse length. Admittedly, the use of such units can make the derivations of some equations somewhat more transparent, but one should be reluctant to risk the loss of cohesion by switching systems of units within a text linking microscopic and macroscopic dosimetry theory. However, having said that, in order to ensure clarity of the expressions derived here, the rest-mass and three-vector momentum of a particle are implicitly assumed to be given in units of energy. In other words, instead of writing the total energy of a moving particle as \(E = \sqrt{p^2c^2 + m^2c^4}\) we will write it as \(E = \sqrt{p^2 + m^2}\). For example, the rest-mass of the electron will be given as \(m_e = 511\) keV. This reduces the plethora of powers of \(c\) which often appear in expressions, but at the slight cost of the frequent use of the conversion factor, \(\hbar c = 197.33\) MeV \(\cdot\) fm.

Frequent use of the definitions of the fine structure constant \(\alpha = e^2/4\pi\varepsilon_0\hbar c\) and the classical radius of the electron \(r_0 = e^2/4\pi\varepsilon_0 m_e c^2\) will be made throughout the text in order to simplify expressions and still retain transparency. For example, as a result of these, the magnitude of the electric field due to a point charge \(e\) will be written in the succinct form as,

\[
E(r) = \frac{\alpha e c}{r}. \quad (2.1)
\]

2.3 Mathematical Notations

2.3.1 Vector Notation

Three-component vectors are denoted in bold. If \(\mathbf{x}\) is a three-component vector, then the corresponding unit vector is,

\[
\mathbf{\hat{x}} = \frac{\mathbf{x}}{|\mathbf{x}|}. \quad (2.2)
\]

A four-component vector is denoted in bold italics, e.g., \(\mathbf{X}\). The contravariant components are denoted by superscripts whereas the covariant components are denoted by subscripts. For example,

\[
X^\mu \equiv (x^0, x^1, x^2, x^3) \equiv (x^0, \mathbf{x}). \quad (2.3)
\]

The covariant and contravariant components are related through,

\[
X_\mu = \sum_{\nu=0}^{3} g_{\mu\nu} X^\nu \quad (2.4)
\]

where the metric tensor is,

\[
g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (2.5)
\]

Hence,

\[
X_\mu = (x^0, -\mathbf{x}). \quad (2.6)
\]

The summation convention will be used in which, when an identical superscript and subscript occur, the components are summed over that superscript/subscript. That is,

---


\(^3\)An inconsistency will be admitted with respect to interaction coefficients such as attenuation coefficients and stopping powers where this book will use cgs units (e.g., the photon mass attenuation coefficient has units of square centimeter per gram). These are simply more practical and virtually all numerical tabulations of such quantities are provided in these units.
\[ p_{\mu}X^\mu \equiv \sum_{\mu=0}^{3} p_\mu X^\mu. \] (2.7)

In the event that no ambiguity can arise, this summation will be simplified by omitting the indices so as to write \( p_\mu X^\mu \equiv pX. \) Note also that,

\[ p_\mu X^\mu = p^0 x^0 - p \cdot x. \] (2.8)

The four-vector momentum for a particle of rest-mass \( m \) is,

\[ p^\mu = (E, p) \] (2.9)

where \( E \) is the total energy (sum of kinetic energy and rest-mass) and \( p \) is the three-vector momentum. From the above,

\[ p \cdot p = E^2 - p \cdot p = m^2 \] (2.10)

and, hence, is an invariant. The product of the four-vector momenta of two distinguishable particles A and B is,

\[ p_A \cdot p_B = E_A E_B - p_A \cdot p_B. \] (2.11)

### 2.3.2 Complex Conjugation

Let \( z = x + iy \) be a complex variable. Its complex conjugate is denoted by,

\[ z^* = x - iy. \] (2.12)

### 2.3.3 Hermitian Conjugation

Let \( M \) be a matrix with complex elements \( (M)_{ij} = m_{ij}. \) The Hermitian conjugate of this matrix is denoted by \( M^\dagger \) where \( (M^\dagger)_{ij} = m_{ji}^*. \) That is, the Hermitian conjugate is the transpose of the original matrix and with the elements replaced by their complex conjugates. If \( M = M^\dagger, \) the matrix is referred to as being Hermitian or self-adjoint.

### 2.3.4 Adjoint Operator

The adjoint of the spinor \( \psi(r, t) \) is,

\[ \bar{\psi}(r, t) = \psi^\dagger(r, t) \gamma^0 \] (2.13)

where \( \gamma^0 \) is a Dirac matrix, to be defined later in this chapter.

### 2.4 Relativistic Kinematics of a Two-Body Elastic Collision

#### 2.4.1 Introduction

As summarized above, the absorbed dose to a medium exposed to radiation is due to the transfer of the kinetic energy of a charged particle to the medium as it slows down. For the charged particles and kinetic energies of interest to nuclear medicine, these energy transfers are predominantly through interactions with atomic electrons. The kinematics of the scattered projectile and recoil target resulting from these interactions are the subject of this subsection.

An elastic scatter between two bodies is that in which the sum of the kinetic energies of the bodies pre- and postcollision is the same. There are no internal degrees of freedom present (such as atomic or nuclear excitation) that can channel away kinetic energy and transfer it to potential energy. Figure 2.2 shows a two-body scatter in which a particle of rest-mass \( m_1, \) total energy \( E_1, \) three-vector momentum \( p_1 \) and kinetic energy \( T_1 \) is incident to a particle at rest in the laboratory reference frame with a rest-mass \( m_2. \) The pre- and postcollision four-vector momenta of the particles are,

\[ p_1 = (E_1, p_1) \] (2.14)

\[ p_2 = (m_2, 0) \] (2.15)

\[ p'_1 = (E'_1, p'_1) \] (2.16)

\[ p'_2 = (E'_2, p'_2). \] (2.17)
2.4.2 Kinetic Energy of the Recoil Particle

2.4.2.1 Derivation

The conservation of four-vector momenta in the scatter of Fig. 2.2 is,

\[ p_1 + p_2 = p'_1 + p'_2 \]  

(2.18)

By isolating and squaring the four-vector momentum of the scattered particle and recalling its invariance,

\[ p'_1^2 = (p_1 + p_2 - p'_2)^2 \]

\[ m_1^2 = m_1^2 + 2m_2^2 + 2(p_1 \cdot p_2 - p_1' \cdot p_2' - p_2' \cdot p_2'). \]  

(2.19)

After further algebraic manipulation,

\[ p_1 p'_2 \cos \phi = (E'_2 - m_2)(E_1 + m_2). \]  

(2.20)

Solving for the total energy of the recoil particle,

\[ E'_2 = m_2 \frac{(E_1 + m_2)^2 + p_1^2 \cos^2 \phi}{(E_1 + m_2)^2 - p_1^2 \cos^2 \phi} \]  

(2.21)

and the corresponding kinetic energy \( T'_2 = E'_2 - m_2 \) is,

\[ T'_2 = 2m_2 \frac{p_1^2 \cos^2 \phi}{(E_1 + m_2)^2 - p_1^2 \cos^2 \phi}. \]  

(2.22)

2.4.2.2 Maximum Recoil Kinetic Energy

Equation (2.22) provides the kinetic energy of the recoil particle as a function of the recoil particle’s mass, the incident projectile’s total energy and momentum and the recoil angle, \( \phi \). In many instances, we will be interested in only the maximum recoil kinetic energy (i.e., the maximum energy transferred). This will clearly occur for the condition of \( \phi = 0 \),

\[ T'_{2,\text{max}} = 2m_2 \frac{p_1^2}{m_1^2 + m_2^2 + 2m_2 \sqrt{p_1^2 + m_1^2}}. \]  

