Quantum Mechanics II

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Voorwoord

Het college Quantummechanica II wordt dit najaar verzorgd door Prof. Piet Mulders met assistentie van Drs. Alessandro Bacchetta bij het werkcollege.

Het college beslaat de hoofdstukken 6 t/m 11 van het boek *Quantum Mechanics* van F. Mandl (Cambridge University Press). Deze aantekeningen geven soms een iets andere kijk op de stof, maar bevatten nauwelijks stof die niet ook in het boek te vinden is.

Piet Mulders
September 2000

Literature

1. F. Mandl, *Quantum Mechanics*, Wiley 1992
2. C. Cohen-Tannoudji, B. Diu and F. Laloë, *Quantum Mechanics I and II*, Wiley 1977
3. J.J. Sakurai, *Modern Quantum Mechanics*, Addison-Wesley 1991
4. E. Merzbacher, *Quantum Mechanics*, Wiley 1998
5. B. Bransden and C. Joachain, *Quantum Mechanics*, Prentice hall 2000

Material covered in lectures

	Collegestof in boek (aantekeningen)	Werkcollege
Week 1 (7/9)	herhaling QM1, 5.3 (1-2)	5.1, 5.2, 5.3
Week 2 (11/9)	5.1, 5.2, 5.8, 5.4 (1-3)	5.4, 5.5, 5.6, 5.7
Week 3 (21/9)	5.5, 5.6, 5.7, 6.3 (3-4)	5.8, 5.9, 6.5, 6.6
Week 4 (28/9)	6.1, 6.2	6.1, 6.2, 6.3, 6.4
Week 5 (5/10)	7.1, 7.2, 7.3	7.1, 7.2, 7.3, 7.4
Week 6 (12/10)	7.4, 7.5	7.5, 7.6, 7.7, 7.8
Week 7 (19/10)	8.1, 8.2, 8.3	8.1, 8.2, 8.3, 8.4
Week 8 (2/11)	9.1, 9.2, 9.3 (5-6)	9.1, 9.2, 9.3, 9.4
Week 9 (9/11)	9.4, 9.5 (7-10)	9.5, 9.6
Week 10 (16/11)	10.1, 10.2 (11-13)	10.1, 10.2, 10.3
Week 11 (23/11)	10.3, 11.1 (14-16)	10.4, 10.5
Week 12 (30/11)	11.2, 11.3 (17-19)	11.1, 11.2, 11.3
Week 13 (7/12)	11.4, 11.5 (20-23)	11.4, 11.5
Tentamen mondeling		

Contents

1 Spin

1.1 Definition

In quantum mechanics spin is introduced as an observable defined via the vector operator $\boldsymbol{s}$. These (three) hermitean operators satisfy commutation relations

$$[s_i, s_j] = i\hbar\epsilon_{ijk}\, s_k, \tag{1}$$

similar to the commutation relations for the angular momentum operator $\boldsymbol{\ell} = \boldsymbol{r} \times \boldsymbol{p}$. The spin operators $\boldsymbol{s}$ commute with the operators $\boldsymbol{r}$ and $\boldsymbol{p}$ and thus also with $\boldsymbol{\ell}$. That's it. All the rest follows from these commutation relations.

1.2 Rotation invariance

Earlier we have seen that, without spin, rotation invariance required specific commutation relations with $\boldsymbol{\ell}$. In fact *scalar* quantities S and *vectors* $\boldsymbol{V}$ under rotations behaved like

$$[\ell_i, S] = 0, \tag{2}$$
$$[\ell_i, V_j] = i\hbar\,\epsilon_{ijk}\, V_k, \tag{3}$$

e.g. scalars $S = \boldsymbol{r}^2$, $\boldsymbol{p}^2$, $\boldsymbol{r}\cdot\boldsymbol{p}$ or $\boldsymbol{\ell}^2$ and vectors $\boldsymbol{V} = \boldsymbol{r}$, $\boldsymbol{p}$ or $\boldsymbol{\ell}$.

Including spin vectors $\boldsymbol{s}$, the notion of behavior under rotations has to be altered, e.g. $[\ell_i, s_j] = 0$ and $[\ell_i, \boldsymbol{\ell}\cdot\boldsymbol{s}] = -i\hbar\,(\boldsymbol{\ell}\times\boldsymbol{s})_i$. It is easy to see that the operator

$$\boldsymbol{j} \equiv \boldsymbol{\ell} + \boldsymbol{s}, \tag{4}$$

satisfies

$$[j_i, S] = 0, \tag{5}$$
$$[j_i, V_j] = i\hbar\,\epsilon_{ijk}\, V_k, \tag{6}$$

not only for the above examples, but now also for the vectors $\boldsymbol{s}$ and $\boldsymbol{j}$ and including scalars like $\boldsymbol{s}^2$ and $\boldsymbol{\ell}\cdot\boldsymbol{s}$.

For a system of many particles the operators $\boldsymbol{r}$, $\boldsymbol{p}$ and $\boldsymbol{s}$ for different particles commute. It is easy to see that the operators

$$\boldsymbol{L} = \sum_{n=1}^{N} \boldsymbol{\ell}_n, \qquad \boldsymbol{S} = \sum_{n=1}^{N} \boldsymbol{s}_n, \qquad \boldsymbol{J} = \sum_{n=1}^{N} \boldsymbol{j}_n = \boldsymbol{L} + \boldsymbol{S}, \tag{7}$$

satisfy commutation relations $[L_i, L_j] = i\hbar\,\epsilon_{ijk}\, L_k$, $[S_i, S_j] = i\hbar\,\epsilon_{ijk}\, S_k$, and $[J_i, J_j] = i\hbar\,\epsilon_{ijk}\, J_k$, while only the operator $\boldsymbol{J}$ satisfies

$$[J_i, S] = 0, \tag{8}$$
$$[J_i, V_j] = i\hbar\,\epsilon_{ijk}\, V_k, \tag{9}$$

for any scalar S or vector $\boldsymbol{V}$.

> *It is easy to show that the inner product $\boldsymbol{a}\cdot\boldsymbol{b}$ of two vectors satisfying the commutation relation in Eq. 9 indeed is a scalar quantity, satifying the commutation relation in Eq. 8.*

An important property is that rotational invariance is one of the basic symmetries of our world.

Rotation invariance of a system of particles requires

$$[\boldsymbol{J}, H] = 0. \tag{10}$$

Besides the behavior under rotations, also the behavior under parity is considered to classify quantities. Vectors behave as $P\,\boldsymbol{V}\,P^{-1} = -\boldsymbol{V}$, *axial vectors as* $P\,\boldsymbol{A}\,P^{-1} = +\boldsymbol{A}$, *a scalar* S *behave as* $P\,S\,P^{-1} = +S$, *and a pseudoscalar* S' *behaves as* $P\,S'\,P^{-1} = -S'$. *Examples of specific quantities are*

vector	*axial vector*	*scalar*	*pseudoscalar*
$\boldsymbol{r}$	$\boldsymbol{\ell}$	$\boldsymbol{r}^2$	$\boldsymbol{s}\cdot\boldsymbol{r}$
$\boldsymbol{p}$	$\boldsymbol{s}$	$\boldsymbol{p}^2$	$\boldsymbol{s}\cdot\boldsymbol{p}$
	$\boldsymbol{j}$	$\boldsymbol{\ell}^2$	
		$\boldsymbol{\ell}\cdot\boldsymbol{s}$	

The hamiltonian is a scalar quantity. Therefore, if we have parity invariance, combinations as $\boldsymbol{s}\cdot\boldsymbol{r}$ *cannot appear but a tensor operator of the form* $(\boldsymbol{s}_1\cdot\boldsymbol{r})(\boldsymbol{s}_2\cdot\boldsymbol{r})$ *is allowed. Note, however, that such an operator does not commute with* $\boldsymbol{\ell}$ *(see Exc. 5.8).*

1.3 spin states

As mentioned above, the commutation relations are all that defines spin. As an operator that commutes with all three spin operators (a socalled Casimir operator) we have $\boldsymbol{s}^2 = s_x^2 + s_y^2 + s_z^2$,

$$[s_i, s_j] = i\hbar\,\epsilon_{ijk}\,s_k, \tag{11}$$

$$[\boldsymbol{s}^2, s_i] = 0. \tag{12}$$

Only one of the three spin operators can be used to label states, for which we without loss of generality can take s_z. In addition we can use $\boldsymbol{s}^2$, which commutes with s_z. We write states $\chi_m^{(s)} = |s,m\rangle$ satisfying

$$\boldsymbol{s}^2|s,m\rangle = \hbar^2\,s(s+1)|s,m\rangle, \tag{13}$$

$$\boldsymbol{s}_z|s,m\rangle = m\hbar\,|s,m\rangle. \tag{14}$$

It is of course a bit premature to take $\hbar^2\,s(s+1)$ as eigenvalue. We need to prove that the eigenvalue of $\boldsymbol{s}^2$ is positive, but this is straightforward as it is the sum of three squared operators. Since the spin operators are hermitean each term is not just a square but also the product of the operator and its hermitean conjugate. In the next step, we recombine the operators s_x and s_y into

$$s_\pm \equiv s_x \pm i\,s_y. \tag{15}$$

The commutation relations for these operators are,

$$[\boldsymbol{s}^2, s_\pm] = 0, \tag{16}$$

$$[s_z, s_\pm] = \pm\hbar\,s_\pm, \tag{17}$$

$$[s_+, s_-] = 2\hbar\,s_z, \tag{18}$$

The first two can be used to show that

$$\begin{gathered}\boldsymbol{s}^2\,s_\pm|s,m\rangle = s_\pm\boldsymbol{s}^2|s,m\rangle = \hbar^2\,s(s+1)\,s_\pm|s,m\rangle,\\ s_z\,s_\pm|s,m\rangle = (s_\pm s_z \pm \hbar\,s_\pm)\,|s,m\rangle = (m\pm1)\hbar\,s_\pm|s,m\rangle,\end{gathered}$$

hence the name step-operators (raising and lowering operator) which achieve

$$s_\pm|s,m\rangle = c_\pm|s,m\pm1\rangle.$$

Furthermore we have $s_\pm^\dagger = s_\mp$ and $\boldsymbol{s}^2 = s_z^2 + (s_+s_- + s_-s_+)/2$, from which one finds that

$$\begin{aligned}|c_\pm|^2 = \langle s,m|s_\pm^\dagger s_\pm|s,m\rangle &= \langle s,m|\boldsymbol{s}^2 - s_z^2 - [s_\pm, s_\mp]/2|s,m\rangle\\ &= \langle s,m|\boldsymbol{s}^2 - s_z^2 \mp \hbar\,s_z|s,m\rangle = s(s+1) - m(m\pm1).\end{aligned}$$

It is convention to define

$$\begin{aligned}s_+|s,m\rangle &= \hbar\sqrt{s(s+1)-m(m+1)}\,|s,m+1\rangle\\ &= = \hbar\sqrt{(s-m)(s+m+1)}\,|s,m+1\rangle \qquad (19)\\ s_-|s,m\rangle &= \hbar\sqrt{s(s+1)-m(m-1)}\,|s,m-1\rangle\\ &= \hbar\sqrt{(s+m)(s-m+1)}\,|s,m-1\rangle. \qquad (20)\end{aligned}$$

This shows that given a state $|s, m\rangle$, we have a whole series of states

$$\ldots |s, m-1\rangle,\ |s, m\rangle,\ |s, m+1\rangle, \ldots$$

But, we can also easily see that since $\boldsymbol{s}^2 - s_z^2 = s_x^2 + s_y^2$ must be an operator with positive definite eigenstates that $s(s+1) - m^2 \geq 0$, i.e. $|m| \leq \sqrt{s(s+1)}$ or strictly $|m| < s+1$. From the second expressions in Eqs 19 and 20 one sees that this inequality requires $m_{max} = s$ as one necessary state to achieve a cutoff of the series of states on the upper side, while $m_{min} = -s$ is required as a necessary state to achieve a cutoff of the series of states on the lower side. Moreover to have both cutoffs the step operators require that the difference $m_{max} - m_{min} = 2\,s$ must be an integer, i.e. the only allowed values of spin quantum numbers are

$$\begin{aligned} s &= 0,\ 1/2,\ 1,\ 3/2, \ldots, \\ m &= s, s-1, \ldots, -s. \end{aligned}$$

Thus for spin states with a given quantum number s, there exist $2s+1$ states.

1.4 Why is ℓ integer

Purely on the basis of the commutation relations, the allowed values for the quantum numbers s and m have been derived. Since the angular momentum operators $\boldsymbol{\ell} = \boldsymbol{r} \times \boldsymbol{p}$ satisfy the same commutation relations, one has the same restrictions on ℓ and m_ℓ, the eigenvalues connected with $\boldsymbol{\ell}^2$ and ℓ_z. However, we have only found integer values for the quantum numbers in our earlier treatment. This is the consequence of restrictions imposed because for $\boldsymbol{\ell}$ we know *more* than just the commutation relations. The operators have been introduced explicitly working in the space of functions, depending on the angles in R^3. One way of seeing where the constraint is coming from is realizing that we want uni-valued functions. The eigenfunctions of $\ell_z = -i\hbar\, d/d\phi$, were found to be

$$Y_\ell^m(\theta, \phi) \propto e^{i\,m\phi}.$$

In order to have the same value for ϕ and $\phi + 2\pi$ we need $\exp(2\pi\, i\, m) = 1$, hence m (and thus also ℓ) can only be integer.

For spin, there are only the commutation relations, thus the spin quantum numbers s can also take half-integer values. Particles with integer spin values are called *bosons* (e.g. pions, photons), particles with half-integer spin values are called *fermions* (e.g. electrons, protons, neutrinos, quarks). For the angular momenta which are obtained as the sum of other operators, e.g. $\boldsymbol{j} = \boldsymbol{\ell} + \boldsymbol{s}$, etc. one can easily see what is allowed. Because the z-components are additive, one sees that for any orbital angular momentum the quantum numbers are integer, while for spin and total angular momentum integer and half-integer are possible.

2 Spin states

2.1 Matrix representations of spin operators

In the space of spin states with a given quantum number s, we can write the spin operators as $(2s+1) \times (2s+1)$ matrices. Let us illustrate this first for spin $s = 1/2$. Define the states

$$\chi^{(1/2)}_{+1/2} \quad \text{or} \quad \chi_\uparrow \quad \text{or} \quad |1/2, +1/2\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

$$\chi^{(1/2)}_{-1/2} \quad \text{or} \quad \chi_\downarrow \quad \text{or} \quad |1/2, -1/2\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Using the definition of the quantum numbers in Eq. 14 one finds that

$$s_z = \hbar \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}, \quad s_+ = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad s_- = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

For spin 1/2 we find the familiar spin matrices, $\boldsymbol{s} = \hbar\boldsymbol{\sigma}/2$,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For spin 1 we define the basis states,

$$\chi^{(1)}_{+1} = |1, +1\rangle \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \chi^{(1)}_{0} = |1, 0\rangle \equiv \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \chi^{(1)}_{-1} = |1, 0\rangle \equiv \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

The spin matrices are then easily found,

$$s_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad s_+ = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}, \quad s_- = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix},$$

from which also s_x and s_y can be constructed.

