Quantum Mechanics

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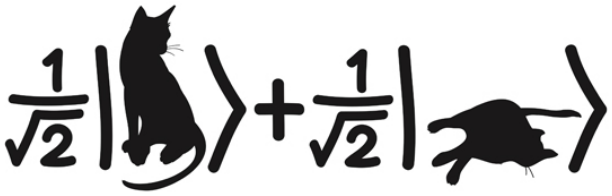

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Chapter 1

Introduction

Those who are not shocked when they first come across quantum theory cannot possibly have understood it.
— Niehls Bohr

I think I can safely say that nobody understands quantum mechanics.
— Richard P. Feynman

Very interesting theory — it makes no sense at all.
— Groucho Marx

1.1 Foundations

Quantum Mechanics (QM) shaped up in the form we know it today during the first quarter of the 20th century by the ingenuity of Heisenberg, Schrödinger, Dirac, von Neumann and many others.

Last course you discussed in detail the historical developments leading to it: Planck's radiation law, the Bohr's atom, the de Broglie's matter waves, the photoelectric effect, etc.

That's the way QM was built but it is not the path we will follow in this course. In the same way as Einstein's Theory of Relativity was formulated from a couple of basic postulates, we will reformulate QM assuming a few *postulates* and then we will elaborate on their logical consequences.

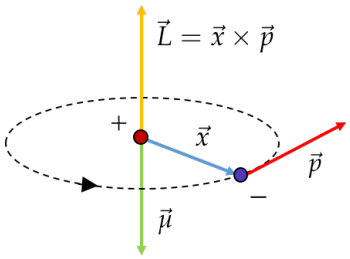
To prepare the ground, in this chapter we will motivate the subject with a simple experiment that illustrates the essence of the quantum theory and will serve as a starting point to introduce the formalism.

1.2 The Stern-Gerlach experiment

The Stern-Gerlach experiment (1921-1922) shows clearly a physical behaviour that Classical Mechanics cannot explain. We will describe it here and in the next chapter we will give the postulates that provide a correct interpretation of the results.

The objective of the experiment was to measure the **magnetic moment** of a silver atom. Suppose first a *classical* hydrogen atom: an electron orbiting a proton of opposite charge with angular momentum $\vec{L}$. The electron mass m is much smaller than the proton mass. Then, the magnetic moment of the system is

$$\vec{\mu} = \frac{q}{2m}\vec{L} \qquad (q = -e) \tag{1.1}$$



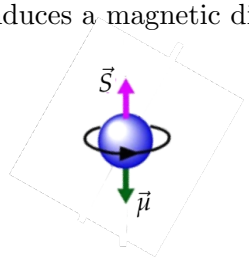
Assume now you send hydrogen atoms at a speed v through a magnetic field $\vec{B}$. The atom has no net electric charge, $Q = 0$. Then its magnetic interaction, $\vec{F} = Q\,\vec{v} \times \vec{B}$, should apparently vanish. However, the relative motion of the proton and the electron creates a non-vanishing magnetic interaction that can be described in terms of the magnetic moment by the Hamiltonian

$$H_{\text{int}} = V = -\vec{\mu} \cdot \vec{B}. \tag{1.2}$$

So, to minimize the energy, the magnetic field tends to align the dipole $\vec{\mu}$ with $\vec{B}$.

In addition to the orbital angular momentum, electrons and protons happen to have an intrinsic angular momentum or spin $\vec{S}$, that is analogue to a rotation around an inner axis.[a] The spin angular momentum also induces a magnetic dipole moment

$$\vec{\mu} = g\frac{q}{2m}\vec{S} \tag{1.3}$$



where g is the gyromagnetic ratio ($g \approx 2$ for the electron). This $\vec{\mu}$ couples to the magnetic field as in (1.2).

A silver atom is made of 47 protons and 47 electrons, whose configuration is such that the total spin and orbital angular momenta tend to cancel each other but actually coincides with the spin of the 47th electron. This means, that the magnetic moment of the silver atom is

$$\vec{\mu} \propto \vec{S} \text{ (spin of the 47th electron)}. \tag{1.4}$$

When silver atoms, heated in a furnace, escape through a small hole and travel across an inhomogeneous magnetic field with a large gradient along the z direction (Fig. 1.1),

$$\vec{B} = (0, 0, B(z)), \tag{1.5}$$

they will experience a force proportional to the vertical component of the magnetic moment μ_z, that will deflect the beams,

$$\vec{F} = -\nabla V = \left(0, 0, \mu_z \frac{\partial B}{\partial z}\right). \tag{1.6}$$

[a] The spin will be discussed in detail in chapter 4.

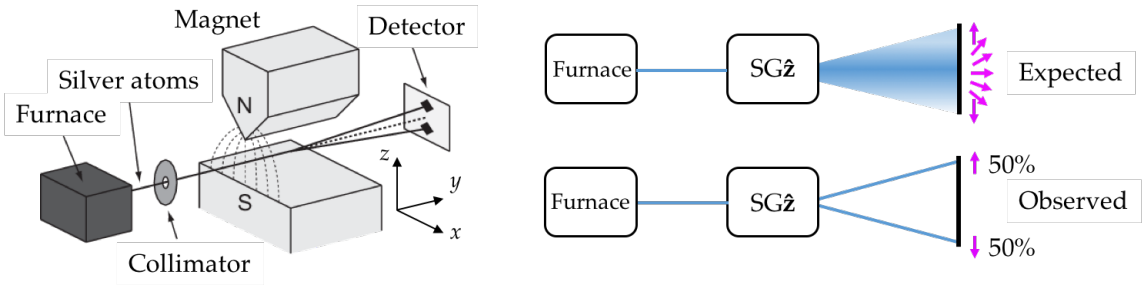


Figure 1.1: Sketch of the Stern-Gerlach experiment (left) and its outcome (right).

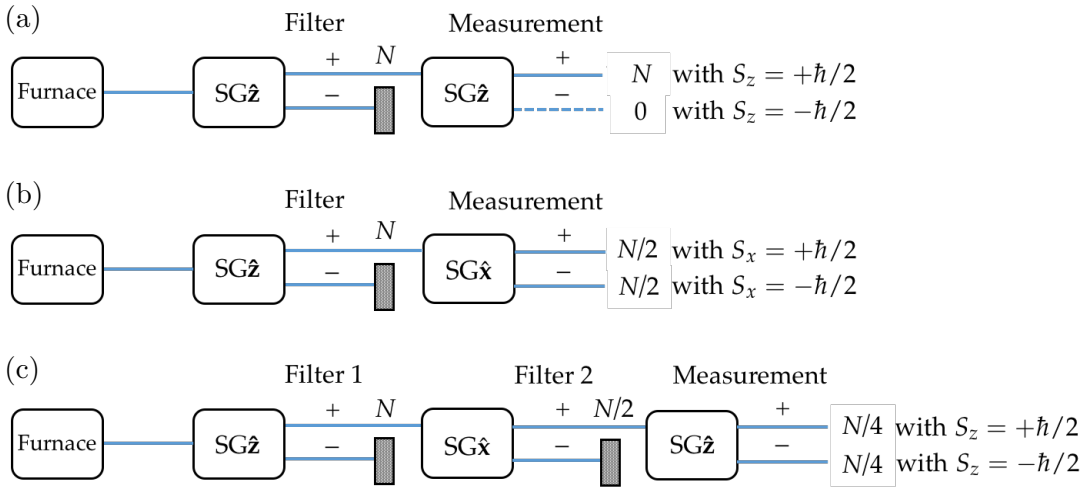


Figure 1.2: Sequential Stern-Gerlach experiments.

Since the magnetic moment orientations are completely random, one would expect a continuum of deviations, as in the upper right corner of Fig. 1.1, with a larger concentration in the central part. However, Stern and Gerlach observed that the original beam splits into *just* two distinct components corresponding to the extremal values

$$S_z = \pm\frac{\hbar}{2}, \tag{1.7}$$

where the reduced Planck constant $\hbar$ is a fundamental unit of angular momentum,

$$\hbar \equiv \frac{h}{2\pi} = 1.0546 \times 10^{-27} \text{ erg s} = 6.5822 \times 10^{-16} \text{ eV s}. \tag{1.8}$$

If instead of orienting the magnetic field in the vertical direction (SG$\hat{\mathbf{z}}$) we do it along any other direction, e.g. the x-axis (SG$\hat{\mathbf{x}}$), a similar result is observed, $S_x = \pm\hbar/2$. This means that the spin angular momentum is **quantized**, namely it may take only discrete values.

In order to try to understand this result, let us perform several sequential Stern-Gerlach experiments (Fig. 1.2). They consist of a chain of SG$\hat{\boldsymbol{\alpha}}$ devices to *measure* the spin along direction $\hat{\alpha}$ or *filter* one of the two spin components $S_\alpha = \pm\hbar/2$ by blocking the other one:

(a) In this experiment nothing very surprising happens, apart from the fact that every SG selects just two possible spin components (quantization). After we filter one of them, say $S_z = +\hbar/2$, by SG$\hat{\boldsymbol{z}}$, we measure that 100% of the atoms have $S_z = +\hbar/2$.

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(b) Now we filter $S_z = +\hbar/2$ and then measure the spin along a different direction S_x. The outcome is 50% of the atoms have either $S_x = \pm\hbar/2$.

Does this mean that half of the atoms filtered after SG$\hat{\boldsymbol{z}}$ have $S_z = +\hbar/2$ and $S_x = +\hbar/2$, and the other half $S_z = +\hbar/2$ and $S_x = -\hbar/2$?

(c) Surprisingly, the answer to the question above is no: if after filtering $S_x = +\hbar/2$ we measure S_z we find $S_z = +\hbar/2$ and $S_z = -\hbar/2$ (again!) with equal frequency.

This illustrates that in Quantum Mechanics one cannot determine S_z and S_x simultaneously, since the selection made by SG$\hat{\boldsymbol{x}}$ destroys the previous information about S_z obtained by SG$\hat{\boldsymbol{z}}$. Both observables are said to be **incompatible**.

Interestingly, there is a classical phenomenon that resembles the situation above, although it does not involve particles but waves! If one sends unpolarized light through two polaroid filters, the first selecting x-axis polarization and the second the (orthogonal) y-axis polarization, no light will be detected afterwards. A fraction of light would pass both filters if the polaroids are not othogonal.

The light polarization is described by a vector $\vec{\epsilon}$, in the plane transverse to the direction of propagation. This vector has a random orientation in the unpolarized case. A polaroid filter selects one of the orientations $\vec{\epsilon}_i$. The amplitude $\mathcal{A}$ of the wave passing two sequential filters is proportional to $\vec{\epsilon}_1 \cdot \vec{\epsilon}_2$ and the intensity of the light is proportional to its modulus squared, $|\mathcal{A}|^2$. We may assume that the two possible values of the silver atom spins, $S_z = \pm\hbar/2$, are "represented" by orthonormal "vectors" or "states" $|S_z\pm\rangle$ and conjecture

$$\vec{\epsilon}_x \rightsquigarrow |S_z+\rangle\,, \qquad\qquad \vec{\epsilon}_y \rightsquigarrow |S_z-\rangle\,. \tag{1.9}$$

The "probability amplitudes" for the transitions in (a) are given by the scalar products:

$$\mathcal{A}(|S_z+\rangle \to |S_z+\rangle) = \langle S_z + | S_z + \rangle = 1, \tag{1.10}$$
$$\mathcal{A}(|S_z+\rangle \to |S_z-\rangle) = \langle S_z + | S_z - \rangle = 0. \tag{1.11}$$

And the probabilities are $|\mathcal{A}|^2$.

How could we represent the states $|S_x\pm\rangle$ for the spins $S_x = \pm\hbar/2$? They must correspond to two orientations orthogonal to each other, but not orthogonal to S_z, that let half of the atoms go through. This means that they must be linear combinations of $|S_z\pm\rangle$,

$$|S_x+\rangle = \frac{1}{\sqrt{2}}\,|S_z+\rangle + \frac{1}{\sqrt{2}}\,|S_z-\rangle\,, \tag{1.12}$$
$$|S_x-\rangle = \frac{1}{\sqrt{2}}\,|S_z+\rangle - \frac{1}{\sqrt{2}}\,|S_z-\rangle\,, \tag{1.13}$$

like when a second polaroid is placed at 45°. Then experiment (b) is justified by

$$\mathcal{A}(|S_z+\rangle \to |S_x+\rangle) = \langle S_z + | S_x + \rangle = \frac{1}{\sqrt{2}}, \tag{1.14}$$
$$\mathcal{A}(|S_z+\rangle \to |S_x-\rangle) = \langle S_z + | S_x - \rangle = \frac{1}{\sqrt{2}}. \tag{1.15}$$

It is important to notice that the amplitude $\mathcal{A}(|S_z+\rangle \to |S_z+\rangle)$ in (a) can be written as the **superposition** of two amplitudes,

$$|S_z+\rangle = \frac{1}{\sqrt{2}}\,|S_x+\rangle + \frac{1}{\sqrt{2}}\,|S_x-\rangle$$

$$\Rightarrow \quad \mathcal{A}(|S_z+\rangle \to |S_z+\rangle) = \frac{1}{\sqrt{2}} \langle S_x + |S_z + \rangle + \frac{1}{\sqrt{2}} \langle S_x - |S_z + \rangle = \frac{1}{2} + \frac{1}{2} = 1. \quad (1.16)$$

Notice that the probability is *not* the sum of probabilities going through states with well defined $S_x = \pm\hbar/2$,

$$p(|S_z+\rangle \to |S_x+\rangle \to |S_z+\rangle) = \frac{1}{2} |\langle S_x + |S_z + \rangle|^2 = \frac{1}{4}, \quad (1.17)$$

$$p(|S_z+\rangle \to |S_x-\rangle \to |S_z+\rangle) = \frac{1}{2} |\langle S_x - |S_z + \rangle|^2 = \frac{1}{4}, \quad (1.18)$$

but that resulting from the *coherent* sum of amplitudes, which includes an *interference* term. Experiment (c) determines (**measures**) the S_x component destroying the coherence.

And how about the states $|S_y\pm\rangle$ corresponding to spins $S_y = \pm\hbar/2$? By symmetry arguments they should behave similarly with respect to $|S_z\pm\rangle$ *and* $|S_x\pm\rangle$ but this cannot happen unless the coefficients of the linear combination are **complex**,

$$|S_y+\rangle = \frac{1}{\sqrt{2}} |S_z+\rangle + \frac{\mathrm{i}}{\sqrt{2}} |S_z-\rangle , \quad (1.19)$$

$$|S_y-\rangle = \frac{1}{\sqrt{2}} |S_z+\rangle - \frac{\mathrm{i}}{\sqrt{2}} |S_z+\rangle , \quad (1.20)$$

in the same way as the right- and left-handed circular polarizations, $\vec{\epsilon}_{R,L}$, are a complex combination of the linear polarizations, $\vec{\epsilon}_{x,y}$.

Therefore, it seems that atoms behave like waves, whose amplitudes can be added and interfere. But "what" is interfering? Perhaps the atoms deflected in one direction somehow interfere with those going in opposite direction? Another weird observation is that the Stern-Gerlach experiment can be conducted sending silver atoms **one by one**, with the same outcome! So we must conclude that every atom interferes with itself!

As a conclusion, we need a **new theory** (Quantum Mechanics) that incorporates the properties found above (quantization, superposition, interference, incompatibility, uncertainty, ...). The new theory will be based in a complex vector (Hilbert) space to describe the physical system states, with observables represented by operators acting on them.

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Chapter 2

Postulates of Quantum Mechanics

2.1 Brief review of Hilbert spaces

A **Hilbert space** $\mathcal{H}$ is a vector space supplied with an inner or *scalar product* that is *complete* respect to the *norm* induced by the scalar product (see below the meaning of these properties). It is a generalization of the very familiar Euclidean spaces, like $\mathbb{R}^3$, to spaces with any finite or infinite number of dimensions.

The vectors in a vector space are elements that can be added and multiplied by a scalar. In a Hilbert space, unlike Euclidean spaces, these scalars are complex numbers:

$$\phi,\ \psi \in \mathcal{H}, \quad c_1,\ c_2 \in \mathbb{C} \Rightarrow c_1\phi + c_2\psi \in \mathcal{H} \quad \text{(linear combination)}. \tag{2.1}$$

We say that a set of vectors $\{\phi_i\}$ is linearly independent if $\sum_i c_i\phi_i = 0 \Rightarrow c_i = 0 \quad \forall i$.

The **scalar product** of any $\phi,\ \psi \in \mathcal{H}$ is a complex number $(\phi, \psi) \in \mathbb{C}$ satisfying:

(i) $(\phi, \psi) = (\psi, \phi)^*$ (hermiticity).

(ii) $(\phi, c_1\psi_1 + c_2\psi_2) = c_1(\phi, \psi_1) + c_2(\phi, \psi_2)$ (linearity of the second entry).
From (i) and (ii) one gets:
$(c_1\phi_1 + c_2\phi_2, \psi) = c_1^*(\phi_1, \psi) + c_2^*(\phi_2, \psi)$ (antilinearity of the first entry).

(iii) $(\phi, \phi) \geq 0$ and $\phi = 0$ when $(\phi, \phi) = 0$.

The scalar product induces a **norm**[a] defined by

$$\|\phi\| = \sqrt{(\phi, \phi)}, \tag{2.2}$$

that generalizes the concept of length (modulus) of a vector and defines a metric (distance between two vectors), given by

$$d(\phi, \psi) = \|\phi - \psi\|. \tag{2.3}$$

[a] The properties of a norm are:

(i) $\|c\phi\| = |c|\|\phi\|$ (homogeneous).

(ii) $\|\phi + \psi\| \leq \|\phi\| + \|\psi\|$ (triangle inequality).

(iii) $\|\phi\| \geq 0$ (positive definite).

The property (ii) follows from the Schwarz inequality: $|(\phi, \psi)|^2 \leq (\phi, \phi)(\psi, \psi)$.

A metric space M is **complete** if every Cauchy sequence in M converges in M. That is, if $\{\psi_n\}$ is a sequence with $d(\psi_m, \psi_n) \to 0$ when $m, n \to \infty$ then there exists a $\eta \in M$ such that $d(\psi_n, \eta) \to 0$ when $n \to \infty$. Complete normed vector spaces are called Banach spaces. A Hilbert space is a Banach space with the norm induced by the scalar product. One also requires that Hilbert spaces associated to physical sytems must be **separable**. This means that they have a countable orthonormal basis.

Let us now introduce linear functionals acting on a vector space V as functions $F : V \to \mathbb{C}$ mapping vectors ϕ to complex numbers $F(\phi)$ satisfying

$$F(a\phi + b\psi) = aF(\phi) + bF(\psi), \quad \phi,\ \psi \in V, \quad a,\ b \in \mathbb{C}. \tag{2.4}$$

Defining the sum of functionals

$$(F + G)(\phi) = F(\phi) + G(\phi), \tag{2.5}$$

the set of linear functionals over V defines another vector space called **dual space** V^*. These elements of the dual space are also called covectors or one-forms. In a Hilbert space $\mathcal{H}$ one can define linear functionals $F_\phi \in \mathcal{H}^*$ from any $\phi \in \mathcal{H}$ by

$$F_\phi(\psi) = (\phi, \psi). \tag{2.6}$$

Then the Riesz representation theorem applies stating that for each $F \in \mathcal{H}^*$ there exists just one vector $\phi_F \in \mathcal{H}$ such that

$$F(\psi) = (\phi_F, \psi) \quad \forall \psi \in \mathcal{H}. \tag{2.7}$$

Therefore, there is a bijective mapping between V and V^* given by the scalar product ($\mathcal{H}$ and $\mathcal{H}^*$ are isomorphic; in particular, they have the same dimension). This suggests the **Dirac's notation**, extensively used in Quantum Mechanics (QM):

$$\begin{aligned} \text{Vector } \psi \in \mathcal{H} \quad &\to \quad \textbf{ket } |\psi\rangle \in \mathcal{H} \\ \text{Functional } F_\phi \in \mathcal{H}^* \quad &\to \quad \textbf{bra } \langle\phi| \in \mathcal{H}^* \\ \text{Action of functional } F_\phi \text{ on } \psi \in \mathcal{H} \quad &\to \quad \textbf{braket } \langle\phi|\psi\rangle = (\phi, \psi) \text{ (scalar product).} \end{aligned}$$

In other words, every ket $|\psi\rangle$ has a corresponding bra $\langle\psi|$, that is unique, and the scalar product (ϕ, ψ) of two vectors (kets) $|\phi\rangle$ and $|\psi\rangle$ is given by the braket $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$.

From now on, until chapter 3, we will work in Hilbert spaces of finite dimension, although many results can be applied to the case of infinite dimensions.

A **basis** is a set of linearly independent vectors $\{|\phi_i\rangle\}$ ($i = 1, \ldots, d = \dim\mathcal{H}$) that allows us to express any vector $|\alpha\rangle \in \mathcal{H}$ as a linear combination (summations extend from $i = 1$ to d unless otherwise stated)

$$|\alpha\rangle = \sum_i |\phi_i\rangle\, \alpha_i = \begin{pmatrix} |\phi_1\rangle & |\phi_2\rangle & \ldots \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{pmatrix}, \quad \alpha_i \in \mathbb{C} \quad \text{or} \quad |\alpha\rangle \doteq \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{pmatrix} \tag{2.8}$$

where the α_i are the components of $|\alpha\rangle$ in the basis $\{|\phi_i\rangle\}$. An **orthonormal basis** $\{|e_i\rangle\}$ fulfills

$$\langle e_k|e_i\rangle = \delta_{ki} \quad \text{(orthonormality relation)}. \tag{2.9}$$

Given a basis $\{|\phi_i\rangle\}$ the Gram-Schmidt process provides an orthornormal basis $\{|e_i\rangle\}$:

$$|e_1\rangle = \frac{|\phi_1\rangle}{\| \, |\phi_1\rangle \, \|}, \quad \| \, |\phi_1\rangle \, \| = \sqrt{\langle\phi_1|\phi_1\rangle}, \tag{2.10}$$

$$|e_{k+1}\rangle = \frac{|\phi_{k+1}\rangle - \sum_{i=1}^{k} |e_i\rangle \, \langle e_i|\phi_{k+1}\rangle}{\| \, |\phi_{k+1}\rangle - \sum_{i=1}^{k} |e_i\rangle \, \langle e_i|\phi_{k+1}\rangle \, \|}. \tag{2.11}$$

In an orthonormal basis the components of a vector are easy to obtain from the scalar product or braket:

$$|\alpha\rangle = \sum_i |e_i\rangle \, \alpha_i \quad \Rightarrow \quad \langle e_k|\alpha\rangle = \sum_i \langle e_k|e_i\rangle \, \alpha_i = \sum_i \delta_{ki}\alpha_i = \alpha_k \tag{2.12}$$

$$\Rightarrow \quad |\alpha\rangle = \sum_i |e_i\rangle \, \langle e_i|\alpha\rangle \quad \Rightarrow \quad I = \sum_i |e_i\rangle\langle e_i| \quad \text{(completeness or closure relation)} \tag{2.13}$$

and the scalar product of two vectors reads:

$$\langle\alpha|\beta\rangle = \sum_i \langle\alpha|e_i\rangle \, \langle e_i|\beta\rangle = \sum_i \langle e_i|\alpha\rangle^* \, \langle e_i|\beta\rangle = \sum_i \alpha_i^*\beta_i. \tag{2.14}$$

In fact, the isomorphism between $\mathcal{H}$ and $\mathcal{H}^*$ is given by the adjoin or dagger relation:

$$\begin{array}{rcl} \mathcal{H} & \longrightarrow & \mathcal{H}^* \\ \{|e_i\rangle\} & \mapsto & \{\langle e_i|\} \quad \text{(so called adjoint basis of } \mathcal{H}^*) \\ |\alpha\rangle & \mapsto & \langle\alpha| = |\alpha\rangle^\dagger = \sum_i \alpha_i^* \, \langle e_i| \quad \text{(by antilinearity of braket's left entry).} \end{array} \tag{2.15}$$

An **operator** A transforms vectors $|\alpha\rangle \in \mathcal{H}$ to other vectors $A\,|\alpha\rangle \in \mathcal{H}$. **Linear** operators satisfy

$$A(a\,|\alpha\rangle + b\,|\beta\rangle) = aA\,|\alpha\rangle + bA\,|\beta\rangle \, . \tag{2.16}$$

Operators can be added and composed (multiplied),

$$(A+B)\,|\alpha\rangle = A\,|\alpha\rangle + B\,|\alpha\rangle \tag{2.17}$$

$$AB\,|\alpha\rangle = A(B\,|\alpha\rangle) \tag{2.18}$$

and the product of operators is associative,

$$A(BC) = (AB)C, \tag{2.19}$$

but not necessarily commutative. To know how an operator acts on all the vectors in $\mathcal{H}$ it is sufficient to know how it acts on a basis of $\mathcal{H}$. Given an orthonormal basis $\{|e_i\rangle\}$,

$$A\,|e_j\rangle = \sum_i |e_i\rangle\langle e_i|\,A\,|e_j\rangle = \sum_i |e_i\rangle \, A_{ij} \quad \Leftrightarrow \quad A_{ij} = \langle e_i|\,A\,|e_j\rangle \quad \text{(matrix element)} \tag{2.20}$$

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one obtains $|\beta\rangle = A\,|\alpha\rangle$ from

$$A\,|\alpha\rangle = A\sum_j |e_j\rangle\,\alpha_j = \sum_{ij} |e_i\rangle\,A_{ij}\alpha_j$$
$$= |\beta\rangle = \sum_i |e_i\rangle\,\beta_i \tag{2.21}$$
$$\Rightarrow \quad \beta_i = \sum_j A_{ij}\alpha_j. \tag{2.22}$$

On the other hand, operators act on bras to the left:

$$A_{ij} = \langle e_i|\,(A\,|e_j\rangle) = (\langle e_i|\,A)\,|e_j\rangle \tag{2.23}$$
$$\Rightarrow \quad \langle e_i|\,A = \sum_j \langle e_i|\,A\,|e_j\rangle\langle e_j| = \sum_j A_{ij}\,\langle e_j| \tag{2.24}$$
$$\Rightarrow \quad \langle\alpha|\,A = \sum_i \alpha_i^*\,\langle e_i|\,A = \sum_{ij} \alpha_i^* A_{ij}\,\langle e_j|$$
$$= \langle\beta| = \sum_j \beta_j^*\,\langle e_j| \tag{2.25}$$
$$\Rightarrow \quad \beta_j^* = \sum_i \alpha_i^* A_{ij}. \tag{2.26}$$

Notice that the vector components are basis-dependent but the "sandwich" $\langle\alpha|\,A\,|\beta\rangle$ and the scalar product $\langle\alpha|\beta\rangle$ are basis-independent:

$$\langle\alpha|\,A\,|\beta\rangle = \sum_{ij} \langle\alpha|e_i\rangle\,\langle e_i|\,A\,|e_j\rangle\,\langle e_j|\beta\rangle = \sum_{ij} \alpha_i^* A_{ij}\beta_j. \tag{2.27}$$

The scalar product of $A\,|\alpha\rangle$ and $|\beta\rangle$ is not $\langle\alpha|\,A\,|\beta\rangle$ but $\langle\alpha|\,A^\dagger\,|\beta\rangle$, that defines the **adjoint operator** $A^\dagger$. This is because the adjoint of $A\,|\alpha\rangle$ is not $\langle\alpha|\,A$ but $\langle\alpha|\,A^\dagger$:

$$A_{ij} = \langle e_i|\,A\,|e_j\rangle \tag{2.28}$$
$$A_{ij}^* = \langle e_j|\,A^\dagger\,|e_i\rangle = A_{ji}^\dagger \tag{2.29}$$
$$\Rightarrow \quad A_{ij}^\dagger = A_{ji}^* \quad \text{or} \quad A^\dagger = A^{T*}. \tag{2.30}$$

Given $|\phi\rangle$, $|\psi\rangle$, a useful way to define a linear operator is $|\phi\rangle\langle\psi|$ (**outer product**) that acting on any $|\eta\rangle \in \mathcal{H}$ gives a vector proportional to $|\phi\rangle$:

$$(|\phi\rangle\langle\psi|)\,|\eta\rangle = |\phi\rangle\,\langle\psi|\eta\rangle\,. \tag{2.31}$$

It is easy to check[b] that

$$(|\phi\rangle\langle\psi|)^\dagger = |\psi\rangle\langle\phi|\,. \tag{2.32}$$

Taking a unit vector $|e_1\rangle$ we obtain a **projector**,

$$P_1 = |e_1\rangle\langle e_1|\,, \quad P_1^2 = P_1\ (\textit{idempotent}), \quad P_1^\dagger = P_1\ (\textit{self-adjoint}), \tag{2.33}$$

that projects any vector $|\alpha\rangle \in \mathcal{H}$ along the vector $|e_1\rangle$,

$$P_1\,|\alpha\rangle = |e_1\rangle\,\langle e_1|\alpha\rangle = |e_1\rangle\,\alpha_1. \tag{2.34}$$

[b] $(|\phi\rangle\langle\psi|)^\dagger\,|\eta\rangle = (\langle\eta|\phi\rangle\,\langle\psi|)^\dagger = |\psi\rangle\,\langle\eta|\phi\rangle^* = |\psi\rangle\,\langle\phi|\eta\rangle = (|\psi\rangle\langle\phi|)\,|\eta\rangle\,, \quad \forall\,|\eta\rangle\,.$

A sum of projectors $\sum_{i=1}^{r} P_i$, with $P_i = |e_i\rangle\langle e_i|$, is also a projector into the subspace spanned by the r unit vectors $|e_i\rangle_{i=1,\dots,r}$. If $\{|e_i\rangle\}$ is an orthonormal basis of $\mathcal{H}$ then the P_i are **orthogonal projectors**,

$$P_i^2 = P_i, \quad P_i P_j = \delta_{ij} P_j. \tag{2.35}$$

We have already seen that in fact $I = \sum_{i=1}^{d} |e_i\rangle\langle e_i|$ since

$$|\alpha\rangle = \sum_{i}^{d} |e_i\rangle \langle e_i|\alpha\rangle , \quad \forall\, |\alpha\rangle \in \mathcal{H}. \tag{2.36}$$

Given a linear operator A, if there exist $a \in \mathbb{C}$ and $|\phi\rangle \in \mathcal{H}$ with $|\phi\rangle \neq 0$ such that

$$A\,|\phi\rangle = a\,|\phi\rangle \tag{2.37}$$

we say that every $|\phi\rangle$ is an **eigenvector** of A with **eigenvalue** a. If $|\phi\rangle_{i=1,\dots,r}$ are linearly independent eigenvectors of A with the same eigenvalue a (degenerate eigenvalue) then obviously any linear combination $\sum_i c_i\,|\phi\rangle_i$ is also an eigenvector. Therefore, the eigenvectors of each eigenvalue form a vector subspace. And, of course, if $A\,|\phi\rangle = a\,|\phi\rangle$ then

$$\langle\phi|\,A^\dagger = a^*\,\langle\phi|\,. \tag{2.38}$$

An operator A is **self-adjoint** if $A^\dagger = A$, namely, if

$$\langle\phi|\,A\,|\psi\rangle = \langle\phi|\,A^\dagger\,|\psi\rangle = \langle\phi|\,A\,|\psi\rangle^*\,, \quad \forall\phi,\ \psi \in \mathcal{H} \tag{2.39}$$

Actually, this is only true in finite dimension, since otherwise the domains of A and $A^\dagger$ may not coincide. In the latter case, we say that A is **Hermitian**, but not self-adjoint. In general, if A is self-adjoint then all its **eigenvalues are real**,[c] and the eigenvectors corresponding to different eigenvalues are orthogonal.[d] Furthermore, an important theorem states that the orthonormal set of the **eigenvectors of a self-adjoint operator** on a Hilbert space of finite dimension is a **basis** of $\mathcal{H}$.

Consider $\mathcal{H}$ of finite dimension, a self-adjoint operator A and an orthonormal basis $\{|\phi_i\rangle\}$ formed by the eigenvectors of A. And let a_i be the corresponding eigenvalues. We define the othogonal projectors to the subspace of eigenvalue a (perhaps degenerate) as

$$P_a = \sum_{i} |\phi_i\rangle\langle\phi_i|\,\delta_{a_i a}. \tag{2.40}$$

Then, one can write A as follows (**spectral decomposition**):

$$A = \sum_{a} a P_a = \sum_{i} a_i\,|\phi_i\rangle\langle\phi_i|\,, \tag{2.41}$$

a diagonal matrix in the basis of eigenvectors. This may be used to define a function f of operators from the same function of complex numbers:

$$f(A) = \sum_{i} f(a_i)\,|\phi_i\rangle\langle\phi_i|\,. \tag{2.42}$$

[c] $A\,|a\rangle = a\,|a\rangle \Rightarrow \langle a|\,A\,|a\rangle = a\,\langle a|a\rangle$ and $\langle a|\,A^\dagger\,|a\rangle = \langle a|\,A\,|a\rangle^* = a^*\,\langle a|a\rangle$. So $A = A^\dagger \Rightarrow a = a^*$.

[d] $A\,|a\rangle = a\,|a\rangle$, $A\,|a'\rangle = a'\,|a'\rangle$, $a, a' \in \mathbb{R}$. Take $\langle a'|\,A\,|a\rangle = a\,\langle a'|a\rangle = a'\,\langle a'|a\rangle \Rightarrow (a - a')\,\langle a'|a\rangle = 0$. Hence, if $a \neq a'$ then $\langle a'|a\rangle = 0$.

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Consider now A and B two **self-adjoint commuting operators**, $[A,B]=AB-BA=0$, in finite dimension. Then there exists a complete set of **simultaneous eigenvectors** of A and B, that is, A and B can be diagonalized simultaneously.

If $A,B,C,\dots$ are self-adjoint operators commuting with each other, then the set of their simultaneous eigenvectors $|a_i,b_j,c_k,\dots\rangle$,

$$A\,|a_i,b_j,c_k,\dots\rangle = a_i\,|a_i,b_j,c_k,\dots\rangle\,, \tag{2.43}$$
$$B\,|a_i,b_j,c_k,\dots\rangle = b_j\,|a_i,b_j,c_k,\dots\rangle\,, \tag{2.44}$$
$$C\,|a_i,b_j,c_k,\dots\rangle = c_k\,|a_i,b_j,c_k,\dots\rangle\,, \quad \text{etc.} \tag{2.45}$$

may be degenerate. But if the subspace of eigenvectors for all possible sets of eigenvalues has dimension one (it is not degenerate) then $A,B,C,\dots$ is a **complete set of commuting (self-adjoint) operators** (CSCO). As a consequence, any operator F commuting with all the members of a CSCO is a function of these operators and

$$F\,|a_i,b_j,c_k,\dots\rangle = f_{ijk\dots}\,|a_i,b_j,c_k,\dots\rangle\,, \quad f_{ijk\dots}=f(a_i,b_j,c_k,\dots). \tag{2.46}$$

Given two orthonormal bases $\{|e_i\rangle\}$ and $\{|\tilde{e}_i\rangle\}$, we may write

$$|\tilde{e}_j\rangle = \sum_i |e_i\rangle\,\langle e_i|\tilde{e}_j\rangle \tag{2.47}$$

and define the **change of basis** operator from $\{|e_i\rangle\}$ to $\{|\tilde{e}_i\rangle\}$ as

$$U=\sum_i |\tilde{e}_i\rangle\langle e_i| \quad\Rightarrow\quad U\,|e_j\rangle = |\tilde{e}_j\rangle\,. \tag{2.48}$$

The operator U is **unitary**, $UU^\dagger = U^\dagger U = \mathbb{I}$. Notice that the basis elements and the vector components transform in an opposite way:

$$|\tilde{e}_j\rangle = \sum_i |e_i\rangle\,\langle e_i|\tilde{e}_j\rangle \quad\Rightarrow\quad |\tilde{e}_j\rangle = \sum_i |e_i\rangle\,U_{ij}\ , \quad U_{ij}=\langle e_i|\tilde{e}_j\rangle = \langle e_i|\,U\,|e_j\rangle \tag{2.49}$$

while for any $|\alpha\rangle\in\mathcal{H}$,

$$\begin{aligned}|\alpha\rangle &= \sum_i |e_i\rangle\,\langle e_i|\alpha\rangle = \sum_i |e_i\rangle\,\alpha_i \\ &= \sum_i |\tilde{e}_i\rangle\,\langle \tilde{e}_i|\alpha\rangle = \sum_i |\tilde{e}_i\rangle\,\tilde{\alpha}_i\ ,\end{aligned} \tag{2.50}$$

$$\langle\tilde{e}_i|\alpha\rangle = \sum_j \langle\tilde{e}_i|e_j\rangle\,\langle e_j|\alpha\rangle \quad\Rightarrow\quad \tilde{\alpha}_i = \sum_j U^\dagger_{ij}\alpha_j, \quad U^\dagger_{ij}=U^*_{ji}=\langle\tilde{e}_i|e_j\rangle \tag{2.51}$$

and in fact U is unitary:

$$\delta_{ik}=\langle e_i|e_k\rangle = \sum_j \langle e_i|\tilde{e}_j\rangle\,\langle\tilde{e}_j|e_k\rangle = \sum_j U_{ij}U^*_{kj} = \sum_j U_{ij}U^\dagger_{jk}. \tag{2.52}$$

On the other hand, the matrix elements of a linear operator A transform as:

$$\begin{aligned}\tilde{A}_{ij} &= \langle\tilde{e}_i|\,A\,|\tilde{e}_j\rangle = \langle e_i|\,U^\dagger AU\,|e_j\rangle = \sum_{kl}\langle e_i|\,U^\dagger\,|e_k\rangle\langle e_k|\,A\,|e_l\rangle\langle e_l|\,U\,|e_j\rangle \\ &= \sum_{kl} U^\dagger_{ik}A_{kl}U_{lj}.\end{aligned} \tag{2.53}$$

If A is a linear operator and $\{|e_i\rangle\}$ is an orthonormal basis then the **trace** of A is

$$\mathrm{Tr}(A) = \sum_i \langle e_i| A |e_i\rangle \quad \text{(sum of the diagonal elements)}. \tag{2.54}$$

Notice that the trace is independent of the basis and satisfies the properties:

(i) $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$.

(ii) $\mathrm{Tr}(U^\dagger AU) = \mathrm{Tr}(A)$ if U is unitary.

(iii) $\mathrm{Tr}(|e_i\rangle\langle e_j|) = \delta_{ij}$.

(iv) $\mathrm{Tr}(|\phi\rangle\langle\psi|) = \langle\psi|\phi\rangle$.

2.2 Pure states

In the previous chapter, with the help of the Stern-Gerlach experiment, we have shown the failure of Classical Mechanics and the need to introduce a new theory able to describe *all* physical phenomena.

It is important to realize that whatever information we have about a physical system is obtained through experimentation. It is useful to divide the experiment in two phases:

- **Preparation**: the experimentalist (or nature) submits the system to some conditions that define its state. For example, the silver atoms in the SG$\hat{\boldsymbol{z}}$ are prepared to have well defined z-component of the magnetic moment after crossing an inhomogeneous magnetic field applied along that direction. By filtering those deflected upward or downward we can select a particular value of the spin.[e]

- **Measurement**: the experimentalist (or nature) interacts with the preparation to determine the value of a particular **observable** (any physical variable that, in principle, can be measured). For example, one can measure the observables S_z or S_x of the atoms previously prepared.

A specific preparation does not necessarily determine the outcome of a subsequent measurement but the *probabilities* of the various possible outcomes. Actually the preparation is independent of the specific measurement that may follow it.

A **state** is the specification of the set of probabilities (or probability distributions) for the measurements of the various observables. The concept of state in QM is very subtle and even controversial. Since it has always been the goal of physics to give an objective realistic description of the world, we are tempted to interpret the state as an element of reality describing the attributes of an individual system. However such assumptions lead to contradictions and must be abandoned. The quantum state description may be taken to refer to a collection of similarly prepared systems.

For the moment we will consider *pure* states, which are those that give maximal (though probabilistic) information about the outcome of the measurements. We will see later, in §2.5, that in general the system is in a *mixed* state, specified by a statistical distribution of pure states. For instance, the ensemble of silver atoms coming directly from the furnace,

[e] See §2.10 for the impossibility of *cloning* quantum states, as if they were keys we want to duplicate.

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before going through any SG device; or a partially polarized (or unpolarized) electron beam.

To construct the physical theory it is necessary to introduce a few basic postulates.

2.2.1 Postulate I

> In QM a physical system is associated to a separable, complex Hilbert space and a pure state of the system at a time t is described by a unit ray[a] represented by a vector (ket) $|\alpha\rangle$ or $|\alpha(t)\rangle$ of the Hilbert space.
>
> [a] A unit ray is a unit vector with arbitrary phase.

Then the superposition principle is guaranteed: if $|\phi\rangle$ and $|\psi\rangle$ are states of the system then $|\eta\rangle = \alpha\,|\phi\rangle + \beta\,|\psi\rangle$, with arbitrary $\alpha, \beta \in \mathbb{C}$, is also a possible state. But not every vector is a pure state (see section §2.9 on superselection rules and chapter 6 on identical particles).

The Hilbert space of the system may have just two dimensions, like in the Stern-Gerlach experiment. Then we may choose an arbitrary basis of two states to represent any other state. For instance, $\{|S_z+\rangle, |S_z-\rangle\}$, $\{|S_x+\rangle, |S_x-\rangle\}$ and $\{|S_y+\rangle, |S_y+\rangle\}$ are three bases, and the state $|S_x+\rangle$ in the first basis is given by

$$|S_x-\rangle = \frac{1}{\sqrt{2}}\,|S_z+\rangle - \frac{1}{\sqrt{2}}\,|S_z-\rangle\,. \tag{2.55}$$

A particularly interesting two-dimensional quantum mechanical system is the *qubit*, the quantum computer unit of information. In contrast to the classical bit that can be in just two states 0 or 1, one can prepare a qubit in any arbitrary superposition of $|0\rangle$ and $|1\rangle$.

2.3 Observables

2.3.1 Postulate II

> Every observable of a physical system is represented by a self-adjoint linear operator acting on the associated Hilbert space, whose eigenvalues are the only possible values of the observable.

This justifies several issues:

- The number of eigenvalues of an operator acting on a space of finite dimension is denumerable. Hence, the values of the corresponding observable are quantized.
- A self-adjoint operator has real eigenvalues. The values of physical observables are always real numbers.
- A linear operator respects the superposition principle.
- It is not possible to measure simultaneously two observables represented by non-commuting operators because they cannot be diagonalized in the same basis, they are incompatible.

For instance, the spin of the silver atom in the z-axis or in the x-axis are observables represented by the self-adjoint operators S_z and S_x, respectively. Both of them have eigenvalues $\pm\hbar/2$. Using their spectral decomposition:

$$S_z = \frac{\hbar}{2}\,|S_z+\rangle\langle S_z+| - \frac{\hbar}{2}\,|S_z-\rangle\langle S_z-| \doteq \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \equiv \frac{\hbar}{2}\sigma_3, \tag{2.56}$$

$$S_x = \frac{\hbar}{2}\,|S_x+\rangle\langle S_x+| - \frac{\hbar}{2}\,|S_x-\rangle\langle S_x-| \doteq \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \equiv \frac{\hbar}{2}\sigma_1. \tag{2.57}$$

The matrix form of the operators has been given in the basis $\{|S_z+\rangle, |S_z-\rangle\}$, where

$$|S_z+\rangle \doteq \begin{pmatrix}1\\0\end{pmatrix}, \quad |S_z-\rangle \doteq \begin{pmatrix}0\\1\end{pmatrix}, \tag{2.58}$$

$$|S_x+\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \quad |S_x-\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}. \tag{2.59}$$

Notice that we have chosen an arbitrary phase for each of these states. The observables S_x and S_z are incompatible because $[S_x, S_z] \neq 0$.

2.4 Measurements

2.4.1 Postulate III

> If a physical system is in a pure state described by the normalized vector $|\psi\rangle$, the probability of obtaining an eigenvalue a of an observable represented by the operator A is
>
> $$p_a = \langle\psi|\, P_{A,a}\,|\psi\rangle$$
>
> where $P_{A,a}$ is the projector into the subspace of eigenvalue a.