(2.23)

Massive Projectile and Light Target

For the case of a heavy incident particle incident to a light particle, \( m_1 \gg m_2 \), (e.g., a proton projectile and an electron target), (2.23) reduces to the following expression,

\[ T'_{2,\text{max}} \approx \frac{2p_1^2}{(m_1^2/m_2^2) + 2 \sqrt{p_1^2 + m_1^2}} \]  

(2.24)

for \( m_1 \gg m_2 \).
For the combination of a massive projectile and light target, we are able to consider two further conditions of the projectile momentum. For the case of the projectile having a high incident three-vector momentum such that \( p_1 \gg (m_1^2/m_2) \), this result reduces considerably to,

\[
T_{2,max}' \approx p_1 \\
\approx T_1 \quad \text{for } m_1 \gg m_2, p_1 \gg (m_1^2/m_2).
\]

Thus, even though the projectile is much more massive than the target, it is possible for all of the projectile’s kinetic energy to be transferred to the target should the incident projectile be relativistic. On the other hand, considering the case of a low incident three-vector momentum \( p_1 \ll (m_1^2/m_2) \), for which the above result becomes,

\[
T_{2,max}' \approx 2m_2 \left( \frac{p_1}{m_1} \right)^2 \\
= 2m_2 \gamma_1^2 \beta_1^2 \quad \text{for } m_1 \gg m_2, p_1 \ll (m_1^2/m_2).
\]

**2.4.3 Kinetic Energy of the Scattered Projectile**

There will also be interest in the kinetic energy of the scattered projectile which, in terms of radiation transport, provides us with the knowledge of how much energy remains to be transferred to the medium at a distance from the collision. The spatial resolution explored by a scattering reaction will be inversely proportional to the bombarding particle’s momentum, as follows from the reduced de Broglie wavelength \( \lambda = \hbar c/p \). For example, an electron with a kinetic energy of 1 GeV has a de Broglie wavelength of about 0.2 fm, which is of the order of 10% of the nuclear dimension making such high-energy electrons useful for probing the nucleus and elucidating understanding of its size and spatial structure, as will be shown in Chap. 3.

To evaluate the scattered projectile’s kinetic energy,
\[ p_1'p_2' = p_1(p_1 + p_2 - p_1') \]
\[ = p'_1(p_1 + p_2 - p_1') \]
\[ = p'_1(p_1 + p_1'p_2' - m_1^2). \quad (2.29) \]

Expanding,
\[ E_1m_2 = E_1'p_1 + p_1'p_2 - p_1'. \quad (2.30) \]

Assume that the projectile is an electron with a de Broglie wavelength smaller than nuclear dimensions thus requiring the electron to be highly relativistic or,
\[ E_1m_2 \approx E_1'E_1 + E_1'm_2 - E_1'E_1 \cos \theta. \quad (2.31) \]

Rearranging and solving for the scattered projectile’s total energy,
\[ E_1'(\theta) = \frac{E_1}{1 + \left(\frac{E_1}{m_2}\right)(1 - \cos \theta)}. \quad (2.32) \]

Figure 2.3 shows the ratio of the kinetic energy of the scattered projectile to that prior to the interaction for an electron projectile \((E_1)\) incident to light \((1\text{H})\) and heavy \((^{208}\text{Pb})\) nuclear targets \((m_2)\) as a function of scattering angle for 1 and 10 GeV electrons, the combinations satisfying the above kinematic requirements. For a head-on scatter of \(\theta = 0\), the scattered energy equals that of that incident, a result independent of the mass of the target should the projectile be relativistic. No energy is transferred to the target as a result, which is of little interest. However, the differences in the angular variations of the scattered energy with scattering angle for a relativistic projectile as functions of projectile energy and target mass are certainly of interest and reflect the role of the target mass. For the two cases of the two electron energies of 1 and 10 GeV incident to the \(^{208}\text{Pb}\) target, the target mass is much greater than the total incident energy \(m_2 \gg E_1\) \((m_2 \approx 208 \text{ GeV})\) and the functional dependence upon the scattering angle is suppressed due to the \(E_1/m_2\) factor in the denominator. In other words, for the heavy Pb target, relatively little kinetic energy is taken up by the recoil nucleus, \(E_1'(0)/E_1 \approx 1\) over all scattering angles, and there is little difference in this feature between 1 and 10 GeV electrons. On the other hand, there is a greater dependence of the scattered projectile energy upon scattering angle for the ultrarelativistic electron incident to the relatively light target of a proton. This is indicative of the greater propensity of the light target nucleus to acquire a greater amount of the projectile’s kinetic energy.

### 2.5 Time-Dependent Perturbation Theory

#### 2.5.1 Introduction

In this book, frequent examinations of conditions under which a given quantum state makes a transition to another distinguishable quantum state will be made. The most pertinent examples will be the transition of a radioactive nucleus from one state to another. In such cases, the energy differential between the pre- and posttransition states is manifest in the emission of an energetic particulate radiation (\(\alpha\) particles, electrons or positrons), or electromagnetic radiation (photons), which are the essence of nuclear medicine. Fundamental to the study of such transitions is the ability to calculate the probability per unit time of these transitions occurring. For the examples to be considered in this book, this probability (i.e., the transition rate) is calculated using time-dependent perturbation theory.
2.5.2 Transition Rate

In this section, we will derive the transition rate which is the probability per unit time for a given transition to occur. Consider a basic system which is initially in steady-state but then perturbed by a small time-dependent potential. This perturbation induces the quantum system to a new state and we wish to calculate the probability with which this can occur. The calculation begins with the definition of the total Hamiltonian of the system as,

\[ H = H_0 + \lambda U(t) \quad (2.33) \]

where \( H_0 \) is the steady-state Hamiltonian and \( U(t) \) is the time-dependent perturbation noted above. For calculational purposes, a dimensionless weighting parameter \( \lambda \) is explicitly applied to the perturbation as it will be used later in a power-series expansion in this derivation. We now consider Schrödinger’s description of this quantum state. Schrödinger’s equation for the steady-state component (i.e., without the perturbation) is,

\[ i\hbar \frac{\partial \Psi_0}{\partial t} = H_0 \Psi_0 \quad (2.34) \]

for which the solution can be written as,

\[ \Psi_0 = \sum_k a_{k,0} \psi_k e^{-\frac{E_k t}{\hbar}} \quad (2.35) \]

where \( a_{k,0} \) are constants. As the eigenstates \( \psi_k \) form a complete set, the solution for the complete Hamiltonian (i.e., for the combined steady and perturbed state) is,

\[ \Psi = \sum_k a_k(t) \psi_k e^{-\frac{E_k t}{\hbar}} \quad (2.36) \]

where,

\[ a_k(t = 0) \equiv a_{k,0} \quad (2.37) \]

The coefficients are such that \( |a_k(t)|^2 \) represents the probability of finding the system in the \( k^{th} \)-state at time \( t \). These coefficients can be found by substituting the wavefunction into the Schrödinger equation to give,

\[ i\hbar \left[ \sum_k \left( \frac{da_k(t)}{dt} \psi_k e^{-\frac{E_k t}{\hbar}} - \frac{E_k}{\hbar} a_k(t) \psi_k e^{-\frac{E_k t}{\hbar}} \right) \right] = (H_0 + \lambda U(t)) \sum_k a_k(t) \psi_k e^{-\frac{E_k t}{\hbar}} \]

\[ = (H_0 + \lambda U(t)) \sum_k a_k(t) \psi_k e^{-\frac{E_k t}{\hbar}} \quad (2.38) \]