2.2 Rotated spin states

Instead of the spin states defined as eigenstates of s_z, one might be interested in eigenstates of $\boldsymbol{s} \cdot \hat{\boldsymbol{n}}$, e.g. because one wants to measure it with a Stern-Gerlach apparatus with an inhomogeneous $\boldsymbol{B}$-field in the $\hat{\boldsymbol{n}}$ direction. We can of course just write down these states formally like

$$\chi^{(1/2)}_{+1/2}(\hat{\boldsymbol{n}}) \quad \text{and} \quad \chi^{(1/2)}_{-1/2}(\hat{\boldsymbol{n}})$$

Suppose that we want to write them down in terms of the eigenstates of s_z, given above. To do this we work in the matrix representation discussed in the previous section. Taking $\hat{\boldsymbol{n}} = (\sin\theta, 0, \cos\theta)$, we can easily write down

$$\boldsymbol{s} \cdot \hat{\boldsymbol{n}} = \frac{1}{2}\hbar\,\boldsymbol{\sigma} \cdot \hat{\boldsymbol{n}} = \frac{\hbar}{2} \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}. \tag{21}$$

We find the following two eigenstates and eigenvalues

$$\chi^{(1/2)}_{+1/2}(\hat{\boldsymbol{n}}) = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix} \qquad \text{with eigenvalue} \quad +1/2,$$

$$\chi^{(1/2)}_{-1/2}(\hat{\boldsymbol{n}}) = \begin{pmatrix} -\sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix} \qquad \text{with eigenvalue} \quad -1/2.$$

The probability that given a state with spin along the z-direction a measurement of the spin along the $+\hat{\boldsymbol{n}}$-direction yields the value $+\hbar/2$ is thus given by

$$\left| \chi^{(1/2)\,\dagger}_{+1/2}(\hat{\boldsymbol{n}}) \chi^{(1/2)}_{+1/2} = \right|^2 = \cos^2(\theta/2).$$

In general the rotated eigenstates are written as

$$\chi_m^{(s)}(\hat{\boldsymbol{n}}) = \left(\begin{array}{c} d_{sm}^{(s)}(\theta) \\ \vdots \\ d_{m'm}^{(s)}(\theta) \\ \vdots \\ d_{-sm}^{(s)}(\theta) \end{array} \right). \tag{22}$$

where $d_{m'm}(\theta)$ *are the d-functions. These are in fact just matrix elements of the spin rotation matrix* $\exp(-i\,\theta\,S_y)$ *between states quantized along the z-direction. Extended to include azimuthal dependence it is customary to use the rotation matrix* $e^{-i\,\phi\,S_z}\,e^{-i\,\theta\,S_y}\,e^{-i\,\chi\,S_3}$ *and the functions are called* $D_{m'm}(\phi,\theta,\chi)$.

3 Combination of angular momenta

3.1 Quantum number analysis

We consider situations in which two sets of angular momentum operators play a role, e.g.

- An electron with spin in an atomic $(n\ell)$-orbit (spin $\boldsymbol{s}$ and orbital angular momentum $\boldsymbol{\ell}$ combined into a total angular momentum $\boldsymbol{j} = \boldsymbol{\ell} + \boldsymbol{s}$).
- Two electrons with spin (spin operators $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$, combined into $\boldsymbol{S} = \boldsymbol{s}_1 + \boldsymbol{s}_2$).
- Two electrons in atomic orbits (orbital angular momenta $\boldsymbol{\ell}_1$ and $\boldsymbol{\ell}_2$ combined into total orbital angular momentum $\boldsymbol{L} = \boldsymbol{\ell}_1 + \boldsymbol{\ell}_2$).
- Combining the total orbital angular momentum of electrons in an atom ($\boldsymbol{L}$) and the total spin ($\boldsymbol{S}$) into the total angular momentum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$.

Let us discuss as the generic example

$$\boldsymbol{J} = \boldsymbol{j}_1 + \boldsymbol{j}_2. \tag{23}$$

We have states characterized by the direct product of two states,

$$|j_1, m_1\rangle \otimes |j_2, m_2\rangle, \tag{24}$$

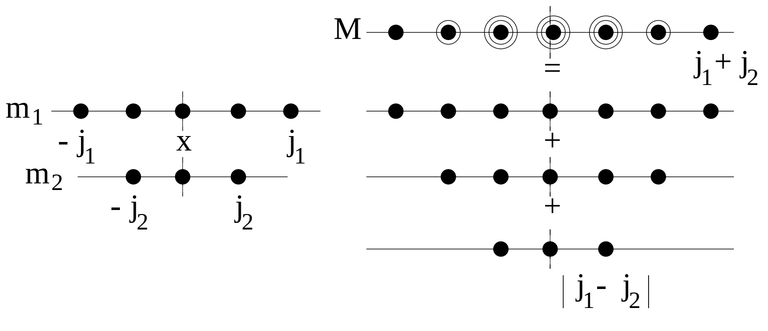
which we can write down since not only $[\boldsymbol{j}_1^2, j_{1z}] = [\boldsymbol{j}_2^2, j_{2z}] = 0$, but also $[j_{1m}, j_{2n}] = 0$. The sum-operator $\boldsymbol{J}$ obviously is not independent, but since the $\boldsymbol{J}$-operators again satisfy the well-known angular momentum commutation relations we can look for states characterized by the commuting operators $\boldsymbol{J}^2$ and J_z, $|\ldots; J, M\rangle$. It is easy to verify that of the four operators characterizing the states in Eq. 24, $[\boldsymbol{J}^2, j_{1z}] \neq 0$ and $[\boldsymbol{J}^2, j_{2z}] \neq 0$ (Note that $\boldsymbol{J}^2$ contains the operator combination $2\boldsymbol{j}_1 \cdot j_2$, which contains operators like j_{1x}, which do not commute with j_{1z}). It is easy to verify that one does have

$$[\boldsymbol{J}^2, \boldsymbol{j}_1^2] = [\boldsymbol{J}^2, \boldsymbol{j}_2^2] = 0,$$
$$[J_z, \boldsymbol{j}_1^2] = [J_z, \boldsymbol{j}_2^2] = 0,$$

and thus we can relabel the $(2j_1+1)(2j_2+1)$ states in Eq. 24 into states characterized with the quantum numbers

$$|j_1, j_2; J, M\rangle. \tag{25}$$

The basic observation in the relabeling is that $J_z = j_{1z} + j_{2z}$ and hence $M = m_1 + m_2$. This leads to the following scheme, in which in the left part the possible m_1 and m_2-values are given and the upper right part the possible sum-values for M including their degeneracy.



1. Since $|m_1| \leq j_1$ and $|m_2| \leq j_2$, the maximum value for M is $j_1 + j_2$. This state is unique.
2. Since $J_+ = j_{1+} + j_{2+}$ acting on this state is zero, it corresponds to a state with $J = j_1 + j_2$. Then, there must exist other states (in total $2J+1$), which can be constructed via $J_- = j_{1-} + j_{2-}$ (in the scheme indicated as the first set of states in the right part below the equal sign).

3. In general the state with $M = j_1 + j_2 - 1$ is twofold degenerate. One combination must be the state obtained with J_- from the state with $M = j_1 + j_2$, the other must be orthogonal to this state and again represents a 'maximum M'-value corresponding to $J = j_1 + j_2 - 1$.
4. This procedure goes on till we have reached $M = |j_1 - j_2|$, after which the degeneracy is equal to the $\min\{2j_1 + 1, 2j_2 + 1\}$, and stays constant till the M-value reaches the corresponding negative value.

Thus

Combining two angular momenta j_1 and j_2 we find resulting angular momenta J with values

$$J = j_1 + j_2,\ j_1 + j_2 - 1, \ldots, |j_1 - j_2|, \tag{26}$$

going down in steps of one.

Note that the total number of states is (as expected)

$$\sum_{J=|j_1-j_2|}^{j_1+j_2} (2J+1) = (2j_1+1)(2j_2+1). \tag{27}$$

Furthermore we have in combining angular momenta:

half-integer with half-integer ⟶ integer
integer with half-integer ⟶ half-integer
integer with integer ⟶ integer

3.2 Clebsch-Gordon coefficients

The actual construction of states just follows the steps outlined above. Let us illustrate it for the case of combining two spin 1/2 states. We have four states according to labeling in Eq. 24,

$$\begin{aligned} |s_1, m_1\rangle \otimes |s_2, m_2\rangle : \qquad & |1/2, +1/2\rangle \otimes |1/2, +1/2\rangle \equiv |\uparrow\uparrow\rangle, \\ & |1/2, +1/2\rangle \otimes |1/2, -1/2\rangle \equiv |\uparrow\downarrow\rangle, \\ & |1/2, -1/2\rangle \otimes |1/2, +1/2\rangle \equiv |\downarrow\uparrow\rangle, \\ & |1/2, -1/2\rangle \otimes |1/2, -1/2\rangle \equiv |\downarrow\downarrow\rangle. \end{aligned}$$

1. The highest state has $M = 1$ and must be the first of the four states above. Thus for the labeling $|s_1, s_2; S, M\rangle$
$$|1/2, 1/2; 1, +1\rangle = |\uparrow\uparrow\rangle. \tag{28}$$
2. Using $S_- = s_{1-} + s_{2-}$ we can construct the other $S+1$ states.
$$\begin{aligned} & S_-|1/2, 1/2; 1, +1\rangle = \hbar\sqrt{2}\,|1/2, 1/2; 1, 0\rangle, \\ & (s_{1-} + s_{2-})|\uparrow\uparrow\rangle = \hbar(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \end{aligned}$$
and thus
$$|1/2, 1/2; 1, 0\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\Big). \tag{29}$$
Continuing with S_- (or in this case using the fact that we have the lowest nondegenerate M-state) we find
$$|1/2, 1/2; 1, -1\rangle = |\downarrow\downarrow\rangle. \tag{30}$$

3. The state with $M = 0$ is twofold degenerate. One combination is already found in the above procedure. The other is made up of the same two states appearing on the right hand side in Eq. 29. Up to a phase, it is found by requiring it to be orthogonal to the state $|1/2, 1/2; 1, 0\rangle$ or by requiring that $S_+ = s_{1+} + s_{2+}$ gives zero. The result is

$$|1/2, 1/2; 0, 0\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\Big). \tag{31}$$

   The convention for the phase is that the higher m_1-value appears with a positive sign.

It is easy to summarize the results in a table, where one puts the states $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$ in the different rows and the states $|j_1, j_2; J, M\rangle$ in the different columns, i.e.

$j_1 \times j_2$	$\vdots$ J $\vdots$
	$\vdots$ M $\vdots$
$\cdots\ \cdots$	
$m_1\ m_2$	
$\cdots\ \cdots$	

For the above case we have

1/2 × 1/2		1	1	0	1
		1	0	0	-1
+1/2	+1/2	1			
+1/2	−1/2		$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	
−1/2	+1/2		$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$	
−1/2	−1/2				1

Note that the recoupling matrix is block-diagonal because of the constraint $M = m_1 + m_2$. The coefficients appearing in the matrix are the socalled Clebsch-Gordan coefficients. We thus have

$$|j_1, j_2; J, M\rangle = \sum_{m_1, m_2} C(j_1, m_1, j_2, m_2; J, M)\, |j_1, m_1\rangle \otimes |j_2, m_2\rangle. \tag{32}$$

Represented as a matrix as done above, it is unitary (because both sets of states are normed). Since the Clebsch-Gordan coefficients are choosen real, the inverse is just the transposed matrix, or

$$|j_1, m_2\rangle \otimes |j_2, m_2\rangle = \sum_{J,M} C(j_1, m_1, j_2, m_2; J, M)\, |j_1, j_2; J, M\rangle. \tag{33}$$

In some cases (like combining two spin 1/2 states) one can make use of symmetry arguments. If a particular state has a well-defined symmetry under permutation of states 1 and 2, then all M-states belonging to a particular J-value have the same symmetry (because $j_{1\pm} + j_{2\pm}$ does not alter the symmetry. This could have been used for the 1/2 × 1/2 case, as the highest total M is symmetric, all $S = 1$ states are symmetric. This is in this case sufficient to get the state in Eq. 29.

We will give two other examples. The first is

1 × 1/2		3/2	3/2	1/2	3/2	1/2	3/2
		+3/2	+1/2	+1/2	−1/2	−1/2	−3/2
+1	+1/2	1					
+1	−1/2		$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{2}{3}}$			
0	+1/2		$\sqrt{\frac{2}{3}}$	$-\sqrt{\frac{1}{3}}$			
0	−1/2				$\sqrt{\frac{2}{3}}$	$\sqrt{\frac{1}{3}}$	
−1	+1/2				$\sqrt{\frac{1}{3}}$	$-\sqrt{\frac{2}{3}}$	
−1	−1/2						1

for instance needed to obtain the explicit states for an electron with spin in an (2p)-orbit coupled to a total angular momentum $j = 3/2$ *(indicated as* $2p_{3/2}$*) with* $m = 1/2$ *is*

$$\phi(\boldsymbol{r},t) = \frac{u_{2p}(r)}{r}\left(\sqrt{\frac{1}{3}}\,Y_1^1(\theta,\phi)\,\chi_\downarrow + \sqrt{\frac{2}{3}}\,Y_1^0(\theta,\phi)\,\chi_\uparrow\right).$$

The second is

1 × 1		2	2	1	2	1	0	2	1	2
		+2	+1	+1	0	0	0	−1	−1	−2
+1	+1	1								
+1	0		$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$						
0	+1		$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$						
+1	−1				$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{3}}$			
0	0				$\sqrt{\frac{2}{3}}$	0	$-\sqrt{\frac{1}{3}}$			
+1	−1				$\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{3}}$			
0	−1							$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	
−1	0							$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$	
−1	−1									1

This example, useful in the combination of two spin 1 particles or two electrons in p-waves, illustrates the symmetry of the resulting wave functions.

3.3 An example: the Helium atom

As a first-order description of the helium atom, one can consider the independent-electron approximation, starting with a hamiltonian in which the electron-electron interaction is neglected, as well as any interactions involving the spin of the electrons. In that case one has a separable hamiltonian and for each of the electrons the solutions are given by hydrogen-like states ($Z = 2$), characterized by $(n\ell)$. Let us investigate the possible ground-state configurations, $(1s)^2$ and the first excited levels $(1s)(2p)$ and $(1s)(2s)$.