If a is a non-degenerate eigenvalue of A and $|a\rangle$ is the corresponding normalized eigenvector then

$$P_{A,a} = |a\rangle\langle a| \quad \Rightarrow \quad p_a = |\,\langle a|\psi\rangle\,|^2. \tag{2.60}$$

In general, let $\{|a_i\rangle\}$ be an orthonormal basis of the subspace of eigenvalue a. Then

$$P_{A,a} = \sum_i |a_i\rangle\langle a_i| \quad \Rightarrow \quad p_a = \sum_i |\,\langle a_i|\psi\rangle\,|^2. \tag{2.61}$$

Notice that:

- If the state of the system was already in the subspace of eigenvalue a,

  $$|\psi\rangle \in \mathcal{H}_a \quad \Rightarrow \quad p_a = \langle\psi|\, P_{A,a}\,|\psi\rangle = \langle\psi|\psi\rangle = 1. \tag{2.62}$$

  If $|\psi\rangle \in \mathcal{H}_a^{\perp}$ (orthogonal subspace) then $p_a = \langle\psi|\, P_{A,a}\,|\psi\rangle = 0$. The probability is $p_a \in (0,1)$ otherwise.

- The sum of probabilities to obtain any possible value is one, as it should be, since the eigenvectors form a complete set,

  $$I = \sum_a P_{A,a} \quad \Rightarrow \quad \sum_a p_a = \sum_a \langle\psi|\, P_{A,a}\,|\psi\rangle = \langle\psi|\psi\rangle = 1. \tag{2.63}$$

And what is the state after the measurement?

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2.4.2 Postulate IV

If a physical system is in a pure state described by the normalized vector $|\psi\rangle$ and one measures A obtaining a, the system is left in the state

$$|\psi'\rangle = \frac{P_{A,a}\,|\psi\rangle}{\|P_{A,a}\,|\psi\rangle\,\|}.$$

In other words, after the measurement, the state of the system is projected into a particular state of the subspace with eigenvalue a. It is often said that the state $|\psi\rangle$ *collapses* to the eigenstate $|\psi'\rangle$ of A. But one can also view it in a different way: There is no measurement without *interaction* with the measuring instrument (another system). Hence, we must always consider our system as a part of a composite system. As we will see in section §2.6, the states of the Hilbert space of this composite system are vectors of the tensor product of the Hilbert spaces of its subsystems. Some of these states are *entangled*, i.e. they cannot be written as the product of a vector of each space, they are a non separable combination. For instance,

$$\frac{1}{\sqrt{2}}\,|\uparrow\rangle\,|+\rangle + \frac{1}{\sqrt{2}}\,|\downarrow\rangle\,|-\rangle\,. \tag{2.64}$$

Now, assume that the *interaction entangles* the measuring instrument with the system we wish to study.[f] Let us take that, after crossing SG$\hat{\boldsymbol{z}}$, $|\uparrow\rangle\,|+\rangle$ is the state for the atoms deviated upward with $S_z = +\hbar/2$ and the opposite for $|\downarrow\rangle\,|-\rangle$. The entangled state (2.64) is none of them but a superposition.[g] The fact is we do not really know whether the atom is in state $|+\rangle$ or $|-\rangle$, since we just measure that it leaves the SG as $|\uparrow\rangle$ or $|\downarrow\rangle$ after experiencing countless (uncontrolled) interactions with the magnetic field. This *partial knowledge* causes the *decoherence*. Thus interaction allows for the creation of superpositions (entangled states), and at the same time breaks the coherence of its subsystems.

Let's apply these postulates to our sequence of Stern-Gerlach experiments (Fig. 1.1):

(a) $|\psi\rangle = |S_z{+}\rangle$

$$p_{S_z,+} = |\,\langle S_z + |S_z + \rangle\,|^2 = 1, \qquad \Rightarrow \quad |\psi'\rangle = |S_z{+}\rangle\,; \tag{2.65}$$

$$p_{S_z,-} = |\,\langle S_z + |S_z - \rangle\,|^2 = 0 \qquad (|S_z{-}\rangle \text{ never happens}). \tag{2.66}$$

(b) $|\psi\rangle = |S_z{+}\rangle$

$$p_{S_x,+} = |\,\langle S_z + |S_x + \rangle\,|^2 = \frac{1}{2}, \qquad |\psi'\rangle = |S_x{+}\rangle\,; \tag{2.67}$$

$$p_{S_x,-} = |\,\langle S_z + |S_x - \rangle\,|^2 = \frac{1}{2}, \qquad |\psi'\rangle = |S_x{-}\rangle\,. \tag{2.68}$$

(c) $|\psi\rangle = |S_x{+}\rangle$ (after filtering one half of the atoms in (b))

$$p_{S_z,+} = |\,\langle S_x + |S_z + \rangle\,|^2 = \frac{1}{2}, \qquad |\psi'\rangle = |S_z{+}\rangle\,; \tag{2.69}$$

$$p_{S_z,-} = |\,\langle S_x + |S_z - \rangle\,|^2 = \frac{1}{2}, \qquad |\psi'\rangle = |S_z{-}\rangle\,. \tag{2.70}$$

[f] Why? How? This view is not a solution of but another way to formulate the measurement problem.

[g] If you replace the states $|\uparrow\rangle$, $|\downarrow\rangle$ by unbroken or broken poisson flask and $|+\rangle$, $|-\rangle$ by cat alive or dead, this describes the famous Schrödinger's cat states.

2.4.3 Expectation value and uncertainty relations

Consider a macroscopic object, like a bar, whose length L we want to measure. The procedure consists of taking several measurements and then averaging. Suppose that, within the precision of the ruler, we obtain L_1 (n_1 times), L_2 (n_2 times), etc. If the total number of measurements is n then the mean value of the bar length is

$$\langle L\rangle = \sum_i L_i \frac{n_i}{n} \tag{2.71}$$

where n_i/n is the relative frequency of every result. We expect that $\langle L\rangle$ approaches the actual value of L for large n.

If you want to measure an observable A in a pure quantum state $|\psi\rangle$ of a physical system you must prepare many replicas of the system in the same state and then measure A. According to the postulates, the result of every measurement is an eigenvalue a_i of A and the mean value of all measurements,

$$\langle A\rangle_\psi = \sum_a a p_a = \sum_a a \langle\psi| P_{A,a} |\psi\rangle = \langle\psi| \sum_a a P_{A,a} |\psi\rangle = \langle\psi| A |\psi\rangle . \tag{2.72}$$

This is called the *expectation value* of the observable A in the pure state $|\psi\rangle$.

We can also define the *uncertainty* of A in the state $|\psi\rangle$ as the dispersion (mean square displacement) of the different measurements around the expectation value,

$$\begin{aligned}\Delta_\psi A &= \left[\langle\psi| (A - \langle A\rangle_\psi)^2 |\psi\rangle\right]^{\frac{1}{2}} \\ &= \left[\langle A^2\rangle_\psi + \langle A\rangle_\psi^2 - 2\langle A\rangle_\psi^2\right]^{\frac{1}{2}} \\ &= \left[\langle A^2\rangle_\psi - \langle A\rangle_\psi^2\right]^{\frac{1}{2}} .\end{aligned} \tag{2.73}$$

The uncertainty of an observable in a pure state is zero if it is an eigenvector of the observable. This is because

$$A |\psi\rangle = a |\psi\rangle \Rightarrow A^2 |\psi\rangle = a^2 |\psi\rangle \Rightarrow \Delta_\psi A = \left[\langle A^2\rangle_\psi - \langle A\rangle_\psi^2\right]^{\frac{1}{2}} = 0. \tag{2.74}$$

It is easy to show [exercise] that for a pure state $|\psi\rangle$ the product of the uncertainties of two observables A and B is

$$\Delta_\psi A \, \Delta_\psi B \geq \frac{1}{2} |\langle\psi| [A, B] |\psi\rangle| . \tag{2.75}$$

These *uncertainty relations* are a generalization of the position-momentum uncertainty relations we will find later (3.71). They have important consequences: if two observables *do not commute*, $[A, B] \neq 0$, it is impossible to measure simultaneously both of them with full precission in any state. That's why we say *they are incompatible*.

2.4.4 Complete Set of Compatible Observables

When two observables A and B are compatible their corresponding self-adjoint operators commute, $[A, B] = 0$. Then there exists a basis of eigenvectors $\{|a_i b_i\rangle\}$ of A and B that is common to A and B simultaneously,

$$A |a_i, b_i\rangle = a_i |a_i, b_i\rangle , \tag{2.76}$$

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$$B\,|a_i, b_i\rangle = b_i\,|a_i, b_i\rangle\,. \tag{2.77}$$

Two (or more) compatible observables define a complete set (CSCO) if any pair of eigenvectors in the common basis differs at least in one eigenvalue. Then the eigenvalues label *unambiguously* (up to a complex phase) the vectors of the basis, i.e. the states of the system that can be measured simultaneously by all the observables in the CSCO.

A characterization of a CSCO is:

(i) They are compatible (commute).

(ii) The basis of common eigenvectors is unique (up to phases).

(iii) The set is minimal. Then the description of the system is not redundant. This condition was not assumed above but it is often imposed.

– Example 1:

$$A \doteq \begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix}, \quad B \doteq \begin{pmatrix} 1 & & \\ & 0 & \\ & & 0 \end{pmatrix} \quad \Rightarrow \quad \text{basis } \{|1,1\rangle\,, |1,0\rangle\,, |-1,0\rangle\} \tag{2.78}$$

A and B *are* a CSCO. The eigenvalues of one of them break the degeneracy of the other.

– Example 2:

$$C \doteq \begin{pmatrix} 1 & & \\ & 0 & \\ & & -1 \end{pmatrix}, \quad D \doteq \begin{pmatrix} 1 & & \\ & 2 & \\ & & 2 \end{pmatrix} \quad \Rightarrow \quad \text{basis } \{|1,1\rangle\,, |0,2\rangle\,, |-1,2\rangle\} \tag{2.79}$$

C and D are *not* a CSCO because it is not minimal (C is enough to label the basis states).

2.5 Density matrix

The formalism developed so far applies to pure states. We have seen that the quantum mechanical predictions are probabilistic, they are understood as the results of the measurements over a collection of identically prepared physical systems, all described by the same vector of a Hilbert space $|\alpha\rangle$.

We will now consider the most general case, a statistical ensemble of N pure states $\{|\alpha_i\rangle\}$ with frequencies $0 \leq w_i \leq 1$ (there are $N_i = w_i N$ in each pure state) and

$$\sum_i w_i = 1. \tag{2.80}$$

The $|\alpha_i\rangle$ do not need to be orthogonal and N is arbitrary (nothing to do with the dimension of the Hilbert space). A system chosen randomly from this statistical ensemble is said to be in a *mixed* state.

The mixed state is described by a *density matrix*,

$$\rho = \sum_i w_i\,|\alpha_i\rangle\langle\alpha_i| \tag{2.81}$$

that gives the expectation value (average) of an observable A measured over the statistical ensemble. In fact,

$$\begin{aligned}\langle A\rangle_\rho = \frac{\sum_i N_i \langle A\rangle_{\alpha_i}}{N} &= \sum_i w_i \langle\alpha_i| A |\alpha_i\rangle \\ &= \sum_a \sum_{a'} \sum_i w_i \langle\alpha_i|a'\rangle \langle a'| A |a\rangle \langle a|\alpha_i\rangle \\ &= \sum_a \sum_{a'} \sum_i w_i \langle a|\alpha_i\rangle \langle\alpha_i|a'\rangle \langle a'| A |a\rangle \\ &= \sum_a \sum_{a'} \rho_{aa'} A_{a'a} = \mathrm{Tr}(\rho A) \end{aligned} \tag{2.82}$$

where $|a\rangle$ and $|a'\rangle$ are eigenvectors of A, that satisfy $\sum_a |a\rangle\langle a| = \sum_{a'} |a'\rangle\langle a'| = I$. Notice that a complex phase of $|\alpha_i\rangle$ in (2.81) is, of course, irrelevant. The density matrix has the following properties:

(i) $\rho = \rho^\dagger$ (self-adjoint).

(ii) $\mathrm{Tr}(\rho) = 1$, since

$$\begin{aligned}\mathrm{Tr}(\rho) &= \sum_i w_i \sum_a \langle a|\alpha_i\rangle \langle\alpha_i|a\rangle = \sum_i w_i \sum_a \langle\alpha_i|a\rangle \langle a|\alpha_i\rangle = \sum_i w_i \langle\alpha_i|\alpha_i\rangle \\ &= \sum_i w_i = 1. \end{aligned} \tag{2.83}$$

(iii) $\mathrm{Tr}(\rho^2) \leq 1$, since

$$\begin{aligned}\mathrm{Tr}(\rho^2) &= \sum_i \sum_j \sum_a w_i w_j \langle a|\alpha_i\rangle \langle\alpha_i|\alpha_j\rangle \langle\alpha_j|a\rangle \\ &= \sum_i \sum_j \sum_a w_i w_j \langle\alpha_i|\alpha_j\rangle \langle\alpha_j|a\rangle \langle a|\alpha_i\rangle \\ &= \sum_i \sum_j w_i w_j \langle\alpha_i|\alpha_j\rangle \langle\alpha_j|\alpha_i\rangle \\ &= \sum_i \sum_j w_i w_j |\langle\alpha_i|\alpha_j\rangle|^2 \\ &\leq \sum_i \sum_j w_i w_j = \Big(\sum_i w_i\Big)^2 = 1. \end{aligned} \tag{2.84}$$

The equality occurs when $w_i = 0\ \forall i \neq j$ and $w_j = 1$ (pure state) $\Rightarrow \rho = |\alpha_j\rangle\langle\alpha_j|$.

(iv) $\langle\psi|\rho|\psi\rangle \geq 0$, $\forall |\psi\rangle \in \mathcal{H}$, since

$$\langle\psi|\rho|\psi\rangle = \sum_i w_i |\langle\alpha_i|\psi\rangle|^2 \geq 0. \tag{2.85}$$

On the other hand, the probability to obtain a non-degenerate value a of the observable A in a random element of the ensemble described by ρ is

$$p_a = \sum_i w_i \langle\alpha_i|a\rangle \langle a|\alpha_i\rangle = \sum_i w_i \langle a|\alpha_i\rangle \langle\alpha_i|a\rangle = \langle a|\rho|a\rangle \tag{2.86}$$

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since w_i is the probability to choose $|\alpha_i\rangle$ and $\langle\alpha_i|a\rangle\langle a|\alpha_i\rangle$ is the probability to obtain a if we have chosen $|\alpha_i\rangle$. Using $P_{A,a} = |a\rangle\langle a|$ we can write this result as

$$\begin{aligned} p_a = \sum_i w_i \langle\alpha_i| P_{A,a} |\alpha_i\rangle &= \sum_i w_i \langle\alpha_i| P_{A,a}^2 |\alpha_i\rangle \\ &= \sum_{a'}\sum_i w_i \langle\alpha_i| P_{A,a} \left|a'\right\rangle\!\left\langle a'\right| P_{A,a} |\alpha_i\rangle \\ &= \sum_{a'}\sum_i w_i \left\langle a'\right| P_{A,a} |\alpha_i\rangle\langle\alpha_i| P_{A,a} \left|a'\right\rangle \\ &= \mathrm{Tr}(P_{A,a}\,\rho P_{A,a}) \\ &= \mathrm{Tr}(\rho P_{A,a}) \end{aligned} \tag{2.87}$$

This expression is also valid if a is degenerate, with a basis of eigenvectors $\{|a_{(j)}\rangle\}$,

$$P_{A,a} = \sum_j |a_{(j)}\rangle\langle a_{(j)}| \tag{2.88}$$

$$p_a = \sum_i w_i \sum_j \langle\alpha_i| P_{A,a} |\alpha_i\rangle = \sum_j \langle a_{(j)}| \rho |a_{(j)}\rangle = \mathrm{Tr}(\rho P_{A,a}). \tag{2.89}$$

If we *measure* A to all the elements of the ensemble and *select* those with eigenvalue a, what is the density matrix of the resulting ensemble? According to postulate IV, if we pick up $|\alpha_i\rangle$ and obtain a, the state collapses into $|\alpha_i'\rangle$, which is an eigenstate of A given by

$$|\alpha_i\rangle \longrightarrow \left|\alpha_i'\right\rangle = \frac{P_{A,a}|\alpha_i\rangle}{\|P_{A,a}|\alpha_i\rangle\|} \tag{2.90}$$

And according to postulate III, the probability to obtain a in the state $|\alpha_i\rangle$ is

$$p_{a,i} = \langle\alpha_i| P_{A,a} |\alpha_i\rangle = \|P_{A,a}|\alpha_i\rangle\|^2. \tag{2.91}$$

(When we measure A on some $|\alpha_i\rangle$, this probability may be zero, of course).

Then, after the measurement on the ensemble (mixed state) described by ρ we get:

$$\rho = \sum_i w_i |\alpha_i\rangle\langle\alpha_i| \rightsquigarrow \sum_i w_i \left|\alpha_i'\right\rangle\!\left\langle\alpha_i'\right| p_{a,i} = \sum_i w_i \frac{P_{A,a}|\alpha_i\rangle\langle\alpha_i| P_{A,a}}{\|P_{A,a}|\alpha_i\rangle\|^2} p_{a,i} = P_{A,a}\,\rho P_{A,a} \tag{2.92}$$

that must be normalized to get a proper density matrix of unit trace:

$$\rho \longrightarrow \rho_{A,a} = \frac{P_{A,a}\,\rho P_{A,a}}{\mathrm{Tr}(\rho P_{A,a})} \tag{2.93}$$

since $\mathrm{Tr}(P_{A,a}\,\rho P_{A,a}) = \mathrm{Tr}(\rho P_{A,a})$. Therefore:

- If the initial ρ described a mixed state then the resulting $\rho_{A,a}$ describes another mixed state.
- If the initial ρ described a pure state $|\alpha\rangle$, and the probability to obtain a on $|\alpha\rangle$ is not zero, then the resulting $\rho_{A,a}$ describes the pure state $|\alpha'\rangle$ where it will collapse:

$$\rho = |\alpha\rangle\langle\alpha| \longrightarrow \rho_{A,a} = \left|\alpha'\right\rangle\!\left\langle\alpha'\right|, \qquad \left|\alpha'\right\rangle = \frac{P_{A,a}|\alpha\rangle}{\|P_{A,a}|\alpha\rangle\|}. \tag{2.94}$$

Putting together the results (2.81), (2.89) and (2.93) we get a generalized version of the postulates:

Postulate I'
In QM a physical system is associated to a complex Hilbert space and any state of the system is described by a linear operator ρ, called density matrix, that satisfies

$$\rho = \rho^\dagger, \quad \mathrm{Tr}(\rho) = 1, \quad \langle\psi|\,\rho\,|\psi\rangle \geq 0, \ \forall\psi \in \mathcal{H}.$$

Postulate II' (same as Postulate II)
Every observable of a physical system is represented by a self-adjoint linear operator acting on the associated Hilbert space, whose eigenvalues are the only possible values of the observable.

Postulate III'
If a physical system is in state described by the density matrix ρ, the probability of obtaining an eigenvalue a of an observable A is

$$p_a = \mathrm{Tr}(\rho P_{A,a}).$$

Postulate IV'
If a physical system is in a mixed state described by the density matrix ρ and one filters the eigenvalue a of an observable A, the system is left in a mixed state described by the density matrix

$$\rho_{A,a} = \frac{P_{A,a}\,\rho P_{A,a}}{\mathrm{Tr}(\rho P_{A,a})}.$$

Pure states are special cases of mixed states. A state is pure if its density matrix has the form $\rho = |\psi\rangle\langle\psi|$ for some $|\psi\rangle \in \mathcal{H}$. A pure state is characterized by $\rho^2 = \rho$ ($\Rightarrow \mathrm{Tr}(\rho^2) = 1$). Otherwise, it is a not a pure state.

If the state is not pure, it is specified by the set of coefficients in (2.81) where more than one w_i is different from zero. Then the decomposition is not unique. For example, the following density matrices are *the same* For example, the following density matrices are *the same* (same $\langle\psi|\,\rho\,|\psi\rangle\,, \forall\,|\psi\rangle$) but they are made of a mixture of but they are made of a mixture of *different* pure states:

$$\rho = a\,|u\rangle\langle u| + (1-a)\,|v\rangle\langle v|\,, \quad 0 < a < 1, \quad \{|u\rangle\,, |v\rangle\} \text{ orthonormal}, \tag{2.95}$$

$$\rho = \frac{1}{2}\,|x\rangle\langle x| + \frac{1}{2}\,|y\rangle\langle y|\,,$$
$$\text{with } |x\rangle = \sqrt{a}\,|u\rangle - \sqrt{1-a}\,|v\rangle\,, \quad |y\rangle = \sqrt{a}\,|u\rangle + \sqrt{1-a}\,|v\rangle\,. \tag{2.96}$$

We do not have a maximal information of the state since we do not know what the mixture is made of.

Let us illustrate with an example the difference between a *coherent* superposition of pure states (another pure state) and a *incoherent* mixture of pure states (mixed state). Consider the following two states:

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- The pure state $|S_x+\rangle$, that can be written as the superposition of eigenstates of S_z,

$$|S_x+\rangle = \frac{1}{\sqrt{2}}|S_z+\rangle + \frac{1}{\sqrt{2}}|S_z-\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \tag{2.97}$$

$$\Rightarrow \quad \rho_1 = |S_x+\rangle\langle S_x+| \doteq \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix} \tag{2.98}$$

  in the basis $\{|S_z+\rangle, |S_z-\rangle\}$. The density matrix ρ_1 is an alternative way of describing this state. Notice that it corresponds to a pure state because

$$\rho_1^2 = \rho_1. \tag{2.99}$$

- The mixed state

$$\rho_2 = \frac{1}{2}|S_z+\rangle\langle S_z+| + \frac{1}{2}|S_z-\rangle\langle S_z-| \doteq \frac{1}{2}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix} \tag{2.100}$$

  ($\rho_2^2 \neq \rho_2$).

In both states the probability to find either $S_z = \pm\hbar/2$ is the same,

$$P_{S_z,+} = |S_z+\rangle\langle S_z+| \doteq \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}, \quad P_{S_z,-} = |S_z-\rangle\langle S_z-| \doteq \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix} \tag{2.101}$$

$$\rho_1: \quad p_{S_z+} = \mathrm{Tr}(\rho_1 P_{S_z,+}) = \frac{1}{2}, \quad p_{S_z-} = \mathrm{Tr}(\rho_1 P_{S_z,-}) = \frac{1}{2}, \tag{2.102}$$

$$\rho_2: \quad p_{S_z+} = \mathrm{Tr}(\rho_2 P_{S_z,+}) = \frac{1}{2} \quad p_{S_z-} = \mathrm{Tr}(\rho_2 P_{S_z,-}) = \frac{1}{2} \tag{2.103}$$

and the expectation value (average) of S_z is also the same,

$$S_z \doteq \frac{\hbar}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} \tag{2.104}$$

$$\langle S_z\rangle_{\rho_1} = \mathrm{Tr}(\rho_1 S_z) = 0, \quad \Delta_{\rho_1} S_z = \sqrt{\langle S_z^2\rangle_{\rho_1} - \langle S_z\rangle_{\rho_1}^2} = \frac{\hbar}{2} \tag{2.105}$$

$$\langle S_z\rangle_{\rho_2} = \mathrm{Tr}(\rho_2 S_z) = 0, \quad \Delta_{\rho_2} S_z = \sqrt{\langle S_z^2\rangle_{\rho_2} - \langle S_z^2\rangle_{\rho_2}^2} = \frac{\hbar}{2}. \tag{2.106}$$

But in contrast to ρ_2, the state ρ_1 has a well defined spin orientation (along the x-axis),

$$P_{S_x,+} = |S_x+\rangle\langle S_x+| \doteq \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}, \quad P_{S_x,-} = |S_x-\rangle\langle S_x-| \doteq \frac{1}{2}\begin{pmatrix}1 & -1\\-1 & 1\end{pmatrix} \tag{2.107}$$

$$\rho_1: \quad p_{S_x+} = \mathrm{Tr}(\rho_1 P_{S_x,+}) = 1, \quad p_{S_x-} = \mathrm{Tr}(\rho_1 P_{S_x,-}) = 0 \tag{2.108}$$

$$\rho_2: \quad p_{S_x+} = \mathrm{Tr}(\rho_2 P_{S_x,+}) = \frac{1}{2}, \quad p_{S_x-} = \mathrm{Tr}(\rho_2 P_{S_x,-}) = \frac{1}{2} \tag{2.109}$$

In fact,

$$S_x \doteq \frac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} \tag{2.110}$$

$$\langle S_x\rangle_{\rho_1} = \mathrm{Tr}(\rho_1 S_x) = \frac{\hbar}{2}, \quad \Delta_{\rho_1} S_x = \sqrt{\langle S_x^2\rangle_{\rho_1} - \langle S_x\rangle_{\rho_1}^2} = 0 \tag{2.111}$$

$$\langle S_x\rangle_{\rho_2} = \mathrm{Tr}(\rho_2 S_x) = 0, \quad \Delta_{\rho_2} S_x = \sqrt{\langle S_x^2\rangle_{\rho_2} - \langle S_x\rangle_{\rho_2}^2} = \frac{\hbar}{2}. \tag{2.112}$$

Actually ρ_1 represents a *polarized* beam (along the x-axis) and ρ_2 an *unpolarized* beam. The silver atoms exiting the furnace in the Stern-Gerlach experiment are in the mixed state ρ_2 (unpolarized), but those filtered by SG$\hat{\boldsymbol{x}}$ are in the pure state ρ_1 (polarized).

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- We could also prepare a *partially polarized* beam along the z-axis,

$$\rho_3 = w_1 \, |S_z+\rangle\langle S_z+| + w_2 \, |S_z-\rangle\langle S_z-| \doteq \begin{pmatrix} w_1 & 0 \\ 0 & w_2 \end{pmatrix} \tag{2.113}$$

with $w_1 + w_2 = 1$ ($w_i \neq 0$, $w_1 \neq w_2$). This is also a mixed state ($\rho_3^2 \neq \rho_3$) that has

$$\rho_3: \quad p_{S_z+} = \mathrm{Tr}(\rho_3 P_{S_z,+}) = w_1, \quad p_{S_z-} = \mathrm{Tr}(\rho_3 P_{S_z,-}) = w_2 \tag{2.114}$$

$$p_{S_x+} = \mathrm{Tr}(\rho_3 P_{S_x,+}) = \frac{1}{2}, \quad p_{S_x-} = \mathrm{Tr}(\rho_3 P_{S_x,-}) = \frac{1}{2} \tag{2.115}$$

$$\langle S_z\rangle_{\rho_3} = \mathrm{Tr}(\rho_3 S_z) = \frac{\hbar}{2}(w_1 - w_2), \quad \Delta_{\rho_3} S_z = \sqrt{\langle S_z^2\rangle_{\rho_3} - \langle S_z\rangle_{\rho_3}^2} = \hbar\sqrt{w_1 w_2} \tag{2.116}$$

$$\langle S_x\rangle_{\rho_3} = \mathrm{Tr}(\rho_3 S_x) = 0, \quad \Delta_{\rho_3} S_x = \sqrt{\langle S_x^2\rangle_{\rho_1} - \langle S_x\rangle_{\rho_3}^2} = \frac{\hbar}{2}. \tag{2.117}$$

- Of course, $|S_z+\rangle$, $|S_y+\rangle = \frac{1}{\sqrt{2}}(|S_z+\rangle + \mathrm{i}\,|S_z-\rangle)$ and in general

$$|(\theta,\varphi)\rangle = \cos(\theta/2)\,|S_z+\rangle + \mathrm{e}^{\mathrm{i}\varphi}\sin(\theta/2)\,|S_z-\rangle\,, \tag{2.118}$$

with $\theta \in [0,\pi]$, $\varphi \in [0,2\pi]$, are other examples of pure states, polarized along the direction $\hat{n}(\theta,\varphi)$. Check that their corresponding density matrices fulfill $\rho^2 = \rho$. The spin along $\hat{n}$ can be determined with full precision: we have *maximal information* about them. In contrast, the spin cannot be determined along any direction without uncertainty when measured over the mixed states ρ_2 or ρ_3.

2.6 Composite systems. Entanglement

A composite system of two subsystems with Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ is associated the Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ (tensor product). This space consists of all the ordered pairs $|u\rangle \otimes |v\rangle \equiv |u\rangle\,|v\rangle \equiv |uv\rangle$, with $|u\rangle \in \mathcal{H}_1$, $|v\rangle \in \mathcal{H}_2$, *and* their linear combinations. By definition, if $c \in \mathbb{C}$,

$$c(|u\rangle \otimes |v\rangle) = (c\,|u\rangle) \otimes |v\rangle = |u\rangle \otimes (c\,|v\rangle) \tag{2.119}$$

$$(|u_1\rangle + |u_2\rangle) \otimes |v\rangle = |u_1\rangle \otimes |v\rangle + |u_2\rangle \otimes |v\rangle \tag{2.120}$$

$$|u\rangle \otimes (|v_1\rangle + |v_2\rangle) = |u\rangle \otimes |v_1\rangle + |u\rangle \otimes |v_2\rangle\,. \tag{2.121}$$

The states that can be written as the direct product of one vector $|u\rangle \in \mathcal{H}_1$ and one vector $|v\rangle \in \mathcal{H}_2$ are called separable states. The linear combination of two or more separable states are called *entangled* states.

If $\{|u_i\rangle\}$ and $\{|v_j\rangle\}$ are bases of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, then $\{|u_i\rangle \otimes |v_j\rangle\}$, $i = 1,\ldots,n$, $j = 1,\ldots,m$, is a basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$ (that has dimension $m \times n$),

$$|\psi\rangle = \sum_{ij} \alpha_{ij}\,|u_i\rangle \otimes |v_j\rangle\,, \quad \forall\,|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2. \tag{2.122}$$

The scalar product in $\mathcal{H}_1 \otimes \mathcal{H}_2$ is defined by

$$\left(\sum_{ij} \alpha_{ij}\,|u_i\rangle \otimes |v_j\rangle\,, \sum_{ij} \beta_{ij}\,|u_i\rangle \otimes |v_j\rangle\right) = \sum_{ijkl} \alpha_{ij}^* \beta_{kl}\,\langle u_i|u_k\rangle\,\langle v_j|v_l\rangle$$

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$$= \sum_{ij} \alpha_{ij}^* \beta_{ij} \quad \text{(if both are orthonormal bases).} \tag{2.123}$$

If A, B are operators acting on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, we define the operator $A \otimes B$ acting on $\mathcal{H}_1 \otimes \mathcal{H}_2$ by

$$(A \otimes B)(|u\rangle \otimes |v\rangle) = (A\,|u\rangle) \otimes (B\,|v\rangle). \tag{2.124}$$

In fact, every linear operator C on $\mathcal{H}_1 \otimes \mathcal{H}_2$ can be written as

$$C = \sum_{ij} c_{ij} A_i \otimes B_j, \tag{2.125}$$

with A_i and B_j operators on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively.

Consider an observable A acting *just* on the subsystem $\mathcal{H}_1$. Then it is of the form $A \otimes I_{\mathcal{H}_2}$ on $\mathcal{H}_1 \otimes \mathcal{H}_2$ and

$$A\,|u_i v_j\rangle = (A\,|u_i\rangle)\,|v_j\rangle\,. \tag{2.126}$$

We can write the expected value of A in a state of density matrix ρ of the composite system as its expected value in the subsystem $\mathcal{H}_1$ with **reduced density matrix** $\rho^{\mathcal{H}_1}$,

$$\begin{aligned} \mathrm{Tr}(\rho A) = \sum_{ij} \langle u_i v_j|\,\rho A\,|u_i v_j\rangle &= \sum_{ij} \langle u_i v_j|\,\rho\,|v_j\rangle\,A\,|u_i\rangle \\ &= \sum_i \langle u_i| \left(\sum_j \langle v_j|\,\rho\,|v_j\rangle \right) A\,|u_i\rangle = \mathrm{Tr}_{\mathcal{H}_1}(\rho^{\mathcal{H}_1} A) \end{aligned} \tag{2.127}$$

where we have introduced the *partial trace* of ρ (or any other operator) as

$$\rho^{\mathcal{H}_1} \equiv \mathrm{Tr}_{\mathcal{H}_2}(\rho) = \sum_j \langle v_j|\,\rho\,|v_j\rangle\,. \tag{2.128}$$

We see that the reduced density matrix, defined as the partial trace of the density matrix of a composite system, describes the state of a subsystem when we ignore the information about the rest of the system. Since, in principle, we lose part of the information, the reduced density matrix of a pure state may be a mixed state. This happens in particular when the state of the composite system is an entangled state.

For example, consider a four-dimensional system $S = S_1 \otimes S_2$ composed of two subsystems of bases $\{|\uparrow\rangle, |\downarrow\rangle\}$ and $\{|+\rangle, |-\rangle\}$. Assume the system is in an entangled state

$$\begin{aligned} |\psi\rangle &= \frac{1}{\sqrt{2}}\,|\uparrow\rangle\,|+\rangle + \frac{1}{\sqrt{2}}\,|\downarrow\rangle\,|-\rangle \\ &\equiv \frac{1}{\sqrt{2}}\,|\uparrow +\rangle + \frac{1}{\sqrt{2}}\,|\downarrow -\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \end{aligned} \tag{2.129}$$

that we have expressed for convenience in the basis $\{|\uparrow +\rangle, |\uparrow -\rangle, |\downarrow +\rangle, |\downarrow -\rangle\}$. The density matrix describing the composite system in that state is

$$\rho = |\psi\rangle\langle\psi| \doteq \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \tag{2.130}$$

that, of course, fulfills $\rho^2 = \rho$, because $|\psi\rangle$ is a pure state. Now, the reduced density matrix of subsystem S_1 is the partial trace

$$\begin{aligned}\rho^{S_1} \equiv \mathrm{Tr}_{S_2}(\rho) &= \langle +| \rho |+\rangle + \langle -| \rho |-\rangle \\ &= \langle +|\psi\rangle \langle\psi|+\rangle + \langle -|\psi\rangle \langle\psi|-\rangle = \frac{1}{2} |\uparrow\rangle\langle\uparrow| + \frac{1}{2} |\downarrow\rangle\langle\downarrow| . \end{aligned} \tag{2.131}$$

Notice that ρ^{S_1} does not describe a pure but a mixed state ($\mathrm{Tr}[(\rho^{S_1})^2] < \mathrm{Tr}(\rho^{S_1}) = 1$): half of the times the subsystem is in the state $|\uparrow\rangle$ and the other half in the state $|\downarrow\rangle$, but never in a coherent superposition. The *coherence is lost*, just because we ignore (have not measured) all the details of the complementary system(s). In practice, this is always what happens when we measure an observable in a non-isolated system: the system is entangled with the measuring apparatus, trillion trillions atoms whose state is impossible to determine. This inevitable partial knowledge leads to a Schrödinger's cat that is either dead or alive, and not in a coherent superposition.

In general, a bipartite pure state ρ is entangled if and only if its reduced states are mixed rather than pure.

2.7 Quantum dynamics: the Schrödinger equation

How does a quantum system change with time?

2.7.1 Postulate V

Postulate V
In the time interval between two consecutive measurements (*closed* system), pure states remain pure, and the time evolution is described by the *Schrödinger equation*,

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle = H(t) |\psi(t)\rangle , \tag{2.132}$$

where $H(t)$ is an observable called the *Hamiltonian* of the system.

The Schrödinger equation is *deterministic*. Given the quantum state at a time t_1 it is known at any later (or earlier) time t_2. Notice that in QM time is not an observable, it is a parameter. In contrast, the position is an observable. This is at odds with the theory of Special Relativity, where space and time are treated on an equal footing.

An important property of the Schrödinger equation is that, during the evolution between two measurements, the norm of the states does not change,

$$\begin{aligned}\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle\psi(t)|\psi(t)\rangle &= \left[\mathrm{i}\hbar \frac{\mathrm{d}\,\langle\psi(t)|}{\mathrm{d}t}\right] |\psi(t)\rangle + \langle\psi(t)| \left[\mathrm{i}\hbar \frac{\mathrm{d}\,|\psi(t)\rangle}{\mathrm{d}t}\right] \\ &= -\langle\psi(t)| H(t) |\psi(t)\rangle + \langle\psi(t)| H(t) |\psi(t)\rangle = 0 \end{aligned} \tag{2.133}$$

where we have used that $H(t)$ is Hermitian. On the other hand, the Schrödinger equation is linear. Therefore, the time evolution must be described by a unitary operator[h]

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle , \quad U^\dagger U = U U^\dagger = I. \tag{2.134}$$

[h] Recall that if U is unitary and $|\psi'\rangle = U|\psi\rangle$ then the norm is preserved, $\langle\psi'|\psi'\rangle = \langle\psi| U^\dagger U |\psi\rangle = \langle\psi|\psi\rangle$.

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From the relations

$$|\psi(t_3)\rangle = U(t_3,t_2)\,|\psi(t_2)\rangle\,, \quad |\psi(t_2)\rangle = U(t_2,t_1)\,|\psi(t_1)\rangle\,, \tag{2.135}$$

one gets

$$U(t,t) = I, \tag{2.136}$$
$$U(t_3,t_1) = U(t_3,t_2)U(t_2,t_1), \tag{2.137}$$
$$U(t_2,t_1) = U^{-1}(t_1,t_2) = U^\dagger(t_1,t_2) \quad \Leftarrow \quad U(t_2,t_1)U(t_1,t_2) = I. \tag{2.138}$$

Notice that, as anticipated above, the time evolution of a state of a closed system is *reversible*. If $t > t_0$,

$$|\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle\,, \quad |\psi(t_0)\rangle = U^\dagger(t,t_0)\,|\psi(t)\rangle\,. \tag{2.139}$$

There is no loss of information. In contrast, the measurement process (collapse of the state) is not a unitary, reversible process. Since this is produced by the interaction with an *external* apparatus, the system will be no longer closed. However, as we have seen, one can include the measuring apparatus as a part of the (composite) system. Then the time evolution will be unitary and reversible and there is no need to introduce the bizarre collapse.

The evolution of a mixed state $\rho(t) = \sum_i w_i\,|\alpha_i(t)\rangle\langle\alpha_i(t)|$ also follows from (2.132),

$$\begin{aligned} \mathrm{i}\hbar\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} &= \sum_i w_i \left\{ \mathrm{i}\hbar \left[\frac{\mathrm{d}\,|\alpha_i(t)\rangle}{\mathrm{d}t}\right] \langle\alpha_i(t)| + |\alpha_i(t)\rangle \left[\mathrm{i}\hbar\frac{\mathrm{d}\,\langle\alpha_i(t)|}{\mathrm{d}t}\right] \right\} \\ &= \sum_i w_i \left\{ H(t)\,|\alpha_i(t)\rangle\,\langle\alpha_i(t)| - |\alpha_i(t)\rangle\,\langle\alpha_i(t)|\,H(t) \right\}, \end{aligned} \tag{2.140}$$

assuming time-independence of the frequencies, and hence

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[\rho(t), H(t)]. \tag{2.141}$$

In general, the expectation values change with time,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\,\langle\psi(t)|\,A\,|\psi(t)\rangle &= \left[\frac{\mathrm{d}\,\langle\psi(t)|}{\mathrm{d}t}\right] A\,|\psi(t)\rangle + \langle\psi(t)|\,A \left[\frac{\mathrm{d}\,|\psi(t)\rangle}{\mathrm{d}t}\right] + \langle\psi(t)|\,\frac{\partial A}{\partial t}\,|\psi(t)\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\,\langle\psi|\,[A,H]\,|\psi\rangle + \langle\psi|\,\frac{\partial A}{\partial t}\,|\psi\rangle\,. \end{aligned} \tag{2.142}$$

The self-adjoint operator H is called Hamiltonian, but in QM there is no prescription to obtain it. It has clearly the dimensions of energy, thanks to the introduction of the dimensionful constant $\hbar$ in (2.132). In systems with a quantum analog one can usually (not always) infer its form from the corresponding classical Hamiltonian (see §2.8).

2.7.2 Time evolution operator

Substituting (2.134) into (2.132) we get the Schrödinger equation for the time evolution operator U,

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0) = H(t)U(t,t_0) \tag{2.143}$$

where we have used that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\{U(t,t_0)\left|\psi(t_0)\right\rangle\right\} = \frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0)\left|\psi(t_0)\right\rangle \tag{2.144}$$

because $|\psi(t_0)\rangle$ does not depend on t. Then, using the properties of U,

$$\begin{aligned} \mathrm{d}U(t,t_0) &= -\frac{\mathrm{i}}{\hbar}H(t)U(t,t_0)\mathrm{d}t \\ \Rightarrow \quad U(t+\delta t,t_0) - U(t,t_0) &= -\frac{\mathrm{i}}{\hbar}H(t)U(t,t_0)\delta t \end{aligned} \tag{2.145}$$

and taking $t_0 = t$,

$$U(t+\delta t,t) = I - \frac{\mathrm{i}}{\hbar}H(t)\delta t. \tag{2.146}$$

This is the expression for an infinitesimal time evolution. It reveals that $H/\hbar$ is the *generator* of time translations (when $H \neq H(t)$). Let us find the evolution operator for an arbitrary time interval.

- If $H \neq H(t)$, the differential equation (2.143), with $U(t_0,t_0) = I$, is easy to solve,

$$U(t,t_0) = \exp\left\{-\frac{\mathrm{i}}{\hbar}H(t-t_0)\right\}. \tag{2.147}$$

- If $H = H(t)$ one can check that the solution is the Dyson series,

$$U(t,t_0) = I + \sum_{n=1}^{\infty}\left(-\frac{\mathrm{i}}{\hbar}\right)^n \int_{t_0}^{t}\mathrm{d}t_1 \int_{t_0}^{t_1}\mathrm{d}t_2 \ldots \int_{t_0}^{t_{n-1}}\mathrm{d}t_n\, H(t_1)H(t_2)\ldots H(t_n). \tag{2.148}$$

  If $[H(t),H(t')] = 0$ it simplifies to

$$U(t,t_0) = \exp\left\{-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t\, H(t)\right\}. \tag{2.149}$$

2.7.3 Stationary states and constants of motion

Consider a time-independent Hamiltonian $H \neq H(t)$. Since H is self-adjoint it can be diagonalized,

$$H\left|E_n\right\rangle = E_n\left|E_n\right\rangle, \quad E_n \in \mathbb{R}. \tag{2.150}$$

The eigenvalues E_n are the allowed energies or energy levels and the $|E_n\rangle$ the energy eigenstates of the system. The time evolution (2.147) of the energy eigenstates is trivial,

$$U(t,t_0)\left|E_n\right\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t-t_0)}\left|E_n\right\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n(t-t_0)}\left|E_n\right\rangle. \tag{2.151}$$

The only change is an irrelevant global phase, so the state remains the same. Hence, the energy eigenstates are *stationary*. One can write the time evolution operator in the basis of energy eigenstates (spectral resolution of U) as

$$U(t,t_0) = \sum_m\sum_n \left|E_m\right\rangle\!\left\langle E_m\right|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t-t_0)}\left|E_n\right\rangle\!\left\langle E_n\right| = \sum_n \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n(t-t_0)}\left|E_n\right\rangle\!\left\langle E_n\right|. \tag{2.152}$$

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The time evolution of a generic state $|\psi\rangle = \sum_i c_i |E_i\rangle$ is

$$|\psi(t)\rangle = U(t,t_0)|\psi\rangle = \sum_i \sum_n c_i \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n(t-t_0)} |E_n\rangle \langle E_n|E_i\rangle = \sum_i c_i \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_i(t-t_0)} |E_i\rangle \,. \tag{2.153}$$

Since the components change by different phases,

$$c_i \longrightarrow c_i \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_i(t-t_0)}, \tag{2.154}$$

the state $|\psi\rangle$ is not stationary unless it is an energy eigenstate.

On the other hand, according to (2.142), we say that a time-independent observable A that commutes with H is a *constant of motion* since its expectation value in any state $|\psi\rangle$ does not change with time,

$$\frac{\partial A}{\partial t} = 0, \quad [A,H] = 0 \quad \Rightarrow \quad \mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle_\psi = 0. \tag{2.155}$$

In particular, since $[H,H] = 0$, a time-independent Hamiltonian is a constant of motion, and the average energy $\langle H\rangle_\psi$ does not change with time even if $|\psi\rangle$ is not a stationary state. And if $|\psi\rangle$ is stationary then any time-dependent observable is a constant of motion.

2.7.4 Time evolution pictures

So far, we have considered that states evolve with time and observables (unless explicitly dependent on time) stay constant,

$$|\alpha\rangle \xrightarrow{t} U|\alpha\rangle \,, \quad A \xrightarrow{t} A. \tag{2.156}$$

This is called the **Schrödinger picture**. However, since after all we just deal with the results of our observations (measurements), we could view things in an alternative way.