Isolating the term associated with the free Hamiltonian from that of the perturbation gives

\[ \sum_k a_k(t) E_k \psi_k e^{-\frac{E_k t}{\hbar}} = H_0 \sum_k a_k(t) \psi_k e^{-\frac{E_k t}{\hbar}} \quad (2.39) \]

\[ i\hbar \sum_k \frac{da_k(t)}{dt} \psi_k e^{-\frac{E_k t}{\hbar}} = \lambda \sum_k U(t) a_k(t) \psi_k e^{-\frac{E_k t}{\hbar}}. \]

\[ (2.40) \]

Ignore the trivial result of (2.39) and instead examine the effect of the perturbation upon the system as described by (2.40). For ease of presentation, the Dirac notation is used so that by multiplying both sides of (2.40) by the bra \( \langle \psi_f | \) and by the ket \( | \psi_f \rangle \) and integrating over space, gives,

\[ i\hbar \sum_k \int d^3r \frac{da_k(t)}{dt} \langle \psi_f | \psi_k \rangle e^{-\frac{E_k t}{\hbar}} \]

\[ = \lambda \sum_k \int d^3r \langle \psi_f | U(t) | \psi_k \rangle a_k(t) e^{-\frac{E_k t}{\hbar}}. \]

\[ (2.41) \]

Using the orthonormality of states, \( \langle \psi_n | \psi_m \rangle = \delta_{mn} \), we have

\[ i\hbar \frac{da_k}{dt} e^{-\frac{E_k t}{\hbar}} = \lambda \sum_k U_{fk}(t) a_k(t) e^{-\frac{E_k t}{\hbar}}. \]

\[ (2.42) \]

where the matrix element is simplified to,

\[ U_{fk}(t) \equiv \langle \psi_f | U(t) | \psi_k \rangle \]

\[ (2.43) \]

Rearranging this result,

\[ \frac{da_k}{dt} = -\frac{i}{\hbar} \lambda \sum_k U_{fk}(t) a_k(t) e^{-\frac{i E_k t}{\hbar}}. \]

\[ (2.44) \]
\[ \omega_{nk} \equiv \frac{E_f - E_k}{\hbar}. \quad (2.45) \]

Essential to this derivation is the assumption that the strength of the perturbation is weak so as to allow the coefficients \( a_k(t) \) to be expanded in a power-series in \( \lambda \),

\[ a_k(t) = \sum_{m=0}^{\infty} \lambda^m a_{k,m}(t). \quad (2.46) \]

Substituting this expansion into (2.44) gives,

\[ \sum_{m=0}^{\infty} \lambda^m \frac{d a_{k,m}(t)}{dt} = 0 \quad (2.47) \]

Then, by equating coefficients of equal powers of \( \lambda \),

\[ \frac{d a_{k,0}(t)}{dt} = 0 \quad (2.48) \]

and

\[ \frac{d a_{k,m}(t)}{dt} = -\frac{i}{\hbar} \sum_k U_{k}(t) \lambda^{m+1} a_{k,m-1}(t) e^{i\omega_k t}. \quad (2.49) \]

In order to use these results to calculate the coefficients, assume that the perturbing potential is “switched on” at time \( t = 0 \) and remains constant for \( t > 0 \),

\[ U(t) = U_0 H(t) \quad (2.50) \]

where \( H(t) \) is the Heaviside function. Further assume that the system is in a single and well-defined state \( |\psi_i\rangle \) before the potential is “switched” on,

\[ |a_{i,0}|^2 = 1. \quad (2.51) \]

The remaining coefficients at time \( t \) are then found by integrating (2.49) where, as \( \lambda \) has been previously defined as small, the calculation need only be limited to first order \( m = 1 \),

\[ a_{f,1}(t) = -\frac{i}{\hbar} \int_0^t dt' M_{fi} e^{i\omega_{fi} t'} \]

\[ = -\frac{i}{\hbar} M_{fi} \int_0^t dt' e^{i\omega_{fi} t'} \quad (2.52) \]

where,

\[ M_{fi} = \langle \psi_f | \psi_i \rangle U_0. \quad (2.53) \]

The probability that a transition will be made from state \( |\psi_i\rangle \) to state \( |\psi_f\rangle \) at time \( t \) is the squared modulus of (2.52),

\[ P_{fi}(t) = |a_{f,1}(t)|^2 = 2 \frac{|M_{fi}|^2}{\hbar^2} \left( 1 - \frac{\cos \omega_{fi} t}{\omega_{fi}^2} \right) \quad (2.54) \]

The function \( B(\omega, t) \), which is plotted in Fig. 2.4, is sharply peaked at \( \omega = 0 \) and the sharpness of this peak increases with \( t \). Thus the probability of a transition is greater for a reduced energy difference between the two states.

In many cases of interest, there will in fact be an ensemble of neighboring states around \( |\psi_i\rangle \) with energies around \( E_f \). The transition probability is then determined by integrating over this ensemble of energies,

\[ P_{fi}(t) = \frac{2}{\hbar^2} \int_{-\infty}^{\infty} dE_f |M_{fi}|^2 B(\omega_{fi}, t) \rho_f \quad (2.55) \]

where the number density of states is,

\[ \rho_f = \frac{dN}{dE_f} (E_f). \quad (2.56) \]

This can be integrated simply if it is assumed that the matrix element \( M_{fi} \) and the density of states are
reasonably constant over the region where $B(\omega_{\gamma i}, t)$ is significant, thus allowing them to be extracted from the integral,

$$
\mathcal{P}_{\gamma i}(t) = \frac{2}{\hbar^2 |M_{\gamma i}|^2 \rho_f} \int dE_f B(\omega_{\gamma i}, t)
$$

$$
= \frac{2}{\hbar} |M_{\gamma i}|^2 \rho_f \int_{-\infty}^{\infty} d\omega_f \frac{(1 - \cos \omega_{\gamma i} t)}{\omega_{\gamma i}^2}.
$$

The integral is solved by the substitution of the variable, $y = \omega_f - \omega_i$, to give

$$
\int_{-\infty}^{\infty} d\omega_f \frac{(1 - \cos \omega_{\gamma i} t)}{\omega_{\gamma i}^2} = 2t \int_{-\infty}^{\infty} dy \frac{(1 - \cos yt)}{y^2}. \tag{2.58}
$$

It is straightforward to solve this integral by parts to yield,

$$
\int_{-\infty}^{\infty} dy \frac{(1 - \cos yt)}{y^2} = 2t \int_{0}^{\infty} dy \frac{\sin yt}{y} = \pi t. \tag{2.59}
$$

The probability of the transition is now,

$$
\mathcal{P}_{\gamma i}(t) = \frac{2}{\hbar} |M_{\gamma i}|^2 \rho_f. \tag{2.61}
$$

The transition rate is the probability of the transition occurring per unit time,

$$
\lambda_{\gamma i} = \frac{d\mathcal{P}_{\gamma i}}{dt}. \tag{2.62}
$$

or,

$$
\lambda_{\gamma i} = \frac{2\pi}{\hbar} |M_{\gamma i}|^2 \rho_f. \tag{2.63}
$$

This result is known as Fermi’s Golden Rule Number 2.