- The ground state configurations $(1s)^2$.
  Knowing the two angular momenta involved is sufficient to know the parity of these states, $\Pi = (-)^{\ell_1}(-)^{\ell_2} = +$. The angular momentum recoupling works in the following way.
  - Combining $\ell_1 = 0$ and $\ell_2 = 0$, the only possibility is $L = 0$. The orbital wave function then is symmetric under the interchange of the two electrons 1 and 2.
  - Combining the spins $s_1 = 1/2$ and $s_2 = 1/2$ gives two possibilities, $S = 0$ or $S = 1$. The first possibility is antisymmetric under the interchange of the electrons, the second is symmetric.
  - The total wave function (product of orbital and spin parts) must be antisymmetric for fermions according to the Pauli principle, hence $L = 0$ can only be combined with $S = 0$. This leaves only one possibility for the total angular momentum, $J = 0$. The notation for the only allowed ground state configuration is

    $$(n_1\,\ell_1)(n_2\,\ell_2)\;{}^{2S+1}L_{J^\Pi} = (1s)^2\;{}^1S_{0^+}.$$

- The configurations $(1s)(2p)$ with parity $\Pi = -$.
  - We have $L = 1$, but appearing twice. We can construct the symmetric and antisymmetric combinations,

    $$\phi^{s/a}_{LM_L} = \frac{1}{\sqrt{2}}\left[\frac{u_{1s}(r_1)}{r_1}\,Y_0^0(\Omega_1)\,\frac{u_{2p}(r_2)}{r_2}\,Y_1^{M_L}(\Omega_2) \pm \frac{u_{2p}(r_1)}{r_1}\,Y_1^{M_L}(\Omega_1)\frac{u_{1s}(r_2)}{r_2}\,Y_0^0(\Omega_2)\right]$$

    for the spatial part.
  - The combination of the spins gives again an antisymmetric $S = 0$ and a symmetric $S = 1$ wave function.

  - The allowed configurations are thus obtained by the appropriate antisymmetric combinations of orbital and spin parts,

$$(1s)(2p)\ {}^1P_{1^-} \qquad \text{and} \qquad (1s)(2p)\ {}^3P_{0^-,1^-,2^-}\,.$$

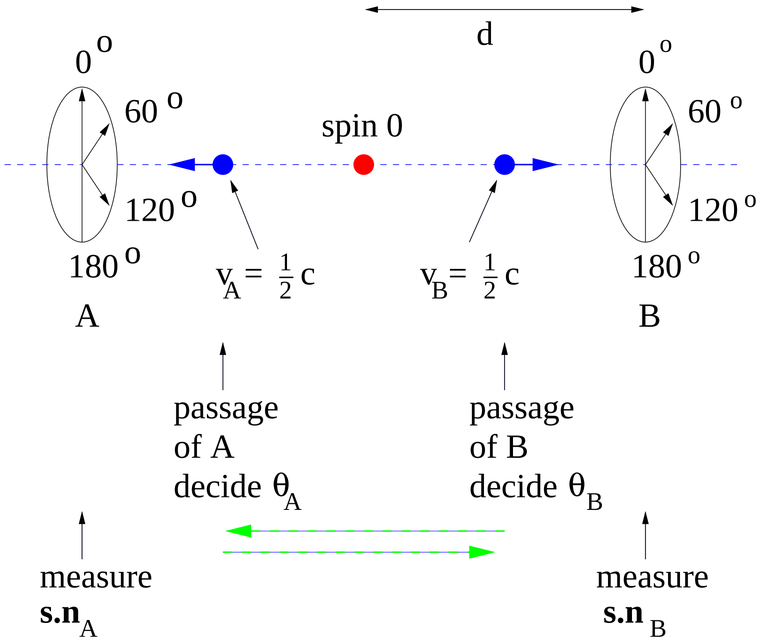
- The configurations $(1s)(2s)$ with parity $\Pi = +$.
  - We have $L = 0$, but now also appearing twice in a symmetric and antisymmetric combination.
  - As above, antisymmetric $S = 0$ and symmetric $S = 1$.
  - This gives the allowed configurations

$$(1s)(2s)\ {}^1S_{0^+} \qquad \text{and} \qquad (1s)(2s)\ {}^3S_{1^+}\,.$$

4 The EPR experiment

4.1 The 'experiment'

One of the best ways to illustrate the 'absurdness' of quantum mechanics when one tries to understand it with classical means is the EPR experiment, proposed by Einstein, Podolsky and Rosen (1935) to show that quantum mechanics should be wrong. A simplified version of the experiment is the decay of a spin 0 system into two spin 1/2 particles with opposite spin. The spin is measured along a direction perpendicular to the motion of the two particles, which are moving apart at (say) half of the speed of light. The angles θ_A and θ_B, along which the spin is measured can be varied, but the actual decision which angles are measured is only taken (at random) when the particles are halfway[1].



The results of the measurements (which in recent years have actually been performed with a variety of particles over macroscopic distances) are as follows:

- Considering only the measurement at A, the probability to measure a spin along $\hat{\boldsymbol{n}}_A$ is $P(\theta_A,+) = 1/2$ and the probability to measure a spin opposite to this is $P(\theta_A,-) = 1/2$. Similarly at B.
- Given a '+'-measurement at A at a given angle θ_A, the following results are found:

$\lvert\theta_A - \theta_B\rvert =$	$0°$	$60°$	$120°$	$180°$
$P(\theta_A,+;\theta_B,+)$	0	1/4	3/4	1
$P(\theta_A,+;\theta_B,-)$	1	3/4	1/4	0

4.2 A classical explanation?

In any 'realistic' theory the information on the potential measurements for particle A should be a property of particle A and hence stored in the particle. Thus to simplify things, only concentrate on three angles ($0°$, $60°$ and $120°$). Any event has particles A and B flying apart with known prescriptions for what to do if they encounters a Stern-Gerlach apparatus under a given angle θ_A. E.g.

Event 1: $\text{memory\_A} = (+-+)$ $\text{memory\_B} = (-+-)$
Event 2: $\text{memory\_A} = (++-)$ $\text{memory\_B} = (--+)$

---

[1] In this way information on the setting of B cannot reach A at the time of measurement

etc. For instance in the first example the prescription tells A that if $\theta_A = 0°$, then a spin measurement yields $+\hbar/2$, if $\theta_A = 60°$, then a spin measurement yields $-\hbar/2$, while if $\theta_A = 120°$, then a spin measurement yields $+\hbar/2$. In each of the events the common origin of A and B is reflected in the complementary prescriptions. This is the only way the first and last colums of the 'experiment' can be explained. Let's now concentrate on the correlations and write some explicit probabilities $P(\theta_A, +; \theta_B, +)$ in terms of the fractions of events with particular memories. We have e.g.

$$\begin{aligned} P(0°,+;120°,+) &= \sum_{\sigma=-\tau} f(+\sigma-;-\tau+) \\ &= f(++-;--+) \;+\; f(+--;-++) \end{aligned} \tag{34}$$

$$P(60°,+;120°,+) = f(++-;--+) \;+\; \underbrace{f(-+-;+-+)}_{\geq 0} \tag{35}$$

$$P(0°,+;60°,+) = \underbrace{f(+-+;-+-)}_{\geq 0} + f(+--;-++), \tag{36}$$

and hence we must have in a realistic theory

$$P(60°,+;120°,+) + P(0°,+;60°,+) \geq P(0°,+;120°,+), \tag{37}$$

which is an explicit example of a Bell inequality. But clearly our 'experiment' above violates this inequality! Thus a realistic theory cannot explain the results in the EPR experiment.

4.3 The quantum-mechanical explanation!

Quantum mechanics can explain the results. Using e.g. the spin states defined with respect to the $\theta = 0$ directions, we know that the AB system is in an antisymmetric (spin zero) state,

$$|AB\rangle = \frac{1}{\sqrt{2}} \left(|A\uparrow\rangle \otimes |B\downarrow\rangle - |A\downarrow\rangle \otimes |B\uparrow\rangle \right) \tag{38}$$

Using the rotated spin states along an arbitrary direction $\hat{\boldsymbol{n}}$, it is straightforward to check the results of the EPR experiment. Given a '+'-measurement at A, the wave function becomes

$$|A\uparrow\rangle \otimes |B\downarrow\rangle$$

and the probability

$$P(0°,+;\theta_B,+) = \left| \langle A\uparrow || A\uparrow\rangle \, \langle \theta_B, + || B\downarrow\rangle \right|^2 = \sin^2(\theta_B/2). \tag{39}$$

For any other angle for θ_A, simply choose this as the quantization axis, to see that the result only depends on $\theta_A - \theta_B$.

5 Time dependent perturbation theory

Mandl, chapter 9

For a hamiltonian without explicit time-dependence, i.e. $H = H(\boldsymbol{r}, \boldsymbol{p}, \ldots)$ one has stationary state solutions of the form $|\phi\rangle\, e^{-iEt/\hbar}$, where $|\phi\rangle$ is time-independent and is a solution of the eigenvalue equation $H|\phi\rangle = E|\phi\rangle$.

> This can be checked by inserting such a solution (with *constant* E) in the Schrödinger equation, $i\hbar\partial|\psi\rangle/\partial t = H(t)|\psi(t)\rangle$, leading to
>
> $$i\hbar\frac{\partial}{\partial t}|\phi\rangle = (H - E)\,|\phi\rangle,$$
>
> If H has no time-dependence a solution satisfying $\partial|\phi\rangle/\partial t = 0$ exists.

As discussed earlier, there are two possibilities

1. One starts (e.g. after a measurement) with $\psi(0) = |\phi_i\rangle$, where ϕ_i is one of the eigenstates of H with eigenvalue/energy E_i. In that case $|\psi(t)\rangle = |\phi_i\rangle\, e^{-iE_it/\hbar}$ and all expectation values of operators (that do not explicitly depend on time) are time-independent.
2. One starts in a mixed state, say $|\psi(0)\rangle = |\phi_1\rangle + |\phi_2\rangle$. In that case one has $|\psi(t)\rangle = |\phi_1\rangle\, e^{-iE_1t/\hbar} + |\phi_2\rangle\, e^{-iE_2t/\hbar}$ or $|\psi(t)\rangle \propto |\phi_1\rangle + |\phi_2\rangle\, e^{-i(E_2-E_1)t/\hbar}$, which leads to oscillations in expectation values with frequency $\sim (E_2 - E_1)/\hbar$.

In the situation that the hamiltonian of a system contains explicit time dependence, i.e. $H = H(\boldsymbol{r}, \boldsymbol{p}, \ldots, t)$ one no longer has stationary state solutions of the form $|\phi\rangle\, e^{-iEt/\hbar}$. It is easy to see that a check as discussed above with a time-dependent $H(t)$ will leave us with a time-dependence in $|\phi\rangle = |\phi(t)\rangle$.

Next consider the case that the time-dependence is contained in a part of the Hamiltonian, which we (in order to study it perturbatively) multiply with a factor λ,

$$H = H_0 + \lambda\, V(t), \tag{40}$$

where H_0 does not have explicit t-dependence, while the second part has a (possible) time-dependence. Assume the problem H_0 to be known, i.e. $H_0|\phi_n\rangle = E_n|\phi_n\rangle$ with eigenstates $|\phi_n\rangle$ and eigen-energies E_n. In doing time-independent perturbation theory (when V is time-independent) one tries to express the true eigenfunctions of H in the complete set ϕ_i. Already in that case one observes that if the system originally is in a state $|\phi_i\rangle$, it will at a later time no longer be in this state, because we have to expand $|\phi_i\rangle$ in the true eigenstates of H, which deviate from the eigenstates of H_0. This problem is more easily dealt with in time-dependent perturbation theory, which, moreover, can also treat time-independent perturbations.

6 Treatment of time-dependent perturbations

We consider as mentioned in the previous section $H = H_0 + \lambda\, V(t)$, with a known (time-independent) part for which the eigenstates and eigen-energies satisfy $H_0|\phi_n\rangle = E_n|\phi_n\rangle$. Using completeness of the states $|\phi_n\rangle$ we know that it is always possible to write

$$|\psi(t)\rangle = \sum_n c_n(t)\,|\phi_n\rangle\, e^{-iE_nt/\hbar}. \tag{41}$$

Note that one could have absorbed the exponential time-dependence in $c_n(t)$, but not doing so is more appropriate in perturbation theory. In the choosen way of proceeding, the time-dependence of c_n is solely a consequence of $\lambda\, V$.

By substituting the expression for $|\psi(t)\rangle$ in the Schrödinger equation,

$$i\hbar\,\frac{\partial}{\partial t}|\psi(t)\rangle = (H_0 + \lambda\, V(t))\,|\psi(t)\rangle, \tag{42}$$

one simply finds

$$i\hbar\,\dot{c}_p(t) = \sum_n \lambda\, V_{pn}(t)\, c_n(t)\, e^{+i\,\omega_{pn}t}, \tag{43}$$

where $V_{pn} = \langle\phi_p|V|\phi_n\rangle$ and $\omega_{pn} = (E_p - E_n)/\hbar$. As promised if $\lambda\, V = 0$, the righthand-side is zero and the coefficients are time-independent.

In the next section we solve the above equations for a simple two-state system. More often, however, one will encounter a perturbative approach.

In the case of perturbation theory, we realize that in trying a solution of the form

$$c_p(t) = c_p^{(0)}(t) + \lambda\, c_p^{(1)}(t) + \ldots, \tag{44}$$

the time-dependence of a specific order is determined by the next lower order,

$$i\hbar\,\dot{c}_p^{(m+1)} = \sum_n V_{pn}(t)\, c_n^{(m)}(t)\, e^{+i\,\omega_{pn}t}. \tag{45}$$

Starting with $c_p(0) = \delta_{pi}$ one immediately sees that the first two orders are given by

$$c_p^{(0)}(\tau) = \delta_{pi}, \tag{46}$$

$$c_p^{(1)}(\tau) = \frac{1}{i\hbar}\int_0^\tau dt\; V_{pi}(t)\, e^{+i\,\omega_{pi}t}. \tag{47}$$

This can straightforwardly been extended and leads to the socalled 'time-ordered' exponential, which we will not discuss here.

The quantity $|c_p(\tau)|^2$ is the probability to find the system in the state $|\phi_p\rangle$, which means the probability for a transition $i \rightarrow p$. The first order result is valid if $|c_p^{(0)}(\tau) + c_p^{(1)}(\tau)|^2 \approx 1$.

6.1 An exactly soluble example

Consider the following hamiltonian for a two-state system,

$$H = -\boldsymbol{\mu} \cdot \boldsymbol{B}(t) = -\gamma\, \boldsymbol{s} \cdot \boldsymbol{B}(t), \tag{48}$$

describing the interaction of a spinning particle (with magnetic moment μ proportional to its spin) in a magnetic field. For instance for an elementary electron $\boldsymbol{\mu} = -(e/m)\, \boldsymbol{s}$ where $\boldsymbol{s} = (\hbar/2)\, \boldsymbol{\sigma}$. For other (composite particles) the factor may be different. However, for any spin 1/2 particle the spin operators can be represented by the Pauli matrices.