The time evolution of the expected value

$$\langle\alpha| A |\beta\rangle \xrightarrow{t} \langle\alpha| U^\dagger A U |\beta\rangle \tag{2.157}$$

can also be interpreted as if the states do not evolve but the observable does,

$$|\alpha\rangle \xrightarrow{t} |\alpha\rangle \,, \quad |\beta\rangle \xrightarrow{t} |\beta\rangle \,, \quad A \xrightarrow{t} U^\dagger A U. \tag{2.158}$$

This is the **Heisenberg picture**. To distinguish both pictures, when necessary, we denote

$$|\alpha\rangle_H = |\alpha(t_0)\rangle_S = U^\dagger |\alpha(t)\rangle_S \tag{2.159}$$

$$A^{(H)}(t) = U^\dagger A^{(S)} U, \quad A^{(H)}(t_0) = A^{(S)}. \tag{2.160}$$

The predictions are identical:

$${}_H\langle\alpha| A^{(H)}(t) |\beta\rangle_H = {}_S\langle\alpha(t)| A^{(S)} |\beta(t)\rangle_S \tag{2.161}$$

and the hamiltonian H has the same form in both pictures,

$$H = U^\dagger H U. \tag{2.162}$$

An observable A in the Heisenberg picture may change with time because of the dynamics of the system or because of its explicit dependence with time. Then, using (2.143), we obtain the *Heisenberg equation of motion*,

$$\begin{aligned}\frac{\mathrm{d}A^{(H)}}{\mathrm{d}t} &= \left[\frac{\mathrm{d}U^\dagger}{\mathrm{d}t}\right] A^{(S)}U + U^\dagger A^{(S)}\left[\frac{\mathrm{d}U}{\mathrm{d}t}\right] + U^\dagger\frac{\partial A^{(S)}}{\partial t}U \\ &= -\frac{\mathrm{i}}{\hbar}U^\dagger[A^{(S)},H]U + U^\dagger\frac{\partial A^{(S)}}{\partial t}U \\ &= -\frac{\mathrm{i}}{\hbar}[A^{(H)},H] + \left(\frac{\partial A}{\partial t}\right)^{(H)} \end{aligned} \tag{2.163}$$

where one usually writes

$$\left(\frac{\partial A}{\partial t}\right)^{(H)} \equiv U^\dagger\frac{\partial A^{(S)}}{\partial t}U. \tag{2.164}$$

The density matrix changes with time in the Schrödinger picture according to (2.141),

$$\frac{\mathrm{d}\rho^{(S)}(t)}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[\rho^{(S)}(t),H(t)] \tag{2.165}$$

but it is constant in the Heisenberg picture,

$$\begin{aligned} & \rho^{(S)}(t_0) = \sum_i \omega_i\,|\alpha_i(t_0)\rangle\langle\alpha_i(t_0)| \\ \Rightarrow\quad & \rho^{(S)}(t) = U(t,t_0)\rho(t_0)U^\dagger(t,t_0) \\ \Rightarrow\quad & \rho^{(H)}(t) = U^\dagger(t,t_0)\rho^{(S)}(t)U(t,t_0) = \rho^{(S)}(t_0) = \rho^{(H)}(t_0) \\ & \Rightarrow\quad \frac{\mathrm{d}\rho^{(H)}(t)}{\mathrm{d}t} = 0. \end{aligned} \tag{2.166}$$

The Heisenberg picture is more similar to the usual description in Classical Mechanics, where the observables (position, momentum, ...) change with time. Actually, the Heisenberg equation of motion has the same form as the Hamilton's equation for a classical variable $A = A(x_1,\ldots,x_N,p_1,\ldots,p_N;t)$,

$$\frac{\mathrm{d}A}{\mathrm{d}t} = [A,H]_P + \frac{\partial A}{\partial t} \tag{2.167}$$

replacing the *Poisson bracket*,

$$[A,B]_P \equiv \sum_i\left(\frac{\partial A}{\partial x_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial x_i}\right) \tag{2.168}$$

by a commutator, namely

$$\text{(classical)}\quad [\cdot,\cdot]_P \longrightarrow -\frac{\mathrm{i}}{\hbar}[\cdot,\cdot]\quad \text{(quantum)}. \tag{2.169}$$

This analogy reinforces the idea that the operator H introduced in (2.132) is in fact the Hamiltonian of the system.

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2.8 Quantization rules

How to build quantum operators that represent the physical observables? Next, we will discuss the *canonical quantization* rules.

2.8.1 Postulate VI

For a physical system in which the Cartesian coordinates are $x_1, x_2, \ldots, x_N$, with corresponding momenta $p_1, p_2, \ldots, p_N$, the operators X_r and P_s, which represent these observables in QM, must satisfy the commutation relations

$$[X_r, X_s] = 0, \quad [P_r, P_s] = 0, \quad [X_r, P_s] = \mathrm{i}\hbar\delta_{rs} I. \tag{2.170}$$

If the system has an observable whose classical expression is $A(x_1, \ldots, x_N, p_1, \ldots, p_N; t)$ then the corresponding operator can be obtained by "conveniently" substituting he variables x_r and p_s by the operators X_r and P_s, respectively.

Here, "conveniently" means the following. Since X and P are noncommuting observables, one should write classical variables like xp as an equivalent combination whose quantum analog is a self-adjoint operator. In fact, the product XP is not self-adjoint, since $X = X^\dagger$, $P = P^\dagger$ and

$$[X, P] = XP - PX = \mathrm{i}\hbar I \Rightarrow (XP)^\dagger = (PX)^\dagger - \mathrm{i}\hbar I = XP - \mathrm{i}\hbar I \neq XP. \tag{2.171}$$

However,

$$xp = \frac{1}{2}(xp + px) \rightsquigarrow \frac{1}{2}(XP + PX) \tag{2.172}$$

is a self-adjoint operator with the same classical expression.

This postulate will look less bizarre when we see in chapter 3 that identifying the momentum with an operator P that satisfies the commutation relations (2.170) is the right way to understand $P/\hbar$ as the generator of spatial translations.

2.9 Superselection rules

Suppose we have an observable whose operator Q commutes (is compatible) with *all* other operators associated to observables in $\mathcal{H}$, $[Q, A] = 0$. Then for any pair of eigenstates of Q with different eigenvalues,

$$Q\,|\psi_1\rangle = q_1\,|\psi_1\rangle\,, \quad Q\,|\psi_2\rangle = q_2\,|\psi_2\rangle\,, \tag{2.173}$$

we have that

$$\begin{aligned} \forall A \quad 0 = \langle\psi_1|\,[Q, A]\,|\psi_2\rangle &= \langle\psi_1|\,QA\,|\psi_2\rangle - \langle\psi_1|\,AQ\,|\psi_2\rangle = (q_1 - q_2)\,\langle\psi_1|\,A\,|\psi_2\rangle \\ &\Rightarrow \quad \langle\psi_1|\,A\,|\psi_2\rangle = 0 \quad \text{if} \quad q_1 \neq q_2. \end{aligned} \tag{2.174}$$

This means there are no transitions between whatever two eigenstates with different eigenvalues of Q.

As a consequence, let us see that there is no pure state in $\mathcal{H}$ that is a superposition of states with different values of Q. Suppose that such a pure state $|\psi\rangle$ exists. Then, since the eigenvectors of Q are a basis of $\mathcal{H}$,

$$|\psi\rangle = \sum_i c_i |\psi_i\rangle \quad \text{with} \quad Q|\psi_i\rangle = q_i |\psi_i\rangle . \tag{2.175}$$

Using (2.174) the expectation of any observable A in this state,

$$\langle\psi| A |\psi\rangle = \sum_i |c_i|^2 \langle\psi_i| A |\psi_i\rangle = \mathrm{Tr}(\rho A) \quad \text{with} \quad \rho = \sum_i |c_i|^2 |\psi_i\rangle\langle\psi_i| . \tag{2.176}$$

We see that unless $|\psi\rangle$ has a well-defined value of Q (there is just one $c_i \neq 0$) ρ describes a mixed state (incoherent superposition of pure states) despite $|\psi\rangle \in \mathcal{H}$.

Any observable Q with these properties is called a *superselection observable* and gives rise to *superselection rules*: one can prepare only states with well defined values of Q. States with different values of Q live in *separate* Hilbert spaces $\mathcal{H}_q$. For example, the electric charge, the parity, the baryon and lepton number, ...

2.10 No-cloning theorem

In §2.2 we emphasized that a quantum state can not be understood as an element of reality but as a collection of similarly prepared systems. But how to make identical state preparations of a state? Notice that the state, in principle, might be even unknown. Sometimes things are easy: it is possible to prepare the lowest energy state of a system by simply waiting for the system to decay to its ground state. Another way is filtering, the technique used in the Stern-Gerlach experiment.

But we would really like to have a procedure to make exact replicas or *clones* of a prototype of the state, provided it exists. This is a common method in classical physics: the duplication of a key or the copying of a computer file. However, surprisingly, let us see that cloning quantum states is *impossible*.

Suppose we want to build a machine to copy a quantum state. There are only two permissible quantum operations with which we may manipulate the composite system. If we perform an observation, the original state will irreversibly collapse into some eigenstate of the observable, corrupting the information contained in the qubit(s). This is obviously not what we want. Instead, we should use unitary operations. Given $|\psi\rangle$ and a "blank piece of paper" $|b\rangle$,

$$|\psi\rangle \otimes |b\rangle \longrightarrow U(|\psi\rangle \otimes |b\rangle) = |\psi\rangle \otimes |\psi\rangle . \tag{2.177}$$

(Imagine we are so wise as to control the Hamiltonian to make the state evolve this way.) And the same wih another state $|\phi\rangle$,

$$|\phi\rangle \otimes |b\rangle \longrightarrow U(|\phi\rangle \otimes |b\rangle) = |\phi\rangle \otimes |\phi\rangle . \tag{2.178}$$

This looks perfect but, if we take the scalar product of both resulting states,

$$(\langle\phi| \otimes \langle b|)U^\dagger U(|\psi\rangle \otimes |b\rangle) = \langle\phi|\psi\rangle \tag{2.179}$$

$$= (\langle\phi| \otimes \langle\phi|)(|\psi\rangle \otimes |\psi\rangle) = \langle\phi|\psi\rangle^2 , \tag{2.180}$$

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we see that this is only possible if

$$\langle\phi|\psi\rangle = 0 \text{ or } \pm 1, \tag{2.181}$$

namely, if $|\psi\rangle$ and $|\phi\rangle$ are either the same state or they are orthogonal. Therefore, a single universal U cannot clone a general quantum state (arbitrary superpositions of the orthogonal qubits $|0\rangle$ and $|1\rangle$).

Notice that states which are classically different will certainly be orthogonal, so the no-cloning theorem for quantum states is not in conflict with the well-known possibility of copying classical states.

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Chapter 3

The wave function

3.1 Continuous spectrum

So far we have assumed observables with a discrete spectrum of possible values. This is in particular the case of S_z. But there are observables, like the position or the momentum of a free particle, that have a continuum of possible values. As a consequence of postulate III, we will need an operator with a continuous set of eigenvalues. Then the operator will be acting on a Hilbert space of infinite dimension. As we will see in this chapter, most of the results that we have already obtained can be generalized to a continuous spectrum.

Let us revise first the concept of **orthonormal basis**. If A is an operator with a (non-degenerate) discrete spectrum, $A\,|a\rangle = a\,|a\rangle$, then $\{|a\rangle\}$ is an orthonormal basis,

$$\langle a|a'\rangle = \delta_{aa'} \quad \text{(Krönecker delta)}, \quad \delta_{aa'} = \begin{cases} 1 & , \quad a = a' \\ 0 & , \quad a \neq a' \end{cases} \tag{3.1}$$

Consider now a generic operator X with a continuous spectrum, $X\,|x\rangle = x\,|x\rangle$. Then $\{|x\rangle\}$ is an orthonormal basis in the following sense,

$$\langle x|x'\rangle = \delta(x - x') \quad \text{(Dirac delta)}, \quad \delta(x - x') = \begin{cases} \infty & , \quad x = x' \\ 0 & , \quad x \neq x' \end{cases} \tag{3.2}$$

The Dirac delta is strictly not a function, it is a *distribution* that assigns a complex number to each smooth function in $x = x_0$ *constrained to satisfy*

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x - x_0) f(x) = \int_{x_0-\epsilon}^{x_0+\epsilon} \mathrm{d}x\, \delta(x - x_0) f(x) = f(x_0), \tag{3.3}$$

equivalently, a distribution that fulfills

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x - x_0) = 1, \quad \delta(x) = 0, \quad \forall x \neq 0. \tag{3.4}$$

From now on, definite integrals extend from $-\infty$ to ∞ unless otherwise stated.

The Dirac delta can be otained as the limit when $L \to \infty$ or $\epsilon \to 0^+$ of the functions:

$$(a) \quad \delta_L(x) = \frac{1}{2\pi} \int_{-L}^{L} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}kx} = \frac{\sin Lx}{\pi x}, \tag{3.5}$$

$$(b) \quad \delta_\epsilon(x) = \frac{1}{(2\pi\epsilon^2)^{1/2}} \mathrm{e}^{-x^2/(2\epsilon^2)} \quad \text{(Gaussian)}, \tag{3.6}$$

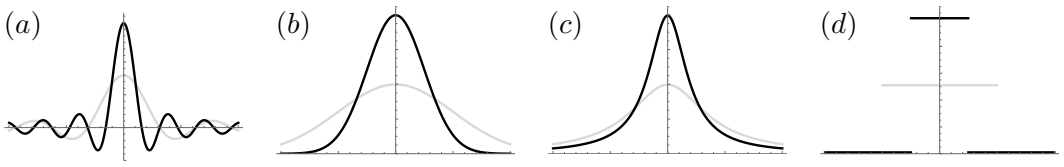

Figure 3.1: Several representations (in some limit) of the Dirac delta function (see text).

$$(c) \quad \delta_\epsilon(x) = \frac{\epsilon/\pi}{x^2+\epsilon^2}, \tag{3.7}$$

$$(d) \quad \delta_\epsilon(x) = \frac{\theta(x+\frac{\epsilon}{2}) - \theta(x-\frac{\epsilon}{2})}{\epsilon} \to \frac{\mathrm{d}\theta(x)}{\mathrm{d}x}, \quad \theta(x) = \text{Heaviside step function.} \tag{3.8}$$

For continuous spectra the **completeness relation** is generalized as follows

$$A: \quad \sum_a |a\rangle\langle a| = I, \qquad X: \quad \int \mathrm{d}x\ |x\rangle\langle x| = I. \tag{3.9}$$

Any vector in the Hilbert space of an operator A can be expressed in the basis of eigenvectors,

$$A: \quad |\psi\rangle = \sum_a |a\rangle\, \langle a|\psi\rangle \equiv \sum_a |a\rangle\, c_a \tag{3.10}$$

where c_a is the component of $|\psi\rangle$ along $|a\rangle$. In the case of X with a continuous spectrum,

$$X: \quad |\psi\rangle = \int \mathrm{d}x\ |x\rangle\, \langle x|\psi\rangle \equiv \int \mathrm{d}x\ |x\rangle\ \psi(x) \tag{3.11}$$

where $\psi(x)$ is the **wave function** of $|\psi\rangle$, analogous to the component of $|\psi\rangle$ along $|x\rangle$. Notice that the vectors in the Hilbert space of A must be normalized,

$$\langle\psi|\psi\rangle = \sum_a \langle\psi|a\rangle\, \langle a|\psi\rangle = \sum_a c_a^* c_a = \sum_a |c_a|^2 = 1. \tag{3.12}$$

Likewise,

$$\langle\psi|\psi\rangle = \int \mathrm{d}x\ \langle\psi|x\rangle\, \langle x|\psi\rangle = \int \mathrm{d}x\, \psi^*(x)\psi(x) = \int \mathrm{d}x\, |\psi(x)|^2 = 1. \tag{3.13}$$

This requires $\psi(x) \in L^2(\mathbb{R})$, a *square-integrable* function in $\mathbb{R}$.

The probability to obtain an eigenvalue a of the observable A on the state $|\psi\rangle$ is

$$\begin{aligned} p_a &= \langle\psi|\, P_{A,a}\, |\psi\rangle = \langle\psi| \left(\sum_{a_i=a} |a_i\rangle\langle a_i| \right) |\psi\rangle \\ &= \sum_i |\, \langle a_i|\psi\rangle\, |^2 \end{aligned} \tag{3.14}$$

for the general case of a degenerate eigenvalue. Analogously, the probability to obtain a value x of the observable X in the interval $[x_0, x_1]$ on the state $|\psi\rangle$ is

$$p_{[x_0,x_1]} = \langle\psi|\, P_{X,[x_0,x_1]}\, |\psi\rangle = \langle\psi| \left(\int_{x_0}^{x_1} \mathrm{d}x\ |x\rangle\langle x| \right) |\psi\rangle$$

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$$= \int_{x_0}^{x_1} \mathrm{d}x\, |\psi(x)|^2. \tag{3.15}$$

Hence, $|\psi(x)|^2$ is the **probability density** to obtain a value x of X that gives the probability to obtain x in the interval $[x, x + \mathrm{d}x]$

Finally, the **braket** of two states

$$\langle\phi|\psi\rangle = \int \mathrm{d}x\, \langle\phi|x\rangle\, \langle x|\psi\rangle = \int \mathrm{d}x\, \phi^*(x)\psi(x) \tag{3.16}$$

is the *overlap* between their wave functions. And for an arbitrary function $F = F(X)$,

$$F(X)\,|x\rangle = F(x)\,|x\rangle\,, \tag{3.17}$$

the **matrix element**

$$\begin{aligned}\langle\phi|\,F(X)\,|\psi\rangle &= \int \mathrm{d}x\ \langle\phi|\,F(X)\,|x\rangle\,\langle x|\psi\rangle = \int \mathrm{d}x\, F(x)\,\langle\phi|x\rangle\,\langle x|\psi\rangle \\ &= \int \mathrm{d}x\, F(x)\phi^*(x)\psi(x).\end{aligned} \tag{3.18}$$

3.2 Position representation

The position of a particle will be given by the eigenvalue of the position operator,

$$\vec{X} = (X_1, X_2, X_3) = (X, Y, Z). \tag{3.19}$$

The (infinite-dimensional) orthonormal basis of eigenvectors of $\vec{X}$ is $\{|\vec{x}\rangle\}$ where $\vec{x}$ labels every point in the 3-dimensional space,

$$\langle\vec{x}\,|\vec{x}'\rangle = \delta^3(\vec{x} - \vec{x}') = \delta(x - x')\delta(y - y')\delta(z - z') \quad \text{(orthonormality)} \tag{3.20}$$

$$\int \mathrm{d}^3x\ |\vec{x}\rangle\langle\vec{x}| = I \qquad \text{(closure)}. \tag{3.21}$$

The wave function in this basis is called the **position representation**,

$$\langle\vec{x}|\psi\rangle \equiv \psi(\vec{x}) = \psi(x, y, z). \tag{3.22}$$

The normalization of the physical states is expressed as

$$1 = \langle\psi|\psi\rangle = \int \mathrm{d}^3x\ \langle\psi|\vec{x}\rangle\,\langle\vec{x}|\psi\rangle = \int \mathrm{d}^3x\, \psi^*(\vec{x})\psi(\vec{x}) = \int \mathrm{d}^3x\, |\psi(\vec{x})|^2. \tag{3.23}$$

The Hilbert space of physical states is formed by the square-integrable functions in $\mathbb{R}^3$, $L^2(\mathbb{R}^3)$. It is remarkable that, in particular, the wave function of $|\vec{x}'\rangle$,

$$\langle\vec{x}\,|\vec{x}'\rangle = \delta^3(\vec{x} - \vec{x}') \tag{3.24}$$

is *not* a square-integrable function and hence does not belong to $\mathcal{H} = L^2(\mathbb{R}^3)$. In order to incorporate it, one must *enlarge* $\mathcal{H}$ to include distributions. This is the so called *rigged* or *equipped* Hilbert space, introduced to account for the continuous spectrum, as was done implicitly in the previous section.

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Furthermore, we should not be concerned that a state described by a delta function cannot be normalized, because it is not physical (but a limiting case), since one cannot measure the position $\vec{x}$ with infinite precision. In practice, when we measure the position X of the state $|\psi\rangle$, it collapses to a state that is actually a superposition of a continuum of eigenstates of X in the interval $[x-\Delta/2, x+\Delta/2]$ where Δ is a narrow (but non zero) range around x that our detector cannot resolve,

$$|\psi\rangle \to \int_{x-\Delta/2}^{x+\Delta/2} \mathrm{d}x' \left|x'\right\rangle \left\langle x'\middle|\psi\right\rangle . \tag{3.25}$$

These can be considered as eigenvectors of a common eigenvalue x, analogous to the case of a degenerate eigenvalue a of an operator A with a discrete spectrum,

$$|\psi\rangle \to \sum_{a_i} |a_i\rangle \langle a_i|\psi\rangle \quad \Rightarrow \quad p_a = \sum_i |\langle a_i|\psi\rangle|^2, \tag{3.26}$$

assuming that $\langle x|\psi\rangle$ does not appreciably change within an infinitesimal interval Δ

$$\Rightarrow \quad p(x) = \int_{x-\Delta/2}^{x+\Delta/2} \mathrm{d}x' \left|\left\langle x'\middle|\psi\right\rangle\right|^2 = \Delta \left|\langle x|\psi\rangle\right|^2. \tag{3.27}$$

Then $\psi(\vec{x})$ is the amplitude and $|\psi(\vec{x})|^2$ is the **probability density** to find a particle at $\vec{x}$.

Let us now introduce the operator that produces a space displacement (**translation**) from the position $\vec{x}$ to $\vec{x}+\vec{x_0}$:

$$T(\vec{x_0})\,|\vec{x}\rangle = |\vec{x}+\vec{x_0}\rangle . \tag{3.28}$$

There is a continuous set of translations, $\vec{x}_0 \in \mathbb{R}^3$, that can be composed (multiplied),

$$T(\vec{x}_1)T(\vec{x}_2) = T(\vec{x}_1+\vec{x}_2). \tag{3.29}$$

They have the mathematical structure of a *Lie group* called T_3. They are represented by unitary transformations acting on $\mathcal{H}$,

$$|\vec{x}\rangle \longrightarrow T(\vec{x}_0)\,|\vec{x}\rangle , \quad \left|\vec{x}'\right\rangle \longrightarrow T(\vec{x}_0)\left|\vec{x}'\right\rangle \tag{3.30}$$

$$\begin{aligned} \langle\vec{x}|\,T^\dagger(\vec{x}_0)T(\vec{x}_0)\left|\vec{x}'\right\rangle &= \left\langle \vec{x}+\vec{x}_0\middle|\vec{x}'+\vec{x}_0\right\rangle \\ &= \delta^3(\vec{x}+\vec{x}_0-\vec{x}'-\vec{x}_0) = \delta^3(\vec{x}-\vec{x}') = \left\langle\vec{x}\middle|\vec{x}'\right\rangle \qquad (3.31) \\ \Rightarrow \quad T^\dagger(\vec{x}_0) &= T^{-1}(\vec{x}_0) = T(-\vec{x}_0). \qquad (3.32) \end{aligned}$$

The elements of a Lie group can be written in terms of the *generators*. Consider first the generator of translations in $\mathbb{R}$,

$$T(x_0)\,|x\rangle = |x+x_0\rangle . \tag{3.33}$$

We define the generator K as the operator such that

$$T(\delta x) \equiv I - \mathrm{i}\delta x\, K \tag{3.34}$$

for an infinitesimal translation δx. K is self-adjoint,

$$T^{-1}(\delta x) = I + \mathrm{i}\delta x\, K, \quad T^\dagger(\delta x) = I + \mathrm{i}\delta x\, K^\dagger \quad \Rightarrow \quad K^\dagger = K, \tag{3.35}$$

and satisfies the differential equation

$$\begin{aligned} T(x+\delta x) &= T(x) + \frac{\mathrm{d}T}{\mathrm{d}x}\delta x \\ T(x+\delta x) &= T(x)T(\delta x) = T(x)\,(I - \mathrm{i}\delta x\, K) = T(x) - \mathrm{i}\delta x\, T(x)K \\ \Rightarrow \quad \frac{\mathrm{d}T}{\mathrm{d}x} &= -\mathrm{i}T\,K \end{aligned} \tag{3.36}$$

with the boundary condition $T(0) = I$. Hence,

$$\begin{aligned} T(x) &= \mathrm{e}^{-\mathrm{i}Kx} \\ &= I - \mathrm{i}Kx + \frac{1}{2!}(-\mathrm{i}Kx)^2 + \dots \\ &= \lim_{N\to\infty}\left(I - \mathrm{i}K\frac{x}{N}\right)^N . \end{aligned} \tag{3.37}$$

A finite translation x is the composition of $N \to \infty$ infinitesimal translations x/N generated by K. The displacement x is the parameter of this one-dimensional Lie group. Next we will investigate how K commutes with the position operator in one dimension:

$$\begin{aligned} & X\,T(\delta x)\,|x\rangle = X\,|x+\delta x\rangle = (x+\delta x)\,|x+\delta x\rangle\,, \\ & T(\delta x)\,X\,|x\rangle = T(\delta x)x\,|x\rangle = x\,|x+\delta x\rangle\,, \\ \Rightarrow \quad & [X, T(\delta x)]\,|x\rangle = \delta x\,|x+\delta x\rangle = \delta x\,T(\delta x)\,|x\rangle \quad \forall\,|x\rangle \\ \Rightarrow \quad & [X, T(\delta x)] = \delta x\,T(\delta x). \end{aligned} \tag{3.38}$$

Writing this expression in terms of the generator, to leading order in δx,

$$[X, T(\delta x)] = [X, I - \mathrm{i}\delta x\, K] = -\mathrm{i}\delta x\,[X, K] \tag{3.39}$$

$$\delta x\,T(\delta x) = \delta x\;(I - \mathrm{i}\delta x\, K) = \delta x\, I, \tag{3.40}$$

we find that

$$[X, K] = \mathrm{i}I \tag{3.41}$$

or

$$[X, \hbar K] = \mathrm{i}\hbar I. \tag{3.42}$$

So, the generator of translations in one dimension, multiplied by $\hbar$, has the same commutation relations (2.170) with X as the momentum $P = \hbar K$.

In $\mathbb{R}^3$ the Lie group of translations has 3 independent generators, $\vec{K}$,

$$T(\delta\vec{x}) = I - \mathrm{i}(\delta x\, K_x + \delta y\, K_y + \delta z\, K_z) = I - \mathrm{i}\delta\vec{x}\cdot\vec{K}. \tag{3.43}$$

One can easily check that the commutation relations of $\vec{X}$ and $\vec{P} = \hbar\vec{K}$ are as in (2.170),

$$[X_r, K_s] = \mathrm{i}\delta_{rs}I \quad \Rightarrow \quad [X_r, P_s] = \mathrm{i}\hbar\delta_{rs}I. \tag{3.44}$$

This is a remarkable result: in QM the **momentum** is the **generator of translations**,

$$\vec{P} = \hbar\vec{K}, \tag{3.45}$$

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since it is represented by the same operator in the Hilbert space,

$$T(\vec{x}) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\vec{P}\cdot\vec{x}}. \tag{3.46}$$

How does the momentum $\vec{P}$ act on the position representation? Consider first $\mathbb{R}$,

$$\begin{aligned} T(\delta x)\,|x\rangle &= |x+\delta x\rangle \\ \text{with } T(\delta x)\,|x\rangle = \left(I - \frac{\mathrm{i}}{\hbar}P\delta x\right)|x\rangle &= |x\rangle - \frac{\mathrm{i}}{\hbar}\delta x P\,|x\rangle \\ \Rightarrow \quad P\,|x\rangle &= \mathrm{i}\hbar\,\frac{|x+\delta x\rangle - |x\rangle}{\delta x}. \end{aligned} \tag{3.47}$$

And for the bra,

$$\langle x|\,P^\dagger = \langle x|\,P = -\mathrm{i}\hbar\,\frac{\langle x+\delta x| - \langle x|}{\delta x}. \tag{3.48}$$

Let's find the wave function of the kets $P\,|\psi\rangle$ in the position representation:

$$\begin{aligned} \langle x|\,P\,|\psi\rangle &= \langle x|\,P\int \mathrm{d}x'\ |x'\rangle\,\langle x'|\psi\rangle \\ &= -\mathrm{i}\hbar\,\frac{\langle x+\delta x| - \langle x|}{\delta x}\int \mathrm{d}x'\ |x'\rangle\,\psi(x') \\ &= -\mathrm{i}\hbar\,\frac{1}{\delta x}\int \mathrm{d}x'\,[\delta(x+\delta x-x') - \delta(x-x')]\psi(x') \\ &= -\mathrm{i}\hbar\,\frac{\psi(x+\delta x)-\psi(x)}{\delta x} \\ &= -\mathrm{i}\hbar\,\frac{\mathrm{d}\psi(x)}{\mathrm{d}x}. \end{aligned} \tag{3.49}$$

We see that P is represented by a *differential operator* in the basis $\{|x\rangle\}$,

$$\begin{aligned} |\psi\rangle &\doteq \langle x|\psi\rangle = \psi(x), \\ P &\doteq -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x} \qquad \Leftarrow \langle x|\,P\,|\psi\rangle = -\mathrm{i}\hbar\,\frac{\mathrm{d}\psi}{\mathrm{d}x}. \end{aligned} \tag{3.50}$$

Proceeding in the same way, in $\mathbb{R}^3$ one obtains

$$\vec{P} \doteq -\mathrm{i}\hbar\vec{\nabla} = -\mathrm{i}\hbar\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right). \tag{3.51}$$

3.3 Momentum representation

Instead of the basis $\{|\vec{x}\rangle\}$ we can use the basis of momentum eigenstates $\{|\vec{p}\rangle\}$,

$$\vec{P}\,|\vec{p}\rangle = \vec{p}\,|\vec{p}\rangle \tag{3.52}$$

This is also an infinite-dimensional orthonormal basis,

$$\langle\vec{p}|\vec{p}\,'\rangle = \delta^3(\vec{p}-\vec{p}\,') = \delta(p_1-p_1')\delta(p_2-p_2')\delta(p_3-p_3') \tag{3.53}$$

$$\int \mathrm{d}^3p\ |\vec{p}\rangle\langle\vec{p}| = I. \tag{3.54}$$

The wave function of a state $|\psi\rangle$ in the **momentum representation** is

$$\hat{\psi}(\vec{p}) \equiv \langle \vec{p}|\psi\rangle \,. \tag{3.55}$$

with

$$1 = \langle\psi|\psi\rangle = \int \mathrm{d}^3p\, \langle\psi|\vec{p}\rangle\, \langle\vec{p}|\psi\rangle = \int \mathrm{d}^3p\, \hat{\psi}^*(\vec{p})\hat{\psi}(\vec{p}) = \int \mathrm{d}^3p\, |\hat{\psi}(\vec{p})|^2. \tag{3.56}$$

Let us see how to express $|\vec{p}\rangle$ in the position representation. Consider first $\mathbb{R}$,

$$P\,|p\rangle = p\,|p\rangle \quad \Rightarrow \quad \langle x|\,P\,|p\rangle = p\,\langle x|p\rangle \,. \tag{3.57}$$

Using (3.50) we find

$$-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\,\langle x|p\rangle = p\,\langle x|p\rangle \quad \Rightarrow \quad \langle x|p\rangle = N\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} \tag{3.58}$$

where N is a normalization constant that we will determine next. Writing the Dirac delta in the form (3.5) and using the property $\delta(ax) = \frac{1}{|a|}\delta(x)$, we have

$$\begin{aligned}
\langle p|p'\rangle = \delta(p-p') = \delta(\hbar(k-k')) &= \frac{1}{\hbar}\delta(k'-k) \\
&= \frac{1}{2\pi\hbar}\int \mathrm{d}x\, \mathrm{e}^{\mathrm{i}x(k'-k)} = \frac{1}{2\pi\hbar}\int \mathrm{d}x\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(p'-p)x} \\
&= \int \mathrm{d}x\, \langle p|x\rangle\, \langle x|p'\rangle = |N|^2 \int \mathrm{d}x\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(p'-p)x} \\
\Rightarrow \quad N &= \frac{1}{(2\pi\hbar)^{1/2}}.
\end{aligned} \tag{3.59}$$

Hence, the wave function of $|p\rangle$ in the position representation is

$$\langle x|p\rangle = \frac{1}{(2\pi\hbar)^{1/2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} \tag{3.60}$$

and in $\mathbb{R}^3$,

$$\langle \vec{x}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}}. \tag{3.61}$$

And then, the wave function of $|\vec{x}\rangle$ in the momentum representation is

$$\langle \vec{p}|\vec{x}\rangle = \langle \vec{x}|\vec{p}\rangle^* = \frac{1}{(2\pi\hbar)^{3/2}}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}}. \tag{3.62}$$

Now we can change from one basis to the other. Consider a state $|\psi\rangle$ in the one-dimensional momentum representation,

$$\begin{aligned}
\hat{\psi}(p) = \langle p|\psi\rangle &= \int \mathrm{d}x\, \langle p|x\rangle\, \langle x|\psi\rangle \\
&= \frac{1}{(2\pi\hbar)^{1/2}}\int \mathrm{d}x\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px}\, \psi(x) = \mathcal{F}[\psi(x)].
\end{aligned} \tag{3.63}$$

We see that $\hat{\psi}(p)$ is the *Fourier transform* of $\psi(x)$. Analogously, $\psi(x)$ is the inverse Fourier transform of $\hat{\psi}(p)$:

$$\psi(x) = \langle x|\psi\rangle = \int \mathrm{d}p\, \langle x|p\rangle\, \langle p|\psi\rangle$$

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$$= \frac{1}{(2\pi\hbar)^{1/2}} \int \mathrm{d}p\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}\, \hat{\psi}(p) = \mathcal{F}^{-1}[\hat{\psi}(p)]. \tag{3.64}$$

The Fourier transform is defined for square-integrable functions *and* for distributions. For example, the wave function of a particle perfectly localized at x_0 is

$$\psi(x) = \langle x|x_0\rangle = \delta(x - x_0) \tag{3.65}$$

$$\hat{\psi}(p) = \mathcal{F}[\delta(x - x_0)] = \frac{1}{(2\pi\hbar)^{1/2}} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px_0} \tag{3.66}$$

whose distribution of momentum is constant (all momenta are equally probable),

$$|\hat{\psi}(p)|^2 = \frac{1}{2\pi\hbar} \quad \forall p \in (-\infty, \infty). \tag{3.67}$$

And the wave function of a particle with a well-defined momentum p_0 is a plane wave,

$$\hat{\psi}(p) = \langle p_0|p\rangle = \delta(p - p_0) \tag{3.68}$$

$$\psi(x) = \mathcal{F}^{-1}[\delta(p - p_0)] = \frac{1}{(2\pi\hbar)^{1/2}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_0 x} \tag{3.69}$$

whose spatial distribution is constant (all positions are equally probable),

$$|\psi(x)|^2 = \frac{1}{2\pi\hbar} \quad \forall x \in (-\infty, \infty). \tag{3.70}$$

These results are as expected because, using the general uncertainty relations (2.75) and the commutation relation of X and P (2.170), one has that the product of uncertainties in position and momentum is

$$\Delta_\psi X\, \Delta_\psi P \geq \frac{\hbar}{2}. \tag{3.71}$$

Hence, if one of them is perfectly known the other must be totally uncertain. In practice, the wave function (3.64) is not a plane wave but a **wave packet**, a superposition of plane waves, with $\hat{\psi}(p)$ a function peaking more or less sharply at $p = p_0$, not quite as $\delta(p - p_0)$. It is instructive to calculate [exercise] the expectation values and uncertainties $\langle X\rangle_\psi$, $\Delta_\psi X$, $\langle P\rangle_\psi$, $\Delta_\psi P$ for different wave packets and check that the Gaussian wave packet,

$$\psi(x) = c_0\, \mathrm{e}^{-\frac{(x-x_0)^2}{2\sigma^2}}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_0 x} \tag{3.72}$$

$$\hat{\psi}(p) = \frac{c_0\, \sigma}{\hbar}\, \mathrm{e}^{-\frac{(p-p_0)^2}{2(\hbar/\sigma)^2}} \tag{3.73}$$

with normalization $c_0^2 = \frac{1}{\sqrt{\pi\sigma^2}}$, is a *minimum uncertainty packet*, that satisfies

$$\Delta_\psi X\, \Delta_\psi P = \frac{\hbar}{2}. \tag{3.74}$$

3.4 Probability density and probability current density

We can now find the Schrödinger equation for the wave function $\psi(\vec{x}, t) = \langle \vec{x}|\psi(t)\rangle$ of a particle of mass m moving in a potential. Starting with (2.132),

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \langle x|\psi(t)\rangle = \langle x|\, H\, |\psi(t)\rangle \tag{3.75}$$

and taking the position representation of a time-independent Hamiltonian, $H \neq H(t)$,

$$H = \frac{P^2}{2m} + V(\vec{X}) \doteq -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}), \tag{3.76}$$

we get the Schrödinger wave equation:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\vec{x},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right)\psi(\vec{x},t). \tag{3.77}$$

In particular, we confirm that energy eigenstates are stationary,

$$\langle x|\, H\,|\psi_E(t)\rangle = E\,\langle x|\psi_E(t)\rangle = E\,\psi_E(\vec{x},t), \tag{3.78}$$

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi_E(\vec{x},t) = E\,\psi_E(\vec{x},t) \quad \Rightarrow \quad \psi_E(\vec{x},t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E(t-t_0)}\psi_E(\vec{x},t_0) \tag{3.79}$$

and satisfy

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right)\psi_E(\vec{x},t) = E\,\psi_E(\vec{x},t). \tag{3.80}$$

Let us see now the evolution with time of the **probability density**

$$\varrho(\vec{x},t) = |\psi(\vec{x},t)|^2 = \psi^*(\vec{x},t)\psi(\vec{x},t), \tag{3.81}$$

$$\begin{aligned}\frac{\partial\varrho}{\partial t} &= \frac{\partial\psi^*}{\partial t}\psi + \psi^*\frac{\partial\psi}{\partial t} = -\frac{1}{\mathrm{i}\hbar}\left[(H\psi)^*\psi - \psi^* H\psi\right] \\ &= -\frac{\mathrm{i}\hbar}{2m}\left(\psi\nabla^2\psi^* - \psi^*\nabla^2\psi\right) = -\vec{\nabla}\cdot\left[\frac{\mathrm{i}\hbar}{2m}\left(\psi\vec{\nabla}\psi^* - \psi^*\vec{\nabla}\psi\right)\right].\end{aligned} \tag{3.82}$$

Hence, the probability density satisfies the *continuity equation*:

$$\frac{\partial\varrho(\vec{x},t)}{\partial t} + \vec{\nabla}\cdot\vec{J}(\vec{x},t) = 0, \tag{3.83}$$

$$\vec{J}(\vec{x},t) \equiv \frac{\mathrm{i}\hbar}{2m}\left(\psi\vec{\nabla}\psi^* - \psi^*\vec{\nabla}\psi\right) = \frac{\hbar}{m}\mathrm{Im}(\psi^*\vec{\nabla}\psi). \tag{3.84}$$

where $\vec{J}$ is the **probability current density**. Integrating this equation over an arbitrary region V of $\mathbb{R}^3$, and applying the divergence (or Gauss's) theorem,

$$\begin{aligned}&\int_V \mathrm{d}V\,\frac{\partial\varrho}{\partial t} + \int \mathrm{d}V\,\vec{\nabla}\cdot\vec{J} = 0 \\ \Rightarrow \quad &\frac{\partial}{\partial t}\int_V \mathrm{d}V\,\varrho + \oint_S \mathrm{d}\vec{S}\cdot\vec{J} = 0\end{aligned} \tag{3.85}$$

we find that flux of the current density through the surface S enclosing the region V gives the total probability that has escaped or entered that region per time unit. If $V = \mathbb{R}^3$ the total probability is constant.

The probability current density integrated over $\mathbb{R}^3$ is the average particle velocity in the state $|\psi\rangle$,

$$\begin{aligned}\langle\vec{v}\rangle_\psi &= \frac{1}{m}\langle\psi|\,\vec{P}\,|\psi\rangle = \frac{1}{m}\int \mathrm{d}^3x\;\langle\psi|x\rangle\,\langle x|\,\vec{P}\,|\psi\rangle \\ &= \frac{1}{m}\int \mathrm{d}^3x\,\psi^*(-\mathrm{i}\hbar\vec{\nabla}\psi) = \int \mathrm{d}^3x\,\left(-\frac{\mathrm{i}\hbar}{m}\psi^*\vec{\nabla}\psi\right)\end{aligned}$$

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$$= \frac{1}{m}\int \mathrm{d}^3x\,(\mathrm{i}\hbar\vec{\nabla}\psi^*)\psi = \int \mathrm{d}^3x\,\left(\frac{\mathrm{i}\hbar}{m}\psi\vec{\nabla}\psi^*\right) \tag{3.86}$$

$$\Rightarrow \quad \int \mathrm{d}^3x\,\vec{J} = \frac{\mathrm{i}\hbar}{2m}\int \mathrm{d}^3x\,\left(\psi\vec{\nabla}\psi^* - \psi^*\vec{\nabla}\psi\right) = \langle\vec{v}\rangle_\psi. \tag{3.87}$$

For an energy eigenstate (3.79), that is stationary, the probability density to find the particle at $\vec{x}$ does not change with time, since

$$\varrho = |\psi_E(\vec{x},t))|^2 = |\psi_E(\vec{x},t_0))|^2 \quad \Rightarrow \quad \frac{\partial\varrho}{\partial t} = \vec{\nabla}\cdot\vec{J} = 0. \tag{3.88}$$

The time evolution of a generic wave function will be described in §3.6.

3.5 Ehrenfest's theorem

We have seen in (2.142) how expectation values change with time. It is remarkable that the expectation values of X and P for a particle of mass m moving in a potential $V(x)$,[a]

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle_\psi = -\frac{\mathrm{i}}{\hbar}\langle[X,H]\rangle_\psi = \frac{1}{m}\langle P\rangle_\psi \tag{3.89}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle_\psi = -\frac{\mathrm{i}}{\hbar}\langle[P,H]\rangle_\psi = -\left\langle\frac{\mathrm{d}V}{\mathrm{d}x}\right\rangle_\psi = \langle F(x)\rangle_\psi \tag{3.90}$$

verify *similar* equations of motion as the the classical variables x and p:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial H}{\partial p} = \frac{p}{m} \tag{3.91}$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial x} = -\frac{\mathrm{d}V}{\mathrm{d}x} = F(x). \tag{3.92}$$

In fact, putting together (3.89) and (3.90) one finds the Ehrenfest's theorem,

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle X\rangle_\psi = \langle F(x)\rangle_\psi \tag{3.93}$$

stating that the center of the wave function $\langle X\rangle_\psi$ moves like a classical particle under the average force $\langle F\rangle_\psi$.

Although, at first glance, it might appear that Ehrenfest's theorem is saying that the quantum mechanical expectation values obey Newton's classical equations of motion, this is not actually the case, because in general

$$\langle F(x)\rangle_\psi \neq F(\langle X\rangle_\psi). \tag{3.94}$$

Exceptions to this inequality are potentials of the form

$$V(x) = -\lambda x^n, \quad F(x) = n\lambda x^{n-1} \tag{3.95}$$

for: $n = 0$ (free particle), $n = 1$ (constant force) or $n = 2$ (harmonic potential). [Exercise]

[a] To check (3.89) and (3.90) notice that

$$[X,P^2] = [X,P]P + P[X,P] = 2\mathrm{i}\hbar P \quad \Leftarrow \quad [A,BC] = [A,B]C + B[A,C],$$

$$[P,V] = PV - VP \doteq -\mathrm{i}\hbar\frac{\mathrm{d}V}{\mathrm{d}x} - \mathrm{i}\hbar V\frac{\mathrm{d}}{\mathrm{d}x} - V\left(-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right) = -\mathrm{i}\hbar\frac{\mathrm{d}V}{\mathrm{d}x}.$$

3.6 Propagator

The time evolution of the wave function can be expressed in terms of the *propagator*. This is a general approach that allows a perturbative treatment. It is frequently applied in Quantum Field Theory, where the propagator is a fundamental concept. We will introduce it here although it will not be used in this course.