Equation (2.63) describes a first-order process and, under some conditions, can yield a zero result. One must account for second-order processes as a result. Consider, for example, the elastic scatter of a photon by a free electron at rest (Compton scatter). There are two scenarios in this interaction. In the first, the primary photon is absorbed by the electron and a
secondary photon with a reduced energy (corresponding to that scattered) is emitted, with the energy difference appearing as the electron’s recoil kinetic energy. In the second scenario, the secondary photon is emitted by the electron and the primary photon is subsequently absorbed. In order to manage such a combination of processes, (2.63) is rearranged to give,

$$\lambda_{fi} = \frac{2\pi}{\hbar} \sum_{n'} \frac{M_{f'n'} M_{i'n'}}{E_i - E_{n'}} \rho_f$$

(2.64)

where the intermediate state of $n'$ differs from the initial and final states by one photon. Equation (2.64), also known as Fermi’s Golden Rule Number 1, allows for the two cases of the absorption of a photon by an electron followed by the emission of a photon or that of the emission of a photon followed by the absorption of a photon.

### 2.6 Quantum Scattering Theory

#### 2.6.1 Introduction

As shown in the diagram of Fig. 2.1, the absorbed dose is the ultimate consequence of the interactions of particles and radiation fields with matter. Photons, in the form of X or γ rays, interact with atomic electrons and nuclei and are absorbed, scattered or, if sufficiently energetic, generate an electron–positron pair through coupling with the nuclear electromagnetic field. On a more fundamental level, the scattering of charged particles sets additional charged particles moving into the medium. In all of these cases, the outcome of the interaction is that an electron or positron is set into motion. As this charged particle moves through the medium, it loses kinetic energy through interactions with matter, the main ones of interest to us being those collisions with atomic electrons individually, with the ensemble of electrons or through violent deflections from its trajectory by the nuclear Coulomb field resulting in the emission of radiation. It is also possible for the charged particle to interact with matter but without the transfer of energy, e.g., elastic Coulomb scattering. Many of the derivations to be faced will be involve understanding the interactions of photons, electrons, and positrons with the medium that they travel through. This subsection develops quantum-mechanical descriptions of how projectiles (photons or particulate) interact with the medium through which they travel.

A quantum-mechanical Hamiltonian can have both discrete and continuous eigenvalues, unlike the classical Hamiltonian which has only continuous eigenvalues. The discrete eigenvalues correspond to bound states of a system which are consequences of an attractive interaction potential confining the system of particles to within a finite volume, the Schrödinger equation in this case being,

$$H \Psi_n = E_n \Psi_n$$

(2.65)

with energy eigenvalues $E_n$ and eigenfunctions $\Psi_n$ for the Hermitian Hamiltonian. In such cases, the wavefunctions of the bound particles decrease rapidly with growing inter-particle spacing. Continuous eigenvalues, on the other hand, correspond to unbound, or scattering, states in which the wavefunctions can extend asymptotically to infinity: an incident particle, modeled by a plane wave, is incident to a potential (e.g., the static Coulomb field of a nucleus) and is then scattered by the potential so that the final state is the combination of the incident and scattered wavefunctions. Whereas the discrete eigenfunction problem corresponds to a single and confined system, the continuous eigenfunction problem describes the interactions between two subsystems (here, the projectile and the target) which are not mutually bound states. The kinematics of a collision between a projectile and a target have been derived. These results provide only the energy and momentum of the two particles in the final state once a scattering or recoil angle has been defined. They do not shed any light on the likelihood of such a final state occurring. The scattering problem is that of interacting systems representing asymptotically-free states which must exist not just during the

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4Collision and scatter have been differentiated by some authors so that the former correspond to multi-channel final states and the latter was linked to a single channel final state. Such a distinction is not made here.
time interval about the collision but also for all time \((t \to \pm \infty)\). As with our previous derivation of perturbation theory, we will treat the Hamiltonian affecting the scattered system as the sum of a free-state Hamiltonian and that of a perturbing potential.

Ultimately, in the solution of the scattering problem, one is required to derive an observable, a physical quantity that can be measured in the laboratory, describing the probability of a given final postscattering state. Here, the observable will be the total cross section of the scatter which is the ratio of the relative decrease, due to scatter, in the number of particles per unit area incident to an ensemble of scattering centers with an areal density of \(\rho\) scattering centers per unit area normalized to the areal density.\(^5\) As the total cross section is proportional to the relative decrease in fluence due to scatter, it is a direct physical measure of the scattering probability. There are further refinements, such as differential cross sections in solid angle and in energy, which provide more detailed information of the scattering process.

This subsection provides a review of those aspects of quantum scattering theory which we will require in later solutions of dosimetry problems. This begins with the derivation of the Born approximation, which is, in fact, a different manifestation of the first-order approximation used in the perturbation theory leading to Fermi’s Golden Rules. The outcome of this derivation is the scattering amplitude which will be shown to be directly linked to the differential cross section in solid angle. As the scattering amplitude is proportional to the Fourier transform of the interaction potential between projectile and target, the Born approximation provides an easy mechanism to solve the many scattering problems we will encounter later. The phase-shift analysis approach to the scattering problem is then reviewed and, inter alia, the Schrödinger equation is solved in spherical coordinates. This will be used in Chap. 3 in solving the bound state problem of the nuclear shell model. Finally, the phase-shift analysis is extended to derive the optical theorem, which provides a simple relationship between the scattering amplitude and the total cross section.

### 2.6.2 Scattering Amplitude

Consider the geometry of Fig. 2.5 in which a particle/wavefunction is incident to a potential centered at the origin \(U(r)\). Assume that the potential is weak. As a result of the interaction between the wavefunction and this potential, it is deflected from its original trajectory and one is interested in the probability of the particle being scattered through the angle \(\theta\) into the differential solid angle element \(d\Omega\) at a distance \(r\) from the scattering center. In order to calculate this probability, first consider the case of a free particle (i.e., one not subject to a potential) with mass \(m\) and the nonrelativistic Hamiltonian,

\[
H_0 = \frac{p^2}{2m}
\]

(2.66)

The eigenvalue equation is, continuing our use of the Dirac notation,

\[
H_0 \psi_0 = E_0 \psi_0
\]

(2.67)

where \(\psi_0\) is the energy eigenfunction of \(H_0\). The wavefunction corresponding to the particle is the scalar product,

\[
\psi_0(r) = \langle r | \psi_0 \rangle
\]

(2.68)

The complete Hamiltonian for the particle when it is in the presence of a potential \(U\) is \(H_0 + U\) and the corresponding Schrödinger equation is,

\[
(H_0 + U) \psi = E \psi
\]

(2.69)

where \(\psi\) is an energy eigenstate of the total Hamiltonian. The scattered wavefunction is given by the scalar product,

\[
\psi(r) = \langle r | \psi \rangle.
\]

(2.70)

The solution to this Schrödinger equation is,

\[
\psi = \psi_0 + \frac{1}{E - H_0 + i\epsilon} U \psi
\]

(2.71)

where \(\epsilon\) is a real, positive small number required to eliminate the singularity that occurs when \(E = H_0\). This is an exact solution, known as the Lippman–Schwinger equation, and which can be solved via

---

\(^5\)The areal density of a scattering medium with physical density \(\rho\) and thickness \(t\) is the product \(\rho t\).
perturbation theory. Using a power-series expansion in \( U \) leads to,

\[
c_{ji} = c_{0ji} + \frac{1}{E/C_0}H_0 \epsilon U c_{0ji} + O(U^2). \tag{2.72}
\]