Considering first the case of a constant magnetic field in (say) the z-direction, i.e. $\boldsymbol{B}_0 = (0, 0, B_0)$. Using the matrix representation for a spin 1/2 particle one has

$$H = -\frac{\gamma B_0}{2}\, \hbar\, \sigma_z = -\frac{\gamma B_0}{2}\, \hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{49}$$

The solutions are easily obtained,

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{with} \quad E_1 = -\frac{\gamma B_0}{2}\, \hbar, \tag{50}$$

$$|\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{with} \quad E_2 = \frac{\gamma B_0}{2}\, \hbar, \tag{51}$$

If the system is in a spin-state along the z-direction, it will stay in this state. If it is in another direction, it will start to oscillate with a frequency $\omega_{12} = (E_1 - E_2)/\hbar = -\gamma\, B_0$.

Next consider the system in a circulating magnetic field in the x-y plane, superimposed on $\boldsymbol{B}_0$, $\boldsymbol{B}(t)$ $= \boldsymbol{B}_0 + \boldsymbol{B}_1(t)$, where $\boldsymbol{B}_1(t) = (B_1 \cos\omega t, B_1 \sin\omega t, 0)$. In that case

$$\begin{aligned} H &= -\frac{\gamma B_0}{2}\, \hbar\, \sigma_z - \frac{\gamma B_1}{2}\, \hbar (\sigma_x \cos\omega t + \sigma_y \sin\omega t) \\ &= -\frac{\gamma B_0}{2}\, \hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{\gamma B_1}{2}\, \hbar \begin{pmatrix} 0 & e^{-i\omega t} \\ e^{+i\omega t} & 0 \end{pmatrix}. \end{aligned} \tag{52}$$

As discussed in the previous section we can assume

$$|\psi(t)\rangle = c_1(t) \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-i\omega_{12}t/2} + c_2(t) \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{+i\omega_{12}t/2} = \begin{pmatrix} c_1(t)\, e^{-i\omega_{12}t/2} \\ c_2(t)\, e^{+i\omega_{12}t/2} \end{pmatrix}, \tag{53}$$

for which insertion in the Schrödinger equation or using the theory in the previous section one finds

$$\begin{aligned} i\hbar \begin{pmatrix} \dot{c}_1(t) \\ \dot{c}_2(t) \end{pmatrix} &= -\frac{\gamma B_1}{2}\, \hbar \begin{pmatrix} 0 & e^{-i(\omega-\omega_{12})t} \\ e^{+i(\omega-\omega_{12})t} & 0 \end{pmatrix} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} \\ &= \hbar \begin{pmatrix} 0 & v(t) \\ v^*(t) & 0 \end{pmatrix} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}, \end{aligned} \tag{54}$$

with $|v| = \gamma B_1/2$. The coupled equations,

$$i\, \dot{c}_1(t) = v(t)\, c_2(t), \tag{55}$$

$$i\, \dot{c}_2(t) = v^*(t)\, c_1(t), \tag{56}$$

can be simply rewritten into a second order differential equation for c_1,

$$\ddot{c}_1 + i(\omega - \omega_{12})\, \dot{c}_1 + |v|^2\, c_1 = 0. \tag{57}$$

This equation has two independent solutions of the form $e^{i\,pt}$ with

$$p = -\frac{1}{2}\, (\omega - \omega_{12}) \pm \frac{1}{2}\, \Delta \tag{58}$$

with $\Delta = \sqrt{(\omega - \omega_{12})^2 + 4|v|^2}$. The general solution can then be written as

$$\begin{aligned} c_1(t) &= e^{-\frac{1}{2}i(\omega-\omega_{12})t}\left(A\,\sin\frac{\Delta\,t}{2} + B\,\cos\frac{\Delta\,t}{2}\right), \\ c_2(t) &= \frac{i}{v(t)}\,\dot{c}_1(t). \end{aligned} \tag{59}$$

Starting off with $c_1(0) = 0$ and $|c_2(0)| = 1$, it is straightforward to check that

$$c_1(t) = A\,e^{\frac{1}{2}\,i\,(\omega-\omega_{12})t}\,\sin\frac{\Delta\,t}{2}, \tag{60}$$

$$|A|^2 = 4\,\frac{|v|^2}{\Delta^2} = \frac{\gamma^2 B_1^2}{(\omega-\omega_{12})^2 + \gamma^2 B_1^2}, \tag{61}$$

$$|c_1(t)|^2 + |c_2(t)|^2 = 1. \tag{62}$$

Thus, given an initial spin aligned parallel or antiparallel to the $\boldsymbol{B}_0$ field, the probability for transition to the other spin state shows oscillations with a frequency Δ, while the magnitude depends on the frequency of the rotating perpendicular $\boldsymbol{B}_1$ field, showing a resonance at $\omega = \omega_{12}$. In that case the spin completely flips from parallel to antiparallel and back with frequency Δ (at resonance we have $\Delta = \gamma B_1$). For further discussion and plots, see Mandl (section 9.2).

7 Fermi's golden rule

We now return to the perturbative treatment of time-dependence and note that also for a time-independent interaction V, transitions occur, if the initial state is not an eigenstate of the full Hamiltonian, but only of H_0. If V is sufficiently weak, we find the result in first order perturbation theory,

$$\begin{aligned} c_p^{(1)}(\tau) &= \frac{V_{pi}}{i\hbar}\int_0^\tau dt\; e^{+i\,\omega_{pi}t} = -\,\frac{V_{pi}}{\hbar\omega_{pi}}\; e^{+i\,\omega_{pi}t}\Big|_0^\tau \\ &= \frac{V_{pi}}{\hbar\omega_{pi}}\left(1-e^{+i\,\omega_{pi}\tau}\right) = -\frac{2\,V_{pi}}{\hbar\omega_{pi}}\,\sin(\omega_{pi}\tau/2)\,e^{+i\,\omega_{pi}\tau/2}, \end{aligned} \tag{63}$$

and thus for $p \neq i$,

$$P^{(1)}_{i\to p}(\tau) = \frac{4\,|V_{pi}|^2}{\hbar^2}\,\frac{\sin^2(\omega_{pi}\tau/2)}{\omega_{pi}^2}. \tag{64}$$

The function

$$f(\omega_{pi}) = \frac{\sin^2(\omega_{pi}\tau/2)}{\omega_{pi}^2}$$

is for increasing times τ ever more strongly peaked around $\omega_{pi} = 0$. The value at zero is $f(0) = \tau^2/4$, the first zeros are at $|\omega_{pi}| = 2\pi/\tau$. Since

$$\int d\omega_{pi}\;\frac{\sin^2(\omega_{pi}\tau/2)}{\omega_{pi}^2} = \frac{\pi\,\tau}{2}, \tag{65}$$

we approximate

$$\frac{\sin^2(\omega_{pi}\tau/2)}{\omega_{pi}^2} = \frac{\pi\,\tau}{2}\,\delta(\omega_{pi}). \tag{66}$$

Then we find[2]

$$P^{(1)}_{i\to p}(\tau) = \tau\,\frac{2\pi}{\hbar}\,|V_{pi}|^2\,\delta(E_p - E_i) \tag{67}$$

or for the transition probability per unit time,

$$\dot{P}^{(1)}_{i\to p} = \frac{2\pi}{\hbar}\,|V_{pi}|^2\,\delta(E_p - E_i) \qquad \text{Fermi's Golden Rule.} \tag{68}$$

Although the allowed final state is selected via the energy delta function, it is often possible that the system can go to many final states, because we are dealing with a continuum. In that case one needs the *density of states* $\rho(E)$, where $\rho(E)\,dE$ is the number of states in an energy interval dE around E. The transition probability per unit time is then given by

$$\dot{P}^{(1)}_{i\to p} = \int dE_f\,\rho(E_f)\,\frac{2\pi}{\hbar}\,|V_{fi}|^2\,\delta(E_f - E_i) = \frac{2\pi}{\hbar}\,|V_{pi}|^2\,\rho(E_p)\Big|_{E_p=E_i} \tag{69}$$

(Fermi's Golden Rule No. 2).

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[2] $\delta(ax) = \frac{1}{|a|}\,\delta(x)$

8 The dipole approximation

As an example of time-dependent perturbations, we discuss the absorption and emission of photons by atoms. In this case one often uses the dipole approximation for the interaction of matter with an electromagnetic field. Here only a very global treatment is presented, to be used in the next section.

We take a plane wave for the scalar and vector potential,

$$\phi = \tilde{\phi}(\boldsymbol{k},\omega)\, \exp[i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)], \tag{70}$$

$$\boldsymbol{A} = \tilde{\boldsymbol{A}}(\boldsymbol{k},\omega)\, \exp[i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)], \tag{71}$$

with $\omega = |\boldsymbol{k}|c$, corresponding with the energy and momentum relation, $E = |\boldsymbol{p}|c$, for a massless photon. Although the physical fields are real, we can work with the plane waves by always taking also the complex conjugate solution into account. The corresponding behavior for the electric and magnetic fields can be obtained from the potentials[3]

$$\boldsymbol{E} = \tilde{\boldsymbol{E}}(\boldsymbol{k},\omega)\, \exp[i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)], \tag{72}$$

$$\boldsymbol{B} = \tilde{\boldsymbol{B}}(\boldsymbol{k},\omega)\, \exp[i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)]. \tag{73}$$

The interaction of matter with an electromagnetic field is given by

$$H_{int} = \int d^3r\ \left[\rho(\boldsymbol{r})\,\phi(\boldsymbol{r}) - \boldsymbol{j}(\boldsymbol{r})\cdot\boldsymbol{A}(\boldsymbol{r})\right], \tag{74}$$

where ρ and $\boldsymbol{j}$ are the charge and current distribution. The dipole approximation is valid when the wave length $\lambda = 2\pi/|\boldsymbol{k}|$ is much larger than the typical size of the system, e.g. for light ($\lambda \approx 6000 \mathring{A}$) and atoms (size $\approx 1 - 10\mathring{A}$). In that case one can restrict oneself to the first nontrivial term in

$$\exp[i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)] = e^{-i\,\omega t}\,(1 + i\,\boldsymbol{k}\cdot\boldsymbol{r} + \ldots). \tag{75}$$

One obtains

$$\begin{aligned} H_{int} &= \int d^3r\ \Big[(1 + i\,\boldsymbol{k}\cdot\boldsymbol{r})\,\rho(\boldsymbol{r})\,\tilde{\phi}(\boldsymbol{k},\omega) - (1 + i\,\boldsymbol{k}\cdot\boldsymbol{r})\,\boldsymbol{j}(\boldsymbol{r})\cdot\tilde{\boldsymbol{A}}(\boldsymbol{k},\omega)\Big] && (76)\\ &= Q\,\tilde{\phi}(\boldsymbol{k},\omega) - \boldsymbol{D}\cdot\tilde{\boldsymbol{E}}(\boldsymbol{k},\omega) - \boldsymbol{\mu}\cdot\tilde{\boldsymbol{B}}(\boldsymbol{k},\omega) + \ldots, && (77)\end{aligned}$$

where we have used that $i\,\boldsymbol{k}\,\tilde{\phi} = -\tilde{\boldsymbol{E}} + (\omega/c)\,\tilde{\boldsymbol{A}}$ and $i\,\boldsymbol{k}\times\tilde{\boldsymbol{A}} = \tilde{\boldsymbol{B}}$. The charge and current distributions give rise to charge, electric and magnetic dipole moments,

$$Q = \int d^3r\ \rho(\boldsymbol{r}) \Longrightarrow \sum_i q_i, \tag{78}$$

$$\boldsymbol{D} = \int d^3r\ \boldsymbol{r}\,\rho(\boldsymbol{r}) \Longrightarrow \sum_i q_i\,\boldsymbol{r}_i, \tag{79}$$

$$\boldsymbol{\mu} = \int d^3r\ \boldsymbol{r}\times\boldsymbol{j}(\boldsymbol{r}) \Longrightarrow \sum_i \frac{q_i}{m_i}\,\boldsymbol{\ell}_i, \tag{80}$$

The results after the arrow in the above equations indicate the results for a number of charges q_i at position $\boldsymbol{r}_i$, i.e. $\rho(\boldsymbol{r}) = \sum_i q_i\,\delta^3(\boldsymbol{r} - \boldsymbol{r}_i)$. For a neutral system the first interaction term disappears and the next important one is the interaction with the electric dipole moment ($\boldsymbol{D}$).

---

[3] Recall that

$$\boldsymbol{E} = -\boldsymbol{\nabla}\Phi - \frac{1}{c}\,\frac{\partial\boldsymbol{A}}{\partial t},$$
$$\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$$

9 Emission and absorption of radiation by atoms

The radiation fields can be obtained from the vector potential

$$\boldsymbol{A} = \boldsymbol{\epsilon}(\boldsymbol{k},\omega)\, \frac{c\,\tilde{E}_0(\boldsymbol{k},\omega)}{i\,\omega}\, \exp[i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)] \tag{81}$$

and $\phi = 0$. The vector $\boldsymbol{\epsilon}$ is called the polarization. One has

$$\boldsymbol{E} = \boldsymbol{\epsilon}\,\tilde{E}_0\, \exp[i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)], \tag{82}$$

$$\boldsymbol{B} = \frac{\boldsymbol{k}\times\boldsymbol{\epsilon}}{|\boldsymbol{k}|}\,\tilde{E}_0\, \exp[i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)]. \tag{83}$$

In the dipole approximation the interaction with matter is given by

$$V(t) = -\boldsymbol{D}\cdot\boldsymbol{E}(t) = -\boldsymbol{D}\cdot\boldsymbol{\epsilon}\,\tilde{E}_0\, e^{-i\,\omega t}. \tag{84}$$

Although we have a time-dependent interaction, we can proceed as in the derivation of Fermi's golden rule. We obtain now

$$c_p^{(1)}(\tau) = \frac{\langle\phi_p|\boldsymbol{D}\cdot\boldsymbol{\epsilon}|\phi_i\rangle\,\tilde{E}_0}{i\hbar}\,\frac{e^{i\,(\omega_{pi}-\omega)\tau} - 1}{i\,(\omega_{pi}-\omega)}, \tag{85}$$

which gives as before rise to a delta function $\delta(\omega - \omega_{pi})$. With ω being the positive photon frequency, this can only describe *absorption* of a photon, $\hbar\omega = E_p - E_i > 0$. As discussed before, also the complex conjugate solution must be considered, which gives the same result with $\omega \to -\omega$. This gives rise to a delta function $\delta(\omega + \omega_{pi})$ and describes the *emission* of a photon, $\hbar\omega = -\hbar\omega_{pi} = E_i - E_p > 0$. The transition probability can be summarized by

$$P_{i\to p}^{(1)}(\tau) = \frac{\tilde{E}_0^2(\omega)}{\hbar^2}\, |\langle\phi_p|\boldsymbol{D}\cdot\boldsymbol{\epsilon}|\phi_i\rangle|^2\, \frac{\pi\,\tau}{2}\, \delta(\omega - |\omega_{pi}|). \tag{86}$$