The propagator $K(\vec{x}_2, t_2; \vec{x}_1, t_1)$ is an *integral operator* that acts on the initial wave function and transforms it to the final one,

$$\psi(\vec{x}_2, t_2) = \int \mathrm{d}^3 x_1 \, K(\vec{x}_2, t_2; \vec{x}_1, t_1) \, \psi(\vec{x}_1, t_1). \tag{3.96}$$

Let us explore its meaning. Suppose a particle perfectly localized initially (t_1) at $\vec{x}_i$. Its wave function is just

$$\psi(\vec{x}_1, t_1) = \delta(\vec{x}_1 - \vec{x}_i). \tag{3.97}$$

According to (3.96), at a time t_2 the wave function develops into

$$\psi(\vec{x}_2, t_2) = \int \mathrm{d}^3 x_1 \, K(\vec{x}_2, t_2; \vec{x}_1, t_1) \, \delta(\vec{x}_1 - \vec{x}_i) = K(\vec{x}_2, t_2; \vec{x}_i, t_1). \tag{3.98}$$

Therefore, the propagator $K(\vec{x}_2, t_2; \vec{x}_1, t_1)$ provides the probability amplitude to find a particle in $\vec{x}_2$ at t_2 *if* the particle was in $\vec{x}_1$ at t_1, namely, it is the probability amplitude for the "propagation" between those points in that interval.

Remember that $|\psi(t_2)\rangle = U(t_2, t_1) \, |\psi(t_1)\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H(t_2 - t_1)} \, |\psi(t_1)\rangle$. Then, taking $|\psi(t_1)\rangle = |\vec{x}_1\rangle$ we have

$$\langle \vec{x}_2 | \psi(t_2) \rangle = K(\vec{x}_2, t_2; \vec{x}_1, t_1) = \langle \vec{x}_2 | \, U(t_2, t_1) \, | \vec{x}_1 \rangle \equiv \langle \vec{x}_2, t_2 | \vec{x}_1, t_1 \rangle \tag{3.99}$$

where $|\vec{x}_1, t_1\rangle$ and $|\vec{x}_2, t_2\rangle$ are position eigenstates in the Heisenberg picture. And in terms of energy eigenstates:[b]

$$\begin{aligned}
\psi(\vec{x}_2, t_2) = \langle \vec{x}_2 | \psi(t_2) \rangle &= \langle \vec{x}_2 | \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H(t_2 - t_1)} \, | \psi(t_1) \rangle = \sum_E \langle \vec{x}_2 | E \rangle \, \langle E | \psi(t_1) \rangle \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} E(t_2 - t_1)} \\
&= \int \mathrm{d}^3 x_1 \, \sum_E \langle \vec{x}_2 | E \rangle \, \langle E | \vec{x}_1 \rangle \, \langle \vec{x}_1 | \psi(t_1) \rangle \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} E(t_2 - t_1)} \\
&= \int \mathrm{d}^3 x_1 \, \sum_E \psi_E(\vec{x}_2) \psi_E^*(\vec{x}_1) \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} E(t_2 - t_1)} \, \psi(\vec{x}_1, t_1) \\
\Rightarrow \quad K(\vec{x}_2, t_2; \vec{x}_1, t_1) &= \sum_E \psi_E(\vec{x}_2) \psi_E^*(\vec{x}_1) \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} E(t_2 - t_1)}.
\end{aligned} \tag{3.100}$$

Restricting ourselves to the case $t_2 > t_1$ we define the *retarded propagator*

$$K_+(\vec{x}_2, t_2; \vec{x}_1, t_1) \equiv \theta(t_2 - t_1) \, \langle \vec{x}_2 | \, U(t_2, t_1) \, | \vec{x}_1 \rangle \tag{3.101}$$

where $\theta(t)$ is the Heaviside step function

$$\theta(t_2 - t_1) = \begin{cases} 1 & , \quad t_2 > t_1 \\ 0 & , \quad t_2 < t_1 \end{cases} \tag{3.102}$$

[b] Replace $\sum_E |E\rangle\langle E|$ with $\int \mathrm{d}E \, |E\rangle\langle E|$ if the energy spectrum is continuous.

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whose derivative is the Dirac delta,

$$\frac{\partial\theta(t_2-t_1)}{\partial t_2}=\delta(t_2-t_1). \tag{3.103}$$

The retarded propagator is the Green's function of the operator $H-\mathrm{i}\hbar\dfrac{\partial}{\partial t}$:

$$\begin{aligned}\left[-\frac{\hbar^2}{2m}\nabla^2_{x_2}+V(\vec{x}_2)-\mathrm{i}\hbar\frac{\partial}{\partial t_2}\right]&\left[\theta(t_2-t_1)\sum_E\psi_E(\vec{x}_2)\psi_E^*(\vec{x}_1)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E(t_2-t_1)}\right]\\ &=\theta(t_2-t_1)\sum_E E\,\psi_E(\vec{x}_2)\psi_E^*(\vec{x}_1)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E(t_2-t_1)}\\ &\quad-\mathrm{i}\hbar\,\delta(t_2-t_1)\sum_E\psi_E(\vec{x}_2)\psi_E^*(\vec{x}_1)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E(t_2-t_1)}\\ &\quad-\mathrm{i}\hbar\,\theta(t_2-t_1)\sum_E\psi_E(\vec{x}_2)\psi_E^*(\vec{x}_1)\left(-\frac{\mathrm{i}}{\hbar}E\right)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E(t_2-t_1)}\\ &=-\mathrm{i}\hbar\,\delta(t_2-t_1)\delta^3(\vec{x}_2-\vec{x}_1)\end{aligned} \tag{3.104}$$

where we have used $H\,\psi_E=E\,\psi_E$, $\delta(t_2-t_1)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E(t_2-t_1)}=1$ and

$$\sum_E\psi_E(\vec{x}_2)\psi_E^*(\vec{x}_1)=\sum_E\langle\vec{x}_2|E\rangle\langle E|\vec{x}_1\rangle=\delta^3(\vec{x}_2-\vec{x}_1). \tag{3.105}$$

Finding K_+ is difficult in general, depending on the form of the potential $V(\vec{x})$. An easily solvable case is the *free propagator*, $V(\vec{x})=0$,

$$\begin{aligned}\langle\vec{x}_2|\,U(t_2,t_1)\,|\vec{x}_1\rangle&=\int\mathrm{d}^3p\;\langle\vec{x}_2|\vec{p}\rangle\langle\vec{p}|\vec{x}_1\rangle\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E(t_2-t_1)}\\ \text{with}\quad\langle\vec{x}|\vec{p}\rangle&=\frac{1}{(2\pi\hbar)^{3/2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}},\quad E=\frac{p^2}{2m}\end{aligned} \tag{3.106}$$

$$\begin{aligned}\Rightarrow\quad K_+^0(\vec{x}_2,t_2;\vec{x}_1,t_1)&=\theta(t_2-t_1)\int\mathrm{d}^3p\,\frac{1}{(2\pi\hbar)^3}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot(\vec{x}_2-\vec{x}_1)}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2m}(t_2-t_1)}\\ &=\theta(t_2-t_1)\mathrm{e}^{-\mathrm{i}\frac{3\pi}{4}}\left[\frac{m}{2\pi\hbar(t_2-t_1)}\right]^{3/2}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\frac{m}{2}\frac{|\vec{x_2}-\vec{x}_1|^2}{t_2-t_1}}\end{aligned} \tag{3.107}$$

where we have used (to the third power in 3 dimensions),

$$\int_{-\infty}^{\infty}\mathrm{d}p\,\mathrm{e}^{-\mathrm{i}(ap^2+2bp)}=\sqrt{\frac{\pi}{a}}\,\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}\mathrm{e}^{\mathrm{i}\frac{b^2}{a}},\quad a>0. \tag{3.108}$$

It is instructive to see [exercise] how a Gaussian wave packet evolves freely with time: its center moves with constant group velocity and the packet broadens being no longer minimal: $\Delta x\,\Delta p>\hbar/2$ (while Δp remains constant).

The free propagator is used as a starting point to find perturbative solutions at order $V^n(\vec{x})$. This is the usual approach in Quantum Field Theory.

3.7 Feynman formulation of Quantum Mechanics: path integral

In Classical Mechanics, dynamics is governed by Hamilton's principle: the trajectory of a system (Fig. 3.2) in the phase space (coordinates and velocities) is an extreme of the *action*

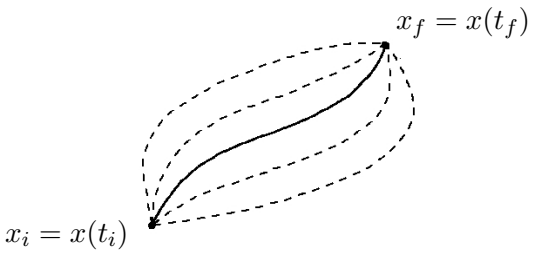

Figure 3.2: Possible trajectories $x(t)$ in the phase space of one particle $(x, \dot{x})$. In Classical Mechanics the particle follows just the one that minimizes the action.

(usually a minimum),

$$\delta S = \delta \int_{t_i}^{t_f} \mathrm{d}t\, L(x, \dot{x}) = 0, \tag{3.109}$$

where the Lagrangian $L(x, \dot{x})$ is a function which contains all physical information concerning the system. If it is conservative,

$$L(x, \dot{x}) = \frac{1}{2} m\dot{x}^2 - V(x). \tag{3.110}$$

From this variational principle one derives the Euler-Lagrange differential equations, whose solutions provide the equations of motion of the system.

In 1933, Dirac pointed out that, in contrast to Classical Mechanics, the action seemed to play no relevant role in QM. He unsuccessfully speculated that the propagator might correspond to $\exp\{\mathrm{i}S/\hbar\}$ where S is the classical action evaluated along the classical trajectory. In 1948, Feynman developed Dirac's idea and accomplished a new formulation of QM based on writing the propagator as the sum over *all possible paths* (not just the classical one) of $\exp\{\mathrm{i}S/\hbar\}$ between the initial and the final state. Somehow, a quantum particle manages to take all paths and the probability amplitude of each one adds up according to the superposition principle of QM.[c]

We have seen (**??**) that in the *canonical formalism*, the propagator is

$$\langle x_f, t_f | x_i, t_i \rangle = \langle x_f | \, \mathrm{e}^{-\mathrm{i}H\Delta t/\hbar} \, | x_i \rangle \, . \tag{3.111}$$

Notice that at every fixed time t, the states $\{|x, t\rangle\}$ form a complete set,

$$I = \int \mathrm{d}x \, |x, t\rangle\langle x, t| \, . \tag{3.112}$$

Let us choose a set of intermediate times $t_n \in \{t_0, t_1, \ldots, t_N\}$ with $t_i \equiv t_0 < t_1 < \cdots < t_N \equiv t_f$ that will be assumed equidistant to simplify,

$$t_n = t_0 + n\delta t \ , \quad \delta t = \frac{t_f - t_i}{N} \ . \tag{3.113}$$

Then the propagator reads

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathrm{d}x_1 \, \langle x_f, t_f | x_1, t_1 \rangle \, \langle x_1, t_1 | x_i, t_i \rangle$$

[c] R. P. Feynman, *Space-time approach to nonrelativistic Quantum Mechanics*, Rev. Mod. Phys. **20** (1948) 367.

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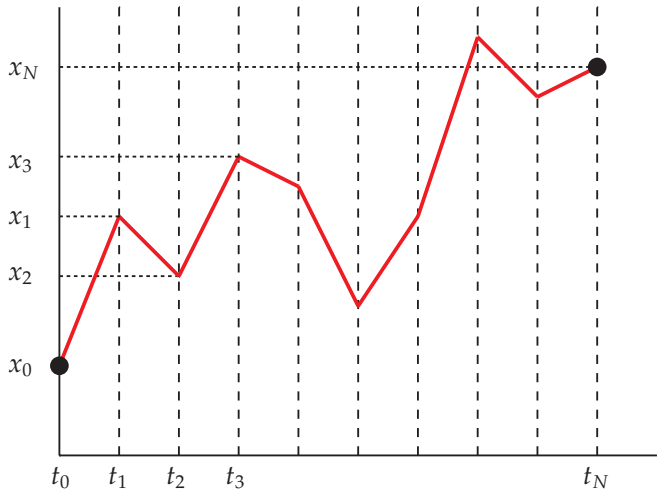

Figure 3.3: Path $x(t)$ defined by the interpolation of $x(t_0) = x_0,\ \ldots,\ x(t_N) = x_N$.

$$
\begin{aligned}
&= \int \mathrm{d}x_1 \mathrm{d}x_2 \, \langle x_f, t_f | x_2, t_2 \rangle \, \langle x_2, t_2 | x_1, t_1 \rangle \, \langle x_1, t_1 | x_i, t_i \rangle \\
&= \int \mathrm{d}x_1 \cdots \mathrm{d}x_{N-1} \prod_{n=0}^{N-1} \langle x_{n+1}, t_{n+1} | x_n, t_n \rangle
\end{aligned} \tag{3.114}
$$

with the notation $x_i \equiv x_0$, $x_f \equiv x_N$. For small enough δt,

$$
\begin{aligned}
\langle x_{n+1}, t_{n+1} | x_n, t_n \rangle &= \langle x_{n+1} | \, \mathrm{e}^{-\mathrm{i}H\delta t/\hbar} \, | x_n \rangle \\
&= \langle x_{n+1} | \, (1 - \mathrm{i}H\delta t/\hbar) \, | x_n \rangle + \mathcal{O}(\delta t)^2 \, .
\end{aligned} \tag{3.115}
$$

In the momentum representation and neglecting terms of order $(\delta t)^2$,

$$
\begin{aligned}
\langle x_{n+1}, t_{n+1} | x_n, t_n \rangle &= \langle x_{n+1} | \, (1 - \mathrm{i}H\delta t/\hbar) \, | x_n \rangle \\
&= \int \mathrm{d}p_n \, \langle x_{n+1} | p_n \rangle \, \langle p_n | \, (1 - \mathrm{i}H\delta t/\hbar) \, | x_n \rangle \\
&= \int \mathrm{d}p_n \, \langle x_{n+1} | p_n \rangle \, [1 - \mathrm{i}H(p_n, x_n)\delta t/\hbar] \, \langle p_n | x_n \rangle \\
&= \int \frac{\mathrm{d}p_n}{2\pi\hbar} \mathrm{e}^{\mathrm{i}p_n(x_{n+1} - x_n)/\hbar} \mathrm{e}^{-\mathrm{i}H(p_n, x_n)\delta t/\hbar} \\
&= \int \frac{\mathrm{d}p_n}{2\pi\hbar} \exp\left\{ \frac{\mathrm{i}}{\hbar} \left[p_n \frac{x_{n+1} - x_n}{\delta t} - H(p_n, x_n) \right] \delta t \right\},
\end{aligned} \tag{3.116}
$$

and substituting in (3.114) in the limit of large N, we have

$$
\begin{aligned}
\langle x_f, t_f | x_i, t_i \rangle = \lim_{N \to \infty} \int \mathrm{d}x_1 \cdots \mathrm{d}x_{N-1} \int \frac{\mathrm{d}p_0}{2\pi\hbar} \cdots \frac{\mathrm{d}p_{N-1}}{2\pi\hbar} \\
\times \exp\left\{ \frac{\mathrm{i}}{\hbar} \sum_{n=0}^{N-1} \left[p_n \frac{x_{n+1} - x_n}{\delta t} - H(p_n, x_n) \right] \delta t \right\}.
\end{aligned} \tag{3.117}
$$

The expression above is an integral over all the possible values of $x_1, \ldots, x_{N-1}$. Every set of values defines a *path*, i.e. a function $x(t)$ given by the interpolation of $x(t_0) = x_0,\ \ldots,\ x(t_N) = x_N$, with fixed x_0 and x_N (Fig. 3.3). There is also an integral over N

momenta $p_0, \ldots, p_{N-1}$. Therefore, we can write the propagator as the discretized version of the *functional integral*

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}x(t)\mathcal{D}p(t) \exp\left\{ \frac{\mathrm{i}}{\hbar} \int_{t_i}^{t_f} \mathrm{d}t \, [p\dot{x} - H(p,x)] \right\} \tag{3.118}$$

where the $x(t)$ have fixed boundary conditions and the momenta $p(t)$ are unbounded.

The potential of a conservative system does not depend on p, so V factors out and we can integrate over the momenta, with the help of (3.108),

$$\int \frac{\mathrm{d}p_n}{2\pi\hbar} \exp\left\{ -p_n^2 \frac{\mathrm{i}\delta t}{2m\hbar} + p_n \frac{\mathrm{i}(x_{n+1} - x_n)}{\hbar} \right\} = \left(\frac{m}{2\pi \mathrm{i}\hbar\delta t} \right)^{1/2} \exp\left\{ \frac{\mathrm{i}m(x_{n+1} - x_n)^2}{2\hbar\delta t} \right\} \tag{3.119}$$

Hence,

$$\begin{aligned} \langle x_f, t_f | x_i, t_i \rangle = \lim_{N\to\infty} \left(\frac{m}{2\pi \mathrm{i}\hbar\delta t} \right)^{N/2} \int \mathrm{d}x_1 \cdots \mathrm{d}x_{N-1} \\ \times \exp\left\{ \frac{\mathrm{i}}{\hbar} \sum_{n=0}^{N-1} \left[\frac{m}{2} \left(\frac{x_{n+1} - x_n}{\delta t} \right)^2 - V(x_n) \right] \delta t \right\} \end{aligned} \tag{3.120}$$

that is the discretized version of the functional integral:

$$\begin{aligned} \langle x_f, t_f | x_i, t_i \rangle &= \int \mathcal{D}x(t) \exp\left\{ \frac{\mathrm{i}}{\hbar} \int_{t_i}^{t_f} \mathrm{d}t \left[\frac{m}{2}\dot{x}^2 - V(x) \right] \right\} \\ &= \int \mathcal{D}x(t) \exp\left\{ \frac{\mathrm{i}}{\hbar} S[x(t)] \right\} \end{aligned} \tag{3.121}$$

where the action $S[x(t)]$ is a *functional* of all possible paths, in terms of the Lagrangian,

$$S[x(t)] = \int_{t_i}^{t_f} \mathrm{d}t \; L(x, \dot{x}) \; , \quad L(x, \dot{x}) = \frac{m}{2}\dot{x}^2 - V(x), \tag{3.122}$$

the result we had advertised. We may interpret $\int \mathcal{D}x(t)$ as a sum over all paths that we usually call *path integral*.

This alternative formulation of QM provides an extremely interesting and intuitive view of quantum processes and allows to derive the classical limit in a very natural way.

As an illustration, let us consider the famous **double slit** experiment. The double-slit experiment was first performed with (sun)light by Thomas Young in 1801 and was key to accept the wave theory of light: the beams passing (diffracting) through two closely separated slits pierced on a plate *interfere* in their way to a screen where they display a fringe pattern of dark and bright bands (Fig. 3.4). In 1927, Davisson and Germer demonstrated that electrons show the same behaviour (using a nickel crystal instead of two slits), which was later extended to atoms and molecules! Similar experiments with low intensity beams of single photons or single electrons sent one by one (using a biprism instead of slits) have been performed with identical results (3.5). The details of the experimental setup are not relevant for us. We will take it as a thought experiment with profound consequences. Richard Feynman in [**?**] called it

> "a phenomenon which is impossible, *absolutely* impossible, to explain in any classical way, and which has in it the heart of quantum mechanics. In reality, it contains the *only* mystery".

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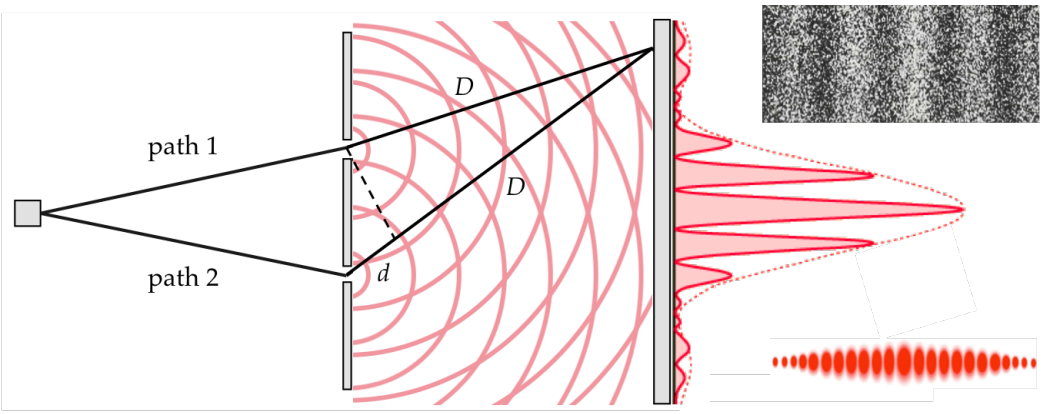

Figure 3.4: Left: Sketch of the double slit experiment for both coherent light and electrons, showing two possible electron paths. Right: Interference fringes for light (bottom), and electron impacts on the screen (up) of the experiment in Fig. 3.5.

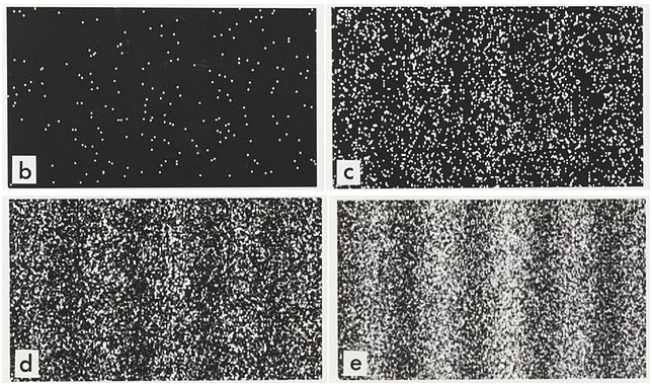

Figure 3.5: Experiment by A. Tonomura *et al.* [*American Journal of Physics* **57** (1989) 117]: (b) 200, (c) 6000, (d) 40000, (e) 140000 electrons are sent one by one through a double slit.

One may think that a flux of electrons behaves like a fluid of many particles interacting with each other and this may cause the accumulation of impacts in bands on the screen resembling an interference pattern. But when sending electrons one by one there is no doubt that somehow *every* electron "interferes" with itself. Even more striking is the fact that if one detects which of the slit each electron goes through, or one closes the other slit, the interference pattern disappears! But how can an electron "know" if the other slit is open? And when both slits are open, how can one electron interfere with another one emitted before or afterwards?

The interpretation of Feynman is perhaps the most satisfactory, though contrary to the common sense.[d] The only thing we know for sure about the electron is that it comes from the source and ends up on the screen, but we have no information about its intermediate positions. So, in between, one can not say if the electron is here or there. Actually *it* is in a cohererent superposition of all possible paths. Of course, classically this makes no sense: nothing can be in more than one state at the same time. To the resulting probability amplitude (path integral) contribute not only *the* classical path but *every* path compatible

[d] "[Quantum theory] describes nature as absurd from the point of view of common sense. And yet it fully agrees with experiment. So I hope you can accept nature as She is — absurd." R. P. Feynman in *QED: the strange theory of light and matter*, Princeton University Press, 1985.

with the boundary conditions. If the electron is detected through one of the slits then the possible paths are restricted in such a way that the interference cancels.

In the *classical limit* ($\hbar \to 0$) one can apply the *stationary phase approximation* to the functional integral (3.121): the *only* contribution to this oscillatory integral, with a rapidly varying phase, is the one that is an extreme of the integrand (the others cancel out),

$$\frac{\delta}{\delta x(t)} S[x(t)]\bigg|_{\text{cl}} = 0. \tag{3.123}$$

We recover Hamilton's principle! The principle of minimal action is just a good approximation of our quantum world in the classical domain.

When we deal with macroscopic systems the action along different paths is always much larger than $\hbar$ so the system obeys the familiar classical rules. Things change when the difference of the action along the possible paths is comparable to $\hbar$. For example, consider two electron paths (Fig. 3.4) with constant velocities $v_1 = D/t$ y $v_2 = (D+d)/t$, and assume $d \ll D$, so $v = v_1 \approx v_2$. Then

$$\left| \exp\left\{ \frac{\mathrm{i}}{\hbar} S[x_1] \right\} + \exp\left\{ \frac{\mathrm{i}}{\hbar} S[x_2] \right\} \right|^2 \propto 1 + \cos \Delta\varphi, \tag{3.124}$$

$$\Delta\varphi = \frac{1}{\hbar}\left(\frac{m v_2^2 t}{2} - \frac{m v_1^2 t}{2} \right) \approx \frac{mDd}{\hbar t} \approx \frac{pd}{\hbar} = 2\pi \frac{d}{\lambda} \tag{3.125}$$

where we have introduced de Broglie's relation $p = h/\lambda$ with $p = mv$. This is exactly the phase difference of two "waves" in a diffraction experiment.

The de Broglie's wavelength assigned to a particle of momentum p should not be taken literally. It is rather an equivalent way of viewing things in the microcosmos.

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Chapter 4

Angular momentum

4.1 Commutation relations of angular momentum

Classically, one defines the angular momentum with respect to the origin of a particle with position $\vec{x}$ and linear momentum $\vec{p}$ as

$$\vec{L} = \vec{x} \times \vec{p}. \tag{4.1}$$

A non-vanishing $\vec{L}$ corresponds to a particle rotating around the origin.

Following postulate VI, the quantum operator representing the angular momentum observable is obtained by substituting the position and momentum operators $\vec{x} \to \vec{X}$ and $\vec{p} \to \vec{P}$,

$$\vec{L} = \vec{X} \times \vec{P} \qquad \text{or} \qquad L_i = \sum_{j=1}^{3}\sum_{k=1}^{3} \epsilon_{ijk} X_j P_k \equiv \epsilon_{ijk} X_j P_k \qquad \text{(self-adjoint)} \tag{4.2}$$

where ϵ_{ijk} is the Levi-Civita symbol,

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } (i,j,k) \text{ is an even permutation of } (1,2,3) \\ -1 & \text{if } (i,j,k) \text{ is an odd permutation of } (1,2,3) \\ 0 & \text{otherwise.} \end{cases} \tag{4.3}$$

and Einstein's notation (summation over repeated indices) will be applied from now on. We will call $\vec{L}$ the *orbital* angular momentum. In the position representation,

$$\vec{L} \doteq -\mathrm{i}\hbar \vec{X} \times \vec{\nabla}, \qquad \langle \vec{L} \rangle_\psi = \langle \psi | \, \vec{L} \, | \psi \rangle \, s - \mathrm{i}\hbar \int \mathrm{d}^3 x \, \psi^*(x) (\vec{x} \times \vec{\nabla}) \psi(x) \tag{4.4}$$

$$L_z \doteq -\mathrm{i}\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right), \quad \langle L_z \rangle_\psi = \langle \psi | \, L_z \, | \psi \rangle = -\mathrm{i}\hbar \int \mathrm{d}^3 x \, \psi^*(x) \left(x \frac{\partial \psi}{\partial y} - y \frac{\partial \psi}{\partial x} \right). \tag{4.5}$$

L_z measures the angular momentum around the z-axis of a system described by the wave function ψ. From the commutation relations $[X_i, P_j] = \mathrm{i}\hbar \delta_{ij} I$ it is straightfoward to derive[a]

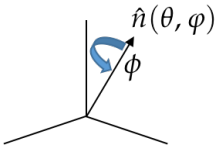
$$[L_i, L_j] = \mathrm{i}\hbar \epsilon_{ijk} L_k. \tag{4.6}$$

[a] Use $[AB, CD] = C[AB, D] + [AB, C]D = C(A[B, D] + [A, D]B) + (A[B, C] + [A, C]B)D$.

4.2 The rotation group

The rotations in the 3-dimensional space form a continuous (Lie) group called $SO(3)$, whose (infinite) elements can be labeled by 3 independent parameters. There are two common parametrizations of the rotations in 3D:

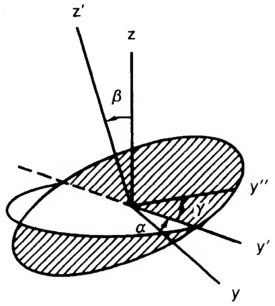
- The *axis-angle* parametrization ($\theta \in [0,\pi]$, $\varphi \in [0,2\pi]$, $\phi \in [0,2\pi]$):



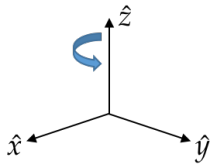
$$R_{\hat{n}}(\phi), \quad \hat{n} = \hat{n}(\theta,\varphi). \tag{4.7}$$

- The *Euler-angle* parametrization ($\alpha \in [0,2\pi]$, $\beta \in [0,\pi]$, $\gamma \in [0,2\pi]$):

$$\begin{aligned} R(\alpha,\beta,\gamma) &\equiv R_{\hat{z}}(\alpha)R_{\hat{y}}(\beta)R_{\hat{z}}(\gamma) \\ &= R_{\hat{z}'}(\gamma)R_{\hat{y}'}(\beta)R_{\hat{z}}(\alpha) \end{aligned} \tag{4.8}$$



Let us consider the subgroup of rotations around the z-axis, $R_z(\phi)$. Choosing the orthonormal basis $\{\hat{x},\hat{y},\hat{z}\}$,

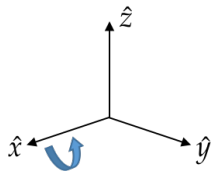


$$\begin{aligned} \hat{x} &\mapsto \cos\phi\,\hat{x} + \sin\phi\,\hat{y} \\ \hat{y} &\mapsto -\sin\phi\,\hat{x} + \cos\phi\,\hat{y} \\ \hat{z} &\mapsto \hat{z} \end{aligned}$$

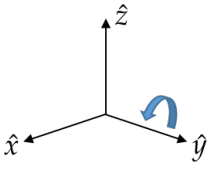
namely

$$\begin{aligned} R_{\hat{z}}(\phi)\begin{pmatrix}\hat{x} & \hat{y} & \hat{z}\end{pmatrix} &= \begin{pmatrix}\hat{x} & \hat{y} & \hat{z}\end{pmatrix}\begin{pmatrix}\cos\phi & -\sin\phi & 0\\ \sin\phi & \cos\phi & 0\\ 0 & 0 & 1\end{pmatrix} \\ \Rightarrow R_{\hat{z}}(\phi) &\doteq \begin{pmatrix}\cos\phi & -\sin\phi & 0\\ \sin\phi & \cos\phi & 0\\ 0 & 0 & 1\end{pmatrix}. \end{aligned} \tag{4.9}$$

Analogously, the rotations around the x-axis and the y-axis are subgroups,



$$\Rightarrow R_{\hat{x}}(\phi) \doteq \begin{pmatrix}1 & 0 & 0\\ 0 & \cos\phi & -\sin\phi\\ 0 & \sin\phi & \cos\phi\end{pmatrix} \tag{4.10}$$



$$\Rightarrow R_{\hat{y}}(\phi) \doteq \begin{pmatrix}\cos\phi & 0 & \sin\phi\\ 0 & 1 & 0\\ -\sin\phi & 0 & \cos\phi\end{pmatrix}. \tag{4.11}$$

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Each subgroup depends on one parameter ϕ. We say that the elements of every subgroup are generated by one *generator*. Let us consider $R_{\hat{z}}(\phi)$. The corresponding generator K_z is obtained doing infinitesimal rotations around the z-axis,

$$R_{\hat{z}}(\delta\phi) \equiv I - \mathrm{i}\delta\phi\, K_z \tag{4.12}$$

$$R_{\hat{z}}(\delta\phi) \doteq \begin{pmatrix} 1 & -\delta\phi & 0 \\ \delta\phi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \Rightarrow K_z \doteq \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{4.13}$$

As we did for translations, we write

$$\begin{aligned} R_{\hat{z}}(\phi+\delta\phi) &= R_{\hat{z}}(\phi)R_{\hat{z}}(\delta\phi) \\ R_{\hat{z}}(\phi) + \frac{\mathrm{d}R_{\hat{z}}}{\mathrm{d}\phi}\delta\phi &= R_{\hat{z}}(\phi)(I - \mathrm{i}\delta\phi\, K_z) \\ \frac{\mathrm{d}R_{\hat{z}}}{\mathrm{d}\phi} &= -\mathrm{i}R_{\hat{z}}(\phi)\, K_z \\ \Rightarrow \quad R_{\hat{z}}(\phi) &= \mathrm{e}^{-\mathrm{i}K_z\phi} \end{aligned} \tag{4.14}$$

where we have used the boundary condition $R_{\hat{z}}(0) = I$. Analogously, the rotations around the x-axis and the y-axis are generated by

$$K_x \doteq \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \quad K_y \doteq \begin{pmatrix} 0 & 0 & \mathrm{i} \\ 0 & 0 & 0 \\ -\mathrm{i} & 0 & 0 \end{pmatrix}. \tag{4.15}$$

One can see that an infinitesimal rotation around the axis $\hat{n} = (n_x, n_y, n_z)$ is given by

$$R_{\hat{n}}(\delta\phi) = I - \mathrm{i}\delta\phi\,(n_x K_x + n_y K_y + n_z K_z) = I - \mathrm{i}\delta\phi\,\hat{n}\cdot\vec{K} \tag{4.16}$$

$$\Rightarrow \quad R_{\hat{n}}(\phi) = \mathrm{e}^{-\mathrm{i}\phi\hat{n}\cdot\vec{K}}. \tag{4.17}$$

The linear combination of generators is another generator. All of them define a 3-dimensional algebra of generators with commutation relations:

$$[K_x, K_y] = \mathrm{i}K_z. \tag{4.18}$$

This means that $\vec{J} = \hbar\vec{K}$ have the same algebra as the angular momentum (4.6),

$$[J_x, J_y] = \mathrm{i}\hbar J_z. \tag{4.19}$$

Hence, in QM the generators of the rotations *are* (represented by the same operators in any Hilbert space as) the three components of the angular momentum divided by $\hbar$,

$$R_{\hat{n}}(\phi) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\phi\hat{n}\cdot\vec{J}} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\phi(n_x J_x + n_y J_y + n_z J_z)}. \tag{4.20}$$

In the widely used Euler-angle parametrization,[b]

$$R(\alpha,\beta,\gamma) = R_{\hat{z}}(\alpha)R_{\hat{y}}(\beta)R_{\hat{z}}(\gamma) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}J_z\alpha}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}J_y\beta}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}J_z\gamma}$$

[b] Notice that indeed the group of rotations is isomorphic to $SO(3)$, the group of 3×3 orthogonal matrices with unit determinant: $RR^T = I$, $\det R = 1$.

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$$\doteq \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} \cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma & -\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma & \cos\alpha\sin\beta \\ \sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma & -\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma & \sin\alpha\sin\beta \\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta \end{pmatrix}. \tag{4.21}$$

The Euler-angle and the axis-angle parametrizations are related by

$$\tan\theta = \frac{\tan\frac{\beta}{2}}{\sin\frac{\alpha+\gamma}{2}}, \quad \varphi = \frac{\pi+\alpha-\gamma}{2}, \quad \cos\phi = 2\cos^2\frac{\beta}{2}\cos^2\frac{\alpha+\gamma}{2} - 1. \tag{4.22}$$

Summarizing, in the Hilbert space $\mathcal{H}$ that describes the state of angular momentum of any system, the operators L_i or J_i representing the angular momentum satisfy (4.19). Under rotations of angle ϕ around the axis $\hat{n}$, the vectors $|\alpha\rangle \in \mathcal{H}$ will change by

$$|\alpha\rangle \mapsto R_{\hat{n}}(\phi)\,|\alpha\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\phi\hat{n}\cdot\vec{J}}\,|\alpha\rangle\,. \tag{4.23}$$

So far, we have found 3×3 matrices that satisfy the commutation relations (4.19),

$$J_x \doteq \hbar\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \quad J_y \doteq \hbar\begin{pmatrix} 0 & 0 & \mathrm{i} \\ 0 & 0 & 0 \\ -\mathrm{i} & 0 & 0 \end{pmatrix}, \quad J_z \doteq \hbar\begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{4.24}$$

Hence there is a 3-dimensional Hilbert space (not necessarily $\mathbb{R}^3$), that we will call $\mathcal{H}^{j=1}$, that describes the angular momentum of *a particular* physical system. In this case, when we measure J_z we will obtain one of the 3 eigenvalues of J_z $(+\hbar, 0, -\hbar)$ and the state of the system will collapse to the corresponding eigenvector $(|jm\rangle = |11\rangle, |10\rangle, |1-1\rangle)$:

$$\det(J_z - \lambda I) = 0 \Rightarrow \lambda \equiv \hbar m = +\hbar, 0, -\hbar \tag{4.25}$$

$$J_z\,|jm\rangle = \lambda\,|jm\rangle \Rightarrow |11\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \mathrm{i} \\ 0 \end{pmatrix}, \quad |10\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad |1-1\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ \mathrm{i} \\ 0 \end{pmatrix} \tag{4.26}$$

(up to arbitrary global phases). We say that this is the *system of angular momentum* $j = 1$.

One can also write $\vec{J}$ *in the basis of eigenvectors of* J_z, where J_z is diagonal. Check that in this new basis $(|11\rangle, |10\rangle, |1-1\rangle)$ the angular momentum operators read

$$J_x \doteq -\frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad J_y \doteq \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & \mathrm{i} & 0 \\ -\mathrm{i} & 0 & \mathrm{i} \\ 0 & -\mathrm{i} & 0 \end{pmatrix}, \quad J_z \doteq \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{4.27}$$

that can be obtained from (4.26) by the change of basis matrix

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & -1 \\ \mathrm{i} & 0 & \mathrm{i} \\ 0 & \sqrt{2} & 0 \end{pmatrix}. \tag{4.28}$$

using $|\tilde{e}_j\rangle = |e_i\rangle\,U_{ij}$ (2.49) with

$$\{|e_i\rangle\} = \{|e_x\rangle, |e_y\rangle, |e_z\rangle\} \tag{4.29}$$

$$\{|\tilde{e}_j\rangle\} = \{|11\rangle, |10\rangle, |1-1\rangle\}. \tag{4.30}$$

4.3 Systems of spin 1/2

Consider now the following three 2×2 complex Hermitian matrices $J_i = \frac{\hbar}{2}\sigma_i$ with σ_i the Pauli matrices,

$$J_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad J_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad J_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.31}$$

that verify the same commutation relations as the angular momentum (4.19). Thus, they are *another* representation of the angular momentum algebra, the generators of the rotations in the 3-dimensional space of another system (spin $\frac{1}{2}$ system) whose 2-dimensional Hilbert space will be called $\mathcal{H}^{j=\frac{1}{2}}$.

When we measure J_z on a state $|\alpha\rangle$ of a spin $\frac{1}{2}$ system we may find one of the two eigenvalues of J_z ($\pm\frac{\hbar}{2}$). We will label the corresponding eigenvectors $|jm\rangle = \left|\frac{1}{2}\frac{1}{2}\right\rangle, \left|\frac{1}{2}-\frac{1}{2}\right\rangle$, that serve as a basis of the Hilbert space. This is actually the original basis (4.31) in which J_z is diagonal. In this basis any $|\alpha\rangle \in \mathcal{H}^{j=\frac{1}{2}}$ is expressed as

$$|\alpha\rangle \doteq \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}, \quad \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{4.32}$$

How does $|\alpha\rangle$ change under rotations?

$$R_{\hat{z}}(\phi) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}J_z\phi} \doteq \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\frac{\phi}{2}} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\frac{\phi}{2}} \end{pmatrix} \tag{4.33}$$

$$\begin{aligned} R_{\hat{y}}(\phi) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}J_y\phi} &\doteq \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma_y\frac{\phi}{2}} \\ &= I - \mathrm{i}\frac{\phi}{2}\sigma_y + \frac{1}{2!}\left(-\mathrm{i}\frac{\phi}{2}\right)^2\sigma_y^2 + \frac{1}{3!}\left(-\mathrm{i}\frac{\phi}{2}\right)^3\sigma_y^3 \ldots \\ &= I\left[1 - \frac{1}{2!}\left(\frac{\phi}{2}\right)^2 + \ldots\right] - \mathrm{i}\sigma_y\left[\frac{\phi}{2} - \frac{1}{3!}\left(\frac{\phi}{2}\right)^3 + \ldots\right] \\ &= I\cos\frac{\phi}{2} - \mathrm{i}\sigma_y\sin\frac{\phi}{2} \\ &= \begin{pmatrix} \cos\frac{\phi}{2} & -\sin\frac{\phi}{2} \\ \sin\frac{\phi}{2} & \cos\frac{\phi}{2} \end{pmatrix}. \end{aligned} \tag{4.34}$$

Notice that a rotation of 2π radians does *not* take the system back to the original state:

$$R_{\hat{z}}(2\pi)\,|\alpha\rangle = R_{\hat{y}}(2\pi)\,|\alpha\rangle \doteq \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = -\,|\alpha\rangle\,. \tag{4.35}$$

A rotation of 4π would be needed for that purpose! Are there *physical* systems with $\hbar/2$ angular momentum? We will see later that *orbital* wave functions cannot have this angular momentum. However, the *intrinsic* angular momentum (*spin*) of the electron, for example, is $\hbar/2$.

From (4.33) and (4.34) one gets how to perform a general rotation of a spin $\frac{1}{2}$ system,

$$R(\alpha,\beta,\gamma) = R_{\hat{z}}(\alpha)R_{\hat{y}}(\beta)R_{\hat{z}}(\gamma) \doteq \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -\mathrm{e}^{-\mathrm{i}\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ \mathrm{e}^{\mathrm{i}\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & \mathrm{e}^{\mathrm{i}\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix}. \tag{4.36}$$

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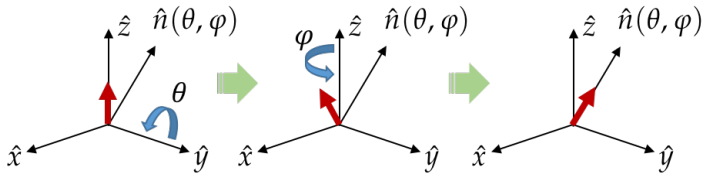
Therefore, rotations in this space are represented by complex unitary 2×2 matrices of unit determinant ($R^\dagger R = I$, $\det R = 1$), that form the group $SU(2)$. The groups $SU(2)$ and $SO(3)$ are *locally* isomorphic: they have the same generators (same algebra). But their *global* properties are different: there are more elements in $SU(2)$ than in $SO(3)$. For instance,

$$SO(3): \; R_{\hat{n}}(0) = R_{\hat{n}}(2\pi) = I \tag{4.37}$$

$$SU(2): \; R_{\hat{n}}(0) \neq R_{\hat{n}}(2\pi) = -I \notin SO(3). \tag{4.38}$$

($SU(2)$ is the universal cover of $SO(3)$, there is a two-to-one relation between them.) Since there are physical systems, like the electron, with spin $\frac{1}{2}$, we will say that the rotation group is $SU(2)$ rather than $SO(3)$.

Rotating the eigenstate $|+\rangle \equiv \left|\frac{1}{2}\frac{1}{2}\right\rangle$ of $J_z = \frac{\hbar}{2}\sigma_z$ (state of spin $+\frac{\hbar}{2}$ in the $\hat{z}$ direction), one can build the state $|+\rangle_{\hat{n}}$ with spin $\frac{\hbar}{2}$ along an arbitrary direction $\hat{n}(\theta, \varphi)$,



$$|+\rangle_{\hat{n}} = R_{\hat{z}}(\varphi) R_{\hat{y}}(\theta) \doteq \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\frac{\varphi}{2}} \cos\frac{\theta}{2} \\ \mathrm{e}^{\mathrm{i}\frac{\varphi}{2}} \sin\frac{\theta}{2} \end{pmatrix}. \tag{4.39}$$

Check that the state $|+\rangle_{\hat{n}}$ is in fact the eigenstate of $\hat{n} \cdot \vec{J}$ with eigenvalue $+\frac{\hbar}{2}$.
In particular (up to global phase) we find the states of Stern-Gerlach experiment:

$$|\pm\rangle_{\hat{x}} = \frac{1}{\sqrt{2}} |+\rangle \pm \frac{1}{\sqrt{2}} |-\rangle, \qquad |\pm\rangle_{\hat{y}} = \frac{1}{\sqrt{2}} |+\rangle \pm \frac{\mathrm{i}}{\sqrt{2}} |-\rangle.$$

4.4 Representations of angular momentum

So far we have constructed two *representations* of angular momentum, $j = \frac{1}{2}$ and $j = 1$. They describe the behaviour of two different systems under spatial rotations. Are there other Hilbert spaces where one can represent the 3 angular momentum operators J_i? One has to find a set of 3 matrices, rotation group generators, that satisfy the commutation relations (4.19).