The first Born approximation for \( c_{ji} \) is the truncation at the first order of \( U \), which is possible following our original assumption of a weak interaction potential. It is also possible to derive the Born approximation, and a solution for the scattered wavefunction in coordinate space, by inserting the free Hamiltonian into the Schrödinger equation and using the canonical relationship

\[
p = -i\hbar \nabla,
\]

in which the momentum is linked to the gradient. This change results in the Helmholtz equation,

\[
\left( \nabla^2 + \frac{2mE}{\hbar^2} \right) \psi_0(r) = \frac{2m}{\hbar^2} U \psi_0(r) \tag{2.73}
\]

where the wave vector is,

\[
k = \frac{\sqrt{2mE}}{\hbar} \tag{2.74}
\]

The solution to the Helmholtz equation is,

\[
\psi(r) = \psi_0(r) + \int d^3r' G(r, r') \frac{r}{\Xi} \psi
\]

where the free particle wavefunction \( \psi_0(r) \) is the solution to the homogeneous equation (i.e., the Schrödinger equation for the free particle),

\[
\left( \nabla^2 + k^2 \right) \psi_0(r) = 0 \tag{2.77}
\]

and \( G(r, r') \) is the Green’s function defined from,

\[
\left( \nabla^2 + k^2 \right) G(r, r') = \delta(r - r') \tag{2.78}
\]

and where \( \delta(r) \) is the Dirac delta function. These yield an expression for the Green’s function of the form,

\[
G(r, r') = -\frac{e^{\pm ik|r-r'|}}{4\pi|r-r'|} \tag{2.79}
\]
and the expression for the scattered wavefunction is,

\[
\psi^\pm(r) = \psi_0(r) - \int \frac{d^3r'}{4\pi|\mathbf{r} - \mathbf{r}'|} \langle \mathbf{r}'| \Xi|\psi \rangle
\]

(2.80)

where the \( \pm \) subscript has been added in order to reflect the sign of the exponent in the Green’s function, the physical interpretation of which will be discussed shortly. From the definition of \( \Xi \), the matrix element contained within the integrand is written as,

\[
\Psi^\pm(r) = \psi_0(r) - \int d^3r' \frac{e^{\pm ik|r-r'|}}{4\pi|\mathbf{r} - \mathbf{r}'|} |\mathbf{r}'\rangle|\Xi|\psi\rangle
\]

(2.81)

\[
\Psi^\pm(r) = \psi_0(r) - \frac{2m}{\hbar c} \int d^3r' \frac{e^{\pm ik|r-r'|}}{4\pi|\mathbf{r} - \mathbf{r}'|} \times \langle \mathbf{r}'|U(r)\delta(r - r')|\psi\rangle
\]

\[
\Psi^\pm(r) = \psi_0(r) - \frac{m}{2\pi(\hbar c)^2} \int d^3r' d^3r'' \frac{e^{\pm ik|r-r'|}}{|\mathbf{r} - \mathbf{r}'|} \times \langle \mathbf{r}'|U(r)\delta(r - r')|\mathbf{r}''\rangle|\psi\rangle
\]

To further the evaluation of the matrix element, the assumption that the scattering potential is weak can be modified by requiring it to be non-zero only in the vicinity of the origin. Then consider this wavefunction only at large distances from the scattering center (i.e., \( r \gg r' \)) in which case, the \( r \)-dependence of the denominator and exponent can be approximated by,

\[
|\mathbf{r} - \mathbf{r}'| = r \sqrt{1 + \frac{r'^2}{r^2} - 2 \frac{r'}{r} \cos \theta}
\]

\[
\approx r \left( 1 - \frac{r'}{r} \cos \theta \right)
\]

(2.82)

where \( \mathbf{r} \) is the unit vector in the direction of \( r \). As a result, the wavefunction expression becomes, for large \( r \),

\[
\psi^\pm(r) = \psi_0(r) - \frac{m}{2\pi(\hbar c)^2} \int d^3r' \frac{e^{\pm ik(r-r')}}{r-r' r \cdot r'} U(r')|\psi(r')\rangle
\]

(2.83)

where the wave vector \( \mathbf{k}' \) (for particles with the same momentum as those incident but scattered along \( \hat{r} \)) is defined as,

\[
\mathbf{k}' = |\mathbf{k}||\hat{r}
\]

(2.84)

If the incident particle were to be treated as a plane wave,

\[
\psi_0(r) = e^{ik\mathbf{r}}
\]

(2.85)

then the wavefunction can be rewritten as,

\[
\psi^\pm(r) = e^{ik\mathbf{r}} - \frac{m}{2\pi(\hbar c)^2} \frac{e^{ikr}}{r} \times \int d^3r' e^{\pm ik'\mathbf{r}'} U(r')|\psi(r')\rangle
\]

(2.86)

The first term is simply the incident plane wave and the second term corresponds to spherical waves propagating away from the scattering center (\( \psi^+(r) \)) and towards the scattering center (\( \psi^-(r) \)). Clearly, the latter solution is nonphysical and will be ignored leaving the physical solution for the wavefunction at large \( r \),

\[
\psi(r) = e^{ik\mathbf{r}} - \frac{m}{2\pi(\hbar c)^2} \frac{e^{ikr}}{r} \times \int d^3r' e^{-ik'\mathbf{r}'} U(r')|\psi(r')\rangle
\]

(2.87)

which is the summation of the incident wave and spherical waves emitted from the scattering center, as shown in Fig. 2.6. From the assumption that the potential \( U(r) \) is negligible at large \( r \), it is possible to approximate the \( |\psi(r')\rangle \) in the integrand by the incident wavefunction \( \psi_0(r') \).
\[ \psi(r) = e^{ikr} - \frac{m}{2\pi\hbar c^2} \frac{e^{ikr}}{r} \int d^3r' e^{-ik'r'} U(r') e^{ik'r'} \]
\[ = e^{ikr} - \frac{m}{2\pi\hbar c^2} \frac{e^{ikr}}{r} \int d^3r' e^{i(k-k'r')} U(r') \]  
(2.88)

which is the first Born approximation. By writing the momentum transfer as,
\[ q = \hbar c (k - k') \]  
(2.89)
the wavefunction can be written in the simpler form,
\[ \psi(r) = e^{ikr} - \frac{m}{2\pi\hbar c^2} \frac{e^{ikr}}{r} \int d^3r' e^{iqr'}/C_{22} \hbar c U(r') \]  
(2.90)

\[ f(q) = -\frac{2m}{q\hbar c} \int d^3r' e^{iqr'}/C_{22} \hbar c U(r'). \]  
(2.91)

The first term is, again, the incident plane wave and the second term is the scattered spherical wave with a magnitude specified by \( f(q) \), which is known as the scattering amplitude. The scattering amplitude is proportional to the Fourier transform of the scattering potential,

\[ f(q) = -\frac{2m}{q\hbar c} \int d^3r' e^{iqr'}/C_{22} \hbar c U(r'). \]  
(2.91)

Most of the scattering problems to be encountered in this book reduce to the calculation of the scattering amplitude as it will be shown to be related to the physical observable of the differential cross section in solid angle.

For example, the potentials that will be encountered here are central or, in other words, azimuthally symmetric. In this case, the integral of (2.91) is,

\[ f(q) = -\frac{2m}{q\hbar c} \int d^3r' e^{iqr'}/C_{22} \hbar c U(r'). \]  
(2.92)

Note that the dimension of the scattering amplitude is that of length.