If one is not working with monochromatic light one has an integral over different frequencies ω. Instead of the intensity of the field $\tilde{E}_0$ one can use the number of incident photons $N(\omega)$ (number/(area×time)). This number is determined by equating the energy densities in a frequency interval $d\omega$,

$$\frac{1}{2}\,\epsilon_0\, E_0^2(\omega)\, d\omega = \frac{N(\omega)\,\hbar\omega}{c}\, d\omega. \tag{87}$$

Integrating over the photon frequencies, one sees that the atom absorps or emits photons of the right frequency leading to a transition rate

$$\dot{P}_{i\to p}^{(1)} = \frac{\pi}{\epsilon_0\,\hbar c}\, |\omega_{pi}|\, N(|\omega_{pi}|)\, |\langle\phi_p|\boldsymbol{D}\cdot\boldsymbol{\epsilon}|\phi_i\rangle|^2. \tag{88}$$

For electrons $\boldsymbol{D} = -\sum_i e\,\boldsymbol{r}_i = -e\,\boldsymbol{R}$. For unpolarized light $\boldsymbol{\epsilon}$ is arbitrary and averaging gives a factor 1/3. In terms of the fine structure constant $\alpha = e^2/4\pi\,\epsilon_0\,\hbar c$ the averaged transition rate is

$$W_{i\to p} = \overline{\dot{P}_{i\to p}^{(1)}} = \frac{4}{3}\,\pi^2\,\alpha\, |\omega_{pi}|\, N(|\omega_{pi}|)\, |\langle\phi_p|\boldsymbol{R}|\phi_i\rangle|^2. \tag{89}$$

Note that by treating also the electromagnetic field quantummechanically one finds in addition to the *stimulated absorption or emission* rate a *spontaneous emission* rate

$$W_{i\to p}^{\text{spont.}} = \frac{4}{3}\,\alpha\,\frac{\omega_{ip}^3}{c^2}\, |\langle\phi_p|\boldsymbol{R}|\phi_i\rangle|^2, \tag{90}$$

governed by the same transition matrix element and thus obeying the same selection rules.

10 Unstable states

In many circumstances one encounters unstable states, i.e. the probability P to find a system in a particular state decreases in time,

$$P(t+dt) = P(t)\;(1-\gamma\,dt) \quad\Longrightarrow\quad \frac{dP}{dt} = -\gamma\,P(t),$$

where γ is the *decay rate* or decay probability per unit time. The solution is

$$P(t) = P(0)\,e^{-\gamma\,t} = P(0)\,e^{-t/T}, \tag{91}$$

with $T = 1/\gamma \equiv \hbar/\Gamma$ the *lifetime*. The quantity Γ is referred to as the *width* of a state. For a decaying state we thus write

$$|\psi_n(t)\rangle \propto e^{-i\,E_n t/\hbar - \gamma_n t/2}. \tag{92}$$

We can expand a decaying state in eigenmodes according to

$$e^{-i\,E_n t/\hbar - \gamma_n t/2}\,\theta(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,c(\omega)\,e^{-i\,\omega t}, \tag{93}$$

with

$$\begin{aligned} c(\omega) &= \int_0^\infty dt\; e^{+i\,(\omega-\omega_n+i\gamma_n/2)t} \\ &= \frac{-i}{\omega-\omega_n+i\gamma_n/2} e^{+i\,(\omega-\omega_n+i\gamma_n/2)t}\Big|_0^\infty \\ &= \frac{i}{\omega-\omega_n+i\gamma_n/2}. \end{aligned} \tag{94}$$

For unstable states the transition amplitude for emission or absorption of a photon is then proportional to

$$\begin{aligned} T(\omega) &= \int \frac{d\omega_1'}{2\pi}\,\frac{d\omega_2'}{2\pi}\,c_2^*(\omega_2')\,c_1(\omega_1')\,2\pi\,\delta(\omega-\omega_1'+\omega_2') \\ &= \int \frac{d\omega'}{2\pi} c_2^*(\omega')\,c_1(\omega'+\omega) \\ &= \int \frac{d\omega'}{2\pi} \int_0^\infty dt_1 \int_0^\infty dt_2\; e^{-i\,(\omega'-\omega_2-i\gamma_2/2)t_2}\; e^{+i\,(\omega'+\omega-\omega_1+i\gamma_1/2)t_1} \\ &= \int_0^\infty dt_1 \int_0^\infty dt_2\; e^{+i\,(\omega_2+i\gamma_2/2)t_2}\; e^{+i\,(\omega-\omega_1+i\gamma_1/2)t_1}\;\delta(t_1-t_2) \\ &= \int_0^\infty dt\; e^{+i\,(\omega-\omega_{12}+i\gamma_{12}/2)t} = \frac{i}{\omega-\omega_{12}+i\gamma_{12}/2}, \end{aligned} \tag{95}$$

where $\omega_{12} = \omega_1 - \omega_2$ and $\gamma_{12} = \gamma_1 + \gamma_2$. Thus the line-intensity becomes instead of a delta-function $\delta(\omega - |\omega_{pi}|)$ proportional to

$$I(\omega) \propto |T(\omega)|^2 \propto \frac{1}{(\omega-\omega_{12})^2 + \gamma_{12}^2/4},$$

or normalizing to the peak intensity

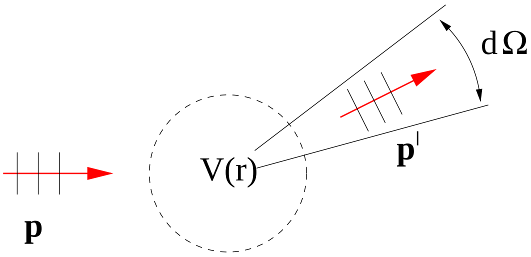
$$I(\omega) = I_0\,\frac{\Gamma_{12}^2/4}{\hbar^2\,(\omega-\omega_{12})^2 + \Gamma_{12}^2/4}, \tag{96}$$

showing the reason for the name width. The quantity Γ_{12} is precisely the width of the peak at half-maximum intensity, when plotting I as a function of the photon energy $\hbar\omega$. The function is known as a Lorentzian distribution or a Breit-Wigner distribution.

11 Introduction to scattering theory

Mandl, chapter 10

The quantummechanical treatment of a scattering problem is that of a particle (with mass m and incoming momentum $\boldsymbol{p}$) scattering in a given potential $V(\boldsymbol{r})$. We assume that the particle is scattered into a final state with momentum $\boldsymbol{p}'$. The latter is the result of a measurement with a detector with opening angle $d\Omega$, located under an angle $(\theta,\,\phi)$ with respect to the incoming momentum.



The number of scattered particles per unit time per solid angle, $n(\theta,\phi)$, is proportional to the incoming flux j_{in}, the number of particles per area per unit time,

$$n(\theta,\phi)\,d\Omega = |\boldsymbol{j}_{in}|\,d\sigma(\theta,\phi). \tag{97}$$

This is the definition of the *differential cross section* $d\sigma$, from which it should be immediately clear that the unit of cross section indeed is that of an area.

Typically cross sections have something to do with the area of the target as seen by the incoming particle, e.g. for proton-proton scattering a characteristic cross section is 40 mb, where 1 barn = 1 b $\equiv 10^{-28}$ m^2. The number 40 mb, indeed, is roughly equal to the area of a proton (with a radius of about 1 fm = 10^{-15} m). Besides the area of the target the cross sections also depends on the strength of the interaction. For instance electromagnetic interactions are typically a factor 100 or $(100)^2$ smaller, e.g. $\sigma_{\gamma p} \approx 100$ μb and $\sigma_{ep} \approx 1\mu$b, corresponding to the presence of the fine structure constant α or α^2 respectively, where $\alpha = e^2/4\pi\epsilon_0\hbar c = 1/137$. Weak interactions, e.g. neutrino-proton scattering, again have much smaller cross section in the order of 10^{-2} pb, indicative for the weakness of the "weak" interactions.

12 Cross section in Born approximation

We use the result of time-dependent perturbation theory to obtain an expression for the cross section, namely the unperturbed situation is the free case, with as possible solutions, the incoming particle in a plane wave, $\phi_i(\boldsymbol{r}) = \sqrt{\rho}\,\exp\left(i\,\boldsymbol{p}\cdot\boldsymbol{r}/\hbar\right)$, with energy $E = \boldsymbol{p}^2/2m$ and the detected final state, $\phi_f(\boldsymbol{r}) = \sqrt{\rho}\,\exp\left(i\,\boldsymbol{p}'\cdot\boldsymbol{r}/\hbar\right)$, with energy $E' = \boldsymbol{p}'^2/2m$. Note that we allow processes in which the energy of the scattered particle changes. writing $Q \equiv E' - E$ one has $Q = 0$ for an elastic scattering process, an energy release, $Q > 0$, for an exothermic process and energy absroption, $Q < 0$, for an endothermic process. The potential V is a perturbation that can cause transitions between these states. Using Fermi's golden rule, we have for the number of particles with momentum $\boldsymbol{p}'$ (of which the direction with respect to $\boldsymbol{p}$ is given by the angles θ, ϕ),

$$n(\theta,\phi)\,d\Omega = \frac{2\pi}{\hbar}\left[\left|\langle\phi_f|V|\phi_i\rangle\right|^2\,\rho(E')\right]_{E'=E+Q}. \tag{98}$$

In order to get $d\sigma$ we need to get the flux $\mathcal{I}$ in the initial state and the density of states $\rho(E')$ in the final state.

- *Initial state flux.*
  The initial state flux is obtained from the wave function in the initial state via the expression for the current,
  $$\boldsymbol{j}(\boldsymbol{r},t) = \frac{\hbar}{2i\,m}\left(\psi^*\,\boldsymbol{\nabla}\psi - (\boldsymbol{\nabla}\psi)^*\psi\right) = \rho\,\frac{\boldsymbol{p}}{m} = \rho\,\boldsymbol{v}. \tag{99}$$
  The incoming flux is along $\boldsymbol{p}$ and, as expected, given by $\mathcal{I} = \rho\,v = \rho\,p/m$ (we use $p = |\boldsymbol{p}|$).

- *Final state density of states.* The final states are plane waves and the density of plane waves is in momentum space given by
  $$\rho(\boldsymbol{p})\,d^3p = \frac{1}{\rho}\,\frac{d^3p}{(2\pi\hbar)^3}. \tag{100}$$
  This can be seen by looking at the expansion of the unit operators in coordinate and momentum space consistent with the choice of the normalization of the plane waves,
  $$\boldsymbol{1} = \int d^3r\;|\boldsymbol{r}\rangle\,\langle\boldsymbol{r}| = \frac{1}{\rho}\int\frac{d^3p}{(2\pi\hbar)^3}\;|\boldsymbol{p}\rangle\,\langle\boldsymbol{p}|. \tag{101}$$
  Another way is to use box normalization, in which case one finds that for one particle in a box with sides L, i.e. $0 \le x \le L$, $0 \le y \le L$ and $0 \le z \le L$ (i.e. density $\rho = 1/L^3$), the wave function is found after imposing periodic boundary conditions,
  $$\phi_p(\boldsymbol{r}) = \frac{1}{L^{3/2}}\,\exp(i\,\boldsymbol{p}\cdot\boldsymbol{r}/\hbar), \tag{102}$$
  with $\boldsymbol{p} = (2\pi\hbar/L)\,(n_x, n_y, n_z)$, showing a density of states in p-space given by $(L/2\pi\hbar)^3$. Rewriting the final state density $\rho(\boldsymbol{p}')$ in terms of E' and Ω' we find
  $$\rho(\boldsymbol{p}')d^3p' = \frac{1}{\rho}\,\frac{p'^2}{(2\pi\hbar)^3}\,dp'\,d\Omega' = \frac{1}{\rho}\,\frac{m\,p'}{(2\pi\hbar)^3}\,dE'\,d\Omega' = \rho(E')\,dE'\,d\Omega'. \tag{103}$$

With the flux and density of final states, we get immediately

$$d\sigma(\theta,\phi) = d\Omega'\left(\frac{m}{2\pi\hbar^2}\right)^2\frac{p'}{p}\left|\int d^3r\;\exp\left(\frac{i}{\hbar}\,(\boldsymbol{p}-\boldsymbol{p}')\cdot\boldsymbol{r}\right)\;V(\boldsymbol{r})\right|^2_{E'=E+Q}, \tag{104}$$

or introducing the Fourier transform

$$\tilde{V}(\boldsymbol{k}) = \int d^3r\;V(\boldsymbol{r})\;\exp(i\,\boldsymbol{k}\cdot r), \tag{105}$$

one obtains the following expression for the differential cross section in the socalled *Born approximation*,

$$\frac{d\sigma}{d\Omega'} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{p'}{p} \left|\tilde{V}(\boldsymbol{q})\right|^2, \tag{106}$$

where $\boldsymbol{q} = (\boldsymbol{p} - \boldsymbol{p}')/\hbar$ is the momentum transfer in the process. Often the differential cross section is azimuthally symmetric and one uses $d\Omega = d\cos\theta\, d\phi = 2\pi\, d\cos\theta$ to obtain $d\sigma/d\theta$. Integrating the differential cross section over all angles one obtains the *total cross section*,

$$\sigma(E) = \int d\Omega\, \frac{d\sigma}{d\Omega}(E, \Omega). \tag{107}$$

Note that in the case of elastic scattering one has $p' = p$ in which case the momentum transfer squared is given by

$$\begin{aligned} \hbar^2 \boldsymbol{q}^2 &= |\boldsymbol{p} - \boldsymbol{p}'|^2 = p^2 + p'^2 + 2\, pp'\, \cos(\theta) \\ &= 2\, p^2 (1 - \cos\theta) = 4\, p^2\, \sin^2(\theta/2). \end{aligned} \tag{108}$$

A dependence of the differential cross section $(d\sigma/d\Omega)(E, \theta)$ on this combination is a test for the validity of the Born approximation. This dependence is in particular applicable for central potentials, $V(\boldsymbol{r}) = V(r)$, in which case the Fourier transform

$$\begin{aligned} \tilde{V}(\boldsymbol{q}) &= \int d^3 r\, V(r)\, \exp(i\, \boldsymbol{q} \cdot \boldsymbol{r}) \\ &= 2\pi \int_0^\infty dr \int_{-1}^{1} d\cos\alpha\ r^2 V(r)\, e^{i\, qr\, \cos\alpha} \\ &= \frac{4\pi}{q} \int_0^\infty dr\ rV(r)\, \sin(qr), \end{aligned} \tag{109}$$

only depends on $q = |\boldsymbol{q}|$.