To label the states of the different representations, and justify our previous notation, let us define the operator

$$[J^2, J_i] = 0, \quad \forall i \quad (J^2 \text{ is a } \textit{Casimir} \text{ operator} = \text{multiple of the identity}). \tag{4.40}$$

It is straightforward to see that J^2 commutes with the 3 generators,

$$[J^2, J_i] = 0, \quad \forall i. \tag{4.41}$$

Then one can take J^2 and one of the J_i, say J_z, as a CSCO and use their simultaneous eigenvectors as a basis of the Hilbert space,

$$J^2 |ab\rangle \equiv \hbar^2 a |ab\rangle, \quad J_z |ab\rangle \equiv \hbar b |ab\rangle. \tag{4.42}$$

To determine the possible values of a and b it is useful to define the *ladder* operatos $J_\pm$,

$$\begin{array}{l} J_+ \equiv J_x + \mathrm{i}J_y \\ J_- \equiv J_x - \mathrm{i}J_y \end{array} \quad \Leftrightarrow \quad \begin{array}{l} J_x \equiv \ \frac{1}{2}(J_+ + J_-) \\ J_y \equiv -\frac{\mathrm{i}}{2}(J_+ - J_-) \end{array}, \quad J_+^\dagger = J_-. \tag{4.43}$$

The commutation relations among the operators J^2, J_+, J_-, J_z are easy to derive from (4.19) and (4.41),

$$[J_+, J_-] = 2\hbar J_z \tag{4.44}$$
$$[J_z, J_\pm] = \pm\hbar J_\pm \tag{4.45}$$
$$[J^2, J_\pm] = 0. \tag{4.46}$$

Then

$$J^2 = J_z^2 + \tfrac{1}{2}J_+J_- + \tfrac{1}{2}J_-J_+ \tag{4.47}$$
$$= J_z^2 - \hbar J_z + J_+J_- \tag{4.48}$$
$$= J_z^2 + \hbar J_z + J_-J_+. \tag{4.49}$$

The strategy to find the basis is the following. Take a vector $|ab\rangle$ and let the algebra operators act on it to obtain new (linearly independent) eigenvectors until the whole basis is obtained.

Notice that if $|ab\rangle$ is an eigenvector of J^2 with eigenvalue $\hbar^2 a$ then $J_+ |ab\rangle$ is also an eigenvector with the same eigenvalue:

$$\begin{aligned} & J^2 |ab\rangle = \hbar^2 a |ab\rangle \\ \Rightarrow \quad & J^2 J_+ |ab\rangle = ([J^2, J_+] + J_+J^2) |ab\rangle = J_+J^2 |ab\rangle = \hbar^2 a\, J_+ |ab\rangle . \end{aligned} \tag{4.50}$$

And $J_+ |ab\rangle$ is also an eigenvector of J_z with eigenvalue $\hbar(b+1)$,

$$\begin{aligned} & J_z |ab\rangle = \hbar b |ab\rangle \\ \Rightarrow \quad & J_z J_+ |ab\rangle = ([J_z, J_+] + J_+J_z) |ab\rangle = (\hbar J_+ + J_+J_z) |ab\rangle = \hbar(b+1)\, J_+ |ab\rangle . \end{aligned} \tag{4.51}$$

Therefore,

$$J_+ |ab\rangle \propto |a\, b+1\rangle . \tag{4.52}$$

The operator J_+ is called the *ascending* operator because it provides vectors of higher J_z. Applying successively J_+,

$$|ab\rangle \xrightarrow{J_+} |a\, b+1\rangle \xrightarrow{J_+} |a\, b+2\rangle \ldots \xrightarrow{J_+} |a\, b_{\max}\rangle . \tag{4.53}$$

There is a last one for which

$$J_+ |a\, b_{\max}\rangle = 0 \tag{4.54}$$

or otherwise we would get an infinite-dimensional Hilbert space (and systems do not have infinite J_z). Analogously, we can act on $|ab\rangle$ with J_- (*descending* operator) and get

$$|ab\rangle \xrightarrow{J_-} |a\, b-1\rangle \xrightarrow{J_-} |a\, b-2\rangle \ldots \xrightarrow{J_-} |a\, b_{\min}\rangle \tag{4.55}$$

with

$$J_- |a\, b_{\min}\rangle = 0. \tag{4.56}$$

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All the basis vectors,

$$\{|a\, b_{\max}\rangle\,, |a\, b_{\max}-1\rangle\,, \ldots, |ab\rangle\,, \ldots, |a\, b_{\min}+1\rangle\,, |a\, b_{\min}\rangle\} \tag{4.57}$$

are eigenvectors of J^2 with the same eigenvalue $\hbar^2 a$. Let us see that a is related to $b_{\max}$ and $b_{\max} = -b_{\min}$. First notice that

$$J^2\,|a\, b_{\max}\rangle = (J_z^2 + \hbar J_z + \cancel{J_-J_+})\,|a\, b_{\max}\rangle = \hbar^2 b_{\max}(b_{\max}+1)\,|a\, b_{\max}\rangle \tag{4.58}$$

and remember that every $|ab\rangle$ is an eigenvector of J^2 with the same eigenvalue. Then it is convenient to change the notation and call

$$\left.\begin{array}{rl} a = b_{\max}(b_{\max}+1) \equiv & j(j+1) \\ b \equiv & m \\ |ab\rangle \equiv & |jm\rangle \end{array}\right\} \quad \Rightarrow \quad \begin{array}{l} J^2\,|jm\rangle = \hbar^2 j(j+1)\,|jm\rangle \\ J_z\,|jm\rangle = \hbar m\,|jm\rangle \end{array} \tag{4.59}$$

and

$$\begin{aligned} |J_\pm\,|jm\rangle\,|^2 &= \langle jm|\,J_\mp J_\pm\,|jm\rangle = \langle jm|\,(J^2 - J_z^2 \mp \hbar J_z)\,|jm\rangle \\ &= \hbar^2[j(j+1) - m(m\pm 1)] \\ \Rightarrow \quad J_\pm\,|jm\rangle &= \hbar\sqrt{j(j+1)-m(m\pm 1)}\,|j\, m\pm 1\rangle\,. \end{aligned} \tag{4.60}$$

where we have used $\langle jm|jm\rangle = 1$ and taken the Condon and Shortley phase convention (later defined in general). We have defined $b_{\max} = j$ and then $J_+\,|jj\rangle = 0$. Let us now define $b_{\min} = l$. Then $J_-\,|jl\rangle = 0$ and

$$j(j+1) - l(l-1) = 0 \quad \Rightarrow \quad l = -j. \tag{4.61}$$

As a consequence, the basis of the Hilbert space $\mathcal{H}^j$ is

$$\{|jj\rangle\,, |j\, j-1\rangle\,, \ldots, |jm\rangle\,, \ldots, |j\ -j+1\rangle\,, |j\ -j\rangle\}. \tag{4.62}$$

What are the possible values of j? We go from $|jj\rangle$ to $|j\ -j\rangle$ through jumps of one unit. Therefore, the difference between j and $-j$ must be a natural number n (number of jumps),

$$j-(-j) = 2j = n = 0, 1, 2, 3, \ldots \quad \Rightarrow \quad j = \frac{n}{2} = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots \tag{4.63}$$

and the dimension of $\mathcal{H}^j$ is $n+1 = 2j+1$. This way we have found the Hilbert spaces describing the possible systems of a given angular momentum, whose bases are

$$\mathcal{H}^{j=0} : \{|00\rangle\}, \tag{4.64}$$

$$\mathcal{H}^{j=\frac{1}{2}} : \{\left|\tfrac{1}{2}\,\tfrac{1}{2}\right\rangle, \left|\tfrac{1}{2}\ -\tfrac{1}{2}\right\rangle\}, \tag{4.65}$$

$$\mathcal{H}^{j=1} : \{|11\rangle\,, |10\rangle\,, |1\ -1\rangle\}, \tag{4.66}$$

$$\mathcal{H}^{j=\frac{3}{2}} : \{\left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle, \left|\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\ -\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\ -\tfrac{3}{2}\right\rangle\}, \text{ etc.} \tag{4.67}$$

Given a value of j, from the action of J_z, J_+ and J_- on the basis vectors $\{|jm\rangle\}$ one can obtain the matrices that represent the J_i, using (4.59) and (4.60). For example, the 4×4 matrices of the $j = \frac{3}{2}$ representation are

$$J_z\,(\left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle, \left|\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\ -\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\ -\tfrac{3}{2}\right\rangle)$$

$$= \left(\left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle, \left|\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\,-\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\,-\tfrac{3}{2}\right\rangle\right)\hbar \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix} \tag{4.68}$$

$$J_+ \left(\left|\tfrac{3}{2}, \tfrac{3}{2}\right\rangle, \left|\tfrac{3}{2}, \tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\,-\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\,-\tfrac{3}{2}\right\rangle\right)$$

$$= \left(\left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle, \left|\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\,-\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\,-\tfrac{3}{2}\right\rangle\right)\hbar \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.69}$$

$$J_- \left(\left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle, \left|\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\,-\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\,-\tfrac{3}{2}\right\rangle\right)$$

$$= \left(\left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle, \left|\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\,-\tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\,-\tfrac{3}{2}\right\rangle\right)\hbar \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \tag{4.70}$$

that implies

$$J_x \doteq \tfrac{1}{2}(J_+ + J_-) = \frac{\hbar}{2} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \tag{4.71}$$

$$J_y \doteq -\tfrac{\mathrm{i}}{2}(J_+ - J_-) = \mathrm{i}\frac{\hbar}{2} \begin{pmatrix} 0 & -\sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & -2 & 0 \\ 0 & 2 & 0 & -\sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \tag{4.72}$$

$$J_z \doteq \hbar \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}. \tag{4.73}$$

These are *irreducible* representations of the generators (there is no basis where these matrices can be simultaneously reduced into smaller diagonal blocks). Taking the tensor product of two representations, j_1 and j_2, one can obtain another (reducible) representation of a higher dimension, $(2j_1+1)(2j_2+1)$,

$$\mathcal{H}^{j_1} : \{|j_1 m_1\rangle\}, \quad \mathcal{H}^{j_2} : \{|j_2 m_2\rangle\}, \tag{4.74}$$

that contains (is the direct sum of) irreducible representations of spin j

$$\mathcal{H} = \mathcal{H}^{j_1} \otimes \mathcal{H}^{j_2} = \bigoplus_j \mathcal{H}^j \quad \text{with} \quad j = |j_1 - j_2|, |j_1 - j_2| + 1, \ldots, j_1 + j_2. \tag{4.75}$$

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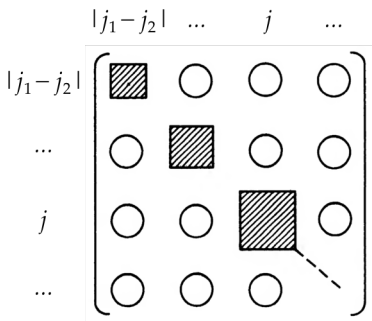
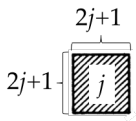
Then

$J_{x,y,z} =$ 

where 

$$\sum_{j=|j_1-j_2|}^{j_1+j_2} 2j+1 = (2j_1+1)(2j_2+1). \tag{4.76}$$

The basis vectors of the *invariant subspaces* with well defined j , $|jm\rangle$, do not have well defined j_1 and j_2 in general, but are combinations (entangled states) of the direct product basis vectors $|j_1m_1\rangle\,|j_2m_2\rangle$ (see §4.7). For example (as we will see in Eqs. (4.127)–(4.130)): $\mathcal{H}^{j=\frac{1}{2}} \otimes \mathcal{H}^{j=\frac{1}{2}} = \mathcal{H}^{j=0} \oplus \mathcal{H}^{j=1}$

$$\mathcal{H}^{j=\frac{1}{2}} \otimes \mathcal{H}^{j=\frac{1}{2}}: \quad \{|+\rangle\,|+\rangle\,, |+\rangle\,|-\rangle\,, |-\rangle\,|+\rangle\,, |-\rangle\,|-\rangle\} \tag{4.77}$$

$$\mathcal{H}^{j=0}: \quad |0\,0\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle\,|-\rangle - |-\rangle\,|+\rangle\right) \tag{4.78}$$

$$\mathcal{H}^{j=1}: \quad \begin{cases} |1\,1\rangle = |+\rangle\,|+\rangle \\ |1\,0\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle\,|-\rangle + |-\rangle\,|+\rangle\right) \\ |1\,-1\rangle = |-\rangle\,|-\rangle \end{cases} \tag{4.79}$$

with $|+\rangle \equiv \left|\frac{1}{2}\,\frac{1}{2}\right\rangle$ and $|-\rangle \equiv \left|\frac{1}{2}\,-\frac{1}{2}\right\rangle$.

Once you know the spin j representation of the angular momentum generators, the *rotation matrices* of the rotation operators $R(\alpha,\beta,\gamma)$ in the basis $\{|jm\rangle\}$ follow by Taylor expanding the exponential of generator J_y,[c]

$$\begin{aligned} D^j_{m'm}(\alpha,\beta,\gamma) &= \left\langle jm'\right| \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}J_z\alpha}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}J_y\beta}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}J_z\gamma} \left|jm\right\rangle \\ &= \mathrm{e}^{-\mathrm{i}m'\alpha}\left\langle jm'\right| \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}J_y\beta} \left|jm\right\rangle \mathrm{e}^{-\mathrm{i}m\gamma} \equiv \mathrm{e}^{-\mathrm{i}(m'\alpha+m\gamma)} d^j_{m'm}(\beta). \end{aligned} \tag{4.80}$$

4.5 Spin and orbital angular momentum

In the Stern-Gerlach experiment we have seen that there are systems whose orbital angular momentum $\vec{L}$ is zero but have a non vanishing angular momentum, that we call spin $\vec{S}$. The spin would be analogous to the intrinsic angular momentum of a *pointlike* particle rotating around an inner axis (classically this has no sense). But there are quantum systems that behave this way: electrons (spin $\frac{1}{2}$), photons (spin 1), gravitons (spin 2), etc.

We have seen that the group of rotations admits representations of $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$. However the orbital wave functions must be invariant under rotations of 2π radians. As a consequence, the orbital angular momentum is restricted to representations of integer $\ell = 0, 1, 2, \ldots$, whereas spin representations may have $s = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$.

[c] This is not so simple for $j > 1$. Nevertheless there are other ways to obtain $d^j_{m'm}(\theta)$ that lead to Wigner's formula (vid. book by Sakurai, p. 223). These matrices are collected in tables for low j in many books.

In general, the total angular momentum of the system is given by the sum of the orbital and the spin angular momenta,

$$\vec{J} = \vec{L} + \vec{S}. \tag{4.81}$$

In section §4.7 we will see how to obtain the irreducible representations contained in the addition of whatever two angular momentum representations j_1 and j_2.

4.6 Spherical harmonics

Let us consider a *spinless* system with spherical symmetry. Then all L_i commute with the Hamiltonian H (the rotated state of an energy eigenstate will have the same energy):

$$H\,|n\rangle = E_n\,|n\rangle\,, \quad [L_i, H] = 0 \quad \Rightarrow \quad H(L_i\,|n\rangle) = L_i H\,|n\rangle = E_n(L_i\,|n\rangle). \tag{4.82}$$

As a consequence, H, L^2 and L_z have a common set of eigenstates,

$$H\,|n\ell m\rangle = E_n\,|n\ell m\rangle \tag{4.83}$$
$$L^2\,|n\ell m\rangle = \hbar^2\,\ell(\ell+1)\,|n\ell m\rangle \tag{4.84}$$
$$L_z\,|n\ell m\rangle = \hbar\,m\,|n\ell m\rangle\,. \tag{4.85}$$

It is convenient to write the wave function $\psi(\vec{x})$ in spherical coordinates,

$$\begin{array}{l} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{array} \qquad \langle\vec{x}|\psi\rangle = \psi(\vec{x}) = \psi(r,\theta,\varphi). \tag{4.86}$$

The orbital angular momentum operators in spherical coordinates are [exercise]:

$$L_x \doteq -\mathrm{i}\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = \mathrm{i}\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right) \tag{4.87}$$
$$L_y \doteq -\mathrm{i}\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) = -\mathrm{i}\hbar\left(\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right) \tag{4.88}$$
$$L_z \doteq -\mathrm{i}\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -\mathrm{i}\hbar\frac{\partial}{\partial\varphi} \tag{4.89}$$
$$L^2 \doteq -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]. \tag{4.90}$$

They do not depend on the radial coordinate r. On the other hand [exercise],

$$P^2 \doteq -\hbar^2\nabla^2 = -\hbar^2\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{L^2}{\hbar^2 r^2}\right). \tag{4.91}$$

Hence, $[L_i, P^2] = 0$ and the (conservative) system is described by a central potential $V(r)$,

$$0 = [L_i, H] = [L_i, V] \quad \Leftrightarrow \quad V = V(r). \tag{4.92}$$

Then the wave function can be separated in a radial part and an angular part,

$$\langle\vec{x}|n\ell m\rangle = R_{n\ell}(r)Y_\ell^m(\theta,\varphi) \tag{4.93}$$

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where both parts are normalized,

$$\langle\psi|\psi\rangle = \int \mathrm{d}^3x\,|\psi(\vec{x})|^2 = \int_0^\infty \mathrm{d}r\,r^2 \int_{-1}^1 \mathrm{d}\cos\theta \int_0^{2\pi} \mathrm{d}\varphi\;|\psi(r,\theta,\varphi)|^2 = 1$$
$$\Rightarrow \quad \int_0^\infty \mathrm{d}r\,r^2|R_{n\ell}(r)|^2 = 1, \quad \int_{-1}^1 \mathrm{d}\cos\theta \int_0^{2\pi} \mathrm{d}\varphi\,|Y_\ell^m(\theta,\varphi)|^2 = 1. \tag{4.94}$$

The *spherical harmonics* are the eigenfunctions of angular momentum in the position representation

$$-\mathrm{i}\hbar\frac{\partial}{\partial\varphi}Y_\ell^m(\theta,\varphi) = \hbar m\,Y_\ell^m(\theta,\varphi) \tag{4.95}$$
$$-\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]Y_\ell^m(\theta,\varphi) = \hbar^2\ell(\ell+1)\,Y_\ell^m(\theta,\varphi) \tag{4.96}$$

satisfying the orthonormality relations

$$\int_{-1}^1 \mathrm{d}\cos\theta \int_0^{2\pi} \mathrm{d}\varphi\,Y_\ell^{m*}(\theta,\varphi)Y_{\ell'}^{m'}(\theta,\varphi) = \delta_{\ell\ell'}\delta_{mm'}. \tag{4.97}$$

They can be found in tables. If the radial dependence of the wave function factors out,

$$\psi(r,\theta,\varphi) = (\langle r|\,\langle\theta\varphi|)\,|\psi\rangle = f(r)\,\Psi(\theta,\varphi) \tag{4.98}$$

then the angular dependence can be expanded in spherical harmonics that give the angular momentum of the system,

$$\Psi(\theta,\varphi) = \sum_{\ell=0}^\infty \sum_{m=-\ell}^{\ell} c_\ell^m\,Y_\ell^m(\theta,\varphi) \tag{4.99}$$

with

$$c_\ell^m = \int_{-1}^1 \mathrm{d}\cos\theta \int_0^{2\pi} \mathrm{d}\varphi\,Y_\ell^{m*}(\theta,\varphi)\,\Psi(\theta,\varphi) \tag{4.100}$$

where $|c_\ell^m|^2$ is the probability to find the system in the state of angular momentum ℓ, m. And the probability density to find the system along the direction (θ,φ) is

$$\int_0^\infty \mathrm{d}r\,r^2\,|\psi(r,\theta,\varphi)|^2 = |\Psi(\theta,\varphi)|^2. \tag{4.101}$$

If the (spinless) system has a well defined orbital angular momentum then the probability density along the direction (θ,φ) is just

$$|Y_\ell^m(\theta,\varphi)|^2. \tag{4.102}$$

4.7 Addition of angular momenta

Suppose we have two spin $\frac{1}{2}$ particles bound together; for example, two quarks in a meson ($\bar{\mathrm{q}}\mathrm{q}$). If the orbital angular momentum $\vec{L}$ of the system is zero ($\ell = 0$), what is the spin of the meson?

Analogously, suppose we have a single particle of spin s turning in a central potential with orbital angular momentum ℓ. What is the Hilbert space associated to the total angular momentum of the particle?

The formalism in both cases is the same. As we have seen in a previous chapter, when we *compose* two quantum systems the resulting Hilbert space is the direct product (or tensor product) of the Hilbert spaces of the two *sub*systems, $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$.

Consider $\vec{J}_1$ and $\vec{J}_2$ the angular momentum operators acting on $\mathcal{H}^{j_1}$ and $\mathcal{H}^{j_2}$, respectively. Then their action on $\mathcal{H} = \mathcal{H}^{j_1} \otimes \mathcal{H}^{j_2}$ is given by

$$\vec{J}_1 \otimes I \equiv \vec{J}_1 \quad \text{and} \quad I \otimes \vec{J}_2 \equiv \vec{J}_2 \tag{4.103}$$

(abusing of the notation) and the total angular momentum is

$$\vec{J} = \vec{J}_1 \otimes I + I \otimes \vec{J}_2 \equiv \vec{J}_1 + \vec{J}_2. \tag{4.104}$$

Notice that, since $\vec{J}_1$ and $\vec{J}_2$ act on different spaces,

$$[\vec{J}_1, \vec{J}_2] = 0 \tag{4.105}$$

and verify separately the generator algebra,

$$[J_{pi}, J_{pj}] = \mathrm{i}\hbar\epsilon_{ijk}J_{pk} \quad (p = 1, 2) \qquad [J_i, J_j] = \mathrm{i}\hbar\epsilon_{ijk}J_k. \tag{4.106}$$

The $(2j_1 + 1)(2j_2 + 1)$ dimensional representation of $\vec{J}$ on $\mathcal{H}$ is reducible, in general, and in the direct product basis $\{|j_1 m_1; j_2 m_2\rangle \equiv |j_1 m_1\rangle\,|j_2 m_2\rangle\}$ can be obtained from

$$\vec{J}\,|j_1 m_1; j_2 m_2\rangle = (\vec{J}_1\,|j_1 m_1\rangle)\,|j_2 m_2\rangle + |j_1 m_1\rangle\,(\vec{J}_2\,|j_2 m_2\rangle). \tag{4.107}$$

We would like to find its irreducible components, going to a basis where the block structure is manifest. Every irreducible prepresentation (irrep) of $\vec{J}$ is labeled by an eigenvalue of J^2, and the corresponding states by the eigenvalues of J_z, where

$$\begin{aligned} J^2 &= J_1^2 \otimes I + I \otimes J_2^2 + (\vec{J}_1 \otimes I) \cdot (I \otimes \vec{J}_2) + (I \otimes \vec{J}_2) \cdot (\vec{J}_1 \otimes I) \\ &= J_1^2 \otimes I + I \otimes J_2^2 + 2 \sum_{i=x,y,z} J_{1i} \otimes J_{2i} \equiv J_1^2 + J_2^2 + 2\vec{J}_1 \cdot \vec{J}_2 \end{aligned} \tag{4.108}$$

$$J_z = J_{1z} \otimes I + I \otimes J_{2z} \qquad \equiv \vec{J}_{1z} + \vec{J}_{2z}. \tag{4.109}$$

Notice that the operators J_1^2, J_2^2, J^2, J_z commute with each other. However, $[J^2, J_{1z}] \neq 0$ and $[J^2, J_{2z}] \neq 0$. Therefore, apart from the original basis, eigenstates of $J_1^2, J_2^2, J_{1z}, J_{2z}$ ($|j_1 m_1; j_2 m_2\rangle$), we can define another basis of eigenstates of J_1^2, J_2^2, J^2, J_z ($|j_1 j_2 j m\rangle$). Given j_1 and j_2, both bases have the same number of vectors $(2j_1 + 1)(2j_2 + 1)$, that can be expressed one in terms of the other,

$$|j_1 j_2 j m\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |j_1 m_1; j_2 m_2\rangle\,\langle j_1 m_1; j_2 m_2 | j_1 j_2 j m\rangle\,. \tag{4.110}$$

The elements of the change of basis matrix

$$\langle j_1 m_1; j_2 m_2 | j m\rangle \tag{4.111}$$

are called *Clebsch-Gordan* coefficients (CGC).

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Clearly, $\langle j_1 m_1; j_2 m_2 | j_1 j_2 j m\rangle = 0$ if $m \neq m_1 + m_2$ since

$$\begin{aligned} 0 &= \langle j_1 m_1; j_2 m_2 |\, 0 \,| jm\rangle \\ &= \langle j_1 m_1; j_2 m_2 |\, (J_z - J_{1z} - J_{2z}) \,| jm\rangle \\ &= \hbar(m - m_1 - m_2)\, \langle j_1 m_1; j_2 m_2 | jm\rangle\,. \end{aligned} \tag{4.112}$$

Hence, $m = m_1 + m_2$ and the maximum value of m is

$$m^{\max} = m_1^{\max} + m_2^{\max} = j_1 + j_2 \quad \Rightarrow \quad j^{\max} = j_1 + j_2. \tag{4.113}$$

Then from (4.110) the "maximum weight" state ($j = j_1 + j_2$, $m = j_1 + j_2$) is

$$|(j_1 + j_2)\,(j_1 + j_2)\rangle = |j_1 j_1; j_2 j_2\rangle\, \langle j_1 j_1; j_2 j_2 | (j_1 + j_2)\,(j_1 + j_2)\rangle \tag{4.114}$$

since only $m_1 = j_1$ and $m_2 = j_2$ contribute. In the Condon and Shortley phase convention,

$$\langle j_1 j_1; j_2 j_2 | (j_1 + j_2)\,(j_1 + j_2)\rangle = 1. \tag{4.115}$$

Acting on this state with J_- we generate the $2(j_1 + j_2) + 1$ states of the irrep $j = j_1 + j_2$. Likewise one proceeds starting with the state $|j_1 j_2\,(j_1 + j_2 - 1)\,(j_1 + j_2 - 1)\rangle$, that is fixed up to a phase because it must be orthogonal to $|j_1 j_2\,(j_1 + j_2)\,(j_1 + j_2 - 1)\rangle$ and has unit norm. And then we repeat the process for the rest of the j until $j = |j_1 - j_2|$. Let us see this with an example: $j_1 = 1$ and $j_2 = \frac{1}{2}$.

- We start by

$$\left|1\tfrac{1}{2}\ \tfrac{3}{2}\tfrac{3}{2}\right\rangle = |11\rangle \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle. \tag{4.116}$$

- Apply J_- to this state:

$$\begin{aligned} J_- \left|1\tfrac{1}{2}\ \tfrac{3}{2}\tfrac{3}{2}\right\rangle &= (J_- |11\rangle) \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + |11\rangle\, (J_- \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle) \\ \sqrt{3}\left|1\tfrac{1}{2}\ \tfrac{3}{2}\tfrac{1}{2}\right\rangle &= \sqrt{2}\,|10\rangle \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + |11\rangle \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle \\ \Rightarrow \quad \left|1\tfrac{1}{2}\ \tfrac{3}{2}\tfrac{1}{2}\right\rangle &= \sqrt{\frac{2}{3}}\,|10\rangle \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + \frac{1}{\sqrt{3}}\,|11\rangle \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle. \end{aligned} \tag{4.117}$$

- Apply to J_- succesively to the states we find:

$$\begin{aligned} J_- \left|1\tfrac{1}{2}\ \tfrac{3}{2}\tfrac{1}{2}\right\rangle &= \sqrt{\frac{2}{3}}(J_- |10\rangle) \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\,|10\rangle\, (J_- \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle) + \frac{1}{\sqrt{3}}(J_- |11\rangle) \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle \\ 2\left|1\tfrac{1}{2}\ \tfrac{3}{2} - \tfrac{1}{2}\right\rangle &= \frac{2}{\sqrt{3}}\,|1-1\rangle \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\,|10\rangle \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\,|10\rangle \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle \\ &= \frac{2}{\sqrt{3}}\,|1-1\rangle \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + 2\sqrt{\frac{2}{3}}\,|10\rangle \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle \\ \Rightarrow \quad \left|1\tfrac{1}{2}\ \tfrac{3}{2} - \tfrac{1}{2}\right\rangle &= \frac{1}{\sqrt{3}}\,|1-1\rangle \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\,|10\rangle \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle. \end{aligned} \tag{4.118}$$

$$\begin{aligned} J_- \left|1\tfrac{1}{2}\ \tfrac{3}{2} - \tfrac{1}{2}\right\rangle &= \frac{1}{\sqrt{3}}\,|1-1\rangle\, (J_- \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle) + \sqrt{\frac{2}{3}}(J_- |10\rangle) \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle \\ \sqrt{3}\left|1\tfrac{1}{2}\ \tfrac{3}{2} - \tfrac{3}{2}\right\rangle &= \frac{1}{\sqrt{3}}\,|1-1\rangle \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle + \frac{2}{\sqrt{3}}\,|1-1\rangle \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle \\ &= \sqrt{3}\,|1-1\rangle \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle \\ \Rightarrow \quad \left|1\tfrac{1}{2}\ \tfrac{3}{2} - \tfrac{3}{2}\right\rangle &= |1-1\rangle \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle. \end{aligned} \tag{4.119}$$

- Now consider the state $\left|1\tfrac{1}{2}\ \tfrac{1}{2}\tfrac{1}{2}\right\rangle$. It must be a unit vector orthogonal to $\left|1\tfrac{1}{2}\ \tfrac{3}{2}\tfrac{1}{2}\right\rangle$. Then

$$\left|1\tfrac{1}{2}\ \tfrac{1}{2}\tfrac{1}{2}\right\rangle = -\frac{1}{\sqrt{3}}\left|10\right\rangle\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\left|11\right\rangle\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle \tag{4.120}$$

  in the phase convention of Condon and Shortley, $\langle j_1 j_1; j_2\, j-j_1|jj\rangle \geq 0$.

- Apply J_- to the previous state:

$$\begin{aligned} J_-\left|1\tfrac{1}{2}\ \tfrac{1}{2}\tfrac{1}{2}\right\rangle &= -\frac{1}{\sqrt{3}}(J_-\left|10\right\rangle)\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle - \frac{1}{\sqrt{3}}\left|10\right\rangle(J_-\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle) + \sqrt{\frac{2}{3}}(J_-\left|11\right\rangle)\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle \\ \left|1\tfrac{1}{2}\ \tfrac{1}{2}-\tfrac{1}{2}\right\rangle &= -\sqrt{\frac{2}{3}}\left|1-1\right\rangle\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle - \frac{1}{\sqrt{3}}\left|10\right\rangle\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle + \frac{2}{\sqrt{3}}\left|10\right\rangle\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle \\ \Rightarrow\quad \left|1\tfrac{1}{2}\ \tfrac{1}{2}-\tfrac{1}{2}\right\rangle &= -\sqrt{\frac{2}{3}}\left|1-1\right\rangle\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + \frac{1}{\sqrt{3}}\left|10\right\rangle\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle. \end{aligned} \tag{4.121}$$

With this procedure we can read the CGC by taking the scalar products

$$\langle j_1 m_1; j_2 m_2|jm\rangle = (\langle j_1 m_1|\,\langle j_2 m_2|)\,|jm\rangle\,. \tag{4.122}$$

For a few values of j_1 and j_2 they are collected in tables of the form

$j_1\otimes j_2$		j	j	$\cdots$
		m	m	$\cdots$
m_1	m_2			
m_1	m_2		CGC	
$\vdots$	$\vdots$			

In the previous example, we have found (empty entries are zero)

$1\otimes\frac{1}{2}$		$\frac{3}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{3}{2}$
		$\frac{3}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$
1	$\frac{1}{2}$	1					
1	$-\frac{1}{2}$		$\frac{1}{\sqrt{3}}$	$\sqrt{\frac{2}{3}}$			
0	$\frac{1}{2}$		$\sqrt{\frac{2}{3}}$	$-\frac{1}{\sqrt{3}}$			
0	$-\frac{1}{2}$				$\sqrt{\frac{2}{3}}$	$\frac{1}{\sqrt{3}}$	
-1	$\frac{1}{2}$				$\frac{1}{\sqrt{3}}$	$-\sqrt{\frac{2}{3}}$	
-1	$-\frac{1}{2}$						1

Analogously, check that for $j_1 = j_2 = \frac{1}{2}$ one obtains (as we had anticipated):

$$\left|\tfrac{1}{2}\tfrac{1}{2}\ 11\right\rangle = \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle \tag{4.123}$$

$$\left|\tfrac{1}{2}\tfrac{1}{2}\ 10\right\rangle = \frac{1}{\sqrt{2}}\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + \frac{1}{\sqrt{2}}\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle \tag{4.124}$$

$$\left|\tfrac{1}{2}\tfrac{1}{2}\ 1-1\right\rangle = \left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle \tag{4.125}$$

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$$\left|\tfrac{1}{2}\tfrac{1}{2}\,00\right\rangle = -\frac{1}{\sqrt{2}}\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + \frac{1}{\sqrt{2}}\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle \tag{4.126}$$

or in a simplified notation,

$$|11\rangle = |+\rangle\,|+\rangle \tag{4.127}$$

$$|10\rangle = \frac{1}{\sqrt{2}}(|+\rangle\,|-\rangle + |-\rangle\,|+\rangle) \tag{4.128}$$

$$|1-1\rangle = |-\rangle\,|-\rangle \tag{4.129}$$

$$|00\rangle = \frac{1}{\sqrt{2}}(|+\rangle\,|-\rangle - |-\rangle\,|+\rangle) \tag{4.130}$$

and hence

$\frac{1}{2}\otimes\frac{1}{2}$		1	1	0	0
		1	0	0	-1
$\frac{1}{2}$	$\frac{1}{2}$	1			
$\frac{1}{2}$	$-\frac{1}{2}$		$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	
$-\frac{1}{2}$	$\frac{1}{2}$		$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	
$-\frac{1}{2}$	$-\frac{1}{2}$				1

We can now explore the physical consequences of this formalism applying it to the two examples at the beginning of the section.

Consider the two spin $\frac{1}{2}$ quarks composing a meson with $\ell = 0$. Suppose they are in a state of total spin $|sm\rangle = |10\rangle$. This is an entangled state where the individual spin states of each quark $\left(|+\rangle \equiv \left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle, |-\rangle \equiv \left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle\right)$ are not well defined,

$$|\psi\rangle = |sm\rangle\,|10\rangle = \frac{1}{\sqrt{2}}(|+\rangle\,|-\rangle + |-\rangle\,|+\rangle). \tag{4.131}$$

If we measure the spin of the first quark, what is the probability to obtain, for instance, $S_{1z} = +\frac{\hbar}{2}$? And what is the state $|\psi'\rangle$ of the system after the measurement? Following the postulates of QM,

$$P_{S_{1z},+} = |+\rangle\langle+| \otimes I_{s_2} \qquad P_{S_{1z},+}\,|\psi\rangle = \frac{1}{\sqrt{2}}\,|+\rangle\,|-\rangle \tag{4.132}$$

$$p_{1_+} = \langle\psi|\,P_{S_{1z},+}\,|\psi\rangle = \frac{1}{2} \qquad \|P_{S_{1z},+}\,|\psi\rangle\,\| = \sqrt{\langle\psi|\,P_{S_{1z},+}\,|\psi\rangle} \tag{4.133}$$

$$|\psi\rangle \to \left|\psi'\right\rangle = \frac{P_{S_{1z},+}\,|\psi\rangle}{\|P_{S_{1z},+}\,|\psi\rangle\,\|} = |+\rangle\,|-\rangle\,. \tag{4.134}$$

Consider now the example of a spin $s = \frac{1}{2}$ particle bound in a central potential with $\ell = 1$. Suppose it is in the following state of total angular momentum j,

$$|\psi\rangle = |jm\rangle = \left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\,|10\rangle\,|-\rangle - \sqrt{\frac{2}{3}}\,|1-1\rangle\,|+\rangle\,. \tag{4.135}$$

Since the orbital angular momentum is well defined, the radial part of the wave function is separable. In contrast, spatial direction and spin can be entangled, as happens here,

$$\langle r\theta\varphi|\psi\rangle = f(r)\left\langle\theta\varphi\right|\left.\tfrac{1}{2}-\tfrac{1}{2}\right\rangle$$

$$= f(r)\left\{\frac{1}{\sqrt{3}}\langle\theta\varphi|10\rangle\,|-\rangle - \sqrt{\frac{2}{3}}\langle\theta\varphi|1-1\rangle\,|+\rangle\right\}$$
$$= f(r)\left\{\frac{1}{\sqrt{3}}Y_1^0(\theta,\varphi)\,|-\rangle - \sqrt{\frac{2}{3}}Y_1^{-1}(\theta,\varphi)\,|+\rangle\right\}. \tag{4.136}$$

What is the angular distribution of the particle, i.e. the probability density to find it along the direction (θ,φ)? Since the radial part factors out and it is normalized,

$$P_{\theta\varphi} = |\theta\varphi\rangle\langle\theta\varphi| \otimes I_{\text{spin}} \tag{4.137}$$
$$P_{\theta\varphi}\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle = |\theta\varphi\rangle\left[\frac{1}{\sqrt{3}}Y_1^0(\theta,\varphi)\,|-\rangle - \sqrt{\frac{2}{3}}Y_1^{-1}(\theta,\varphi)\,|+\rangle\right] \tag{4.138}$$
$$p_{\theta\varphi} = \left\langle\tfrac{1}{2}-\tfrac{1}{2}\right| P_{\theta\varphi}\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle = \frac{1}{3}|Y_1^0(\theta,\varphi)|^2 + \frac{2}{3}|Y_1^{-1}(\theta,\varphi)|^2. \tag{4.139}$$

What is the probability (density) to find particles along the direction (θ,φ) with $S_z = +\frac{\hbar}{2}$?

$$P_{S_z,+} = |\theta\varphi\rangle\langle\theta\varphi| \otimes |+\rangle\langle+| \tag{4.140}$$
$$P_{S_z,+}\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle = -\,|\theta\varphi\rangle\,|+\rangle\sqrt{\frac{2}{3}}Y_1^{-1}(\theta,\varphi) \tag{4.141}$$
$$p_+ = \left\langle\tfrac{1}{2}-\tfrac{1}{2}\right| P_{S_z,+}\left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle = \frac{2}{3}|Y_1^{-1}(\theta,\varphi)|^2. \tag{4.142}$$

But if one filters the particles along the direction (θ,φ), what is the probability that they have $S_z = +\frac{\hbar}{2}$? After the measurement of (θ,φ) the state $|\psi\rangle$ (ignore the radial part) collapses to

$$\left|\psi'\right\rangle = \frac{P_{\theta\varphi}\,|\psi\rangle}{\|P_{\theta\varphi}\,|\psi\rangle\,\|} = |\theta\varphi\rangle\,\frac{\frac{1}{\sqrt{3}}Y_1^0(\theta,\varphi)\,|-\rangle - \sqrt{\frac{2}{3}}Y_1^{-1}(\theta,\varphi)\,|+\rangle}{\sqrt{\frac{1}{3}|Y_1^0(\theta,\varphi)|^2 + \frac{2}{3}|Y_1^{-1}(\theta,\varphi)|^2}} \tag{4.143}$$

The probability to find $S_z = +\frac{\hbar}{2}$ on this state is given by

$$P_{S_z,+} = I_{\text{orbital}} \otimes |+\rangle\langle+| \tag{4.144}$$
$$P_{S_z,+}\left|\psi'\right\rangle = -\frac{\sqrt{\frac{2}{3}}Y_1^{-1}(\theta,\varphi)\,|\theta\varphi\rangle\,|+\rangle}{\sqrt{\frac{1}{3}|Y_1^0(\theta,\varphi)|^2 + \frac{2}{3}|Y_1^{-1}(\theta,\varphi)|^2}} \tag{4.145}$$
$$p = \left\langle\psi'\right| P_{S_z,+}\left|\psi'\right\rangle = \frac{\frac{2}{3}|Y_1^{-1}(\theta,\varphi)|^2}{\frac{1}{3}|Y_1^0(\theta,\varphi)|^2 + \frac{2}{3}|Y_1^{-1}(\theta,\varphi)|^2}. \tag{4.146}$$

As a final comment, notice that the case of two particles of masses m_1 and m_2 and spins $\vec{S}_1$ and $\vec{S}_2$ interacting with each other via a (spin-independent) potential $V(|\vec{x}_1-\vec{x}_2|)$ can be reduced to one particle of mass m and spin $\vec{S} = \vec{S}_1+\vec{S}_2$ bound in a central potential $V(r)$, with

$$m = \frac{m_1 m_2}{M}, \quad M = m_1+m_2, \quad \vec{x} = \vec{x}_1-\vec{x}_2, \quad \vec{x}_{\text{CM}} = \frac{m_1\vec{x}_1+m_2\vec{x}_2}{M}. \tag{4.147}$$

In fact, the system is equivalent to one particle of mass M at the center of mass of the system moving with constant momentum $\vec{p}_{\text{CM}} = M\dot{\vec{x}}_{\text{CM}}$ and one particle of mass m with momentum $\vec{p} = m\dot{\vec{x}}$,

$$H = \frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} + V(|\vec{x}_1-\vec{x}_2|) = \frac{\vec{p}_{\text{CM}}^{\,2}}{2M} + \frac{\vec{p}^{\,2}}{2m} + V(r). \tag{4.148}$$

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Hence, in the center of mass frame,

$$H = \frac{\vec{p}^2}{2m} + V(r). \tag{4.149}$$

4.8 Vector operators

We have already introduced several operators that are vectors, like $\vec{X}$, $\vec{P}$, $\vec{L}$, $\vec{S}$, ..., but we have not yet discussed how they transform under rotations.

In classical physics, a vector $\vec{V}$ is a quantity with 3 components that, by definition, transform under a rotation R like

$$V_i \to R_{ij} V_j. \tag{4.150}$$

It is reasonable to demand that the expectation value of a *vector operator* $\vec{V}$ in QM transforms like a classical vector under rotations,

$$|\psi\rangle \to D(R)\,|\psi\rangle \tag{4.151}$$

$$\langle\psi|\, V_i\, |\psi\rangle \to \langle\psi|\, D^\dagger(R) V_i D(R)\, |\psi\rangle = R_{ij}\, \langle\psi|\, V_j\, |\psi\rangle\,. \tag{4.152}$$

Since this must be true for any state $|\psi\rangle$, this leads to the operator equation

$$D^\dagger(R) V_i D(R) = R_{ij} V_j \tag{4.153}$$

where R is a 3×3 matrix while $D(R)$ and V_i are operators acting on our Hilbert space of arbitrary dimension.

For an infinitesimal rotation $\delta\phi$ around an axis $\hat{n}$,

$$D(R) = I - \frac{\mathrm{i}}{\hbar}\delta\phi\, \hat{n}\cdot\vec{J}, \tag{4.154}$$

the opeator equation above reads

$$V_i - \frac{\mathrm{i}}{\hbar}\delta\phi[V_i,\, \hat{n}\cdot\vec{J}] = R_{ij}(\hat{n};\delta\phi) V_j. \tag{4.155}$$

And remembering that

$$R(\hat{x};\delta\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -\delta\phi \\ 0 & \delta\phi & 1 \end{pmatrix} \quad R(\hat{y};\delta\phi) = \begin{pmatrix} 1 & 0 & \delta\phi \\ 0 & 1 & 0 \\ -\delta\phi & 0 & 1 \end{pmatrix} \quad R(\hat{z};\delta\phi) = \begin{pmatrix} 1 & -\delta\phi & 0 \\ \delta\phi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{4.156}$$

one easily gets that relation (4.152) is equivalent to

$$[V_i, J_j] = \mathrm{i}\hbar\epsilon_{ijk} V_k. \tag{4.157}$$

This can be taken as a defining property of a vector operator. Check that in fact this property is fulfilled by the vector operators we have introduced so far, like $\vec{J}$, $\vec{X}$, $\vec{P}$:

$$V_i = J_i: \qquad [J_i, J_j] = \mathrm{i}\hbar\epsilon_{ijk} J_k \tag{4.158}$$

$$V_i = X_i: \qquad [X_i, L_j] = \mathrm{i}\hbar\epsilon_{ijk} X_k \tag{4.159}$$

$$V_i = P_i: \qquad [P_i, L_j] = \mathrm{i}\hbar\epsilon_{ijk} P_k. \tag{4.160}$$

4.9 Tensor operators

A Cartesian tensor $T_{i_1 i_2 \cdots i_r}$ is a generalization of a vector V_i, that under rotations R transforms as

$$T_{i_1 i_2 \cdots i_r} \to R_{i_1 j_1} R_{i_2 j_2} \cdots R_{i_r j_r} T_{j_1 j_2 \cdots j_r} \tag{4.161}$$

The number of indices r is the rank of the tensor. A scalar is a tensor of rank 0 (no indices; it does not transform). A vector is a tensor of rank 1. A rank 2 tensor is an element (vector) of the direct product of a vector space with itself (another vector space).