### 2.6.3 Scattering Cross Sections

Next, consider the physical observables associated with scattering, the differential and total cross sections. The cross section is a quantitative measure of the complete likelihood of a given interaction occurring between a bombarding beam and a target. An initial intuitive description is given by Fig. 2.7 which shows a flux \( \varphi \) of particles per square centimeter per second incident orthogonally to a medium of differential thickness \( dx \) containing \( N \) “target centers” per cubic centimeter (with an areal density of \( N \) target centers per square centimeter). Assume that only one type of interaction can occur between a bombarding particle and a target center. The interactions between
the incident particles and the target centers will cause a differential flux reduction, $d\phi$, proportional to the incident flux and the areal density of target centers. The relative flux reduction is,

$$\frac{d\phi}{\phi} = -\sigma N dx.$$ (2.94)

The constant of proportionality, $\sigma$, between the relative flux reduction and the areal density of scattering centers has dimensions of area and is referred to as the reaction total cross section per target center. As each target center has a cross-sectional area $s$, the fraction of the total area covered by the target centers is $\sigma N dx$ and any of the bombarding particles that hit these areas are removed from the beam. Integrating over the target thickness $L$ (and neglecting any other changes over this thickness, such as energy loss) leads to the exponential attenuation of the beam through the medium,

$$\phi = \phi_0 e^{-\sigma NL}$$ (2.95)

where $\phi_0$ is the incident flux.

Reaction cross sections in differential form will be required in most of our calculations. For example, consider a process in which an incident particle is scattered by a target center into the direction $(\theta, \phi)$. The differential flux fraction scattered into the differential solid angle element $d\Omega$ centered on the direction $(\theta, \phi)$ is,

$$\frac{d\phi}{\phi} = \frac{d\sigma(\theta, \phi)}{d\Omega} N dx d\Omega.$$ (2.96)

This differential cross section in solid angle is the fractional loss of fluence per areal density per unit solid angle. Similarly, the differential flux fraction within the energy interval between $E$ and $E + dE$ following an interaction is,

$$\frac{d\phi}{\phi} = \frac{d\sigma(E)}{dE} N dx dE.$$ (2.97)

The total cross section, $\sigma$, is obtained by integrating $d\sigma/d\Omega$ over $4\pi$ steradians or by integrating $d\sigma/dE$ over all energies.

The differential cross section with solid angle, $d\sigma/d\Omega$, can be readily shown to be related to the scattering amplitude of the Born approximation due to its definition as the ratio of the number of particles scattered per unit time into the differential solid angle element $d\Omega$ to the number of incident particles per unit time per unit area, or,

$$\frac{d\sigma}{d\Omega} = \frac{r^2 |f(q)|^2 |\psi|^2}{|e^{ikr}|^2} = |f(q)|^2.$$ (2.98)

### 2.6.4 Phase-Shift Analysis

A description of scattering based upon phase shifts of the wavefunctions induced as a result of the interaction with the potential is now provided. Recall from above that, in the Born approximation, the final state is the sum of the incident and scattered wavefunctions. As the spherical coordinate system is more natural for describing the scattering problem, we shall recast this description by expressing the incident plane wave in terms of spherical waves and solve the Schrödinger equation in a region near the scattering center where the potential is non-zero by writing the Laplacian in spherical coordinates

$$\nabla^2 \psi + (k^2 - \Xi)\psi = 0$$ (2.99)

where $k$ and $\Xi$ are given above. The wavefunction is solved by first separating it into radial and angular terms,

$$\Psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$$ (2.100)

and then substituting the expression into the Schrödinger equation,
The radial and angular terms can be isolated by multiplying through by the ratio \( r^2/R(r)Y(0, \phi) \),

\[
\begin{align*}
\frac{Y(0, \phi)}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{R(r)}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) \\
\times \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{R(r)}{r^2 \sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \\
+ (k^2 - \Xi) R(r) Y(0, \phi) = 0
\end{align*}
\]

or,

\[
\begin{align*}
\frac{1}{R(r)} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + r^2 (k^2 - \Xi) \\
= -\left( \frac{1}{Y(0, \phi) \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{Y(0, \phi) \sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right).
\end{align*}
\]

(2.102)

The right- and left-hand sides must both equal the same constant. As the radial equation will be linked to the Bessel equation, this constant will be taken to be \( l(l + 1) \) where \( l \) is an integer equal to 0, 1, 2, . . .

\[
\begin{align*}
\frac{1}{R(r)} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + r^2 (k^2 - \Xi) - l(l + 1) = 0
\end{align*}
\]

(2.104)

or,

\[
\begin{align*}
\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \\
+l(l + 1)Y(0, \phi) = 0.
\end{align*}
\]

(2.105)

(2.103)

The radial equation is first solved for. Following differentiation and rearrangement,

\[
\begin{align*}
r^2 \frac{d^2 R}{dr^2} + 2r \frac{dR}{dr} + [(k^2 - \Xi) r^2 - l(l + 1)] R &= 0 \\
r^2 \frac{d^2 R}{dr^2} + 2r \frac{dR}{dr} + [\lambda^2 r^2 - l(l + 1)] R &= 0
\end{align*}
\]

(2.106)

where

\[
\lambda \equiv \sqrt{k^2 - \Xi} = \frac{\sqrt{2m(E - U)}}{\hbar c}.
\]

By defining \( \rho = \lambda r \), (2.106) reduces to the Bessel equation,

\[
\rho^2 \frac{d^2 R}{d\rho^2} + 2\rho \frac{dR}{d\rho} + [\rho^2 - l(l + 1)] R = 0.
\]

(2.108)

The solution for this equation for a given value of \( l \) is the weighted sum of the spherical Bessel functions of the first and second kind,

\[
R_l(\rho) = A_j j_l(\rho) + B_l y_l(\rho)
\]

or

\[
R_l(\rho) = A_j j_l(\lambda r) + B_l y_l(\lambda r)
\]

(2.109)

where \( j_l(x) \) is the spherical Bessel function of the first kind and \( y_l(x) \) is the spherical Bessel function of the second kind (also referred to as a Neumann function) and which are related to the Bessel functions via

\[
\begin{align*}
\frac{\lambda}{2x} J_{l+\frac{1}{2}}(x) &\quad |l| = 0, 1, 2. \\
\frac{\lambda}{2x} Y_{l+\frac{1}{2}}(x) &\quad |l| = 1, 2.
\end{align*}
\]

(2.110)

(2.111)

These functions are plotted in Fig. 2.8 for \( l = 0, 1, \) and 2. From the asymptotic behavior of these spherical Bessel functions, the radial function is,

\[
\begin{align*}
R_l(r) &= \frac{1}{\lambda r} \left( A_l \sin \left( \lambda r - \frac{l\pi}{2} \right) - B_l \cos \left( \lambda r - \frac{l\pi}{2} \right) \right) \\
&= \frac{\sqrt{A_l^2 + B_l^2}}{\lambda r} \left( \frac{A_l}{\sqrt{A_l^2 + B_l^2}} \sin \left( \lambda r - \frac{l\pi}{2} \right) - \frac{B_l}{\sqrt{A_l^2 + B_l^2}} \cos \left( \lambda r - \frac{l\pi}{2} \right) \right)
\end{align*}
\]

(2.112)
The integration constants, $A_l$ and $B_l$, will be set by the boundary conditions. From the trigonometric identity, $\sin(\alpha - \beta) = \sin \alpha \sin \beta - \cos \alpha \cos \beta$, (2.112) can be written as,

$$R_l(r) = C_l kr \sin \left( \frac{\lambda r}{2} + \delta_l \right).$$  \hspace{1cm} (2.113)

The phase shift for the $l$th partial wave is,

$$\delta_l = -\tan^{-1} \frac{B_l}{A_l}$$  \hspace{1cm} (2.114)

and

$$C_l = \sqrt{A_l^2 + B_l^2}.$$  \hspace{1cm} (2.115)