13 Applications

13.1 The square well potential

As a first application consider the square well potential, $V(r) = V_0$ for $r \leq a$ and zero elsewhere for sufficiently weak potentials at low energies and small angles ($qa \ll 1$). We will come back to the applicability of the Born approximation in a later section. The Fourier transform is given by

$$\begin{aligned}\tilde{V}(\boldsymbol{q}) &= \frac{4\pi\,V_0}{q}\int_0^a dr\ r\,\sin(qr) \\ &= \frac{4\pi\,V_0}{q^3}\int_0^{qa} dx\ x\,\sin(x) \\ &= \frac{4\pi\,V_0}{q^3}\left[\sin qa - qa\,\cos qa\right] \\ &\overset{qa\ll 1}{\longrightarrow} \frac{4\pi\,V_0}{q^3}\left[qa - \frac{1}{3!}(qa)^3 - qa + \frac{1}{2!}(qa)^3 + \ldots\right] = \frac{4\pi}{3}\,V_0 a^3,\end{aligned} \tag{110}$$

leading for $E \to 0$ to

$$\frac{d\sigma}{d\Omega} \approx \frac{1}{9}\left(\frac{2m\,V_0\,a^2}{\hbar^2}\right)^2 a^2 \tag{111}$$

13.2 The Coulomb potential

The integral

$$\tilde{V}(\boldsymbol{q}) = -\frac{Ze^2}{4\pi\epsilon_0}\,\frac{4\pi}{q}\int_0^\infty dr\ \sin(qr) \tag{112}$$

diverges and we need to consider for instance the screened Coulomb potential, multiplied with $\exp(-\mu r)$. In that case one obtains

$$\begin{aligned}\tilde{V}(\boldsymbol{q}) &= -\frac{Ze^2}{4\pi\epsilon_0}\,\frac{4\pi}{q}\int_0^\infty dr\ \sin(qr)\,e^{-\mu r} \\ &= -\frac{Ze^2}{4\pi\epsilon_0}\,\frac{4\pi}{q}\int_0^\infty dr\ \frac{1}{2i}\left(e^{i(q+i\mu)r} - e^{i(q-i\mu)r}\right) \\ &= -\frac{Ze^2}{\epsilon_0}\,\frac{1}{q^2+\mu^2},\end{aligned} \tag{113}$$

allowing even the limit $\mu \to 0$ to be taken. Thus

$$\frac{d\sigma}{d\Omega}(E,\theta) = \left(\frac{m}{2\pi\,\hbar^2}\right)^2\left(\frac{Ze^2}{\epsilon_0}\right)^2\frac{1}{q^4} = \left(\frac{Ze^2}{8\pi\,\epsilon_0\,pv}\right)^2\frac{1}{\sin^4(\theta/2)}. \tag{114}$$

This result is known as the Rutherford cross section.

13.3 Processes near threshold

If the volume integral over the potential exists, one knows that $\tilde{V}(0)$ is finite and one sees that for small values of the momentum transfer one can write

$$\sigma(E)\ \propto\ \frac{p'}{p}\ =\ \sqrt{\frac{E'}{E}}. \tag{115}$$

Thus for an endothermic process (energy absorption or $Q < 0$) one has a threshold value for the incoming energy, $E_{\mathrm{thr}} = |Q|$ and one has for $E \approx E_{\mathrm{thr}}$

$$\sigma(E)\ \propto\ \sqrt{E - E_{\mathrm{thr}}}. \tag{116}$$

For an exothermic process (with energy release $Q > 0$) one can scatter for any (positive) energy E and one has near $E \approx 0$

$$\sigma(E) \;\propto\; \frac{1}{\sqrt{E}}. \tag{117}$$

13.4 Application to two-particle collisions

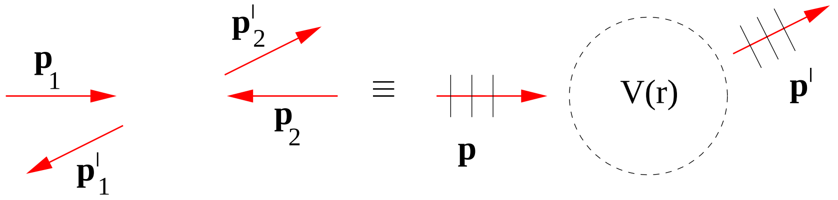
In most applications, the target is not an "external" potential, but rather two particles that collide (*collider experiments*) or one particle that is shot onto another one (*fixed target experiments*). This can in general lead to several possibilities corresponding to several *scattering channels*,

$$\begin{array}{ccll} a+b & \longrightarrow & a+b & \text{(elastic scattering)} \\ & \longrightarrow & c_1+c_2 & \multirow{2}{*}{$\left.\right\}$ (inelastic scattering)} \\ & \longrightarrow & d_1+d_2+d_3 & \end{array} \tag{118}$$

Nevertheless, one can deal with these processes, at least the two → two ones, by considering the problem in the center of mass (CM) system. Considering two particles with momenta $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ and masses m_1 and m_2, for which the only translationally invariant interaction that is allowed must be of the form $V(\boldsymbol{r}_1 - \boldsymbol{r}_2) = V(\boldsymbol{r})$ with $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ the relative coordinate. Since the flux factor is just given by

$$\mathcal{I} = \rho\, |\boldsymbol{v}_1 - \boldsymbol{v}_2| = \rho \left| \frac{\boldsymbol{p}_1}{m_1} - \frac{\boldsymbol{p}_2}{m_2} \right| = \rho\, \frac{\boldsymbol{p}}{\mu}, \tag{119}$$

where $\boldsymbol{p}$ is the relative momentum and μ the reduced mass one sees that the collision of *two* particles indeed can be described by considering the scattering of *one* particle with reduced mass μ having the relative momentum $\boldsymbol{p}$, scattering of the potential $V(\boldsymbol{r})$.



Notes:

- Note that in the scattering of *one* particle in an "external" potential, there is no translation invariance, hence no momentum conservation, while for *two* particles with a potential depending on the relative coordinate there is translation invariance. The latter requires conservation of the total momentum $\boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2$, but not of the relative momentum.
- In the limit that one of the masses becomes very large, the light particle's momentum and mass, indeed, coincide with relative momentum and reduced mass, so one finds (consistently) that the heavy particle can be considered as scattering center.

14 Scattering off a composite system

Consider the scattering of an electron off an extended object, e.g. an atomic nucleus consisting of Z protons (and N neutral neutrons). The hamiltonian is given by

$$H = H_{\rm nucleus} + V, \tag{120}$$

where $H_{\rm atom}(\boldsymbol{r}_1, \boldsymbol{p}_1; \ldots; \boldsymbol{r}_Z, \boldsymbol{p}_Z)$ is the nuclear hamiltonian and V describes the interaction between the scattering electron and the nucleus,

$$V = -\sum_{j=1}^{Z} \frac{e^2}{4\pi\,\epsilon_0\,|\boldsymbol{r} - \boldsymbol{r}_j|}. \tag{121}$$

We consider the nucleus to be initially in a state $|\Phi_A\rangle$ with energy ϵ_A and after the collision in a state $|\Phi_B\rangle$ with energy ϵ_B. Depending on the energy of the incoming electron this will be an elastic or endothermic process with $Q = \epsilon_A - \epsilon_B \le 0$, i.e. part of the energy of the scattering electron is absorbed and brings the nucleus into an excited state. The wave functions of the scattering electron in initial and final states are plane waves characterized by the momenta $\boldsymbol{p} = \hbar\boldsymbol{k}$ and $\boldsymbol{p}' = \hbar\boldsymbol{k}'$, respectively. The full initial state and final state wave functions are taken to be $\Psi_i(\boldsymbol{r}, \boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z) = \sqrt{\rho}\,\exp(i\,\boldsymbol{k}\cdot\boldsymbol{r})\,\Phi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z)$ and $\Psi_f(\boldsymbol{r}, \boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z) = \sqrt{\rho}\,\exp(i\,\boldsymbol{k}'\cdot\boldsymbol{r})\,\Phi_B(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z)$, respectively. The Fourier transform of the potential becomes

$$\begin{aligned} V(\boldsymbol{q}) &= \int d^3r \int \prod_{k=1}^{Z} d^3r_k\ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{r})\,\Phi_B^*(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z) \left(\sum_{j=1}^{Z} \frac{-e^2}{4\pi\,\epsilon_0\,|\boldsymbol{r} - \boldsymbol{r}_j|}\right) \Phi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z) \\ &= -\frac{e^2}{4\pi\,\epsilon_0} \sum_{j=1}^{Z} \int \prod_{k=1}^{Z} d^3r_k \int d^3r\ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{r})\,\Phi_B^* \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_j|}\,\Phi_A \\ &= -\frac{e^2}{4\pi\,\epsilon_0} \sum_{j=1}^{Z} \int \prod_{k=1}^{Z} d^3r_k\ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{r}_j) \int d^3r'\ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{r}')\,\Phi_B^* \frac{1}{r'}\,\Phi_A \\ &= -\frac{e^2}{4\pi\,\epsilon_0}\,\frac{4\pi}{q^2}\,F_{BA}(\boldsymbol{q}), \end{aligned} \tag{122}$$

where we have introduced the nuclear form factor

$$\begin{aligned} F_{BA}(\boldsymbol{q}) &= \sum_{j=1}^{Z} \int \prod_{k=1}^{Z} d^3r_k\ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{r}_j)\,\Phi_B^*(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z)\,\Phi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z) \\ &= \int d^3s\ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{s})\ \underbrace{Z \int \prod_{k=2}^{Z} d^3r_k\ \Phi_B^*(\boldsymbol{s}, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_Z)\,\Phi_A(\boldsymbol{s}, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_Z)}_{\rho_{BA}(\boldsymbol{s})}, \end{aligned} \tag{123}$$

which is the Fourier transform of the one-nucleon (transition) density $\rho_{BA}(\boldsymbol{s})$. We note that the wave functions Φ_A and Φ_B are fully antisymmetric. The result for the cross section is

$$\frac{d\sigma_{BA}}{d\Omega} = \left(\frac{m\,e^2}{2\pi\,\epsilon_0\,\hbar^2\,q^2}\right)^2 \frac{p'}{p}\,|F_{BA}(\boldsymbol{q})|^2. \tag{124}$$

and shows the possibility to determine the distribution of nucleons in a nucleus.

In Chapter 10 of Mandl the equivalent example for the scattering off an atom is considered, for which the full hamiltonian is given by

$$H = -\frac{\hbar^2}{2m}\,\boldsymbol{\nabla}^2 + H_{\rm atom} + V, \tag{125}$$

where $H_{\rm atom}(\boldsymbol{r}_1,\boldsymbol{p}_1;\ldots;\boldsymbol{r}_Z,\boldsymbol{p}_Z)$ is the Z-electron hamiltonian of the atom and V describes the interaction between the scattering electron and the atom,

$$V = -\frac{Ze^2}{4\pi\,\epsilon_0\,r} + \sum_{j=1}^{Z} \frac{e^2}{4\pi\,\epsilon_0\,|\boldsymbol{r}-\boldsymbol{r}_j|}. \tag{126}$$

with $|\Phi_a\rangle$ with energy ϵ_a and $|\Phi_b\rangle$ with energy ϵ_b the initial and final state wave functions. The full initial state and final state wave functions are taken to be $\Psi_i(\boldsymbol{r},\boldsymbol{r}_1,\ldots,\boldsymbol{r}_Z) = \sqrt{\rho}\,\exp(i\,\boldsymbol{k}\cdot\boldsymbol{r})\,\Phi_a(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_Z)$ and $\Psi_f(\boldsymbol{r},\boldsymbol{r}_1,\ldots,\boldsymbol{r}_Z) = \sqrt{\rho}\,\exp(i\,\boldsymbol{k}'\cdot\boldsymbol{r})\,\Phi_b(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_Z)$, respectively. This neglects the antisymmetrization of the scattering electron and the atomic electrons, which will be allright at sufficiently high momentum transfer.

The first of the two contributions of the potential in Eq. 126 is evaluated as the example of the Coulomb potential in the previous section. Since Φ_a and Φ_b are orthonormal solutions, one finds

$$\int d^3r \int \prod_{k=1}^{Z} d^3r_k\;\exp(i\,\boldsymbol{q}\cdot\boldsymbol{r})\,\Phi_b^*(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_Z)\left(-\frac{Ze^2}{4\pi\,\epsilon_0\,r}\right)\Phi_a(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_Z) = -\frac{Ze^2}{4\pi\,\epsilon_0}\,\frac{4\pi}{q^2}\,\delta_{ba} \tag{127}$$

The second contribution is equivalent to the case of the nucleus considered above. The result for the cross section is now

$$\frac{d\sigma_{ba}}{d\Omega} = \left(\frac{m\,e^2}{2\pi\,\epsilon_0\,\hbar^2\,q^2}\right)^2 \frac{p'}{p}\,|Z\delta_{ba} - F_{ba}(\boldsymbol{q})|^2 \tag{128}$$

getting contributions from both nucleus and electrons. The quantity $F_{ba}(\boldsymbol{q})$ is the Fourier transform of the one-electron (transition) density $\rho_{ab}(\boldsymbol{s})$. This shows the possibility to determine electron distributions in an atom.

> Note that the first term is derived treating the nucleus as a point. In fact $Z\,\delta_{ba}$, should read $F_{AA}(\boldsymbol{q})\,\delta_{ba}$ (where A indicates the nuclear groundstate). However as we will see in the next section, for relevant q-values for scattering of the atomic electrons one has $F_{AA}(\boldsymbol{q}) = F_{AA}(0) = 1$.

15 Form factors

Form factors as encountered in the previous section are defined as the Fourier transform of a density,

$$F(\boldsymbol{q}) = \int d^3r \;\exp(i\,\boldsymbol{q}\cdot\boldsymbol{r})\,\rho(\boldsymbol{r}). \tag{129}$$

As before in discussing the potential in momentum space, one has for a spherically symmetric density,

$$F(q) = \frac{4\pi}{q}\int dr\; r\,\rho(r)\,\sin(qr). \tag{130}$$

For a spherical distributions it is trivial to find by expanding the exponential $\exp(i\,\boldsymbol{q}\cdot\boldsymbol{r}) = 1 + i\,\boldsymbol{q}\cdot\boldsymbol{r}$ - $\frac{1}{2}\,(\boldsymbol{q}\cdot\boldsymbol{r})^2 + \ldots$, that

$$F(q) = Q - \frac{1}{6}\,q^2\,\langle r^2\rangle + \ldots, \tag{131}$$

where

$$Q = \int d^3r\;\rho(r), \tag{132}$$

$$\langle r^2\rangle = \int d^3r\; r^2\,\rho(r). \tag{133}$$

This is the reason that the small-$\boldsymbol{q}$ behavior of a form factor can be used to determine the charge radius of an atom or similarly of elementary particles, like pions or nucleons.