The trouble with Cartesian tensors is that, in general, they are reducible representations of the group of rotations. The properties of the tensors are more apparent in the basis of spherical tensors (vectors with well defined angular momentum).

For instance, take the basis $\{|1m\rangle = |11\rangle, |10\rangle, |1-1\rangle\}$ of $\mathbb{R}^3 \sim \mathcal{H}^{j=1}$. The space of rank 2 tensors form a *reducible* representation space that can be written as a direct sum of subspaces with well defined angular momentum j:

$$\mathcal{H}^{j=1} \otimes \mathcal{H}^{j=1} = \mathcal{H}^{j=0} \oplus \mathcal{H}^{j=1} \oplus \mathcal{H}^{j=2} \tag{4.162}$$

Under rotations, the tensors of each subspace $\mathcal{H}^j$ transform to tensors within the same subspace. They are irreducible representations. This means that the 9 components T_{ij} of a rank 2 Cartesian tensor can be decomposed into 3 types of *irreducible* spherical tensors T^k_q with $q = -k, \ldots, k$ that have well defined properties under rotations:

$$T_{ij} = T\delta_{ij} + A_{ij} + S_{ij} \tag{4.163}$$

$$T = \tfrac{1}{3}\sum_i T_{ii} \quad \text{(proportional to trace of the tensor)} \tag{4.164}$$

$$A_{ij} = \tfrac{1}{2}(T_{ij} - T_{ji}) \quad \text{(antisymmetric tensor)} \tag{4.165}$$

$$S_{ij} = \tfrac{1}{2}(T_{ij} + T_{ji}) - T\delta_{ij} \quad \text{(traceless symmetric tensor)} \tag{4.166}$$

$$T = T^0_0, \quad A_{ij} \leftrightarrow T^1_q, \quad S_{ij} \leftrightarrow T^2_q. \tag{4.167}$$

Notice that, in fact, $9 = 3 \times 3 = 1 + 3 + 5$.

The spherical tensors transform under a rotation R like

$$T^k_q \to \sum_{q'} T^k_{q'} D^k(R)_{q'q} \tag{4.168}$$

since

$$\begin{aligned}
|jm\rangle &\to D(R)\,|jm\rangle \\
\sum_{m'=-j}^{j} |jm'\rangle \langle jm'|jm\rangle &\to \sum_{m'=-j}^{j} |jm'\rangle\langle jm'|\, D(R)\,|jm\rangle \\
|jm\rangle &\to \sum_{m'=-j}^{j} |jm'\rangle\, D^j(R)_{m'm} \\
|jm\rangle &\to \sum_{m'=-j}^{j} |jm'\rangle\, D^j(R)_{m'm}
\end{aligned} \tag{4.169}$$

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$$\Leftrightarrow \quad D^j(R)_{m'm} = \langle jm' | \, D(R) \, |jm\rangle \, . \tag{4.170}$$

As we did before for vector operators, we demand that the expectation value of spherical *tensor operators* transforms like a classical tensor,

$$\begin{aligned} |\psi\rangle &\to D(R)\,|\psi\rangle \\ \langle\psi|\, T^k_q \,|\psi\rangle \to \langle\psi|\, D^\dagger(R) T^k_q D(R)\,|\psi\rangle &= \sum_{q'=-k}^{k} \langle\psi|\, T^k_{q'}\,|\psi\rangle\, D^k(R)_{q'q} \qquad (4.171) \\ \Rightarrow \quad D^\dagger(R) T^k_q D(R) &= \sum_{q'=-k}^{k} T^k_{q'}\, D^k(R)_{q'q} \qquad (4.172) \end{aligned}$$

where every T^k_q is an operator (n-dimensional matrix) acting on our n-dimensional Hilbert space, and the right hand side is a linear combination of the $(2k+1)$ matrices $T^k_{q'}$ with coefficients $D^k(R)_{q'q}$.

Taking now an infinitesimal rotation (4.154) we get

$$[\hat{n}\cdot\vec{J},\, T^k_q] = \sum_{q'=-k}^{k} T^k_{q'}\, \langle kq' | \, \hat{n}\cdot\vec{J}\,|kq\rangle \, . \tag{4.173}$$

Therefore, the relation (4.172) is equivalent to

$$[J_z, T^k_q] = \hbar q\, T^k_q \tag{4.174}$$

$$[J_\pm, T^k_q] = \hbar\sqrt{k(k+1) - q(q\pm 1)}\, T^k_{q\pm 1} \tag{4.175}$$

that is the defining property of a (irreducible) spherical tensor operator.

4.10 Wigner-Eckart theorem

The matrix elements of spherical tensor operators satisfy

$$\langle \alpha_2; j_2 m_2 |\, T^k_q \,|\alpha_1; j_1 m_1\rangle = \langle kq; j_1 m_1 | j_2 m_2\rangle \, \langle \alpha_2; j_2 \| T^k \| \alpha_1; j_1\rangle \tag{4.176}$$

where $\langle \alpha_2; j_2 \| T^k \| \alpha_1; j_1\rangle$ is a *reduced matrix element* independent of m_1, m_2 and q. This is the Wigner-Eckart theorem.[d]

This theorem simplifies the calculation of transition amplitudes between different states because once we know the corresponding matrix element for a given transition we obtain the rest just by using a CGC. And it also tells us directly which transitions are forbidden (selection rules).

For example, a trivial case is a transition mediated by a scalar operator,

$$\begin{aligned} \langle \alpha_2; j_2 m_2 |\, T^0_0 \,|\alpha_1; j_1 m_1\rangle &= \langle 00; j_1 m_1 | j_2 m_2\rangle \, \langle \alpha_2; j_2 \| T^0 \| \alpha_1; j_1\rangle \\ &= \delta_{j_1 j_2}\delta_{m_1 m_2} \langle \alpha_2; j_2 \| T^0 \| \alpha_1; j_1\rangle . \end{aligned} \tag{4.177}$$

[d] The proof is a bit convoluted and can be found in Sakurai's book [**?**].

Chapter 5

Symmetries and conservation laws

5.1 Symmetries in Classical Mechanics

Both in classical and quantum mechanics the information about the dynamics of a physical system is in the Lagrangian $L(x_i, \dot{x}_i)$ or the Hamiltonian $H(x_i, p_i)$. A symmetry of the system is a group of *transformations* that leaves H *invariant*. There is a connection between symmetries and conservation laws: for every symmetry there is a quantity that remains *constant* in time (it is conserved). In particular,

- The invariance under spatial translations:

$$H(x_i) = H(x_i + \delta x_i) \quad \Rightarrow \quad \dot{p_i} = -\frac{\partial H}{\partial x_i} = 0 \quad \Rightarrow \quad p_i = \text{const.} \tag{5.1}$$

- The invariance under time translations:

$$H(t) = H(t + \delta t) \quad \Rightarrow \quad \frac{\mathrm{d}H}{\mathrm{d}t} = 0 \quad \Rightarrow \quad E = \text{const.} \tag{5.2}$$

- The invariance under rotations:

$$H(\vec{x}) = H(R\vec{x}) \quad \Rightarrow \quad \vec{L} = \text{const.} \tag{5.3}$$

5.2 Symmetries in Quantum Mechanics

In QM most of the symmetries are associated to *unitary* operators acting on the Hilbert space. We have already seen a few examples:

- Spatial translations:

$$|\alpha\rangle \to |\tilde{\alpha}\rangle = T(\vec{x})\,|\alpha\rangle\,, \quad T(\delta\vec{x}) = I - \frac{\mathrm{i}}{\hbar}\sum_i \delta x_i P_i \tag{5.4}$$

  where the momentum operators P_i are the generators of spatial translations.

- Time translations:

$$|\alpha\rangle \to |\tilde{\alpha}\rangle = U(t, t_0)\,|\alpha\rangle\,, \quad U(t_0 + \delta t_0, t) = I - \frac{\mathrm{i}}{\hbar}\delta t\, H \tag{5.5}$$

  where the Hamiltonian operator H is the generator of time translations.

- Rotations:

$$|\alpha\rangle \to |\tilde{\alpha}\rangle = R_{\hat{n}}(\phi)\,|\alpha\rangle\,, \quad R_{\hat{n}}(\delta\phi) = I - \frac{\mathrm{i}}{\hbar}\delta\phi \sum_i n_i J_i \tag{5.6}$$

  where the angular momentum operators J_i are the generators of rotations.

All the unitary transformations S (with $S^{-1} = S^\dagger$) we have seen so far are *continuous*. They are generated by (a set of) *self-adjoint operators* G (group generators) and specified by a (a set of) parameters x,

$$S(\delta x) = I - \mathrm{i}\delta x\, G \tag{5.7}$$

$$S^{-1}(\delta x) = S(-\delta x) = S^\dagger(\delta x) \quad \Rightarrow \quad I + \mathrm{i}\delta x\, G = I + \mathrm{i}\delta x\, G^\dagger \quad \Rightarrow \quad G = G^\dagger. \tag{5.8}$$

We say that S is a *symmetry* of the system if it commutes with the Hamiltonian H,

$$[S, H] = 0 \quad \Rightarrow \quad SH = HS \quad \text{or} \quad SHS^\dagger = H. \tag{5.9}$$

This implies that $|\psi\rangle$ and $\left|\tilde{\psi}\right\rangle = S\,|\psi\rangle$ have the same energy:

$$\langle H\rangle_\psi = \langle\psi|\,H\,|\psi\rangle = \langle\psi|\,S^\dagger S\,H\,S^\dagger S\,|\psi\rangle = \left\langle\tilde{\psi}\right|\,H\,\left|\tilde{\psi}\right\rangle = \langle H\rangle_{\tilde{\psi}} \tag{5.10}$$

and also, for a continuous symmetry,

$$[S, H] = 0 \quad \Rightarrow \quad [G, H] = 0 \quad \Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\,G\,|\psi\rangle = -\frac{\mathrm{i}}{\hbar}\langle\psi|\,[G, H]\,|\psi\rangle = 0, \tag{5.11}$$

the *generator* of a continuous symmetry is a *constant of motion*.

In general, we also say that any unitary operator is a symmetry even if it does not commute with H, and its generator is not a constant of motion. We call it a *broken symmetry*. And this is extended to any types of symmetries (see below).

Not all symmetries are related to *continuous* and *space-time* transformations. In this chapter we will study two *discrete* symmetries (parity and time reversal) and an *internal* continuous symmetry (isospin).

Unitary transformations (continuous or discrete) statisfy

$$\left\langle\tilde{\beta}\middle|\tilde{\alpha}\right\rangle = \langle\beta|\,U^\dagger U\,|\alpha\rangle = \langle\beta|\alpha\rangle \tag{5.12}$$

and hence they preserve the norm of a vector,

$$\langle\tilde{\alpha}|\tilde{\alpha}\rangle = \langle\alpha|\alpha\rangle\,. \tag{5.13}$$

But the norm is also preserved if we simply impose

$$|\left\langle\tilde{\beta}\middle|\tilde{\alpha}\right\rangle| = |\,\langle\beta|\alpha\rangle\,|. \tag{5.14}$$

and this is all we need to declare $|alpha\rangle \to |\tilde{\alpha}\rangle$ a symmetry transformation. Actually, Wigner's theorem states that any symmetry transformation is represented on the Hilbert space by a *linear and unitary* or *antilinear and antiunitary* transformation. The latter satisfy

$$\left\langle\tilde{\beta}\middle|\tilde{\alpha}\right\rangle = \langle\beta|\alpha\rangle^* = \langle\alpha|\beta\rangle\,. \tag{5.15}$$

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A transformation Θ

$$|\alpha\rangle \to |\tilde{\alpha}\rangle = \Theta\,|\alpha\rangle \ , \quad |\beta\rangle \to \left|\tilde{\beta}\right\rangle = \Theta\,|\beta\rangle \tag{5.16}$$

is said to be *antiunitary* if

$$\left\langle\tilde{\beta}\middle|\tilde{\alpha}\right\rangle = \langle\beta|\alpha\rangle^* \tag{5.17}$$

and *antilinear* if

$$\Theta(c_1\,|\alpha\rangle + c_2\,|\beta\rangle) = c_1^*\Theta\,|\alpha\rangle + c_2^*\Theta\,|\beta\rangle\,. \tag{5.18}$$

An antiunitary operator can be always written as

$$\Theta = UK \tag{5.19}$$

where U is a unitary operator and K is the operator that takes the complex-conjugate of any coefficient that multiplies a ket. Then the antilinearity is obvious. Let us prove the other property:

$$|\tilde{\alpha}\rangle = \Theta\,|\alpha\rangle = UK\sum_{a'}\left|a'\right\rangle\left\langle a'\middle|\alpha\right\rangle = \sum_{a'}\left\langle a'\middle|\alpha\right\rangle^* U\left|a'\right\rangle. \tag{5.20}$$

We do not need to define the action on bras nor it is necessary to define $\Theta^\dagger$. We simply take the adjoint relation between kets and bras:

$$\left|\tilde{\beta}\right\rangle = \Theta\,|\beta\rangle = \sum_{a''}\left\langle a''\middle|\beta\right\rangle^* U\left|a''\right\rangle \quad \Rightarrow \quad \left\langle\tilde{\beta}\right| = \sum_{a''}\left\langle a''\middle|\beta\right\rangle\left\langle a''\right|U^\dagger. \tag{5.21}$$

Then

$$\begin{aligned}\left\langle\tilde{\beta}\middle|\tilde{\alpha}\right\rangle &= \sum_{a'}\sum_{a''}\left\langle a''\middle|\beta\right\rangle\left\langle a'\middle|\alpha\right\rangle^*\left\langle a''\right|U^\dagger U\left|a'\right\rangle = \sum_{a'}\left\langle a'\middle|\beta\right\rangle\left\langle a'\middle|\alpha\right\rangle^* \\ &= \sum_{a'}\left\langle\alpha\middle|a'\right\rangle\left\langle a'\middle|\beta\right\rangle = \langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*\,.\end{aligned} \tag{5.22}$$

We will have to introduce an antiunitary operator to define the time reversal symmetry.

An important observation is the relation between symmetry and *degeneracy*. We have already seen that a symmetry S commutes with the Hamiltonian. Therefore given an energy eigenstate $|n\rangle$ the states $S\,|n\rangle$ (if they are different to $|n\rangle$) are degenerate states with the same energy. For example, if H is invariant under rotations then $[J^2, H] = [J_i, H] = 0$ then the $(2j+1)$ states $|njm\rangle$ with $m = -j, \ldots, j$ have the same energy,

$$H\,|njm\rangle = E_n\,|njm\rangle\,, \tag{5.23}$$

since

$$\begin{aligned}[J_\pm, H] = 0 \quad &\Rightarrow \quad H(J_\pm\,|njm\rangle) = J_\pm H\,|njm\rangle = E_n(J_\pm\,|njm\rangle) \\ &\Rightarrow \quad H\,|nj\,m\pm1\rangle = E_n\,|nj\,m\pm1\rangle\,.\end{aligned} \tag{5.24}$$

This is the case of an atomic electron bound by a potential $V(r) + V_{LS}(r)\,\vec{L}\cdot\vec{S}$. Because r and $\vec{L}\cdot\vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$ are rotationally invariant, there is a $(2j+1)$ degeneracy for each atomic level (fine structure of atomic levels for $\ell \geq 1$). For a Hydrogen atom ($s = \frac{1}{2}$):

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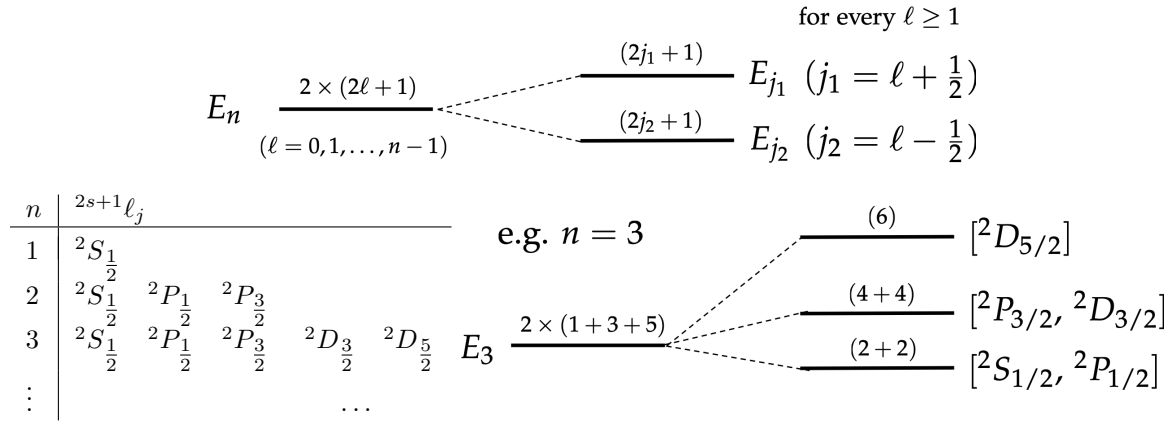


n	$^{2s+1}\ell_j$					
1	$^2S_{\frac{1}{2}}$					
2	$^2S_{\frac{1}{2}}$	$^2P_{\frac{1}{2}}$	$^2P_{\frac{3}{2}}$			
3	$^2S_{\frac{1}{2}}$	$^2P_{\frac{1}{2}}$	$^2P_{\frac{3}{2}}$	$^2D_{\frac{3}{2}}$	$^2D_{\frac{5}{2}}$	
⋮				...		

5.3 Discrete symmetries

5.3.1 Parity

Rotations and spatial translations are continuous transformations, that can be obtained by successive infinitesimal transformations (they can be continuously connected with the identity). Not all symmetries are like this.

In particular, the *parity* transformation or *space inversion* Π is defined as an order 2 operation,

$$\Pi^2 = I \quad \Rightarrow \quad \Pi^{-1} = \Pi^\dagger = \Pi, \tag{5.25}$$

that changes the sign of the expectation value of the position operator $\vec{X}$:

$$|\psi\rangle \to \Pi\,|\psi\rangle \tag{5.26}$$

$$\langle\psi|\,X_i\,|\psi\rangle \to \langle\psi|\,\Pi X_i \Pi\,|\psi\rangle = -\,\langle\psi|\,X_i\,|\psi\rangle \quad \Rightarrow \quad \Pi X_i \Pi = -X_i. \tag{5.27}$$

Notice that $\Pi X_i = -X_i \Pi$ (they do not commute but anticommute) so they do not have a common basis of eigenvectors. In fact,

$$X_i\,\Pi\,|\vec{x}\rangle = -\Pi X_i\,|\vec{x}\rangle = -\Pi x_i\,|\vec{x}\rangle = -x_i\,\Pi\,|\vec{x}\rangle \quad \Rightarrow \quad \Pi\,|\vec{x}\rangle = \eta_I\,|-\vec{x}\rangle \tag{5.28}$$

where η_I is the *intrinsic parity* of the system (state *independent*), with

$$\Pi^2\,|\vec{x}\rangle = |\vec{x}\rangle = \eta_I^2\,|\vec{x}\rangle \quad \Rightarrow \quad \eta_I = \pm 1. \tag{5.29}$$

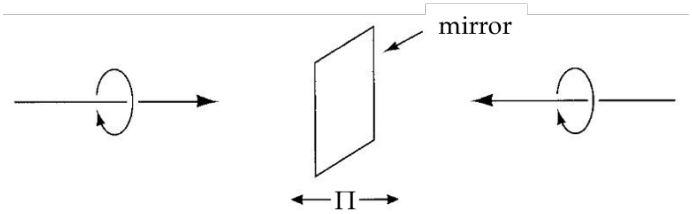
The linear momentum operator also changes sign under parity,

$$\vec{P} = m\frac{\mathrm{d}\vec{X}}{\mathrm{d}t} \quad \Rightarrow \quad \Pi P_i \Pi = -P_i \tag{5.30}$$

while the angular momentum $\vec{J}$ ($\vec{L}$ or $\vec{S}$) does not change (by analogy with $\vec{L} = \vec{X} \times \vec{P}$),

$$\Pi J_i \Pi = J_i \quad \Rightarrow \quad [\Pi, J_i] = 0. \tag{5.31}$$

Therefore, in contrast to position or linear momentum, angular momentum and parity have common eigenstates.. Notice that $\vec{X}$ and $\vec{P}$ are vectors but $\vec{J}$ is a pseudovector or axial-vector. This is consistent with the meaning of a parity transformation, that takes the system to its mirror image (along the perpendicular direction):



What is the parity transform of the wave function in the position representation $\psi(\vec{x}) = \langle\vec{x}|\psi\rangle$ of a system in a state $|\psi\rangle$?

$$\langle\vec{x}|\,\Pi\,|\psi\rangle = \eta_I\,\langle -\vec{x}|\psi\rangle = \eta_I\psi(-\vec{x}) \quad \Rightarrow \quad \Pi\psi(\vec{x}) = \eta_I\psi(-\vec{x}). \tag{5.32}$$

Let us examine the eigenstates of Π. Since $\Pi^2 = I$ they verify

$$\Pi\,|\psi\rangle = \eta\,|\psi\rangle \quad \text{with} \quad \eta = \pm 1 \qquad (\textit{parity} \text{ of the state}) \tag{5.33}$$

and their wave function is

$$\langle\vec{x}|\,\Pi\,|\psi\rangle = \begin{cases} \eta\,\langle\vec{x}|\psi\rangle = \eta\psi(\vec{x}) \\ \eta_I\,\langle -\vec{x}|\psi\rangle = \eta_I\psi(-\vec{x}) \end{cases} \quad \Rightarrow \quad \psi(-\vec{x}) = \eta_\psi\psi(\vec{x}) \quad \text{with} \quad \eta = \eta_I\eta_\psi. \tag{5.34}$$

Therefore the eigenstates of Π in position representation are of two types:

- *Even* or *symmetric* wave functions ($\eta_\psi = +1$): $\psi(-\vec{x}) = \psi(\vec{x})$.
- *Odd* or *antisymmetric* wave functions ($\eta_\psi = -1$): $\psi(-\vec{x}) = -\psi(\vec{x})$.

Clearly, the plane waves $\psi(\vec{x}) = \langle\vec{x}|\vec{p}\rangle = \dfrac{1}{(2\pi\hbar)^{3/2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}}$ do not have well defined parity, but spherical harmonics do:

$$\vec{x} \to -\vec{x}: \quad \left.\begin{array}{l} r \to r \\ \theta \to \pi - \theta \\ \varphi \to \varphi + \pi \end{array}\right\} \quad \Rightarrow \quad Y_\ell^m(\theta,\varphi) \to (-1)^\ell Y_\ell^m(\theta,\varphi). \tag{5.35}$$

Therefore,

$$\Pi\,|\ell m\rangle = (-1)^\ell\,|\ell m\rangle\,. \tag{5.36}$$

This is in agreement with $[\Pi, J_i] = 0$: the orbital angular momentum eigenstates are also eigenstates of parity.

Recall that for a system with intrinsic parity η_I, in a state $|\psi\rangle$ whose wave function has a well defined parity η_ψ (parity eigenstate), the total parity of that state is η,

$$\eta = \eta_I\eta_\psi, \quad \Pi\,|\psi\rangle = \eta\,|\psi\rangle\,. \tag{5.37}$$

If $[\Pi, H] = 0$ then the total parity η is conserved, and the energy eigenstates are also states with well defined parity η.

Remember that a system of two particles with masses m_1 and m_2 is equivalent to one particle of reduced mass $m = m_1m_2/(m_1 + m_2)$ submitted to a central potential $V(|\vec{x}|)$

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where $\vec{x}$ is the position of one of the two particles in their center of mass frame. Then the **composite system** will have an intrinsic parity

$$\eta_I = \eta_1 \eta_2 (-1)^\ell \tag{5.38}$$

where η_1 and η_2 are the intrinsic parities of each particle and ℓ the orbital angular momentum of the reduced system.

One usually defines the spin J of the system (its total angular momentum at rest) and the intrinsic parity P, the so-called spin-parity J^P. The conservation of parity in a reaction (scattering or decay) depends on the type of mediating interaction:

- Strong interactions do *not violate* parity.
- Electromagnetic interactions do *not violate* parity.
- Weak interactions *violate* parity.
- Gravitational interactions do *not violate* parity.

For example, we observe that nuclei with spin-parity J^P decay very fast (strongly) into an α particle (^{4}He) and a lighter nucleus, both of 0^+, preserving parity:

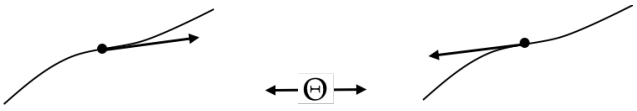
$$J^P \to 0^+ + 0^+ \quad \text{initial parity: } P, \quad \text{final parity: } (-1)^\ell = (-1)^j. \tag{5.39}$$

However, sometimes we also observe (rare) weak decays changing parity, like:

$$\begin{aligned} &^{16}\mathrm{O}\,(2^-) \to {}^{12}\mathrm{C}\,(0^+) + \alpha\,(0^+) \\ &\qquad \text{initial parity: } -1, \quad \text{final parity: } (-1)^\ell = (-1)^j = (-1)^2 = +1. \end{aligned} \tag{5.40}$$

5.3.2 Time reversal

Time reversal changes the direction of the time evolution. Classically, if we have a particle that describes a trajectory $\vec{x}(t)$, a time reversal transformation would show a particle that describes the reversed trajectory:



In QM, the time-reversed state

$$|\tilde{\alpha}\rangle = \Theta\,|\alpha\rangle \tag{5.41}$$

should be called the *motion-reversed* state. That is, if $|\alpha\rangle$ is a state with well defined momentum $\vec{p}$ then $|\tilde{\alpha}\rangle$ is a state with momentum $-\vec{p}$. Likewise, the angular momentum should be reversed. So, up to a possible complex phase,

$$\Theta\,|\vec{x}\rangle = |\vec{x}\rangle \tag{5.42}$$

$$\Theta\,|\vec{p}\rangle = |-\vec{p}\rangle \tag{5.43}$$

$$\Theta\,|jm\rangle = |j\ -m\rangle\,. \tag{5.44}$$

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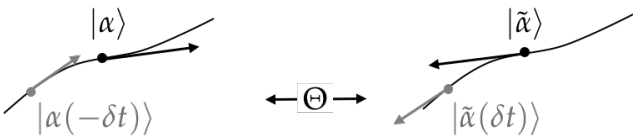
Therefore, if the system is invariant under time-reversal, $|\tilde{\alpha}\rangle = \Theta\,|\alpha\rangle \Rightarrow |\tilde{\alpha}(\delta t)\rangle = \Theta\,|\alpha(-\delta t)\rangle$:



(5.45)

Let us see that the operator Θ must be an *antiunitary* operator:

$$\begin{aligned} |\tilde{\alpha}(\delta t)\rangle &= (I - \tfrac{\mathrm{i}}{\hbar}\delta t H)\,|\tilde{\alpha}\rangle = (I - \tfrac{\mathrm{i}}{\hbar}\delta t H)\Theta\,|\alpha\rangle \\ = \Theta\,|\alpha(-\delta t)\rangle &= \Theta(I - \tfrac{\mathrm{i}}{\hbar}(-\delta t)H)\,|\alpha\rangle \ , \quad \forall\,|\alpha\rangle \\ \Rightarrow \quad & -\mathrm{i}H\Theta = \Theta\mathrm{i}H. \end{aligned} \tag{5.46}$$

If Θ was linear then $\Theta H = -H\Theta$ and the time-reversed state of an energy eigenstate would have negative energy:

$$H\,|E\rangle = E\,|E\rangle \quad \Rightarrow \quad H\,\Theta\,|E\rangle = -\Theta H\,|E\rangle = -E\,\Theta\,|E\rangle \tag{5.47}$$

that would be *unphysical*. Therefore, Θ must be antilinear (antiunitary), $\Theta = UK$, and then

$$-\mathrm{i}H\Theta = \Theta\mathrm{i}H = -\mathrm{i}\Theta H \quad \Rightarrow \quad \Theta H = H\Theta. \tag{5.48}$$

Now Θ and H commute, so they have common eigenvectors.

To derive the commutation relations of Θ with $\vec{X}$, $\vec{P}$ and $\vec{J}$, remember that

$$|\tilde{\alpha}\rangle = \Theta\,|\alpha\rangle \quad \Rightarrow \quad |\alpha\rangle = \Theta^{-1}\,|\tilde{\alpha}\rangle \tag{5.49}$$

and both Θ and Θ^{-1} act on kets only. Then for a given operator A,

$$\begin{aligned} \langle\alpha|\,A\,|\beta\rangle = \langle\beta|\,A^\dagger\,|\alpha\rangle^* &= \left\langle\beta\middle|A^\dagger\alpha\right\rangle^* \\ &= \left\langle\tilde{\beta}\middle|\widetilde{A^\dagger\alpha}\right\rangle = \left\langle\tilde{\beta}\middle|\,\Theta\,\middle|A^\dagger\alpha\right\rangle = \left\langle\tilde{\beta}\middle|\,\Theta A^\dagger\,|\alpha\right\rangle \\ &= \left\langle\tilde{\beta}\middle|\,\Theta A^\dagger\Theta^{-1}\,|\tilde{\alpha}\right\rangle. \end{aligned} \tag{5.50}$$

Therefore, the expectation values of our self-adjoint operators satisfy:

$$\langle\tilde{\alpha}|\,\vec{X}\,|\tilde{\alpha}\rangle \equiv +\,\langle\alpha|\,\vec{X}\,|\alpha\rangle = \langle\tilde{\alpha}|\,\Theta\vec{X}\Theta^{-1}\,|\tilde{\alpha}\rangle \quad \Rightarrow \quad \Theta X_i\Theta^{-1} = X_i \quad \Rightarrow \quad [X_i,\Theta] = 0 \tag{5.51}$$

$$\langle\tilde{\alpha}|\,\vec{P}\,|\tilde{\alpha}\rangle \equiv -\,\langle\alpha|\,\vec{P}\,|\alpha\rangle = -\,\langle\tilde{\alpha}|\,\Theta\vec{P}\Theta^{-1}\,|\tilde{\alpha}\rangle \quad \Rightarrow \quad \Theta P_i\Theta^{-1} = -P_i \tag{5.52}$$

$$\langle\tilde{\alpha}|\,\vec{J}\,|\tilde{\alpha}\rangle \equiv -\,\langle\alpha|\,\vec{J}\,|\alpha\rangle = -\,\langle\tilde{\alpha}|\,\Theta\vec{J}\Theta^{-1}\,|\tilde{\alpha}\rangle \quad \Rightarrow \quad \Theta J_i\Theta^{-1} = -J_i \tag{5.53}$$

As expected, $\vec{X}$ and Θ have common eigenvectors but neither $\vec{P}$ nor $\vec{J}$ do.

What is the action of Θ on the wave function of a spinless system?

$$\begin{aligned} |\psi\rangle &= \int \mathrm{d}^3x'\ |\vec{x}'\rangle\,\langle\vec{x}'|\psi\rangle = \int \mathrm{d}^3x'\ |\vec{x}'\rangle\,\psi(\vec{x}') \\ \Rightarrow \quad \Theta\,|\psi\rangle &= \int \mathrm{d}^3x'\ |\vec{x}'\rangle\,\psi^*(\vec{x}') \\ \Rightarrow \quad \langle\vec{x}|\,\Theta\,|\psi\rangle &= \int \mathrm{d}^3x'\,\delta^3(\vec{x}-\vec{x}')\psi^*(\vec{x}') \end{aligned}$$

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$$\Rightarrow \quad \psi(\vec{x}) \xrightarrow{\Theta} \psi^*(\vec{x}) \quad \text{(the complex conjugate)}. \tag{5.54}$$

How does Θ act on a wave function with well defined (orbital) angular momentum?

$$\langle\theta\varphi|\psi\rangle = Y_\ell^m(\theta,\varphi) \xrightarrow{\Theta} Y_\ell^{m*}(\theta,\varphi) = (-1)^m Y_\ell^{-m}(\theta,\varphi) \tag{5.55}$$

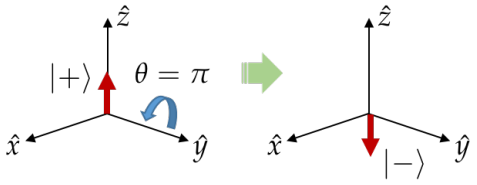
(not an eigenstate of Θ as expected). Therefore

$$\Theta\,|\ell m\rangle = (-1)^m\,|\ell\ -m\rangle\,. \tag{5.56}$$

And what is the action of Θ on a spin state? Notice that Θ changes the sign of the angular momentum, because $\Theta J_i \Theta^{-1} = -J_i$. Therefore the time-reversed of $|+\rangle \equiv \left|\frac{1}{2}\,\frac{1}{2}\right\rangle$ is $|-\rangle \equiv \left|\frac{1}{2}\ -\frac{1}{2}\right\rangle$, up to a complex phase η:

$$\Theta\,|+\rangle = \eta\,|-\rangle\,, \quad |\eta|^2 = 1 \quad \text{(normalized state)}. \tag{5.57}$$

Hence, $\Theta = UK$ is defined by a rotation of π radians about the y axis:



(5.58)

$$\Theta = \eta \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\pi J_y} K, \quad \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\pi J_y} \doteq \mathrm{e}^{-\mathrm{i}\frac{\pi}{2}\sigma_y} = \begin{pmatrix} \cos\frac{\pi}{2} & -\sin\frac{\pi}{2} \\ \sin\frac{\pi}{2} & \cos\frac{\pi}{2} \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$\Rightarrow \quad \Theta = \eta \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K. \tag{5.59}$$

Then (K is irrelevant when acting on basis states):

$$\Theta\,|+\rangle = \eta\,|-\rangle\,, \quad \Theta\,|-\rangle = -\eta\,|+\rangle \tag{5.60}$$

and for any state $c_1\,|+\rangle + c_2\,|-\rangle$ we have

$$\Theta(c_1\,|+\rangle + c_2\,|-\rangle) = \eta(c_1^*\,|-\rangle - c_2^*\,|+\rangle) \tag{5.61}$$

$$\Rightarrow \quad \Theta^2(c_1\,|+\rangle + c_2\,|-\rangle) = -\eta\eta^*(c_1\,|+\rangle + c_2\,|-\rangle) = -(c_1\,|+\rangle + c_2\,|-\rangle). \tag{5.62}$$

Thus, $\Theta^2 = -I$ when acting on a spin $\frac{1}{2}$ state. The same will happen whenever we have a state of $j = \frac{1}{2}, \frac{3}{2}, \ldots$, that changes sign when rotated 2π radians. This is in contrast with the states of integer j, since we have seen that $\Theta\,|\ell m\rangle = (-1)^m\,|\ell - m\rangle$, so $\Theta^2 = I$ on these states. Therefore, we *choose* $\eta = \mathrm{i}$ for states of half-integer spin, so that the general expression, valid for both orbital ($m =$ integer) and spin angular momentum, is

$$\Theta\,|jm\rangle = \mathrm{i}^{2m}\,|j\ -m\rangle\,. \tag{5.63}$$

If the system is time-reversal symmetric then $|E\rangle$ and $\Theta\,|E\rangle$ have the same energy,

$$[\Theta, H] = 0, \quad H\,|E\rangle = E\,|E\rangle \quad \Rightarrow \quad H\,\Theta\,|E\rangle = \Theta H\,|E\rangle = E\,\Theta\,|E\rangle\,. \tag{5.64}$$

And if $|E\rangle$ and $\Theta\,|E\rangle$ were *different* states this energy eigenstate would be *degenerate*. Notice that both states are the same if they differ at most by a phase factor:

$$\Theta\,|E\rangle = \mathrm{e}^{\mathrm{i}\delta}\,|E\rangle \quad \Rightarrow \quad \Theta^2\,|E\rangle = +\,|E\rangle\,. \tag{5.65}$$

This happens only for integer j systems. Therefore $\Theta\,|E\rangle \neq \mathrm{e}^{\mathrm{i}\delta}\,|E\rangle$ for half-integer j systems. So *the energy states are (at least doubly) degenerate if they have half-integer spin.* For instance, the energy levels of a system with an odd total number of fermions (such as electrons, protons and neutrons) are at least doubly degenerate. This is the **Kramers degeneracy**.

5.3.3 About the group and representations of Parity and Time reversal

Π and Θ are order two operations, because they leave the system invariant after applying them twice. Therefore both have the structure of the (abelian) symmetry group Z_2.

What are their **representations** in the Hilbert space of *states* (unit rays)? Remember that two states are the same if their (unit) vectors differ at most by a global phase. The representations must verify:

- ▷ $\Pi^2 |\alpha\rangle = \mathrm{e}^{\mathrm{i}\phi} |\alpha\rangle$ *and* Π is a *unitary* representation.
- ▷ $\Theta^2 |\alpha\rangle = \mathrm{e}^{\mathrm{i}\phi} |\alpha\rangle$ *and* Θ is an *antiunitary* representation.

Let's examine them separately.

Parity

$\Pi^2 = \mathrm{e}^{\mathrm{i}\phi} I$, but since Π is unitary one can absorb a phase $\mathrm{e}^{\mathrm{i}\phi/2}$ replacing $\Pi \to \Pi'$:

$$\Pi' = \mathrm{e}^{-\mathrm{i}\phi/2}\Pi \quad \Rightarrow \quad \Pi'^2 = \mathrm{e}^{-\mathrm{i}\phi}\Pi^2 = I. \tag{5.66}$$

So we can always take $\Pi^2 = I$ without loss of generality.

Time reversal

$\Theta^2 = \mathrm{e}^{\mathrm{i}\phi} I$, but now $\Theta = UK$ (antiunitary) and then $\Theta^2 = UKUK = UU^*$. And since U is unitary then $U^\dagger U = I \Rightarrow U^T U^* = I$. Therefore:

$$\Theta^2 = UU^* = \mathrm{e}^{\mathrm{i}\phi} I = \mathrm{e}^{\mathrm{i}\phi} U^T U^* \quad \Rightarrow \quad U = \mathrm{e}^{\mathrm{i}\phi} U^T \tag{5.67}$$

$$\Rightarrow \quad U = \mathrm{e}^{\mathrm{i}\phi}(\mathrm{e}^{\mathrm{i}\phi} U^T)^T = \mathrm{e}^{2\mathrm{i}\phi} U \quad \Rightarrow \quad \mathrm{e}^{2\mathrm{i}\phi} = 1 \quad \Rightarrow \quad \mathrm{e}^{\mathrm{i}\phi} = \pm 1 \tag{5.68}$$

$$\Rightarrow \quad \Theta^2 = \pm I. \tag{5.69}$$

So there are *two types of distinct representations of* Θ. Two relevant **comments** are in order:

(1) The representation of Θ with $\Theta^2 = UU^* = -I$ *cannot be one-dimensional.* This is not in contradiction with the fact that *unitary* representations of an *abelian group* must be one-dimensional, because this is antiunitary.

(2) Recall that $\Theta = UK$ reverses the angular momentum $\vec{J}$: $\Theta J_i = -J_i \Theta_i$. In the Condon and Shortley convention $J_\pm$ are real matrices, so $J_x = \frac{1}{2}(J_+ + J_-)$ and J_z are real but $J_y = -\frac{\mathrm{i}}{2}(J_+ - J_-)$ is pure imaginary. Since K changes the sign of J_y but not that of J_x and J_z, we need that U changes the sign of J_x and J_z leaving J_y untouched. Then U *must be a rotation of* π *about the* y*–axis* (up to a global phase η):

$$U = \eta \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\pi J_y}, \quad |\eta|^2 = 1, \quad \Theta = UK. \tag{5.70}$$

This explains the connection between the time reversal and spin representations:

$$\Theta^2 = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}2\pi J_y} = \begin{cases} +I, & \text{if } j \text{ integer} \\ -I, & \text{if } j \text{ half-integer} \end{cases} \tag{5.71}$$

And, as we have already seen, Θ can be represented by

$$\Theta |jm\rangle = \mathrm{i}^{2m} |j\ -m\rangle . \tag{5.72}$$

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5.4 Isospin

All the symmetries we have discussed so far are *space-time symmetries*: they transform the system into a different space time configuration (time or spatial translation, rotation, space or time inversion).

However, there are other symmetries, called *internal symmetries* of different nature. We will describe here just the *isospin symmetry* and skip the most important internal symmetries, the so called *gauge symmetries*.

Consider a proton p and a neutron n. The proton has a positive electric charge and the neutron has no electric charge. But other than that they are very similar: nearly the same mass ($m_{\rm p} = 0.938$ GeV/c^2, $m_{\rm n} = 0.939$ GeV/c^2), the same spin and parity ($\frac{1}{2}^+$). When they combine to form nuclei the (attractive) strong interaction among protons and neutrons is the same and much more important than the (repulsive) electromagnetic interaction among protons.[a] Therefore, one may suppose that $|{\rm p}\rangle$ and $|{\rm n}\rangle$ are two *isospin* states of the same quantum system (the nucleon), like $|+\rangle$ and $|-\rangle$ are two *spin* states of a the same spin $\frac{1}{2}$ particle. The states $|{\rm p}\rangle$ and $|{\rm n}\rangle$ would be related by a (isospin) symmetry transformation, just like $|+\rangle$ and $|-\rangle$ are related by a rotation. Let us examine the analogy in more detail.

The rotations acting on the two-dimensional Hilbert space of a spin $\frac{1}{2}$ system are $SU(2)$ matrices that mix the two possible spin eigenstates ($|+\rangle$, $|-\rangle$). If the system is invariant under rotations, $[J_i, H] = 0$, these spin states are dynamically equivalent and the angular momentum (generators of rotations in space) is conserved.

The hypothesis is that there is a similar symmetry relating the two states of a nucleon, proton and neutron. This is not a space-time symmetry but an internal one. The "isospin" symmetry, also matrices of $SU(2)$, mixes $|{\rm p}\rangle$ and $|{\rm n}\rangle$, eigenstates of isospin $t = \frac{1}{2}$. If the system is invariant under these transformations, their generators T_i (analogous to J_i) verify $[T_i, H] = 0$, the two isospin states of the nucleon are dynamically equivalent and the isospin (generators of this kind of "rotations in flavour space") is conserved.

In general, particles have spin; they are vectors of $\mathcal{H}^{s=0,\frac{1}{2},1,\cdots}$. Analogously, hadrons (particles that experience strong interactions) have isospin; they are vectors of $\mathcal{H}^{t=0,\frac{1}{2},1,\cdots}$. Therefore, the Hilbert space describing a spin $\frac{1}{2}$ nucleon is $\mathcal{H}^{s=\frac{1}{2}} \otimes \mathcal{H}^{t=\frac{1}{2}}$, with basis $\{|+\rangle, |-\rangle\} \otimes \{|{\rm p}\rangle = \left|\frac{1}{2}\ +\frac{1}{2}\right\rangle, |{\rm n}\rangle = \left|\frac{1}{2}\ -\frac{1}{2}\right\rangle\}$. And, for instance, the Hilbert space describing the spin 0, isospin triplet of pions ($\pi^0, \pi^\pm$) is $\mathcal{H}^{s=0} \otimes \mathcal{H}^{t=1}$ with basis $\{|00\rangle\} \otimes \{|\pi^+\rangle = |1\ +1\rangle, \left|\pi^0\right\rangle = |1\,0\rangle, |\pi^-\rangle = |1\ -1\rangle\}$.