For completeness, we solve for the angular component of the wavefunction expression by differentiating and expanding to give,

\[
\frac{\partial^2 Y}{\partial \theta^2} + \cot \theta \frac{\partial Y}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} + l(l+1)Y(\theta, \phi) = 0
\]

and, then, by using another separation of variables, $Y(\theta, \phi) = \Theta(\theta) \Phi(\phi)$,

$$\Phi(\phi) \frac{d^2 \Theta(\theta)}{d\theta^2} + \Phi(\phi) \cot \theta \frac{d\Theta(\theta)}{d\theta} + \frac{\Theta(\theta)}{\sin^2 \theta} \frac{d^2 \Phi(\phi)}{d\phi^2} + l(l+1)\Theta(\theta)\Phi(\phi) = 0$$

Finally, by multiplying through by $\sin^2 \theta$ and dividing by $\Theta(\theta)\Phi(\phi)$, and isolating the angular terms,

$$\sin^2 \theta \left( \frac{1}{\Theta(\theta)} \frac{d^2 \Theta(\theta)}{d\theta^2} + \cot \theta \frac{d\Theta(\theta)}{d\theta} + l(l+1) \right) = -\frac{1}{\Phi(\phi)} \frac{d^2 \Phi(\phi)}{d\phi^2}$$

(2.117)

As both sides of the equation are each a function of a single angular variable, they must both be equal to the same constant. As the left-hand side of (2.117) can be written as Legendre’s differential equation, this constant can be specified to be $m^2$,

$$\frac{1}{\Phi(\phi)} \frac{\partial^2 \Phi(\phi)}{\partial \phi^2} = -m^2$$  \hspace{1cm} (2.118)

$$\frac{d^2 \Theta(\theta)}{d\theta^2} + \cot \theta \frac{d\Theta(\theta)}{d\theta} + (l(l+1) - m^2 \csc^2 \theta) \Theta(\theta) = 0.$$  \hspace{1cm} (2.119)

Equation (2.118) has the general solution,

$$\Phi(\phi) = k_1 e^{im \phi + k_2}.$$  \hspace{1cm} (2.120)

As $\Phi(\phi)$ is required to be single valued, $m$ must be an integer or zero. By defining $\mu = \cos \theta$, (2.119) is recast as,

$$\left( 1 - \mu^2 \right) \frac{d^2 \Theta}{d\mu^2} - 2\mu \frac{d\Theta}{d\mu} + \left( l(l+1) - \frac{m^2}{1-\mu^2} \right) \Theta = 0.$$  \hspace{1cm} (2.121)
This is the associated Legendre differential equation, the solutions of which are the associated Legendre polynomials of the first kind, \( P_m(\mu) \), with the requirement that \( |m| \leq l \). A special case arises for \( m = 0 \),

\[
(1 - \mu^2) \frac{d^2 \Theta}{d\mu^2} - 2\mu \frac{d\Theta}{d\mu} + l(l + 1)\Theta = 0
\]  

(2.122)

which is the Legendre differential equation with solutions given by the Legendre polynomials, \( P_l(\mu) \),

\[
P_l(\mu) = \frac{(-1)^l}{2^l l!} \frac{d^l}{d\mu^l} \left( (1 - \mu^2)^l \right).
\]  

(2.123)

The first three Legendre polynomials are,

\[
\begin{align*}
P_0(\mu) &= 1 \\
P_1(\mu) &= \mu \\
P_2(\mu) &= \frac{3\mu^2 - 1}{2}.
\end{align*}
\]  

(2.124)

The Legendre polynomials are orthogonal and have the recurrence relation,

\[
(l + 1)P_{l+1}(\mu) = (2l + 1)\mu P_l(\mu) - lP_{l-1}(\mu).
\]  

(2.125)

The associated Legendre polynomials can be calculated from the Legendre polynomials via,

\[
P_m(\mu) = (1 - \mu^2)^{|m|/2} \frac{d^{|m|}}{d\mu^{|m|}} P_l(\mu).
\]  

(2.126)

Combining this with the angular solutions gives the spherical harmonic,

\[
Y_{lm}(\theta, \phi) = k_{lm} P_{lm}(\theta) e^{im\phi}
\]  

(2.127)

where,

\[
k_{lm} = (-1)^m \sqrt{\frac{2l + 1}{4\pi} \frac{(l - m)!}{(l + m)!}}
\]  

(2.128)

The final form of the wavefunction with the radial and angular terms combined is,

\[
\psi(r, \theta, \phi) = R_l(r) Y_{lm}(\theta, \phi) = (A_l j_l(\lambda r) + B_l y_l(\lambda r)) Y_{lm}(\theta, \phi).
\]  

(2.129)

### 2.6.5 Optical Theorem

An important relationship between the scattering amplitude and the total reaction cross section is derived by considering the simple case of azimuthal symmetry (i.e., no \( \phi \)-dependence) so that the wavefunction at a distance can be expanded as a summation of Legendre polynomials,

\[
\psi(r) = \psi(r, \theta) = \sum_{l=0}^{\infty} R_l(r) P_l(\cos \theta).
\]  

(2.130)

By inserting the asymptotic form of the radial function, we achieve,

\[
\psi(r, \theta) = \sum_{l=0}^{\infty} C_l \left[ e^{i(\lambda - \lambda + \delta)} - e^{-i(\lambda - \lambda + \delta)} \right] P_l(\cos \theta).
\]  

(2.131)

As the incident plane wave can be described by the identity,

\[
\psi_0(r) = e^{ikr} = e^{ikr \cos \theta} = \sum_{l=0}^{\infty} i^l(2l + 1) j_l(\lambda r) P_l(\cos \theta)
\]  

(2.132)

Then the difference between (2.131) and (2.132) must be the scattered wavefunction,

\[
\sum_{l=0}^{\infty} C_l \frac{e^{i(\lambda - \lambda + \delta)} - e^{-i(\lambda - \lambda + \delta)}}{2ikr} P_l(\cos \theta)
\]

\[
- \sum_{l=0}^{\infty} i^l(2l + 1) \frac{e^{i(\lambda - \lambda + \delta)} - e^{-i(\lambda - \lambda + \delta)}}{2ikr} P_l(\cos \theta) = f(\theta) e^{ikr}.
\]  

(2.133)
By equating the coefficients of the exponentials,
\[ C_l = (2l + 1) i \delta_l = (2l + 1) e^{i \delta_l} \] (2.134)

The scattering amplitude is then given by the summation,
\[ f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) e^{i \delta_l} \sin \delta_l P_l(\cos \theta). \] (2.135)

In order to obtain an expression for the total cross section, one first recalls that the differential cross section in solid angle is the squared-magnitude of the scattering amplitude,
\[ \frac{d\sigma}{d\Omega} = |f(\theta)|^2 \] (2.136)

The total cross section is obtained by integrating over 4π steradians,
\[ \sigma = \int d\phi \int d(\cos \theta) \frac{d\sigma}{d\Omega} = \frac{2\pi}{k^2} \sum_{l=0}^{\infty} \sum_{l' = 0}^{\infty} (2l + 1)(2l' + 1) e^{i(\delta_l - \delta_{l'})} \sin \delta_l \sin \delta_{l'} \times \int d(\cos \theta) P_l(\cos \theta) \sin^2 \delta_l \] (2.137)

where the orthonormality of the Legendre polynomials has been used. However, note that the imaginary part of the scattering amplitude for \( \theta = 0 \) is,
\[ \text{Im} f(0) = \frac{1}{k} \text{Im} \left( \sum_{l=0}^{\infty} (2l + 1) e^{i \delta_l} P_l(1) \right) = \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l. \] (2.138)

Substituting this into the expression for the total cross section gives,
\[ \sigma = \frac{4\pi}{k} \text{Im} f(0) \] (2.139)
which is known as the optical theorem. The total cross section is a measure of the reduction in flux which results from the destructive interference between the incident and scattered wavefunctions for \( \theta = 0 \).