Some examples of form factors corresponding to specific densities are:

- A uniform density
$$\rho(r) = \rho_0 \qquad \text{for } x \le R \tag{134}$$
(and zero elsewhere). If $\rho_0 = 3/4\pi\,a^3$, i.e. the integrated density is one, the Fourier transform is given in terms of the Bessel function j_1,
$$F(q) = \frac{3\,j_1(qR)}{qR}, \tag{135}$$
where
$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}. \tag{136}$$
Note that
$$\frac{3\,j_1(x)}{x} \approx 1 - \frac{1}{10}\,x^2 + \ldots, \tag{137}$$
and, indeed, the charge radius of a uniform distribution is $\langle r^2\rangle = \frac{3}{5}\,R^2$.
- A (normalized) Yukawa distribution
$$\rho(r) = \frac{\mu^2}{4\pi}\,\frac{e^{-\mu r}}{r}, \tag{138}$$
has as form factor
$$F(q) = \frac{\mu^2}{q^2+\mu^2} = \frac{1}{1+q^2/\mu^2}, \tag{139}$$
which is called a *monopole* form factor. We have encountered this example already in a previous section where we derived the momentum space screened Coulomb potential.
- The form factor of the exponential distribution
$$\rho(r) = \frac{\mu^3}{8\pi}\,e^{-\mu r}, \tag{140}$$

is simply found by differentiation of the Yukawa form factor with respect to μ,

$$e^{-\mu r} = -\frac{d}{d\mu}\left(\frac{e^{-\mu r}}{r}\right).$$

This gives

$$F(q) = \frac{1}{\left(1 + q^2/\mu^2\right)^2}, \tag{141}$$

which is called a *dipole* form factor.

- Finally a normalized Gaussian distribution

$$\rho(r) = \rho_0\, e^{-\frac{1}{2}\, r^2/R^2} \tag{142}$$

has also a Gaussian form factor

$$F(q) = e^{-\frac{1}{2}\, q^2\, R^2}. \tag{143}$$

16 Scattering solutions

Mandl, chapter 11

In this section we will attack the scattering of a potential in a different way, namely by solving the Schrödinger equation. The time-independent Schrödinger equation can be rewritten as

$$\left(\boldsymbol{\nabla}^2 + k^2\right)\psi(\boldsymbol{r}) = \frac{2m}{\hbar^2}\,V(\boldsymbol{r})\,\psi(\boldsymbol{r}), \tag{144}$$

where $E = \hbar^2 k^2/2m$. This is a linear equation of which the righthandside is referred to as *source* term. There is a whole family of solutions of such an equation. Given a solution of the above *inhomogeneous* equation, one can obtain all solutions by adding any of the possible solutions of the *homogeneous* equation,

$$\left(\boldsymbol{\nabla}^2 + k^2\right)\psi_{\rm hom}(\boldsymbol{r}) = 0. \tag{145}$$

The solutions of the homogeneous equation are well-known, namely the plane waves,

$$\phi_k(\boldsymbol{r}) = \exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}), \tag{146}$$

characterized by a wave vector $\boldsymbol{k}$.

Another systematic way of obtaining the solutions of the homogeneous equation is by considering the radial Schrödinger equation, i.e. writing

$$\psi(\boldsymbol{r}) = \frac{u(r)}{r}\,Y_\ell^m(\theta,\phi), \tag{147}$$

the radial wave function $u(r)$ satisfies for the homogeneous equation

$$\left(\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + k^2\right)u(r) = 0. \tag{148}$$

There are two type of solutions of this equation

- Regular solutions: spherical Bessel functions of the first kind: $u(r) = kr\,j_\ell(kr)$.
  Properties:

$$\begin{aligned} j_0(z) &= \frac{\sin z}{z}, \\ j_\ell(z) &= z^\ell\left(-\frac{1}{z}\frac{d}{dz}\right)^\ell \frac{\sin z}{z} \quad \overset{z\rightarrow 0}{\longrightarrow} \quad z^\ell, \\ & \qquad\qquad\qquad\qquad \overset{z\rightarrow\infty}{\longrightarrow} \quad \frac{\sin(z-\ell\pi/2)}{z}. \end{aligned}$$

- Irregular solutions: spherical Bessel functions of the second kind: $u(r) = kr\,n_\ell(kr)$.
  Properties:

$$\begin{aligned} n_0(z) &= -\frac{\cos z}{z}, \\ n_\ell(z) &= -z^\ell\left(-\frac{1}{z}\frac{d}{dz}\right)^\ell \frac{\cos z}{z} \quad \overset{z\rightarrow 0}{\longrightarrow} \quad z^{-(\ell+1)}, \\ & \qquad\qquad\qquad\qquad \overset{z\rightarrow\infty}{\longrightarrow} \quad -\frac{\cos(z-\ell\pi/2)}{z}. \end{aligned}$$

Equivalently one can use linear combinations, known as Hankel functions,

$$\begin{aligned} kr\,h_\ell^{(1)}(kr) = kr\,(j_\ell(kr) + i\,n_\ell(kr)) \quad &\overset{z\rightarrow\infty}{\longrightarrow} \quad (-i)^{\ell+1}\,e^{i\,kr}, \\ kr\,h_\ell^{(2)}(kr) = kr\,(j_\ell(kr) - i\,n_\ell(kr)) \quad &\overset{z\rightarrow\infty}{\longrightarrow} \quad (i)^{\ell+1}\,e^{-i\,kr}. \end{aligned}$$

A specific example of an expansion into these spherical solutions, is the expansion of the plane wave,

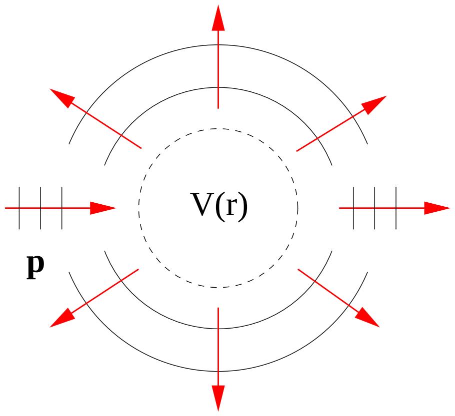
$$\exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}) = e^{i\,kz} = e^{i\,kr\,\cos\theta} = \sum_{\ell=0}^{\infty}(2\ell+1)\,i^{\ell}\,j_\ell(kr)\,P_\ell(\cos\theta), \tag{149}$$

where the Legendre polynomials P_ℓ can be also expressed in Y_ℓ^0,

$$P_\ell(\cos\theta) = \sqrt{\frac{4\pi}{2\ell+1}}\,Y_\ell^0(\theta).$$

17 Asymptotic solution

In order to construct solutions of the Schrödinger equation that describe a scattering process, one wants the appropriate asymptotic behavior, which includes a plane wave part, describing the incoming part and outgoing spherical waves, describing the scattering part, pictorially represented below



We thus require the following asymptotic form,

$$\psi(\boldsymbol{r}) \quad \xrightarrow{r\to\infty} \quad \exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}) + \frac{e^{i\,kr}}{r}\,f(k;\theta,\phi). \tag{150}$$

We have seen in the previous chapter that for $r \to \infty$, this is a solution of the homogeneous equation.

> It can also simply be checked that the above represents a solution if $r \to \infty$, by inserting it into the homogeneous equation. In order to select the leading part for large r one needs to use that $\boldsymbol{\nabla} f(k;\theta,\phi) \propto 1/r$ and $\boldsymbol{\nabla}^2 f(k;\theta,\phi) \propto 1/r^2$.

For the asymptotic solution the current corresponding to the first part is given by

$$\boldsymbol{j}_{in} = \frac{\hbar\boldsymbol{k}}{m}, \tag{151}$$

while the second part up to $\mathcal{O}(1/r)$ corresponds with a radially outward directed flux of magnitude

$$j_r = -\frac{i\hbar}{2m}\left[\psi^*\frac{d}{dr}\psi - \left(\frac{d}{dr}\psi^*\right)\psi\right] = \frac{\hbar k}{m}\,\frac{|f(k;/\theta,\phi)|^2}{r^2}. \tag{152}$$

From it, one derives the cross section using that

$$|j_{in}|\,d\sigma(\theta,\phi) = n(\theta,\phi)\,d\Omega = j_r\,r^2\,d\Omega, \tag{153}$$

i.e.

$$\frac{d\sigma}{d\Omega} = |f(k;\theta,\phi)|^2. \tag{154}$$

The above considerations require a careful analysis of the forward direction ($\theta = 0$), where the interference term becomes important. For an acceptable asymptotic scattering solution one must have that $\int d\Omega\; j_r|_{r=R} = 0$ for large R, i.e. that there is no loss of probability. This leads to the *optical theorem* or Bohr-Peierls-Placzek relation,

$$\mathcal{I}m\,f_{el}(\theta = 0) = \frac{k}{4\pi}\,\sigma_T, \tag{155}$$

where σ_T is the total cross section and f_{el} is the scattering amplitude for elastic scattering.

In order to derive this result, one can just consider the full current. Keeping only the dominant contributions when $r \to \infty$, this is given by

$$j_r = \frac{\hbar k}{m}\left\{\cos\theta + \frac{|f|^2}{r^2} + \mathcal{R}e\left[(1+\cos\theta)\,\frac{e^{ikr(1-\cos\theta)}}{r}\,f\right]\right\}$$

Integrating over the polar angle (writing $\cos\theta \equiv X$) gives for the interference term:

$$\begin{aligned}
&\mathcal{R}e\int_{-1}^{1} dX\;(1+X)\,\frac{e^{i\,kr(1-X)}}{r}\,f \\
&\qquad = \mathcal{R}e\int_{-1}^{1} d\left(e^{i\,kr(1-X)}\right)\;\frac{(1+X)f}{-i\,kr^2} \\
&\qquad = \mathcal{R}e\left(\frac{2\,f(k;\theta=0)}{-i\,kr^2}\right) - 2\mathcal{R}e\int_{-1}^{1} dX\;\frac{e^{i\,kr(1-X)}}{-i\,kr^2}\,\frac{d}{dX}\,[(1+X)f] \\
&\qquad = -\frac{2\,\mathcal{I}m\,f(k;\theta=0)}{kr^2} + \mathcal{O}\left(\frac{1}{r^3}\right).
\end{aligned}$$

The interference term thus actually only contributes at forward angles if $r \to \infty$. Neglecting any contribution disappearing faster than $1/r^2$ the integral over the angles gives

$$\int d\Omega\; j_r\Big|_{r=R} = \frac{1}{R^2}\left[\int d\Omega\;|f|^2 - \frac{4\pi}{k}\,\mathcal{I}m\,f(k;\theta=0)\right],$$

yielding the optical theorem. In fact the result is only derived if the total cross section is given by the integration over $|f|^2$, but it should be clear that flux conservation needs only to hold if we integrate over elastic and inelastic channels, while the interference only occurs for the elastic channel. We will encounter the result again in the section on partial wave expansions.

18 The integral equation for the scattering amplitude

In order to solve the inhomogeneous equation with which we started, we solve the Green's function equation

$$\left(\boldsymbol{\nabla}^2 + k^2\right) G(\boldsymbol{r},\boldsymbol{r}') = -\delta^3(\boldsymbol{r}-\boldsymbol{r}'). \tag{156}$$

> With the help of the Green's function an inhomogeneous solution for
>
> $$\left(\boldsymbol{\nabla}^2 + k^2\right) \psi(\boldsymbol{r}) = \rho(\boldsymbol{r}),$$
>
> can be written down, namely
>
> $$\psi(\boldsymbol{r}) = -\int d^3r'\; G(\boldsymbol{r},\boldsymbol{r}')\,\rho(\boldsymbol{r}').$$
>
> By choosing an 'appropriate' Green's function one can built in boundary conditions. Note that the difference between any two Green's function is a solution of the homogeneous equation.

It is not difficult to check that two particular Green's functions in our case are

$$G^{(\pm)}(\boldsymbol{r}-\boldsymbol{r}') = -\frac{\exp\left(\pm i\,k|\boldsymbol{r}-\boldsymbol{r}'|\right)}{4\pi\,|\boldsymbol{r}-\boldsymbol{r}'|}. \tag{157}$$

In particular $G^{(+)}$ has the correct asymptotic behavior as discussed in the previous section. As an *exact* solution valid for all r, we can write

$$\psi(\boldsymbol{r}) = \exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}) - \frac{m}{2\pi\,\hbar^2}\int d^3r'\;\frac{\exp\left(\pm i\,k|\boldsymbol{r}-\boldsymbol{r}'|\right)}{|\boldsymbol{r}-\boldsymbol{r}'|}\,V(\boldsymbol{r}')\,\psi(\boldsymbol{r}'). \tag{158}$$

This result is the desired integral representation of the inhomogenous Schrödinger equation, which has the advantages that the boundary conditions for interpretation as a scattering solution have been built in. It is therefore a good starting point for approximations

The result for $f(k;\theta,\phi)$ is obtained by taking the limit for $r \to \infty$ in the integral equation, in particular

$$\begin{aligned} |\boldsymbol{r}-\boldsymbol{r}'| = r\sqrt{1 - 2\,\frac{\boldsymbol{r}\cdot\boldsymbol{r}'}{r^2} + \frac{r'^2}{r^2}} \;&\approx\; r\left[1 - \frac{\boldsymbol{r}\cdot\boldsymbol{r}'}{r^2} + \ldots\right], \\ \frac{\exp\left(\pm i\,k|\boldsymbol{r}-\boldsymbol{r}'|\right)}{|\boldsymbol{r}-\boldsymbol{r}'|} \;&\approx\; \frac{e^{i\,kr}}{r}\,\exp\left(i\,\boldsymbol{k}'\cdot\boldsymbol{r}'\right) + \ldots, \end{aligned}$$

where $\boldsymbol{k}' \equiv k\hat{\boldsymbol{r}}$. This gives

$$\psi(\boldsymbol{r}) \quad \overset{r\to\infty}{\longrightarrow} \quad \exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}) - \frac{e^{i\,kr}}{r}\,\frac{m}{2\pi\,\hbar^2}\int d^3r'\;\exp\left(-i\,\boldsymbol{k}'\cdot\boldsymbol{r}'\right)\,V(\boldsymbol{r}')\,\psi(\boldsymbol{r}'). \tag{159}$$

and thus the exact expression is

$$f(k;\theta,\phi) = -\frac{m}{2\pi\,\hbar^2}\int d^3r'\;\exp\left(-i\,\boldsymbol{k}'\cdot\boldsymbol{r}'\right)\,V(\boldsymbol{r}')\,\psi(\boldsymbol{r}'). \tag{160}$$

19 The Born approximation and beyond

The Born approximation is obtained by using perturbation methods, namely to approximate in the above expression $\psi(\boldsymbol{r}') = \exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}')$, yielding the result

$$f(k;\theta,\phi) = -\frac{m}{2\pi\,\hbar^2}\int d^3r'\;\exp(i\,\boldsymbol{q}\cdot\boldsymbol{r}')\;V(\boldsymbol{r}'), \tag{161}$$

where $\boldsymbol{q} = \boldsymbol{k}-\boldsymbol{k}'$. This gives for the cross section the same result as we found using Fermi's golden rule.