The isospin symmetry is actually an *approximate symmetry* that organizes the hadrons into multiplets of $SU(2)$. But it is still useful when isospin violation is negligible. In reactions mediated by strong interactions isospin is conserved (like angular momentum is conserved under rotations when interactions are due to a central potential). Then the probability amplitude to obtain a given final state is determined by which is its component with same isospin as the initial one (it will depend on Clebsch-Gordan coefficients). And if the reaction produces a final state of different isospin than the initial state (isospin is violated), then it will be mediated by a linear combination of spherical tensors T^k_q with $k \neq 0$, and one can use the Wigner-Eckart theorem to relate the matrix elements of the

[a] Strong interactions are responsible for the nucleus stability.

different final states,

$$\langle \alpha_2; t_2 m_2 |\, T^k_q \,| \alpha_1; t_1 m_1 \rangle = \langle kq; t_1 m_1 | t_2 m_2 \rangle \, \langle \alpha_2; t_2 \| T^k \| \alpha_1; t_1 \rangle. \tag{5.73}$$

Let us see how it works.

The probability of a reaction to occur is described by the cross section σ, which is proportional to the modulus squared of the so called scattering amplitude $\mathcal{A}$ between the initial state $|i\rangle$ and the final state $|f\rangle$ (see chapter 8),

$$\sigma(i \to f) \propto |\mathcal{A}(i \to f)|^2. \tag{5.74}$$

The amplitude, in turn, is in first approximation proportional to the matrix element:

$$\mathcal{A}(i \to f) \propto \langle f |\, V \,| i \rangle \tag{5.75}$$

where the initial state is of the form

$$|i\rangle = |i_{\text{orbital}}\rangle \otimes |i_{\text{spin}}\rangle \otimes |i_{\text{isospin}}\rangle \otimes \cdots \tag{5.76}$$

and similarly the final state $|f\rangle$. If the Hamiltonian H is invariant under isospin transformations (electromagnetic or strong interactions) then the isospin will be conserved,

$$\mathcal{A}(i \to f) \propto \langle f |\, V \,| i \rangle \propto \langle f_{\text{isospin}} | i_{\text{isospin}} \rangle \,. \tag{5.77}$$

For example, consider the following proton-deuteron (strong) reactions (the deuteron is a nucleus of ^{2}H with isospin $|00\rangle$) producing a pion and a member of the isospin doublet $\{|{}^3\text{He}\rangle = \left|\tfrac{1}{2}\,\tfrac{1}{2}\right\rangle, |{}^3\text{H}\rangle = \left|\tfrac{1}{2}\,-\tfrac{1}{2}\right\rangle\}$, the nuclei of ^{3}He and tritium, respectively:

(1) $\text{p} + \text{d} \to \pi^+ + {}^3\text{H}$. The total isospin states are

$$|i_{\text{isospin}}\rangle = \left|\tfrac{1}{2}\,+\tfrac{1}{2}\right\rangle |00\rangle = \left|\tfrac{1}{2}\,+\tfrac{1}{2}\right\rangle \tag{5.78}$$

$$|f_{\text{isospin}}\rangle = |1\,+1\rangle \left|\tfrac{1}{2}\,-\tfrac{1}{2}\right\rangle = \tfrac{1}{\sqrt{3}} \left|\tfrac{3}{2}\,+\tfrac{1}{2}\right\rangle + \sqrt{\tfrac{2}{3}} \left|\tfrac{1}{2}\,+\tfrac{1}{2}\right\rangle \tag{5.79}$$

and

$$\sigma_1 \propto |\, \langle f_{\text{isospin}} | i_{\text{isospin}} \rangle \,|^2 = \left| \sqrt{\frac{2}{3}} \right|^2 = \frac{2}{3}. \tag{5.80}$$

(2) $\text{p} + \text{d} \to \pi^0 + {}^3\text{He}$. The total isospin states are

$$|i_{\text{isospin}}\rangle = \left|\tfrac{1}{2}\,+\tfrac{1}{2}\right\rangle |00\rangle = \left|\tfrac{1}{2}\,+\tfrac{1}{2}\right\rangle \tag{5.81}$$

$$|f_{\text{isospin}}\rangle = |1\,0\rangle \left|\tfrac{1}{2}\,+\tfrac{1}{2}\right\rangle = \sqrt{\tfrac{2}{3}} \left|\tfrac{3}{2}\,+\tfrac{1}{2}\right\rangle - \tfrac{1}{\sqrt{3}} \left|\tfrac{1}{2}\,+\tfrac{1}{2}\right\rangle \tag{5.82}$$

and

$$\sigma_2 \propto |\, \langle f_{\text{isospin}} | i_{\text{isospin}} \rangle \,|^2 = \left| -\frac{1}{\sqrt{3}} \right|^2 = \frac{1}{3}. \tag{5.83}$$

Therefore,

$$\frac{\sigma(\text{p} + \text{d} \to \pi^+ + {}^3\text{H})}{\sigma(\text{p} + \text{d} \to \pi^0 + {}^3\text{He})} = 2. \tag{5.84}$$

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Chapter 6

Systems of identical particles

6.1 Indistinguisible particles

Particles are identical if they cannot be distinguished from one another.

In classical physics it is possible to keep track of individual particles even if they may look alike (Fig. 6.1). In principle, one can know their positions and follow their trajectories separately. In addition, the probability to find two identical particles in exactly the same position (in this case we would be unable to distinguish them) is zero, since there is a continuum of locations.

Figure 6.1: The paths of classical identical particles can be tracked.

In quantum mechanics, however, identical particles are *truly* indistinguisible. All the information we have about a system of identical particles is provided by a complete set of commuting observables (CSCO). Then we cannot label them or follow their individual trajectories (positions and momenta) because this would disturb the system (Fig. 6.2). Furthermore, since the only values of the physical observables (eigenvalues of the CSCO) are quantized, it may be possible that two particles are in the same state. We will see that this has far-reaching consequences.

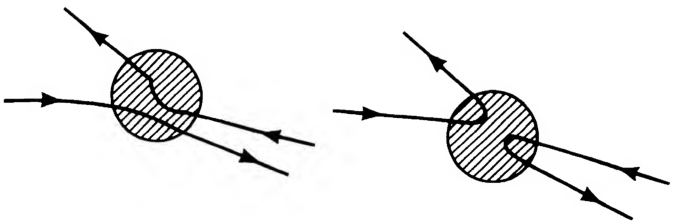

Figure 6.2: Indistinguisable paths of the quantum system of two identical particles.

6.2 Symmetry under permutations

Let us consider two identical particles (later we will generalize to n identical particles) characterized by their eigenvalues with respect to the same CSCO $(A, B, \dots)$:

$$\left|a'b'\dots\right\rangle \equiv \left|a'\right\rangle, \quad A\left|a'\right\rangle = a'\left|a'\right\rangle \quad \text{and} \quad \left|a''b''\dots\right\rangle \equiv \left|a''\right\rangle, \quad A\left|a''\right\rangle = a''\left|a''\right\rangle \tag{6.1}$$

(to simplify the notation we label the ket just by the eigenvalues of A).

The system of both particles is described by the tensor product

$$\left|a'\right\rangle \otimes \left|a''\right\rangle = \left|a'a''\right\rangle \tag{6.2}$$

where it is understood that the first eigenvalue corresponds to particle 1 and the second to particle 2. How does an observable A act on the system?

$$A = A_1 \otimes I + I \otimes A_2 \tag{6.3}$$

$$\begin{aligned} A\left|a'a''\right\rangle &= A_1\left|a'\right\rangle \otimes I\left|a''\right\rangle + I\left|a'\right\rangle \otimes A_2\left|a''\right\rangle \\ &= a'\left|a'a''\right\rangle + a''\left|a'a''\right\rangle \\ &= (a' + a'')\left|a'a''\right\rangle. \end{aligned} \tag{6.4}$$

Notice that the states $|a'a''\rangle$ and $|a''a'\rangle$ are mathematically different (orthogonal) but one cannot distinguish them by measuring any observable in the CSCO, since they have the same eigenvalues,

$$A\left|a''a'\right\rangle = (a' + a'')\left|a''a'\right\rangle. \tag{6.5}$$

Therefore if we measure A and obtain $a' + a''$ we do not know a priori whether the state ket is $|a'a''\rangle$, $|a''a'\rangle$ or any linear combination,

$$\alpha\left|a'a''\right\rangle + \beta\left|a''a'\right\rangle. \tag{6.6}$$

This is known as **exchange degeneracy**. It presents a difficulty because, unlike the single particle case, a specification of the eigenvalue of a CSCO does not completely determine the state. We will see in the next section how nature solves this problem, but before let us review the mathematics we need to study the *permutation symmetry*.

The permutations of n objects form the *symmetric group*, called S_n, with $n!$ elements. A permutation $p \in S_n$ is denoted by

$$p = \begin{pmatrix} 1 & 2 & \cdots & n \\ p_1 & p_2 & \cdots & p_n \end{pmatrix} \tag{6.7}$$

although the alternative *cycle* notation is more economical. For example,

$$\begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \end{pmatrix} \equiv (12)(34), \quad \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 3 & 1 & 4 \end{pmatrix} \equiv (123). \tag{6.8}$$

The advantage of cycles is that if they are disjoint their product can be specified in any order, and any rotation of a given cycle specifies the same cycle,

$$(12)(34) = (34)(12), \quad (123) = (231) = (312). \tag{6.9}$$

Read (123) as $1 \to 2$, $2 \to 3$, $3 \to 1$. For example, the $3! = 6$ permutations in S_3 are

$$S_3 = \left\{ e, \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix} \right\}$$
$$= \{e, (12), (23), (13), (123), (132)\}\,. \tag{6.10}$$

The permutations can be composed (multiplied), form right to left. For example:

$$(123)(132) = (1)(2)(3) = e, \quad (13)(12) = (123). \tag{6.11}$$

They form a group. In general, permutations do not commute,

$$(12)(13) = (132), \quad (13)(12) = (123). \tag{6.12}$$

Any permutation p can be written as a product of r *transpositions* (ij). The parity of the permutation p is $(-1)^r = \pm 1$ that will be denoted as $(-1)^p$. For example,

$$e \text{ and } (123) = (12)(23) \text{ are even } (+1); \quad (12) \text{ and } (13)(245) \text{ are odd } (-1). \tag{6.13}$$

A cycle of length $r+1$ can be written as the product of r transpositions:

$$(i_1 i_2 \dots i_{r+1}) = (i_1 i_2)(i_2 i_3) \cdots (i_r i_{r+1}) \quad \Rightarrow \quad \text{parity } = (-1)^r \tag{6.14}$$

Notice that however this *decomposition is not unique*. For example:

$$(12)(23) = (231) = (123) \quad \text{and also} \quad (13)(12) = (123). \tag{6.15}$$

We define the action of the permutations of S_n on a system of n identical particles as

$$(12)\left|a'a''\right\rangle = \left|a''a'\right\rangle, \quad (132)\left|a'a''a'''\right\rangle = \left|a''a'''a'\right\rangle, \quad \text{etc.} \tag{6.16}$$

Let us go back to the system of two identical particles. One can define two operators,

$$s = \frac{1}{2}[e + (12)] \quad \text{(symmetrizer)} \tag{6.17}$$

$$a = \frac{1}{2}[e - (12)] \quad \text{(antisymmetrizer)}. \tag{6.18}$$

They are orthogonal projectors ($s^2 = s$, $a^2 = a$, $s\,a = 0$) into invariant subspaces of vectors that are symmetric or antisymmetric, respectively, under the exchange of the two particles,

$$s\left|a'a''\right\rangle = \frac{1}{2}(\left|a'a''\right\rangle + \left|a''a'\right\rangle) \tag{6.19}$$

$$a\left|a'a''\right\rangle = \frac{1}{2}(\left|a'a''\right\rangle - \left|a''a'\right\rangle). \tag{6.20}$$

Since the states of the system must be normalized we will define

$$\left|a'a''\right\rangle_s \equiv \frac{1}{\sqrt{2}}(\left|a'a''\right\rangle + \left|a''a'\right\rangle), \quad (12)\left|a'a''\right\rangle_s = +\left|a'a''\right\rangle_s \tag{6.21}$$

$$\left|a'a''\right\rangle_a \equiv \frac{1}{\sqrt{2}}(\left|a'a''\right\rangle - \left|a''a'\right\rangle), \quad (12)\left|a'a''\right\rangle_a = -\left|a'a''\right\rangle_a. \tag{6.22}$$

In the general case of n identical particles, one defines

$$s = \frac{1}{n!}\sum_{p \in S_n} p \qquad \text{(symmetrizer)} \tag{6.23}$$

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$$a = \frac{1}{n!}\sum_{p\in S_n}(-1)^p\, p \quad \text{(antisymmetrizer)} \tag{6.24}$$

that project into invariant subspaces of vectors that are *totally* symmetric or antisymmetric, respectively, under the exchange of *any* pair of particles (transpositions),

$$s\left|a'a''a'''\dots\right\rangle \xrightarrow{\text{normalized}} \left|a'a''a'''\dots\right\rangle_s, \quad (ij)\left|a'a''a'''\dots\right\rangle_s = +\left|a'a''a'''\dots\right\rangle_s \tag{6.25}$$

$$a\left|a'a''a'''\dots\right\rangle \xrightarrow{\text{normalized}} \left|a'a''a'''\dots\right\rangle_a, \quad (ij)\left|a'a''a'''\dots\right\rangle_a = -\left|a'a''a'''\dots\right\rangle_a. \tag{6.26}$$

For example, consider the system of 3 identical particles in the states $|a'\rangle$, $|a''\rangle$ and $|a'''\rangle$, find $|a'a''a'''\rangle_s$ and $|a'a''a'''\rangle_a$ and check that $(23)\,|a'a''a'''\rangle_{s(a)} = +(-)\,|a'a''a'''\rangle_{s(a)}$.

The Hilbert space of a system of two identical particles of spins s_i and isospins t_i is $\mathcal{H} = \mathcal{H}^{\text{space}} \otimes \mathcal{H}^{\text{spin}} \otimes \mathcal{H}^{\text{isospin}} \otimes \cdots$ where every factor is also the tensor product of the corresponding Hilbert spaces of each particle. For example, consider a system of two identical particles of spin $\frac{1}{2}$ and isospin $\frac{1}{2}$,

$$\mathcal{H}^{\text{space}} : \{|\psi_1\rangle\} \otimes \{|\psi_2\rangle\} = \{|\psi_1\psi_2\rangle\} \tag{6.27}$$

$$\mathcal{H}^{\text{spin}} : \{|+\rangle, |-\rangle\} \otimes \{|+\rangle, |-\rangle\} = \{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\} \tag{6.28}$$

$$\mathcal{H}^{\text{isospin}} : \{|u\rangle, |d\rangle\} \otimes \{|u\rangle, |d\rangle\} = \{|uu\rangle, |ud\rangle, |du\rangle, |dd\rangle\}. \tag{6.29}$$

To antisymmetrize the state $|\psi_1\psi_2\rangle \otimes |+-\rangle \otimes |ud\rangle$:

$$(12)\,|\psi_1\psi_2\rangle \otimes |+-\rangle \otimes |ud\rangle = |\psi_2\psi_1\rangle \otimes |-+\rangle \otimes |du\rangle \tag{6.30}$$

$$\frac{1}{2}[e-(12)]\,|\psi_1\psi_2\rangle \otimes |+-\rangle \otimes |ud\rangle \xrightarrow{\text{normalized}} \frac{1}{\sqrt{2}}[|\psi_1\psi_2\rangle \otimes |+-\rangle \otimes |ud\rangle - |\psi_2\psi_1\rangle \otimes |-+\rangle \otimes |du\rangle]. \tag{6.31}$$

6.3 Symmetrization postulate

We have seen that states differing by a permutation of two identical particles, though being different (orthogonal), would be indistinguishable by any observation (exchange degeneracy). To reconcile this with the fact that a state must be fully determined by a CSOC, one has to introduce the following postulate (in full agreement with experiment):

Symmetrization postulate
The states of a system of identical particles must be either totally symmetric or antisymmetric under the exchange of any pair.

Since the only one-dimensional invariant subspaces under the exchange of two particles are the totally symmetric and the totally antisymmetric vectors, this postulate guarantees that the states of systems of identical particles are perfectly determined by a complete set of observations.

On the other hand, in the context of relativistic quantum field theory one can prove the following theorem, that otherwise would be part of the symmetrization postulate:

Spin-statistics connection
The states of a system of identical particles are totally symmetric (antisymmetric) under the exchange of any pair if their spin is integer (half-integer).

One can show that systems of identical particles with totally symmetric wave functions obey the *Bose-Einstein statistics* (these particles are called *bosons*) and those with totally antisymmetric wave functions obey the *Fermi-Dirac statistics* (these particles are called *fermions*). Therefore, this theorem establishes a connection between the spin and the bosonic of fermionic behaviour (statistics) of identical particles: the spin of a boson is integer and the spin of a fermion is half-integer.

A corolary of the symmetrization postulate and the spin-statistics connection theorem is that there are only fermions and bosons in nature.[a]

An immediate consequence of the symmetrization postulate is that identical fermions satisfy the *Pauli exclusion principle*: two of them cannot ocupy the same state, since $|\cdots a' \cdots a' \cdots\rangle_a = 0$. This is why there can only be one electron of a given spin component (two of opposite spins) per energy level in an atomic orbital. This is key to understand the electronic configuration of atoms and hence the periodic table of the chemical elements, the cornerstone of the whole of chemistry. And thanks to Pauli exclusion principle, some types of stars (white dwarfs and neutron stars) may avoid the gravitational collapse.

One may say that fermions are "less sociable" than bosons, since they "avoid" being in the same state as an alike partner. Bosons, in turn, are more "friendly"; they do not mind to be altogether in the same state and actually they do if they can. For instance, at very low temperature they form *Bose-Einstein condensates*, with many particles in the minimum energy state, that gives the system very perculiar properties like superfluidity or superconductivity.

Consider two identical particles, each of them in two possible states + or −. Then:

- Classically, think of two balls labeled with a sign; there are 4 possible configurations: 1/2 with both "states" equal ($|\oplus\oplus\rangle$, $|\ominus\ominus\rangle$) and 1/2 that are different ($|\oplus\ominus\rangle$, $|\ominus\oplus\rangle$).
- If they behave as bosons, they must be in symmetric configurations (symmetric state of the system) and there are 3 possibilities: 2/3 have same quantum numbers ($|{+}{+}\rangle$, $|{-}{-}\rangle$) and 1/3 has different quantum numbers $\left(\frac{1}{\sqrt{2}}(|{+}{-}\rangle + |{-}{+}\rangle)\right)$.
- If they behave as fermions, they must be in antisymmetric configurations (antisymmetric state of the system) and there is just 1 possibility, that, of course, has different quantum numbers $\left(\frac{1}{\sqrt{2}}(|{+}{-}\rangle - |{-}{+}\rangle)\right)$.

This illustrates that bosons are more friendly than classical identical particles (2/3 versus 1/2 of the cases they are in the same state in our example) while fermions are antisocial, never in the same state.

How does a permutation act on the wave function of identical particles? For example,

$$(123)\psi(\vec{x}_1, \vec{x}_2, \vec{x}_3) = \langle \vec{x}_1, \vec{x}_2, \vec{x}_3 | \, (123) \, |\psi\rangle \tag{6.32}$$

[a] However, in two-dimensional systems there are "quasiparticles" called *anyons* that obey intermediate statistics. They play an important role in the fractional quantum Hall effect.

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We know that on the ket,

$$(123)\,|\vec{x}_1,\vec{x}_2,\vec{x}_3\rangle = |\vec{x}_3,\vec{x}_1,\vec{x}_2\rangle \tag{6.33}$$

but notice that in the wave function $p=(123)$ acts on the bra. Then, from

$$\begin{aligned}\delta^3(x_1-\vec{x}_1')\delta^3(x_2-\vec{x}_2')\delta^3(x_3-\vec{x}_3') &= \left\langle \vec{x}_1,\vec{x}_2,\vec{x}_3\middle|\vec{x}_1',\vec{x}_2',\vec{x}_3'\right\rangle \\ &= \langle \vec{x}_1,\vec{x}_2,\vec{x}_3|\,(123)(132)\left|\vec{x}_1',\vec{x}_2',\vec{x}_3'\right\rangle \\ &= \langle \vec{x}_1,\vec{x}_2,\vec{x}_3|\,(123)\left|\vec{x}_2',\vec{x}_3',\vec{x}_1'\right\rangle \end{aligned} \tag{6.34}$$

where we have used $p^{-1}=(132)$, we have that

$$\langle \vec{x}_1,\vec{x}_2,\vec{x}_3|\,(123) = \langle \vec{x}_2,\vec{x}_3,\vec{x}_1| \quad\Rightarrow\quad (123)\psi(\vec{x}_1,\vec{x}_2,\vec{x}_3) = \psi(\vec{x}_2,\vec{x}_3,\vec{x}_1) \tag{6.35}$$

where the arguments of the wave functions are exchanged by the *inverse permutation*.

6.4 System of two electrons

Consider a system of two electrons ($s=\frac{1}{2}$). The first electron is described by a ket of

$$\mathcal{H}_1 = \mathcal{H}_1^{\text{space}}\otimes\mathcal{H}_1^{\text{spin}} : \{|\psi_1^{\text{space}}\rangle\}\otimes\left\{\left|\psi_1^{\text{spin}}\right\rangle\right\} \tag{6.36}$$

where $|\psi_1^{\text{space}}\rangle$ gives the position $\vec{x}$ of electron 1, whose wave function (space part) is $\psi_1(\vec{x})\equiv\langle\vec{x}|\psi_1^{\text{space}}\rangle$ in the position representation, and $\left|\psi_1^{\text{spin}}\right\rangle = |+\rangle$ or $|-\rangle$. And similarly for the second electron. The system of the two electrons is described by

$$\begin{aligned}|\psi\rangle\in\mathcal{H} = \mathcal{H}_1\otimes\mathcal{H}_2 &: \{|\psi^{\text{space}}\rangle\}\otimes\left\{\left|\psi^{\text{spin}}\right\rangle\right\} \\ &= \mathcal{H}^{\text{space}}\otimes\mathcal{H}^{\text{spin}} : \{|\psi_1^{\text{space}}\psi_2^{\text{space}}\rangle\}\otimes\left\{\left|\psi_1^{\text{spin}}\psi_2^{\text{spin}}\right\rangle\right\}\end{aligned} \tag{6.37}$$

where $|\psi^{\text{space}}\rangle$ gives the positions $\vec{x_1}$ of electron 1 an $\vec{x_2}$ of electron 2, whose wave function (space part) is $\psi(\vec{x_1},\vec{x_2})\equiv\langle\vec{x_1},\vec{x}_2|\psi^{\text{space}}\rangle = \psi_1(\vec{x}_1)\psi_2(\vec{x}_2)$, and $\left|\psi^{\text{spin}}\right\rangle$ is any linear combination of $\{|{+}{+}\rangle, |{+}{-}\rangle, |{-}{+}\rangle, |{-}{-}\rangle\}$.

The positions of both electrons could be entangled and also their spins (to make a state with well defined total spin) and also the positions with the total spin. Let us see that *if the total spin is well defined*, $[H,S^2]=0$, then the symmetrization implies that positions and spin states are separable. Because the electrons are fermions, we must *antisymmetrize* and normalize the possible states:

$$(\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|{+}{+}\rangle)_a = \frac{1}{\sqrt{2}}[\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)-\psi_1(\vec{x}_2)\psi_2(\vec{x}_1)]\,|{+}{+}\rangle \tag{6.38}$$

$$(\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|{-}{-}\rangle)_a = \frac{1}{\sqrt{2}}[\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)-\psi_1(\vec{x}_2)\psi_2(\vec{x}_1)]\,|{-}{-}\rangle \tag{6.39}$$

$$(\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|{+}{-}\rangle)_a = \frac{1}{\sqrt{2}}[\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|{+}{-}\rangle-\psi_1(\vec{x}_2)\psi_2(\vec{x}_1)\,|{-}{+}\rangle] \tag{6.40}$$

$$(\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|{-}{+}\rangle)_a = \frac{1}{\sqrt{2}}[\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|{-}{+}\rangle-\psi_1(\vec{x}_2)\psi_2(\vec{x}_1)\,|{+}{-}\rangle]. \tag{6.41}$$

(Last two are not separable but their (total) spin is not well defined.)

Remember that the total spin of the system of two electrons can be $s = 0$ or $s = 1$ with

$$|0\,0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) \tag{6.42}$$

$$|1\ +1\rangle = |++\rangle\,, \quad |1\,0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle), \quad |1\ -1\rangle = |--\rangle\,. \tag{6.43}$$

Notice that the members of the spin multiplet have the same properties under exchange. This is because $S_\pm = S_{1\pm} + S_{2\pm}$ and (12) commute (for any spin). In our system of two identical spin $\frac{1}{2}$ fermions the spin state with $s = 0$ is antisymmetric and the spin states with $s = 1$ are symmetric under exchange.

Can we write the four antisymmetric states above as states with well defined spin without spoiling the symmetrization? We just need to combine a symmetric space part and an antisymmetric spin state *or* viceversa. A symmetric (antisymmetric) space part of the wave function is:

$$\psi_\pm(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}}[\psi_1(\vec{x}_1)\psi_2(\vec{x}_2) \pm \psi_1(\vec{x}_2)\psi_2(\vec{x}_1)]. \tag{6.44}$$

Then we see that the first two are already as needed:

$$\psi_-(\vec{x}_1, \vec{x}_2)\,|1\ +1\rangle = (\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|++\rangle)_a \tag{6.45}$$

$$\psi_-(\vec{x}_1, \vec{x}_2)\,|1\ -1\rangle = (\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|--\rangle)_a \tag{6.46}$$

and we can combine the other two into:

$$\psi_-(\vec{x}_1, \vec{x}_2)\,|1\,0\rangle = \frac{1}{\sqrt{2}}\Big[\,(\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|+-\rangle)_a + (\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|-+\rangle)_a\,\Big] \tag{6.47}$$

$$\psi_+(\vec{x}_1, \vec{x}_2)\,|0\,0\rangle = \frac{1}{\sqrt{2}}\Big[\,(\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|+-\rangle)_a - (\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\,|-+\rangle)_a\,\Big] \tag{6.48}$$

As a particular case, in the *center of mass frame* (CoM),

$$\vec{r} = \vec{x}_1 - \vec{x}_2, \quad \psi(\vec{x}_1, \vec{x}_2) = \psi(\vec{r}), \quad (12)\psi(\vec{r}) = \psi(-\vec{r}). \tag{6.49}$$

Then

$$\psi(\vec{r}) = \pm\psi(-\vec{r}) \quad \Leftrightarrow \quad \psi(\vec{r}) \propto Y_\ell^m(\hat{r}), \quad Y_\ell^m(\hat{r}) = (-1)^\ell Y_\ell^m(-\hat{r}). \tag{6.50}$$

Therefore, in this case the space (orbital) part of the wave function is symmetric (antisymmetric) if ℓ is even (odd).

To summarize, the (antisymmetric) states of a two-electron system are

- Space (orbital) part of the wave function symmetric and spin state antisymmetric:

$$\psi_+(\vec{x}_1, \vec{x}_2) = \psi_+(\vec{x}_2, \vec{x}_1) \quad (\ell \text{ even in CoM}) \quad \text{and} \quad s = 0: \quad |00\rangle\,. \tag{6.51}$$

- Space (orbital) part of the wave function antisymmetric and spin state symmetric:

$$\psi_-(\vec{x}_1, \vec{x}_2) = -\psi_-(\vec{x}_2, \vec{x}_1) \quad (\ell \text{ odd in CoM}) \quad \text{and} \quad s = 1: \quad |1m_s\rangle\,. \tag{6.52}$$

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6.5 Exchange correlation

Consider two free *identical* particles with momenta $\vec{k}$ and $\vec{k}'$. The space part of the space wave function of the system must be symmetric or antisymmetric under exchange,

$$\begin{aligned}\psi_\pm(\vec{x}_1,\vec{x}_2) &\sim \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{x}_1}\mathrm{e}^{\mathrm{i}\vec{k}'\cdot\vec{x}_2} \pm \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{x}_2}\mathrm{e}^{\mathrm{i}\vec{k}'\cdot\vec{x}_1}\right)\\ &= \frac{1}{\sqrt{2}}\mathrm{e}^{\mathrm{i}(\vec{k}+\vec{k}')\cdot\vec{R}}\left(\mathrm{e}^{\mathrm{i}(\vec{k}-\vec{k}')\cdot\vec{r}/2} \pm \mathrm{e}^{-\mathrm{i}(\vec{k}-\vec{k}')\cdot\vec{r}/2}\right)\end{aligned} \tag{6.53}$$

with $\vec{R} = \frac{1}{2}(\vec{x}_1+\vec{x}_2)$ and $\vec{r} = \vec{x}_1 - \vec{x}_2$. Then the probability density to find a particle in a space region is *correlated* with the position of the other one:

$$|\psi_+(\vec{x}_1,\vec{x}_2)|^2 = 2\cos^2\frac{(\vec{k}-\vec{k}')\cdot\vec{r}}{2} \quad\Rightarrow\quad \vec{r}=0 \quad \text{favoured} \tag{6.54}$$

$$|\psi_-(\vec{x}_1,\vec{x}_2)|^2 = 2\sin^2\frac{(\vec{k}-\vec{k}')\cdot\vec{r}}{2} \quad\Rightarrow\quad \vec{r}=0 \quad \text{impossible.} \tag{6.55}$$

Likewise, in a more general case of two particles with wave functions (space parts) $\psi_1(\vec{x})$ and $\psi_2(\vec{x})$, the space part of the wave function of the system if they are identical must be

$$\psi_\pm(\vec{x}_1,\vec{x}_2) = \frac{1}{\sqrt{2}}[\psi(\vec{x}_1,\vec{x}_2) \pm \psi(\vec{x}_2,\vec{x}_1)] \quad \text{with} \quad \psi(\vec{x}_1,\vec{x}_2) = \psi_1(\vec{x}_1)\psi_2(\vec{x}_2) \tag{6.56}$$

and then

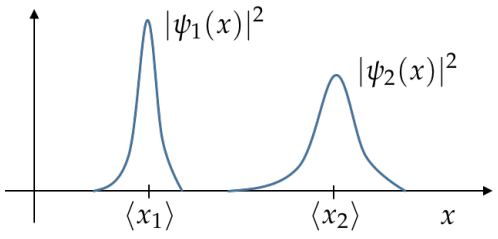
$$\begin{aligned}|\psi_\pm(\vec{x}_1,\vec{x}_2)|^2 &= \frac{1}{2}\left[|\psi(\vec{x}_1,\vec{x}_2)|^2 + |\psi(\vec{x}_2,\vec{x}_1)|^2 \pm 2\mathrm{Re}\left(\psi(\vec{x}_1,\vec{x}_2)\psi^*(\vec{x}_2,\vec{x}_1)\right)\right]\\ &= \frac{1}{2}\Big[|\psi_1(\vec{x}_1)|^2|\psi_2(\vec{x}_2)|^2 + |\psi_1(\vec{x}_2)|^2|\psi_2(\vec{x}_1)|^2\\ &\qquad \pm 2\mathrm{Re}\left(\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\psi_1^*(\vec{x}_2)\psi_2^*(\vec{x}_1)\right)\Big].\end{aligned} \tag{6.57}$$

The last term is known as the **exchange density**.

If the wave functions $\psi_1(\vec{x})$ and $\psi_2(\vec{x})$ do *not overlap* (see figure), then the probability density to find one particle at $\vec{x} = \vec{x}_1 \sim \langle x_1\rangle$ and the other at $\vec{x} = \vec{x}_2 \sim \langle x_2\rangle$ is

$$|\psi_\pm(\vec{x}_1,\vec{x}_2)|^2 + |\psi_\pm(\vec{x}_2,\vec{x}_1)|^2 = 2|\psi_\pm(\vec{x}_1,\vec{x}_2)|^2 = |\psi_1(\vec{x}_1)|^2|\psi_2(\vec{x}_2)|^2 \tag{6.58}$$

where we have used that



$$\psi_1(x_2) \sim 0, \quad \psi_2(x_1) \sim 0. \tag{6.59}$$

Therefore, in that case (not very dense systems of identical particles) the exchange-density term is unimportant and there is no need to symmetrize or antisymmetrize the states.

6.6 Creation and annihilation operators

6.6.1 Harmonic oscillator

Consider the simple harmonic oscillator, a particle of mass m in one dimension submitted to an attractive force proportional to the distance. The Hamiltonian of the system is

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2, \quad k \equiv m\omega^2 \tag{6.60}$$

and the classical trajectories of the particle (solutions of the equations of motion) are oscillations of angular frequency $\omega = 2\pi\nu$.

In QM, x and p become self-adjoint operators X and P with $[X, P] = \mathrm{i}\hbar I$. An elegant method introduced by Dirac that allows to find the energy eigenvalues and eigenvectors of this quantum system consists of defining the operators a and $a^\dagger$:

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(X + \mathrm{i}\frac{P}{m\omega}\right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(X - \mathrm{i}\frac{P}{m\omega}\right) \tag{6.61}$$

$$\Rightarrow \quad X = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \quad P = -\mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger), \tag{6.62}$$

with

$$[X, P] = \mathrm{i}\hbar I \quad \Rightarrow \quad [a, a^\dagger] = I. \tag{6.63}$$

Then the Hamiltonian reads

$$H = \hbar\omega(a^\dagger a + \tfrac{1}{2}) = \hbar\omega(N + \tfrac{1}{2}), \tag{6.64}$$

where we have introduced the self-adjoint operator

$$N = a^\dagger a. \tag{6.65}$$

Because H is just a linear function of N, both can be diagonalized simultaneously. We denote the energy eigenstates $|n\rangle$ by the eigenvalues of N, so

$$N|n\rangle = n|n\rangle \quad \text{and} \quad H|n\rangle = E_n|n\rangle, \quad E_n = (n + \tfrac{1}{2})\hbar\omega. \tag{6.66}$$

To appreciate the physical meaning of a, $a^\dagger$ and N, notice that

$$[N, a] = [a^\dagger a, a] = a^\dagger[a, a] + [a^\dagger, a]a = -a, \quad [N, a^\dagger] = a^\dagger \tag{6.67}$$

and then

$$Na^\dagger|n\rangle = ([N, a^\dagger] + a^\dagger N)|n\rangle = (n + 1)a^\dagger|n\rangle \tag{6.68}$$

$$Na|n\rangle = ([N, a] + aN)|n\rangle = (n - 1)a|n\rangle. \tag{6.69}$$

Therefore, $a^\dagger|n\rangle$ and $a|n\rangle$ are also eigenstates of N with eigenvalue $n + 1$ and $n - 1$, respectively. That is why we call $a^\dagger$ (a) the *creation* (*annihilation*) *operators* of *oscillation modes* of energy $\hbar\omega$. On the other hand,

$$a|n\rangle = c|n - 1\rangle, \quad \langle n|a^\dagger a|n\rangle = |c|^2 = \langle n|N|n\rangle = n \quad \Rightarrow \quad a|n\rangle = \sqrt{n}|n - 1\rangle \tag{6.70}$$

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and from $|n\rangle = \dfrac{1}{\sqrt{n+1}} a\,|n+1\rangle$,

$$a^\dagger\,|n\rangle = \frac{1}{\sqrt{n+1}} a^\dagger a\,|n+1\rangle \quad \Rightarrow \quad a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,. \tag{6.71}$$

If we apply a successively,

$$a^2\,|n\rangle = \sqrt{n(n-1)}\,|n-2\rangle\,, \quad a^3\,|n\rangle = \sqrt{n(n-1)(n-2)}\,|n-3\rangle\,, \quad \ldots \tag{6.72}$$

we would find states with (unacceptable) negative energy and (also unacceptable) norm, because

$$n = \langle n|\,N\,|n\rangle = (\langle n|\,a^\dagger)(a\,|n\rangle) > 0, \tag{6.73}$$

unless n is a *non-negative integer*. Then the sequence terminates at $n = 0$ and the ground state of the system $|0\rangle$ has a (non-zero!) energy

$$E_0 = \tfrac{1}{2}\hbar\omega. \tag{6.74}$$

Hence, $N = a^\dagger a$ is the *number operator*, the state $|0\rangle$ is called the *vacuum* (assumed normalized, $\langle 0|0\rangle = 1$) because it has no modes, and $|n\rangle$ is the state of n modes that can be obtained applying $a^\dagger$ on the vacuum n times,

$$a^\dagger\,|0\rangle = |1\rangle \Rightarrow \quad |1\rangle = a^\dagger\,|0\rangle \tag{6.75}$$

$$a^\dagger\,|1\rangle = \sqrt{2}\,|2\rangle \Rightarrow \quad |2\rangle = \frac{1}{\sqrt{2}} a^\dagger\,|1\rangle = \frac{1}{\sqrt{2}}(a^\dagger)^2\,|0\rangle \tag{6.76}$$

$$a^\dagger\,|2\rangle = \sqrt{3}\,|3\rangle \Rightarrow \quad |3\rangle = \frac{1}{\sqrt{3}} a^\dagger\,|2\rangle = \frac{1}{\sqrt{6}}(a^\dagger)^3\,|0\rangle \tag{6.77}$$

$$\ldots \qquad \Rightarrow \quad |n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n\,|0\rangle\,. \tag{6.78}$$

We can now obtain the energy eigenfunctions in the position representation from

$$a = \frac{1}{\sqrt{2}}(\alpha X + \frac{\mathrm{i}}{\hbar\alpha} P) \quad \text{with} \quad \alpha \equiv \sqrt{\frac{m\omega}{\hbar}}. \tag{6.79}$$

Exchanging variables,

$$\tilde{X} \equiv \alpha X, \quad X\,|x\rangle = x\,|x\rangle \quad \Rightarrow \quad \tilde{X}\,|x\rangle = \alpha x\,|x\rangle \equiv \tilde{x}\,|x\rangle \tag{6.80}$$

the momentum operator in the position representation is

$$P \doteq -\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}x} = -\mathrm{i}\hbar\alpha \frac{\mathrm{d}}{\mathrm{d}\tilde{x}} \tag{6.81}$$

and the wave function of vacuum follows from

$$a\,|0\rangle = 0 \quad \Rightarrow \quad \frac{1}{\sqrt{2}}\left(\tilde{x} + \frac{\mathrm{d}}{\mathrm{d}\tilde{x}}\right)\psi_0(\tilde{x}) = 0 \tag{6.82}$$

whose (normalized) solution is

$$\psi_0(\tilde{x}) = A\mathrm{e}^{-\frac{\tilde{x}^2}{2}} \quad \Rightarrow \quad \psi_0(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}}}\mathrm{e}^{-\frac{\alpha^2 x^2}{2}}. \tag{6.83}$$

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Likewise, from

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n\,|0\rangle \quad \Rightarrow \quad \psi_n(\tilde{x}) = \frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}\left(\tilde{x} - \frac{\mathrm{d}}{\mathrm{d}\tilde{x}}\right)^n \psi_0(\tilde{x})$$
$$\Rightarrow \quad \psi_n(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}\,n!\,2^n}}\,H_n(\alpha x)\,\mathrm{e}^{-\frac{\alpha^2 x^2}{2}} \tag{6.84}$$

where $H_n(t)$ is the n^{th}-order Hermite polynomial:

$$H_n(t) \equiv \mathrm{e}^{t^2/2}\left(t - \frac{\mathrm{d}}{\mathrm{d}t}\right)^n \mathrm{e}^{-t^2/2}. \tag{6.85}$$

6.6.2 Identical bosons

The method of creation and annihilation operators introduced above to solve the harmonic oscillator problem is very convenient to study the systems of identical particles.

Let us define $|n\rangle$ as the state of the system with n identical bosons, all of them in the *same* quantum state $|\alpha\rangle$ (for example: $|\alpha\rangle$ the state of $E = \hbar\omega$). We introduce the *annihilation operator* a such that it gives the state with one particle less:

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle \tag{6.86}$$

The adjoint is the creation operator $a^\dagger$,

$$\langle n|\,a^\dagger = \sqrt{n}\,\langle n-1| \quad \Rightarrow \quad \langle n|\,a^\dagger a\,|n\rangle = n \quad \Rightarrow \quad a^\dagger a\,|n\rangle = n\,|n\rangle\,. \tag{6.87}$$

Hence, $N = a^\dagger a$ is the *number operator* that *counts* the number of particles and $a^\dagger$ is the *creation operator* that adds one particle in the same state:

$$|n\rangle = \frac{1}{\sqrt{n+1}}a\,|n+1\rangle \quad \Rightarrow \quad a^\dagger\,|n\rangle = \frac{1}{\sqrt{n+1}}a^\dagger a\,|n+1\rangle = \sqrt{n+1}\,|n+1\rangle\,. \tag{6.88}$$

Now we can derive the commutation relations:

$$\left.\begin{array}{l} aa^\dagger\,|n\rangle = \sqrt{n+1}\,a\,|n+1\rangle = (n+1)\,|n\rangle \\ a^\dagger a\,|n\rangle = \sqrt{n}\,a^\dagger\,|n-1\rangle = n\,|n\rangle \end{array}\right\} \quad \Rightarrow \quad [a, a^\dagger] = I. \tag{6.89}$$

The state $|0\rangle$ with no particles (assumed normalized, $\langle 0|0\rangle = 1$) is called the vacuum, with $a\,|0\rangle = 0$. The state with n particles can be written as

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n\,|0\rangle \tag{6.90}$$

that is, of course, a symmetric state under the exchange.

Now let us generalize this formalism to the case of n identical bosons, with n_1 at the same state $|\alpha_1\rangle$, n_2 at the same state $|\alpha_2\rangle$, etc. (for example: $|\alpha_i\rangle$ the states of $E_i = \hbar\omega_i$)

$$|n_1, n_2, \cdots\rangle \tag{6.91}$$

that is understood to be symmetrized (symmetric under the exchange of any pair). The n_i are the *occupation numbers* and $n = \sum_i n_i$. We define the annihilation (a_i) and creation ($a_i^\dagger$) operators of particles in the state $|\alpha_i\rangle$ as

$$a_i\,|n_1, \cdots, n_i, \cdots\rangle = \sqrt{n_i}\;|n_1, \cdots, n_i - 1, \cdots\rangle \tag{6.92}$$

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$$a_i^\dagger \left|n_1, \cdots, n_i, \cdots\right\rangle = \sqrt{n_i+1}\ \left|n_1, \cdots, n_i+1, \cdots\right\rangle . \tag{6.93}$$

The number operator $N_i = a_i^\dagger a_i$ gives the occupation of state $|\alpha_i\rangle$,

$$a_i^\dagger a_i \left|n_1, \cdots, n_i, \cdots\right\rangle = n_i\ \left|n_1, \cdots, n_i, \cdots\right\rangle . \tag{6.94}$$

The annihilation and creation operators satisfy the commutation relations:

$$[a_i, a_j^\dagger] = \delta_{ij} I, \quad [a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0. \tag{6.95}$$

Then any state of the system of n identical bosons can be written as:

$$|n_1, n_2, \cdots\rangle = \frac{1}{\sqrt{n_1! n_2! \cdots}} (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} \cdots |0\rangle \tag{6.96}$$

with $|0\rangle \equiv |0, 0, \cdots\rangle$ the vacuum state (no bosons). This state is symmetric under the exchange of any pair of particles.

The Hilbert space $\mathcal{H}_B$ of a system of identical bosons is called *Fock space of bosons*, whose states are symmetric under exchange and can be written in the occupation number formalism described above,

$$\mathcal{H}_B = \mathcal{H}_S^0 \oplus \mathcal{H}_S^1 \oplus \mathcal{H}_S^2 \oplus \mathcal{H}_S^3 \oplus \cdots = \bigoplus_{n=0}^{\infty} \mathcal{H}_S^n \tag{6.97}$$

where the basis of $\mathcal{H}_S^n$ is the set of symmetric states $|n_1 n_2 \cdots\rangle$ with $n = \sum_i n_i$. The states of $\mathcal{H}_S^n$ could also be obtained by symmetrizing the tensors of $\mathcal{H}^n = \mathcal{H} \otimes \mathcal{H} \otimes \cdots$, n times ($\mathcal{H}_S^n \subset \mathcal{H}^n$) where $\mathcal{H}$ is the Hilbert space of one particle.[b] $\mathcal{H}_S^0$ is formed by just on state, the vacuum. $\mathcal{H}_S^1 = \mathcal{H}$ is the system of one particle. $\mathcal{H}_S^{n\geq 2}$ is the system of n identical bosons, whose states are symmetric under exchange.

In particular, this formalism describes a system of oscillators with a discrete spectrum of energies $E_i = \hbar\omega_i \equiv \alpha_i$. When there is a continuum of oscillator modes of energy E, we have $a_i = a(\omega_i) \to a(\omega = E/\hbar)$ that defines a *quantum field theory* (bosonic fields).