### 2.7 Dirac’s Equation

#### 2.7.1 Introduction

Dirac’s equation will be the foundation of subsequent discussions regarding the interactions of electrons with the electromagnet field and of the phenomena of the creation and annihilation of positrons. This section is intended to be only an overview of the derivation and characteristics of the Dirac equation to be called upon later.

This discussion begins by considering Schrödinger’s equation which is nonrelativistic and, as a descriptor for free particles, was derived from the quantum-mechanical interpretation of energy and momentum as operators,
\[ E \rightarrow i\hbar \frac{\partial}{\partial t} \] (2.140)
\[ \mathbf{p} \rightarrow -i\hbar \mathbf{\nabla}. \] (2.141)

Note that the constants of \( \hbar \) and \( \hbar c \) have been used in order to maintain our convention that the units of both energy and momentum are those of energy. Substituting these operator expressions into the nonrelativistic relationship between energy and momentum,
\[ E = \frac{\left| \mathbf{p} \right|^2}{2m} \] gives the Schrödinger equation,
\[ i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{(\hbar c)^2}{2m} \nabla^2 \psi(x, t). \] (2.142)
Early attempts at forming a relativistically invariant analog to this Schrödinger equation began with the relativistic relationship between energy and momentum,

\[ E^2 = p^2 + m^2. \]  

(2.143)

If the operator forms of energy and momentum are substituted into this relationship, then the Klein–Gordon equation is obtained,

\[ \Delta^2 + m^2/c = 0. \]  

(2.144)

where the operator \( \Delta \equiv h^2 \partial^2/\partial t^2 - (hc)^2 \nabla^2 \) has been defined. This attempt at forming a relativistic result confronted immediate problems. First, the energy-momentum relationship of (2.143) allowed negative-energy solutions, \( E = \pm \sqrt{p^2 + m^2} \). Although this was a difficulty later confronted and surmounted by Dirac in his interpretation of antiparticles, this conundrum was at first assumed to be fatal to this attempt. Second, the Klein–Gordon equation is second-order in that the time derivative leads to a probability density for the wavefunction that was not positive-definite. As a result, the solution represented by the Klein–Gordon equation was rejected, although it was “rehabilitated” in later times as a descriptor of spinless particles (scalar or pseudoscalar wavefunctions) such as the pion.

However, the above result has shown that, in order to derive the required relativistic form of a solution, the use of a first-order time derivative was required.

### 2.7.2 Derivation of Dirac’s Equation

Recognizing the requirement for a first-order time derivative, Dirac began with a linear ansatz of the form,

\[ E\psi = (\alpha p + \beta m)\psi. \]  

(2.145)

The operators \( \alpha \) and \( \beta \) are required in order to be consistent with the relativistic relationship between energy and momentum given by (2.143),

\[ E^2 = (\alpha p)^2 + (\beta m)^2 + (\beta m \alpha p + \alpha p \beta m). \]  

(2.146)

Equating terms to those of (2.143), one finds the requirements, following Dirac’s proposal that (2.146) be regarded as a matrix equation with the four matrices \( \alpha_i \) and \( \beta \) obeying the algebra, of,

\[ \alpha_i^2 = \beta^2 = 1 \]  

(2.147)

\[ \alpha_i \alpha_j + \alpha_j \alpha_i = 2\delta_{ij} \]  

(2.148)

\[ \alpha_i \beta + \beta \alpha_i = 0. \]  

(2.149)

In order to construct these four matrices, a number of conditions must be met. First, they must be Hermitian in order for the Hamiltonian to be so. Second, the eigenvalues of the \( \alpha \) and \( \beta \) matrices are \( \pm 1 \). Finally, from their anti-commutation property, the traces of the matrices must be zero. These last two conditions allow the dimensions of the matrices to be specified. As the trace of a matrix is also the sum of its eigenvalues, the number of positive and negative eigenvalues must be equal, requiring that the dimensions of the \( \alpha \) and \( \beta \) matrices be even. A dimension of 2 is insufficient and the smallest even-numbered dimension for which these matrices can be realized is 4. Hence,

\[ \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad i = 1, 2, 3 \]  

(2.150)

\[ \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]  

(2.151)

where \( \sigma_i \) are the 2 \( \times \) 2 Pauli matrices and \( \mathbf{1} \) is the 2 \( \times \) 2 identity matrix. In order to write the Dirac result in a covariant form, we introduce the notation of,

\[ \gamma^0 = \beta \]  

(2.152)

\[ \gamma^i \equiv \beta \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} \quad i = 1, 2, 3. \]  

(2.153)

An additional matrix is defined as,

\[ \gamma_5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3 = \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}. \]  

(2.154)

One can then write the Dirac equation as,

\[ (\gamma^0 E - \gamma \cdot \mathbf{p} - m \mathbf{1})\psi = 0 \]  

(2.155)
where $\mathbf{p}^\mu = (E, \mathbf{p})$ and the covariant is,

$$P_\mu \equiv g_{\mu\nu}P^\nu = (E, -\mathbf{p}).$$  \hfill (2.156)

Equation (2.155) can be rewritten in the form,

$$(\gamma^\mu p_\mu - m\mathbf{1})\psi = 0.$$  \hfill (2.157)

One now has the $\psi(X)$ as a wavefunction with space–time and spinor degrees of freedom,

$$\psi(X) = \begin{pmatrix} \psi_1(X) \\ \psi_2(X) \\ \psi_3(X) \\ \psi_4(X) \end{pmatrix}. \hfill (2.158)$$

There are two solutions to the Dirac equation,

$$\psi_+(x, t) = u e^{-i p_x x^\mu}$$
$$= u e^{-i (\mathbf{p} \cdot \mathbf{x} - mc)}$$  \hfill (2.159)

where $u$ is defined as a Dirac spinor and $\hbar$ and $\hbar c$ have been inserted in order to make the exponent dimensionally correct. This solution corresponds to a positive energy. The negative-energy solution is,

$$\psi_-(x, t) = v e^{i p_x x^\mu}$$
$$= v e^{i (\mathbf{p} \cdot \mathbf{x} + mc)}.$$  \hfill (2.160)

$\psi_-(x, t)$ is the wavefunction of a positron or, in the Feynman picture, an electron moving backward in time with momentum $-\mathbf{p}$. The Dirac spinors are,

$$u(p, s) = \sqrt{E + m} \left( \begin{array}{c} \chi_s \\ \sigma \mathbf{p} / \sqrt{E + m} \chi_s \end{array} \right)$$  \hfill (2.161)

$$v(p, s) = \sqrt{E + m} \left( \begin{array}{c} \sigma \mathbf{p} / \sqrt{E + m} \chi_s \\ \chi_s \end{array} \right) \hfill (2.162)$$

where

$$\hat{\mathbf{e}} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$  \hfill (2.163)

and where $\chi_s$ is the (nonrelativistic) Pauli two-component spinor for a spin-$\frac{1}{2}$ particle. Note that another variable, $s$, has been introduced and which describes the spin orientation of the particle. Equation (2.161) describes the particle (electron) states and (2.162) describes the antiparticle (positron) states.
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