We can go beyond the first order result by introducing the scattering amplitude T. It is defined by

$$V\psi \equiv T\phi,$$

where ψ is the scattering solution and ϕ the incoming plane wave part of it. One then finds that the integral equation, $V\psi = V\phi + V\,\tilde{G}\,V\psi$ turns into $T\phi = V\phi + V\,\tilde{G}\,T\phi$, i.e. an equation for T,

$$T = V + V\,\tilde{G}\,T, \tag{162}$$

the socalled *Lippmann-Schwinger* equation. Here $\tilde{G}$ is the Green's function with factor $-2m/\hbar^2$ absorbed, which is the inverse of $E - H_0$. The exact expression for the scattering amplitude f is thus given by

$$f(k;\theta,\phi) = -\frac{m}{2\pi\,\hbar^2}\,\langle\boldsymbol{p}'|T|\boldsymbol{p}\rangle. \tag{163}$$

The lowest order (Born approximation) result is the first term in the expansion obtained from Eq. 162,

$$T = V + V\,\tilde{G}\,V + V\,\tilde{G}\,V\,\tilde{G}\,V + \ldots.$$

To judge the validity of the Born approximation one requires that the scattering term in the wave function is small, i.e.

$$\frac{m}{2\pi\,\hbar^2}\left|\int d^3r'\;\frac{\exp(i\,k|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|}\;V(\boldsymbol{r}')\,\psi(\boldsymbol{r}')\right| \ll 1. \tag{164}$$

The disturbance of the plane wave is near $r \approx 0$, while for selfconsistency $\psi(\boldsymbol{r})$ should be dominantly plane wave, thus

$$\begin{aligned}
\left|\int d^3r'\;\frac{\exp(i\,kr' + i\,\boldsymbol{k}\cdot\boldsymbol{r}')}{r'}\;V(\boldsymbol{r}')\right| &\ll \frac{2\pi\,\hbar^2}{m}\\
\left|2\pi\int_{-1}^{1} dX\int dr'\;r'\,e^{i\,kr'(1+X)}\;V(r')\right| &\ll \frac{2\pi\,\hbar^2}{m},\\
\left|\int dr'\;\left(e^{2i\,kr'}-1\right)V(r')\right| &\ll \frac{\hbar^2 k}{m} = \hbar v.
\end{aligned}$$

We see two limits in which the Born approximation is applicable

- Weak potentials with a finite range.
  Starting with the second of the above estimates, we see for a potential with average depth V_0 and range a one has after bringing the absolute value under the integral $V_0\,a^2 \ll \hbar^2/m$, i.e.

  $$V_0 \ll \frac{\hbar^2}{m\,a^2}, \tag{165}$$

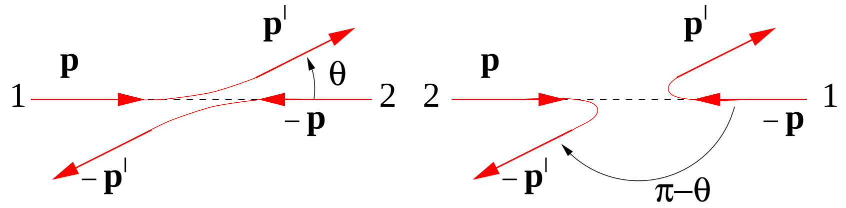
  a condition where an approximately equal sign usually is already ok.

- High energies (but nonrelativistic!).
  In the last of the three expressions the exponential is fast-varying for high momenta k and can be neglected, so $V_0\,a \ll \hbar^2\,k/m$, i.e.

  $$ka \gg \frac{m\,V_0\,a^2}{\hbar^2} \qquad \text{or} \qquad E \gg \frac{m\,V_0^2\,a^2}{\hbar^2}. \tag{166}$$

20 Identical particles

We already discussed how to treat the scattering of two particles in the center of mass frame. In the case that one has two identical particles the scattering in the following two situations both leads to the same final state,



Thus if ψ_{12} is the wave function in which particle 1 is coming from the left and is scattered over an angle θ and ψ_{21} is the wave function in which particle 1 is coming from the right and is scattered over an angle $\pi-\theta$,

$$\psi_{12}(\boldsymbol{r}) = e^{i\,kz} + f(k;\theta,\phi)\,\frac{e^{i\,kr}}{r}, \tag{167}$$

$$\psi_{21}(\boldsymbol{r}) = e^{-i\,kz} + f(k;\pi-\theta,\phi+\pi)\,\frac{e^{i\,kr}}{r}, \tag{168}$$

one has the same final state. One should use the appropriately symmetrized or antisymmetrized wave functions, leading to (omitting ϕ-dependence)

$$n(\theta,\phi)\,d\Omega = \frac{\hbar k}{\mu}\,\left|f(k;\theta) \pm f(k;\pi-\theta)\right|^2\,d\Omega$$

In the cross section,

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \left|f(k;\theta) \pm f(k;\pi-\theta)\right|^2 \\ &= \left|f(k;\theta)\right|^2 + \left|f(k;\pi-\theta)\right|^2 \pm 2\,\mathcal{R}e\left[f^*(k;\theta)\,f(k;\pi-\theta)\right],\end{aligned} \tag{169}$$

the (third) interference term gives rise to oscillations. Note that in order to determine the total cross section one has to integrate over the range $0 \le \theta \le \pi/2$ in order to avoid double counting. Note that the cross sections at angles θ and $\pi-\theta$ are identical. For destructive interference (a minus sign) the cross section is zero at $\theta = 90$ degrees.

For example in the (hypothetical) scattering process of two pions the amplitudes interfere constructively as pions are bosons (spin 0 particles) and the wave function must be symmetric. When scattering two electrons (spin 1/2 particles) off each other the total wave function is antisymmetric, but the symmetry of the scattering solution depends on the spin state. In the spin 0 state (singlet) the spin wave function is antisymmetric, while in the spin 1 state (triplet) the spin wave function is symmetric. Hence

$$\frac{d\sigma_s}{d\Omega} = |f_s(\theta) + f_s(\pi-\theta)|^2, \tag{170}$$

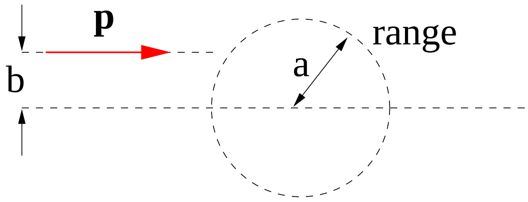
$$\frac{d\sigma_t}{d\Omega} = |f_t(\theta) - f_t(\pi-\theta)|^2, \tag{171}$$

If one scatters unpolarized electrons, the initial state has a probability 1/4 to be in the singlet state, 3/4 to be in the triplet state, thus for a spin-independent potential

$$\frac{d\sigma}{d\Omega} = \frac{1}{4}\,\frac{d\sigma_s}{d\Omega} + \frac{3}{4}\,\frac{d\sigma_t}{d\Omega} = |f(k;\theta)|^2 + |f(k;\pi-\theta)|^2 - \mathcal{R}e\left[f(k;\theta)\,f^*(k;\pi-\theta)\right]. \tag{172}$$

21 Partial wave expansion

At low energies a particle scattering off a target with impact parameter b has an angular momentum $\hbar\sqrt{\ell(\ell+1)} = p\,b$,



If the potential has a finite range a the angular momenta that are important correspond to $b \le a$. From this we obtain $\hbar\ell \le pa = \hbar ka$ or $\ell \le ka$. Therefore it is especially at low energies convenient to expand into different partial waves, eigenstates of angular momentum, because the lower partial waves dominate. Also for central potentials, which satisfy $[\boldsymbol{L}, V(r)] = 0$, it is useful to expand in partial waves, since each angular momentum state in that case is a proper scattering solution.

Starting off with the plane wave, we have

$$e^{ikz} = \sum_\ell (2\ell+1)\, i^\ell\, j_\ell(kr)\, P_\ell(\cos\theta). \tag{173}$$

As already mentioned it only contains the ϕ-independent spherical harmonics, namely $Y_\ell^0(\theta) = \sqrt{(2\ell+1)/4\pi}\, P_\ell(\cos\theta)$. Assuming azimuthal symmetry the scattering amplitude only depends on θ and also can be expanded in Legendre polynomials,

$$f(k;\theta) = \sum_\ell (2\ell+1)\, f_\ell(k)\, P_\ell(\cos\theta). \tag{174}$$

Thus one obtains

$$\psi_{sc}(\boldsymbol{r}) \quad \overset{r\to\infty}{\longrightarrow} \quad \sum_\ell (2\ell+1)\, P_\ell(\cos\theta)\, i^\ell \underbrace{\left[j_\ell(kr) + (-i)^\ell \,\frac{e^{i\,kr}}{r}\, f_\ell(k)\right]}_{\psi_{sc}^{(\ell)}(r)}. \tag{175}$$

Rewriting the scattering wave in the following way,

$$\begin{aligned} \psi_{sc}^{(\ell)}(\boldsymbol{r}) \quad &\overset{r\to\infty}{\longrightarrow} \quad \frac{\sin(kr-\ell\pi/2)}{kr} + (-i)^\ell\, \frac{e^{i\,kr}}{r}\, f_\ell(k) \\ &= \quad \frac{1}{2i\,k}\left[-\frac{e^{-i(kr-\ell\pi/2)}}{r} + \frac{e^{i(kr-\ell\pi/2)}}{r}\,(1+2i\,kf_\ell(k))\right], \end{aligned} \tag{176}$$

Conservation of flux tells us that the incoming and outgoing fluxes should be equal in magnitude, i.e.

$$1 + 2i\,kf_\ell(k) \equiv e^{2i\,\delta_\ell(k)}, \tag{177}$$

where $\delta_\ell(k)$ is called the *phase shift*. Going back and expressing $f_\ell(k)$ in the phase shift it is easy to see that

$$f_\ell(k) = \frac{e^{2i\,\delta_\ell(k)} - 1}{2i\,k} = \frac{e^{i\,\delta_\ell(k)}\,\sin\delta_\ell(k)}{k}, \tag{178}$$

and

$$\psi_{sc}^{(\ell)}(\boldsymbol{r}) \quad \overset{r\to\infty}{\longrightarrow} \quad e^{i\,\delta_\ell(k)}\,\frac{\sin(kr-\ell\pi/2+\delta_\ell(k))}{kr}. \tag{179}$$

22 Cross sections and partial waves

At this point it is useful to slightly generalize the result of the previous section. If also inelastic scattering is possible a particular ℓ-wave amplitude is parametrized

$$1 + 2i\,kf_\ell(k) \equiv \eta_\ell\,e^{2i\,\delta_\ell(k)}, \tag{180}$$

where η_ℓ is called the *elasticity.* One then has for the elastic cross section

$$\frac{d\sigma_{el}}{d\Omega} = |f(k;\theta)|^2 = 4\pi \sum_{\ell,\ell'} \sqrt{(2\ell+1)(2\ell'+1)}\,f_\ell(k)\,f_{\ell'}(k)\,Y_\ell^{0*}(\theta)\,Y_{\ell'}^0(\theta). \tag{181}$$

Integrating over angles the orthonormality of the Y_ℓ^m's can be used to get

$$\sigma_{el} = \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\,\sin^2\delta_\ell(k) \tag{182}$$

Via the optical theorem, which relates the forward scattering amplitude to the total cross section one finds

$$\sigma_T = \frac{2\pi}{k^2}\sum_\ell (2\ell+1)\,(1-\eta_\ell\,\cos 2\delta_\ell), \tag{183}$$

which indeed is identical for purely elastic scattering ($\eta_\ell = 1$). The difference is the inelastic cross section,

$$\sigma_{inel} = \frac{\pi}{k^2}\sum_\ell (2\ell+1)\,(1-\eta_\ell^2). \tag{184}$$

23 Calculating the phase shift from the potential

The easiest illustration of the calculation of the phase shift is the calculation for a square well, $V(r) = V_0$ for $r \leq a$ and zero elsewhere. We immediately know that for $r \geq a$ the solution must be the asymptotic solution. Inside the square well we use the radial Schrödinger equation to get the radial wave function $u(r)$. Thus for

$$\psi_{\ell m}(\boldsymbol{r}) = \frac{u_\ell(r)}{r}\, Y_\ell^m(\theta,\phi), \tag{185}$$

we have

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r)\right] u_\ell(r) = E\, u_\ell(r). \tag{186}$$

Knowing that $u_\ell(0) = 0$ we obtain for s-waves ($\ell = 0$)

$$\begin{aligned} r \leq a \qquad & u(r) = A\,\sin Kr \qquad \text{with } K = \sqrt{\frac{2m}{\hbar^2}\,(E - V_0)}, \\ r \geq a \qquad & u(r) = B\,\sin(kr + \delta_0) \quad \text{with } k = \sqrt{\frac{2m}{\hbar^2}\,E}, \end{aligned}$$

Matching the logarithmic derivative $(du/dr)/u(r)$ at $r = a$ gives

$$\tan(ka + \delta_0) = \frac{k}{K}\,\tan Ka \tag{187}$$

or

$$\begin{aligned} \tan\delta_0(k) \quad &= \quad \frac{\frac{k}{K}\,\tan Ka - \tan ka}{1 + \frac{k}{K}\,\tan Ka\,\tan ka} && (188) \\ &\xrightarrow{ka \ll 1} \quad \frac{ka\left[\frac{\tan Ka}{Ka} - 1\right]}{1 + (ka)^2\,\frac{\tan Ka}{Ka}}, && (189) \\ &\xrightarrow{Ka \ll 1} \quad ka\left[\frac{\tan Ka}{Ka} - 1\right] \approx \frac{K^2\,a^3}{3}\,k && (190) \end{aligned}$$

For low energies, where s-waves are the dominant contribution, the above result and its limits can be used to understand many qualitative features in the cross section, e.g. the disappearance of the cross section at specific energies, because of a zero in $1 - \tan Ka/Ka$ (the Ramsauer-Townsend effect) or the behavior of the cross section near threshold for weak potentials. The first two coefficients of the phase shift in an expansion in the momentum,

$$\delta_0(k) = a_0\,k + \frac{1}{2}\,r_e\,k^2 + \ldots, \tag{191}$$

have specific names, namely *scattering length* and *effective range*, respectively.