6.6.3 Identical fermions

The occupation number formalism can also be adapted to describe a system of identical fermions, whose states are antisymmetric under exchange. Then obviously

$$\left|n_1, n_2, \ldots\right\rangle, \quad n_i = 0 \text{ or } 1. \tag{6.98}$$

To introduce annihilation (η) and creation ($\eta^\dagger$) operators of fermionic states we define

$$\eta\left|0\right\rangle = 0, \quad \eta\left|1\right\rangle = \left|0\right\rangle, \quad \eta^\dagger\left|0\right\rangle = \left|1\right\rangle, \quad \eta^\dagger\left|1\right\rangle = 0 \tag{6.99}$$

and

$$\eta_i \left|n_1, \cdots n_i, \cdots\right\rangle = (-1)^{\nu_i} n_i\ \left|n_1, \cdots, 1-n_i, \cdots\right\rangle \tag{6.100}$$

$$\eta_i^\dagger \left|n_1, \cdots n_i, \cdots\right\rangle = (-1)^{\nu_i} (1-n_i)\ \left|n_1, \cdots, n_i+1, \cdots\right\rangle \tag{6.101}$$

[b] Notice that every $\mathcal{H}$ can be the tensor product of other Hilbert spaces (e.g. $\mathcal{H}^{\text{space}} \otimes \mathcal{H}^{\text{spin}} \otimes \cdots$) but this formalism is particularly useful when the states are labeled by the eigenvalues of just one observable, like the energy.

where

$$\nu_i = \sum_{k=1}^{i-1} n_k. \tag{6.102}$$

Then the number operator $N_i = \eta_i^\dagger \eta_i$ gives the occupancy of state $|\alpha_i\rangle$,

$$\eta_i^\dagger \eta_i \, |n_1, \cdots n_i, \cdots\rangle = n_i^2 \; |n_1, \cdots n_i, \cdots\rangle = n_i \, |n_1, \cdots n_i, \cdots\rangle \, . \tag{6.103}$$

And one can easily derive the anticommutation relations:

$$\{\eta_i, \eta_j^\dagger\} = \delta_{ij} I, \quad \{\eta_i, \eta_j\} = \{\eta_i^\dagger, \eta_j^\dagger\} = 0. \tag{6.104}$$

where $\{A, B\} \equiv AB + BA$. As expected,

$$\{\eta_i^\dagger, \eta_i^\dagger\} = 0 \quad \Rightarrow \quad (\eta_i^\dagger)^2 = 0 \tag{6.105}$$

and therefore two fermions cannot be in the same state (Pauli exclusion principle).

Any state of the system of identical fermions can be written as:

$$|n_1, n_2, \cdots\rangle = (\eta_1^\dagger)^{n_1} (\eta_2^\dagger)^{n_2} \cdots |0\rangle \, . \tag{6.106}$$

These states span the *Fock space of fermions*.

This formalism of creation and annihilation operators for identical fermions is applied in quantum field theory (fermionic fields), where fermions have a continuous spectrum of energies.

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Chapter 7

Approximation methods

Few systems in quantum mechanics can be solved exactly. So we are forced to adopt approximate solutions that can be obtained by different types of methods, numerical (with the help of a computer) or analytical: perturbative, variational, WKB, etc. Here we will discuss the perturbative approximations.

7.1 Stationary perturbations

7.1.1 Nondegenerate case

Let us consider a *time-independent* Hamiltonian, that can be separated into two parts:

$$H = H^0 + \lambda V \tag{7.1}$$

where we know the eigenvalues and eigenstates of H^0:

$$H^0 \left|\psi_i^{(0)}\right\rangle = E_i^{(0)} \left|\psi_i^{(0)}\right\rangle . \tag{7.2}$$

H^0 does *not* have to be the free Hamiltonian.
For example, we know the exact solutions of the hydrogen atom,

$$H^0 = \frac{p^2}{2m} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r} \tag{7.3}$$

and V could be the interaction with an external magnetic field. Then, we suppose that V is a *perturbation* that changes a *little* the eigenvalues and eigenvectors of H. We assume the *analyticity* of H around $\lambda = 0$, namely there is a smooth transition between the solutions for $\lambda = 0$ and those we are looking for ($\lambda = 1$) so that

$$H\left|\psi_i(\lambda)\right\rangle = E_i(\lambda)\left|\psi_i(\lambda)\right\rangle . \tag{7.4}$$

with

$$\boxed{\left|\psi_i(\lambda)\right\rangle = \sum_{n=0}^{\infty} \lambda^n \left|\psi_i^{(n)}\right\rangle , \qquad E_i(\lambda) = \sum_{k=0}^{\infty} \lambda^k E_i^{(k)}} \tag{7.5}$$

Inserting this into the Schrödinger equation above we have:[a]

$$(H^0+\lambda V)\sum_{n=0}^{\infty}\lambda^n\left|\psi_i^{(n)}\right\rangle=\sum_{n=0}^{\infty}\sum_{k=0}^{\infty}\lambda^{n+k}E_i^{(n)}\left|\psi_i^{(k)}\right\rangle;$$

$$H^0\left|\psi_i^{(0)}\right\rangle+\sum_{n=1}^{\infty}\lambda^n\left(H^0\left|\psi_i^{(n)}\right\rangle+V\left|\psi_i^{(n-1)}\right\rangle\right)=E_i^{(0)}\left|\psi_i^{(0)}\right\rangle+\sum_{n=1}^{\infty}\lambda^n\sum_{k=0}^{n}E_i^{(k)}\left|\psi_i^{(n-k)}\right\rangle \tag{7.6}$$

and hence, comparing powers of λ,

$$\left(H^0-E_i^{(0)}\right)\left|\psi_i^{(0)}\right\rangle=0\quad\text{(this we knew already)}, \tag{7.7}$$

$$\left(H^0-E_i^{(0)}\right)\left|\psi_i^{(n)}\right\rangle=-V\left|\psi_i^{(n-1)}\right\rangle+\sum_{k=1}^{n}E_i^{(k)}\left|\psi_i^{(n-k)}\right\rangle,\quad n\geq 1. \tag{7.8}$$

Remember that the states $\left|\psi_i^{(0)}\right\rangle$ are normalized,

$$\left\langle\psi_i^{(0)}\middle|\psi_i^{(0)}\right\rangle=1. \tag{7.9}$$

To simplify the calculations, let us choose *for the moment* the normalization

$$\left\langle\psi_i^{(0)}\middle|\psi_i(\lambda)\right\rangle=1 \tag{7.10}$$

also for $\lambda\neq 0$, so that

$$1=\left\langle\psi_i^{(0)}\middle|\psi_i(\lambda)\right\rangle=\left\langle\psi_i^{(0)}\middle|\psi_i^{(0)}\right\rangle+\sum_{n=1}^{\infty}\lambda^n\left\langle\psi_i^{(0)}\middle|\psi_i^{(n)}\right\rangle$$

$$\Rightarrow\quad\left\langle\psi_i^{(0)}\middle|\psi_i^{(n)}\right\rangle=0,\quad\forall n\geq 1. \tag{7.11}$$

Then muliplying the equation (7.8) by $\left\langle\psi_i^{(0)}\right|$ we have that for $n\geq 1$:

$$\left\langle\psi_i^{(0)}\middle|\left(H^0-E_i^{(0)}\right)\middle|\psi_i^{(n)}\right\rangle=-\left\langle\psi_i^{(0)}\middle|V\middle|\psi_i^{(n-1)}\right\rangle+\sum_{k=1}^{n}E_i^{(k)}\left\langle\psi_i^{(0)}\middle|\psi_i^{(n-k)}\right\rangle;$$

$$0=-\left\langle\psi_i^{(0)}\middle|V\middle|\psi_i^{(n-1)}\right\rangle+\sum_{k=1}^{n}E_i^{(k)}\delta_{nk}$$

$$\Rightarrow\quad\boxed{E_i^{(n)}=\left\langle\psi_i^{(0)}\middle|V\middle|\psi_i^{(n-1)}\right\rangle,\quad n\geq 1} \tag{7.12}$$

And multiplying (7.8) by $\left\langle\psi_j^{(0)}\right|$ with $j\neq i$ we have:

$$\left\langle\psi_j^{(0)}\middle|\left(H^0-E_i^{(0)}\right)\middle|\psi_i^{(n)}\right\rangle=-\left\langle\psi_j^{(0)}\middle|V\middle|\psi_i^{(n-1)}\right\rangle+\sum_{k=1}^{n}E_i^{(k)}\left\langle\psi_j^{(0)}\middle|\psi_i^{(n-k)}\right\rangle;$$

$$\left(E_j^{(0)}-E_i^{(0)}\right)\left\langle\psi_j^{(0)}\middle|\psi_i^{(n)}\right\rangle=-\left\langle\psi_j^{(0)}\middle|V\middle|\psi_i^{(n-1)}\right\rangle+\sum_{k=1}^{n-1}E_i^{(k)}\left\langle\psi_j^{(0)}\middle|\psi_i^{(n-k)}\right\rangle$$

[a] We replace $\sum_{n=0}^{\infty}\sum_{k=0}^{\infty}\lambda^{n+k}E_i^{(k)}\left|\psi_i^{(n)}\right\rangle=\sum_{n=0}^{\infty}\lambda^n\sum_{k=0}^{n}E_i^{(k)}\left|\psi_i^{(n-k)}\right\rangle$.

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$$\Rightarrow \quad \left\langle \psi_j^{(0)} \middle| \psi_i^{(n)} \right\rangle = \frac{1}{E_i^{(0)} - E_j^{(0)}} \left[\left\langle \psi_j^{(0)} \middle| V \middle| \psi_i^{(n-1)} \right\rangle - \sum_{k=1}^{n-1} E_i^{(k)} \left\langle \psi_j^{(0)} \middle| \psi_i^{(n-k)} \right\rangle \right] \tag{7.13}$$

and then (remember that $\left\langle \psi_i^{(0)} \middle| \psi_i^{(n)} \right\rangle = 0$, $\forall n \geq 1$):

$$\left| \psi_i^{(n)} \right\rangle = \sum_j \left| \psi_j^{(0)} \right\rangle \left\langle \psi_j^{(0)} \middle| \psi_i^{(n)} \right\rangle$$

$$\Rightarrow \quad \boxed{\left| \psi_i^{(n)} \right\rangle = \sum_{j \neq i} \frac{1}{E_i^{(0)} - E_j^{(0)}} \left| \psi_j^{(0)} \right\rangle \left[\left\langle \psi_j^{(0)} \middle| V \middle| \psi_i^{(n-1)} \right\rangle - \sum_{k=1}^{n-1} E_i^{(k)} \left\langle \psi_j^{(0)} \middle| \psi_i^{(n-k)} \right\rangle \right]} \tag{7.14}$$

Therefore from (7.12) and (7.14) we have:

$$n = 1: \qquad E_i^{(1)} = \left\langle \psi_i^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle \tag{7.15}$$

$$\left| \psi_i^{(1)} \right\rangle = \sum_{j \neq i} \left| \psi_j^{(0)} \right\rangle \frac{\left\langle \psi_j^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle}{E_i^{(0)} - E_j^{(0)}} \tag{7.16}$$

$$\begin{aligned} n = 2: \qquad E_i^{(2)} &= \left\langle \psi_i^{(0)} \middle| V \middle| \psi_i^{(1)} \right\rangle \\ &= \sum_{j \neq i} \frac{\left\langle \psi_j^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle \left\langle \psi_i^{(0)} \middle| V \middle| \psi_j^{(0)} \right\rangle}{E_i^{(0)} - E_j^{(0)}} \\ &= \sum_{j \neq i} \frac{\left| \left\langle \psi_j^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle \right|^2}{E_i^{(0)} - E_j^{(0)}} \end{aligned} \tag{7.17}$$

etc.

One expects that taking just the first terms will be a good approximation as long as

$$\frac{\left| \left\langle \psi_j^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle \right|}{\left| E_i^{(0)} - E_j^{(0)} \right|} \ll 1, \quad j \neq i. \tag{7.18}$$

Then, from (7.5) and for our case of interest ($\lambda = 1$) we have that up to first order :

$$E_i = E_i^{(0)} + \left\langle \psi_i^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle + \dots \tag{7.19}$$

$$|\psi_i\rangle = \left| \psi_i^{(0)} \right\rangle + \sum_{j \neq i} \left| \psi_j^{(0)} \right\rangle \frac{\left\langle \psi_j^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle}{E_i^{(0)} - E_j^{(0)}} + \dots \tag{7.20}$$

This was obtained with the normalization $\left\langle \psi_i^{(0)} \middle| \psi_i(\lambda) \right\rangle = 1$ that implies $\langle \psi_i(\lambda)) | \psi_i(\lambda) \rangle \neq 1$. However, we *must* normalize the states canonically:

$$|\psi_i(\lambda)\rangle \to \left| \overline{\psi}_i(\lambda) \right\rangle = Z_i^{\frac{1}{2}}(\lambda) \, |\psi_i(\lambda)\rangle \tag{7.21}$$

$$\text{with} \quad \left\langle \overline{\psi}_i(\lambda) \middle| \overline{\psi}_i(\lambda) \right\rangle = 1 \quad \Rightarrow \quad Z_i(\lambda) = \langle \psi_i(\lambda) | \psi_i(\lambda) \rangle^{-1} . \tag{7.22}$$

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From $\left\langle \psi_i^{(0)} \middle| \psi_i^{(n)} \right\rangle = 0$ for $n \geq 1$ (7.11) and the expression (7.16) for $\left| \psi_i^{(1)} \right\rangle$ above we have:

$$\begin{aligned}
\langle \psi_i(\lambda) | \psi_i(\lambda) \rangle &= \left\langle \psi_i^{(0)} \middle| \psi_i^{(0)} \right\rangle \\
&\quad + \lambda \left(\left\langle \psi_i^{(0)} \middle| \psi_i^{(1)} \right\rangle + \left\langle \psi_i^{(1)} \middle| \psi_i^{(0)} \right\rangle \right) \\
&\quad + \lambda^2 \left(\left\langle \psi_i^{(0)} \middle| \psi_i^{(2)} \right\rangle + \left\langle \psi_i^{(2)} \middle| \psi_i^{(0)} \right\rangle + \left\langle \psi_i^{(1)} \middle| \psi_i^{(1)} \right\rangle \right) + \dots \\
&= 1 + \lambda^2 \left\langle \psi_i^{(1)} \middle| \psi_i^{(1)} \right\rangle + \dots \\
&= 1 + \lambda^2 \sum_{j \neq i} \sum_{k \neq i} \frac{\left\langle \psi_j^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle^*}{E_i^{(0)} - E_j^{(0)}} \frac{\left\langle \psi_k^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle}{E_i^{(0)} - E_k^{(0)}} \left\langle \psi_j^{(0)} \middle| \psi_k^{(0)} \right\rangle + \dots \\
&= 1 + \lambda^2 \sum_{j \neq i} \frac{\left| \left\langle \psi_j^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle \right|^2}{\left(E_i^{(0)} - E_j^{(0)} \right)^2} + \dots
\end{aligned} \tag{7.23}$$

Therefore, one should replace:

$$\boxed{|\psi_i(\lambda)\rangle \to Z_i^{\frac{1}{2}}(\lambda) \, |\psi_i(\lambda)\rangle \quad \text{with} \quad Z_i(\lambda) = 1 - \lambda^2 \sum_{j \neq i} \frac{\left| \left\langle \psi_j^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle \right|^2}{\left(E_i^{(0)} - E_j^{(0)} \right)^2} + \dots} \tag{7.24}$$

that will give $\mathcal{O}(\lambda^2)$ order corrections to the perturbative series, beyond the first order approximation we have shown in (7.19) and (7.20).

7.1.2 Degenerate case

If H^0 has *degenerate eigenvalues*, namely same energies $E_i^{(0)} = E_j^{(0)}$ for some eigenvectors $\left| \psi_i^{(0)} \right\rangle \neq \left| \psi_j^{(0)} \right\rangle$, then the expressions above are divergent and cannot be used. Notice that any combination of those states has the same energy according to the unperturbed Hamiltonian *but* we assume the interaction V *will break the degeneracy*. So we must diagonalize V in the degenerate subspace of H^0 to find the appropriate combinations $\left\{ \left| \psi_{i,a}^{(0)} \right\rangle \right\}$ that will be the right basis to start our perturbation theory

$$E_{i,a} = E_i^{(0)} + E_{i,a}^{(1)} + \dots \tag{7.25}$$

Then we separate the contributions of the degenerate eigenstates of H^0 ($E_j^{(0)} = E_i^{(0)}$) from the rest, that were found before in (7.19) and (7.20):

$$E_i = E_i^{(0)} + E_i^{(1)} + \dots \qquad \text{with } E_i^{(1)} = \left\langle \psi_i^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle \tag{7.26}$$

$$\begin{aligned}
|\psi_i\rangle = \left| \psi_i^{(0)} \right\rangle &+ \sum_{\substack{j \neq i \\ E_j^{(0)} \neq E_i^{(0)}}} \left| \psi_j^{(0)} \right\rangle \frac{\left\langle \psi_j^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle}{E_i^{(0)} - E_j^{(0)}} \\
&+ \sum_{\substack{j \neq i \\ E_j^{(0)} = E_i^{(0)}}} \left| \psi_j^{(0)} \right\rangle \frac{1}{E_i^{(1)} - E_j^{(1)}} \sum_{\substack{k \neq i \\ E_k^{(0)} \neq E_i^{(0)}}} \frac{\left\langle \psi_j^{(0)} \middle| V \middle| \psi_k^{(0)} \right\rangle \left\langle \psi_k^{(0)} \middle| V \middle| \psi_i^{(0)} \right\rangle}{E_i^{(0)} - E_k^{(0)}} + \dots
\end{aligned} \tag{7.27}$$

Example: Calculate to first order in perturbation theory the energy eigenvalues and eigenstates of a system described by the Hamiltonian $H = H^0 + V$ with

$$H^0 \doteq \begin{pmatrix} \Delta & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \Delta \end{pmatrix}, \quad V \doteq \begin{pmatrix} 0 & 0 & \epsilon \\ 0 & 0 & \epsilon \\ \epsilon & \epsilon & 0 \end{pmatrix} \tag{7.28}$$

in the basis $\{|e_1\rangle, |e_2\rangle, |e_3\rangle\}$ of H^0 eigenstates. There is a degenerate eigenvalue, $E_1^{(0)} = E_3^{(0)} = \Delta$. We must diagonalize V in the the subspace $\mathcal{H}_\Delta : \{|e_1\rangle, |e_3\rangle\}$:

$$P_\Delta = |e_1\rangle\langle e_1| + |e_3\rangle\langle e_3|, \quad V = \epsilon\left(|e_1\rangle\langle e_3| + |e_2\rangle\langle e_3| + |e_3\rangle\langle e_1| + |e_3\rangle\langle e_2|\right) \tag{7.29}$$

$$P_\Delta H^0 P_\Delta = \Delta P_\Delta \doteq \begin{pmatrix} \Delta & 0 \\ 0 & \Delta \end{pmatrix}, \quad P_\Delta V P_\Delta = \epsilon\left(|e_1\rangle\langle e_3| + |e_3\rangle\langle e_1|\right) \doteq \begin{pmatrix} 0 & \epsilon \\ \epsilon & 0 \end{pmatrix}. \tag{7.30}$$

Diagonalization:

$$\begin{vmatrix} -\lambda & \epsilon \\ \epsilon & -\lambda \end{vmatrix} = \lambda^2 - \epsilon^2 = 0 \quad \Rightarrow \quad \begin{cases} \lambda = +\epsilon: & |u_1\rangle = \frac{1}{\sqrt{2}}(|e_1\rangle + |e_3\rangle) \\ \lambda = -\epsilon: & |u_3\rangle = \frac{1}{\sqrt{2}}(|e_1\rangle - |e_3\rangle) \end{cases} \tag{7.31}$$

So the right basis to start the perturbation theory is:

$$\{|u_1\rangle, |e_2\rangle, |u_3\rangle\} \equiv \left\{\left|\psi_1^{(0)}\right\rangle, \left|\psi_2^{(0)}\right\rangle, \left|\psi_3^{(0)}\right\rangle\right\} \tag{7.32}$$

with

$$|e_1\rangle = \frac{1}{\sqrt{2}}\left(\left|\psi_1^{(0)}\right\rangle + \left|\psi_3^{(0)}\right\rangle\right) \tag{7.33}$$

$$|e_2\rangle = \left|\psi_2^{(0)}\right\rangle \tag{7.34}$$

$$|e_3\rangle = \frac{1}{\sqrt{2}}\left(\left|\psi_1^{(0)}\right\rangle - \left|\psi_3^{(0)}\right\rangle\right) \tag{7.35}$$

In this new basis H^0 has, of course, the same form and

$$V = \epsilon\left(|e_1\rangle\langle e_3| + |e_2\rangle\langle e_3| + |e_3\rangle\langle e_1| + |e_3\rangle\langle e_2|\right) \doteq \epsilon \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & -1 \end{pmatrix} \tag{7.36}$$

$$\left\langle \psi_i^{(0)} \right| V \left| \psi_j^{(0)} \right\rangle = V_{ij} \tag{7.37}$$

Now we can use the general expressions to obtain the energy eigenvalues:

$$E_i^{(0)} = E_i^{(0)} + E_i^{(1)} + \ldots \tag{7.38}$$

$$E_i^{(1)} = \left\langle \psi_i^{(0)} \right| V \left| \psi_i^{(0)} \right\rangle \tag{7.39}$$

$$E_1^{(0)} = \Delta \qquad E_1^{(1)} = \epsilon \tag{7.40}$$

$$E_2^{(0)} = 0 \qquad E_2^{(1)} = 0 \tag{7.41}$$

$$E_3^{(0)} = \Delta \qquad E_3^{(1)} = -\epsilon \tag{7.42}$$

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And the energy eigenstates:

$$|\psi_i\rangle = \left|\psi_i^{(0)}\right\rangle + \left|\psi_i^{(1)}\right\rangle + \dots \tag{7.43}$$

$$\left|\psi_i^{(1)}\right\rangle = \sum_{\substack{j\neq i \\ E_j^{(0)}\neq E_i^{(0)}}} \left|\psi_j^{(0)}\right\rangle \frac{\left\langle\psi_j^{(0)}\right| V \left|\psi_i^{(0)}\right\rangle}{E_i^{(0)} - E_j^{(0)}} \tag{7.44}$$

$$+ \sum_{\substack{j\neq i \\ E_j^{(0)}= E_i^{(0)}}} \left|\psi_j^{(0)}\right\rangle \frac{1}{E_i^{(1)} - E_j^{(1)}} \sum_{\substack{k\neq i \\ E_k^{(0)}\neq E_i^{(0)}}} \frac{\left\langle\psi_j^{(0)}\right| V \left|\psi_k^{(0)}\right\rangle \left\langle\psi_k^{(0)}\right| V \left|\psi_i^{(0)}\right\rangle}{E_i^{(0)} - E_k^{(0)}} \tag{7.45}$$

$$\left|\psi_1^{(0)}\right\rangle = \frac{1}{\sqrt{2}}(|e_1\rangle + |e_3\rangle) \tag{7.46}$$

$$\left|\psi_2^{(0)}\right\rangle = |e_2\rangle \tag{7.47}$$

$$\left|\psi_3^{(0)}\right\rangle = \frac{1}{\sqrt{2}}(|e_1\rangle - |e_3\rangle) \tag{7.48}$$

$$\begin{aligned}\left|\psi_1^{(1)}\right\rangle &= \left|\psi_2^{(0)}\right\rangle \frac{\left\langle\psi_2^{(0)}\right| V \left|\psi_1^{(0)}\right\rangle}{E_1^{(0)} - E_2^{(0)}} \\ &+ \left|\psi_3^{(0)}\right\rangle \frac{1}{E_1^{(1)} - E_3^{(1)}} \frac{\left\langle\psi_3^{(0)}\right| V \left|\psi_2^{(0)}\right\rangle \left\langle\psi_2^{(0)}\right| V \left|\psi_1^{(0)}\right\rangle}{E_1^{(0)} - E_2^{(0)}} \\ &= \left|\psi_2^{(0)}\right\rangle \frac{\frac{\epsilon}{\sqrt{2}}}{\Delta - 0} + \left|\psi_3^{(0)}\right\rangle \frac{1}{\epsilon - (-\epsilon)} \frac{-\frac{\epsilon}{\sqrt{2}}\frac{\epsilon}{\sqrt{2}}}{\Delta - 0} \\ &= \frac{\epsilon}{\sqrt{2}\Delta}\left|\psi_2^{(0)}\right\rangle + \frac{\epsilon}{4\Delta}\left|\psi_3^{(0)}\right\rangle\end{aligned} \tag{7.49}$$

$$\begin{aligned}\left|\psi_2^{(1)}\right\rangle &= \left|\psi_1^{(0)}\right\rangle \frac{\left\langle\psi_1^{(0)}\right| V \left|\psi_2^{(0)}\right\rangle}{E_2^{(0)} - E_1^{(0)}} + \left|\psi_3^{(0)}\right\rangle \frac{\left\langle\psi_3^{(0)}\right| V \left|\psi_2^{(0)}\right\rangle}{E_2^{(0)} - E_3^{(0)}} \\ &= \left|\psi_1^{(0)}\right\rangle \frac{\frac{\epsilon}{\sqrt{2}}}{0 - \Delta} + \left|\psi_3^{(0)}\right\rangle \frac{-\frac{\epsilon}{\sqrt{2}}}{0 - \Delta} \\ &= -\frac{\epsilon}{\sqrt{2}\Delta}\left|\psi_1^{(0)}\right\rangle + \frac{\epsilon}{\sqrt{2}\Delta}\left|\psi_3^{(0)}\right\rangle\end{aligned} \tag{7.50}$$

$$\begin{aligned}\left|\psi_3^{(1)}\right\rangle &= \left|\psi_2^{(0)}\right\rangle \frac{\left\langle\psi_2^{(0)}\right| V \left|\psi_3^{(0)}\right\rangle}{E_3^{(0)} - E_2^{(0)}} \\ &+ \left|\psi_1^{(0)}\right\rangle \frac{1}{E_3^{(1)} - E_1^{(1)}} \frac{\left\langle\psi_1^{(0)}\right| V \left|\psi_2^{(0)}\right\rangle \left\langle\psi_2^{(0)}\right| V \left|\psi_3^{(0)}\right\rangle}{E_3^{(0)} - E_2^{(0)}} \\ &= \left|\psi_2^{(0)}\right\rangle \frac{-\frac{\epsilon}{\sqrt{2}}}{\Delta - 0} + \left|\psi_1^{(0)}\right\rangle \frac{1}{-\epsilon - \epsilon} \frac{-\frac{\epsilon}{\sqrt{2}}\frac{\epsilon}{\sqrt{2}}}{\Delta - 0} \\ &= -\frac{\epsilon}{\sqrt{2}\Delta}\left|\psi_2^{(0)}\right\rangle + \frac{\epsilon}{4\Delta}\left|\psi_1^{(0)}\right\rangle\end{aligned} \tag{7.51}$$

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7.2 Time-dependent perturbations

7.2.1 The interaction picture

Let us now discuss *time-dependent* perturbations. The typical situation is the following. Suppose that the Hamiltonian is

$$H = H^0 + V(t) \quad \text{with} \quad V(t<0) = 0 \tag{7.52}$$

and the system is initially ($t = 0$) in an eigenstate $\left|i^0\right\rangle$ of H^0. Once we switch on the perturbation $V(t \geq 0) \neq 0$ the state $\left|i^0\right\rangle$ becomes non-stationary, it will change, and we are interested in the probability that after a time t it goes to a final state $\left|f^0\right\rangle$ (transition probability). Notice that both states are by definition eigenstates of H^0.

The problem is usually formulated in the so called *interaction picture* (or Dirac picture), half the way between the Schrödinger and the Heisenberg pictures. Remember that in the Schrödinger picture the operators remain constant but the states evolve with time:

$$\mathcal{O} \equiv \mathcal{O}_S = \text{const}, \quad \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\alpha(t)\right\rangle_S = H\left|\alpha(t)\right\rangle_S \quad \Rightarrow \quad \left|\alpha(t)\right\rangle_S = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}\left|\alpha(0)\right\rangle_S \tag{7.53}$$

whereas in the Heisenberg picture the states remain constant but the operators evolve with time:

$$\left|\alpha\right\rangle_H = \text{const}, \quad \mathcal{O}_H(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}O_H(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht} \tag{7.54}$$

so that the expectation values are independent of the time evolution picture:

$${}_H\!\left\langle\alpha\right|\mathcal{O}_H(t)\left|\beta\right\rangle_H = {}_S\!\left\langle\alpha(t)\right|\mathcal{O}\left|\beta(t)\right\rangle_S, \quad \text{with} \quad \mathcal{O} = \mathcal{O}_H(0), \quad \left|\alpha\right\rangle_H = \left|\alpha(0)\right\rangle_S. \tag{7.55}$$

The interaction picture is useful when the spectrum of eigenvalues and eigenvectors of the unperturbed system described by H^0 is known. In that case one can *subtract* from a state the part of the evolution due to H^0. In particular, in the interaction picture we define

$$\left|\alpha(t)\right\rangle_I \equiv e^{\frac{\mathrm{i}}{\hbar}H^0t}\left|\alpha(t)\right\rangle_S. \tag{7.56}$$

Let us see how $\left|\alpha(t)\right\rangle_I$ evolves with time:

$$\begin{aligned}
\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\alpha(t)\right\rangle_I &= \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left(e^{\frac{\mathrm{i}}{\hbar}H^0t}\left|\alpha(t)\right\rangle_S\right) \\
&= -H^0e^{\frac{\mathrm{i}}{\hbar}H^0t}\left|\alpha(t)\right\rangle_S + \mathrm{i}\hbar\, e^{\frac{\mathrm{i}}{\hbar}H^0t}\frac{\mathrm{d}}{\mathrm{d}t}\left|\alpha(t)\right\rangle_S \\
&= -H^0e^{\frac{\mathrm{i}}{\hbar}H^0t}\left|\alpha(t)\right\rangle_S + e^{\frac{\mathrm{i}}{\hbar}H^0t}\underbrace{(H^0+V)}_{H}\left|\alpha(t)\right\rangle_S \\
&= e^{\frac{\mathrm{i}}{\hbar}H^0t}V\left|\alpha(t)\right\rangle_S \\
&= \underbrace{e^{\frac{\mathrm{i}}{\hbar}H^0t}Ve^{-\frac{\mathrm{i}}{\hbar}H^0t}}_{V_I(t)}\underbrace{e^{\frac{\mathrm{i}}{\hbar}H^0t}\left|\alpha(t)\right\rangle_S}_{\left|\alpha(t)\right\rangle_I}.
\end{aligned} \tag{7.57}$$

Therefore in the interaction picture the states evolve according to the perturbation:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\alpha(t)\right\rangle_I = V_I(t)\left|\alpha(t)\right\rangle_I \tag{7.58}$$

(*Schrödinger equation in the interaction picture*) and the operators, including V, evolve according to the unperturbed Hamiltonian:

$$\mathcal{O}_I(t) \equiv e^{\frac{\mathrm{i}}{\hbar}H^0t}\mathcal{O}e^{-\frac{\mathrm{i}}{\hbar}H^0t} \quad (\mathcal{O} \text{ in the interaction picture}) \tag{7.59}$$

$$\Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{O}_I = -\frac{\mathrm{i}}{\hbar}[\mathcal{O}_I, H^0]. \tag{7.60}$$

If $V = 0$ we recover the Heisenberg picture.

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7.2.2 Dyson series

Our next objective is to solve the Schrödinger equation in the interaction picture in terms of a time-evolution linear operator $\widetilde{U}(t)$:

$$|\alpha(t)\rangle_I \equiv \widetilde{U}(t)\,|\alpha(0)\rangle_I\,. \tag{7.61}$$

Substituting this in (7.58) we have

$$\mathrm{i}\hbar\frac{\mathrm{d}\widetilde{U}(t)}{\mathrm{d}t} = V_I(t)\,\widetilde{U}(t) \tag{7.62}$$

with the boundary condition $\widetilde{U}(0) = I$ whose solution is

$$\begin{aligned}\mathrm{i}\hbar\int_0^t \mathrm{d}t_1\,\frac{\mathrm{d}\widetilde{U}(t_1)}{\mathrm{d}t_1} &= \int_0^t \mathrm{d}t_1\,V_I(t_1)\,\widetilde{U}(t_1)\\ \Rightarrow\quad \widetilde{U}(t) &= I - \frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t_1\,V_I(t_1)\,\widetilde{U}(t_1).\end{aligned} \tag{7.63}$$

This is the integral version of the Schrödinger equation for the time-evolution operator $\widetilde{U}(t)$.

If V is "small" we can solve this equation by iterations. At the zeroth order $\widetilde{U}(t) = I$, so

$$\widetilde{U}(t) = I - \frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t_1\,V_I(t_1) + \mathcal{O}(V^2). \tag{7.64}$$

Inserting now

$$\widetilde{U}(t_1) = I - \frac{\mathrm{i}}{\hbar}\int_0^{t_1} \mathrm{d}t_2\,V_I(t_2) \tag{7.65}$$

in (7.63) we have

$$\widetilde{U}(t) = I - \frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t_1\,V_I(t_1) + \left(-\frac{\mathrm{i}}{\hbar}\right)^2\int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\,V_I(t_1)V_I(t_2) + \mathcal{O}(V^3). \tag{7.66}$$

Then it is straightforward that the term of order n of the *Dyson series* is:

$$\left(-\frac{\mathrm{i}}{\hbar}\right)^n\int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\cdots\int_0^{t_{n-1}}\mathrm{d}t_n\,V_I(t_1)V_I(t_2)\cdots V_I(t_n). \tag{7.67}$$

The Dyson series can be expressed in a more compact form using the *time-ordered product* of operators defined as:

$$T\{A(t_1)B(t_2)\} = \begin{cases} A(t_1)B(t_2) & \text{if } t_1 \geq t_2\\ B(t_2)A(t_1) & \text{if } t_1 < t_2\end{cases} \tag{7.68}$$

that puts first the latter operator. Using T it is easy to see that:

$$\left(-\frac{\mathrm{i}}{\hbar}\right)^2\int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\,V_I(t_1)V_I(t_2) = \frac{1}{2}\left(-\frac{\mathrm{i}}{\hbar}\right)^2\int_0^t \mathrm{d}t_1\int_0^{t}\mathrm{d}t_2\,T\{V_I(t_1)V_I(t_2)\} \tag{7.69}$$

and for the order n:

$$\begin{aligned}&\left(-\frac{\mathrm{i}}{\hbar}\right)^n\int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\cdots\int_0^{t_{n-1}}\mathrm{d}t_n\,V_I(t_1)V_I(t_2)\cdots V_I(t_n)\\ &\qquad = \frac{1}{n!}\left(-\frac{\mathrm{i}}{\hbar}\right)^n\int_0^t \mathrm{d}t_1\int_0^{t}\mathrm{d}t_2\cdots\int_0^{t}\mathrm{d}t_n\,T\{V_I(t_1)V_I(t_2)\cdots V_I(t_n)\}.\end{aligned} \tag{7.70}$$

Hence the Dyson series can be written as the following time-ordered exponential:

$$\boxed{\widetilde{U}(t) = T\left\{\exp\left[-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\,V(t')\right]\right\}} \tag{7.71}$$

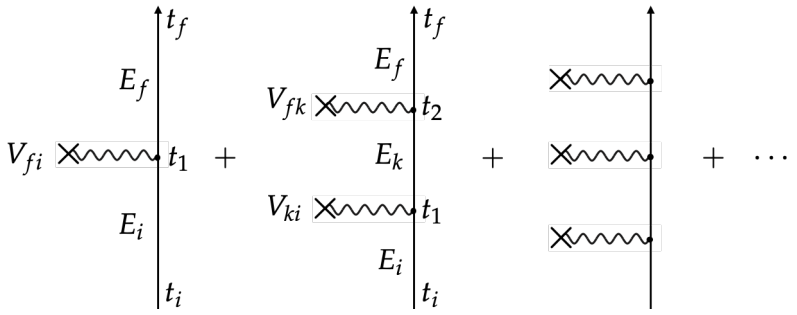

Figure 7.1: Pictorial view of the transition amplitude from the Dyson series.

7.2.3 Transition probability

The time-evolution operator in the interaction picture $\widetilde{U}$ is related to the the time-evolution operator in the Schrödinger picture by

$$U(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0 t}\widetilde{U}(t) \tag{7.72}$$

since it satisfies the equation

$$\begin{aligned}
\mathrm{i}\hbar\frac{\mathrm{d}U(t)}{\mathrm{d}t} &= H^0\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0 t}\widetilde{U}(t) + \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0 t}V_I(t)\widetilde{U}(t) \\
&= H^0\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0 t}\widetilde{U}(t) + \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0 t}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t}V\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0 t}\widetilde{U}(t) \\
&= (H^0 + V)\,U(t) \\
&= H\,U(t)
\end{aligned} \tag{7.73}$$

Notice that $\widetilde{U}(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t}U(t)$ is not the same as "U_I" (U in the interaction picture)!

Therefore, the probability amplitude that a state $\left|i^0\right\rangle$ at $t = 0$ goes to a final state $\left|f^0\right\rangle$ after a time t due to a perturbation V is given by

$$\mathcal{A}(i \to f; t) = \left\langle f^0\right| U(t)\left|i^0\right\rangle = \langle f|\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0 t}\widetilde{U}(t)\,|i\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_f t}\,\langle f|\,\widetilde{U}(t)\,|i\rangle\,. \tag{7.74}$$

Here and in the following superindices 0 are dropped to alleviate the notation. The matrix elements $\langle f|\,\widetilde{U}(t)\,|i\rangle$ can be calculated perturbatively using the Dyson series:

$$\mathcal{A}(i \to f; t) = \sum_{n=0}^{\infty}\mathcal{A}^{(n)}(i \to f; t) \tag{7.75}$$

$$\begin{aligned}
\mathcal{A}^{(n)}(i \to f; t) &= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_f t}\left(-\frac{\mathrm{i}}{\hbar}\right)^n\int_0^t \mathrm{d}t_n\int_0^{t_n}\mathrm{d}t_{n-1}\cdots\int_0^{t_2}\mathrm{d}t_1\;\langle f|\,V_I(t_n)V_I(t_{n-1})\cdots V_I(t_1)\,|i\rangle \\
&= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_f t}\left(-\frac{\mathrm{i}}{\hbar}\right)^n\sum_{k_{n-1}}\sum_{k_{n-2}}\cdots\sum_{k_1}\int_0^t \mathrm{d}t_n\int_0^{t_n}\mathrm{d}t_{n-1}\cdots\int_0^{t_2}\mathrm{d}t_1 \\
&\quad\times \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_f - E_{k_{n-1}})t_n}\left\langle f\right| V(t_n)\left|\psi_{k_{n-1}}\right\rangle \\
&\quad\times \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_{k_{n-1}} - E_{k_{n-2}})t_{n-1}}\left\langle\psi_{k_{n-1}}\right| V(t_{n-1})\left|\psi_{k_{n-2}}\right\rangle\cdots \\
&\quad\times \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_{k_1} - E_i)t_1}\left\langle\psi_{k_1}\right| V(t_1)\left|i\right\rangle
\end{aligned} \tag{7.76}$$

where we have redefined the integration variables so that $t > t_n > t_{n-1} > \cdots > t_2 > t_1 > 0$, we have inserted $n-1$ times the resolution of the identity:

$$I = \sum_k |\psi_k\rangle\langle\psi_k| \quad \text{with} \quad H^0\,|\psi_k\rangle = E_k\,|\psi_k\rangle \tag{7.77}$$

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and we have substituted:

$$V_I(t_k) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t_k} V(t_k) \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0 t_k}. \tag{7.78}$$

The amplitude can be represented pictorially as in Fig. 7.1 with $t_i = 0$, $t_f = t$.

The **transition probability** is then:

$$w_{i\to f}(t) = |\mathcal{A}(i \to f; t)|^2 = |\langle f| \widetilde{U}(t) |i\rangle|^2. \tag{7.79}$$

that can be calculated order by order in perturbation theory using the Dyson series.

7.2.4 Constant perturbation: Fermi's golden rule

This is the simplest example,

$$V(t) = V\,\theta(t) = \begin{cases} 0 & \text{if } t < 0 \\ V & \text{if } t \geq 0. \end{cases} \tag{7.80}$$

where V is independent of t but may depend on $\vec{x}$, $\vec{p}$ and $\vec{s}$. Then at first order we have, for $f \neq i$,

$$\begin{aligned} \langle f| \widetilde{U}(t) |i\rangle &= -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t' \ \langle f| \mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t'} V \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0 t'} |i\rangle = -\frac{\mathrm{i}}{\hbar}\langle f| V |i\rangle \int_0^t \mathrm{d}t' \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_f - E_i)t'} \\ &= \begin{cases} -\dfrac{\mathrm{i}}{\hbar} V_{fi}\, t & ; \quad \text{if } \Delta E = 0 \\ \dfrac{V_{fi}}{\Delta E}\left(1 - \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Delta E\, t}\right) & ; \quad \text{if } \Delta E \neq 0 \end{cases} \end{aligned} \tag{7.81}$$

with

$$V_{fi} = \langle f| V |i\rangle, \quad \Delta E = E_f - E_i. \tag{7.82}$$

Hence, for $\Delta E \neq 0$, the (first order) **Born approximation** is:

$$w_{i\to f\neq i}(t) = \frac{4|V_{fi}|^2}{(\Delta E)^2}\sin^2\frac{\Delta E\, t}{2\hbar}, \quad w_{i\to i}(t) = 1 - \sum_f w_{i\to f\neq i}(t). \tag{7.83}$$

This transition probability (Fig. 7.2) oscillates for $\Delta E \neq 0$, grows with t^2 when $\Delta E \to 0$,

$$\lim_{\Delta E\to 0} w_{i\to f}(t) = \frac{|V_{fi}|^2}{\hbar^2} t^2 \tag{7.84}$$

and is negligible when $\Delta E > 2\pi\hbar/t$. Of course the probability must be $w_{i\to f} < 1$, so the Born approximation fails when t is too large.

On the other hand, if we call Δt the interval during which the perturbation has been turned on, a transition with appreciable probability is possible only if

$$\Delta E \sim \frac{\hbar}{\Delta t} \quad \Leftrightarrow \quad \Delta E\, \Delta t \sim \hbar \tag{7.85}$$

where by ΔE we mean the energy change involved in a transition. If Δt is small we can tolerate a good amount of energy non-conservation. If Δt is large only transitions with very approximate energy conservation are most likely to occur. This provides a kind of time-energy uncertainty relation.

The fact that the transition probability for $i \to f$ it not linear but grows quadratically with time when $E_f \approx E_i$ may look unreasonable. We will see that this is actually not the case.

In realistic situations final states that are so close form a continuous spectrum in the neighbourhood of E_i. This may happen in the scattering of a plane wave by a finite range potential

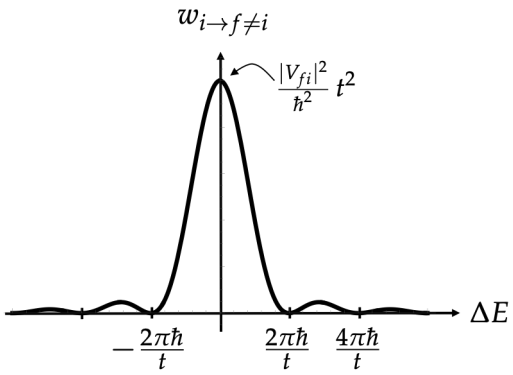

Figure 7.2: Transition probability for $i \to f \neq i$ as a function of $\Delta E = E_f - E_i$ at fixed t.

(the final state has a continuum of possible scattering angles; see next chapter), or in the ionization of an atom (see example at the end of this chapter). In such cases we are interested in the sum (integration) of transition probabilities over final states with $E \approx E_i$.

Let us represent by ν the set of variables describing the final state that take values in the continuum, including the energy E (with respect to H^0) and perhaps other variables α. We are interested in the transition probability from an initial state $|i\rangle$ of the discrete spectrum of H^0 to a continuous set of states $[f]$ characterized by $\Delta\nu$, with normalization $\langle\nu|\nu'\rangle = \delta(\nu - \nu')$. The projector into this set of final states is:

$$P_{\Delta\nu} = \int_{\Delta\nu} \mathrm{d}\nu\ |\nu\rangle\langle\nu| = \int_{\Delta\alpha} \mathrm{d}\alpha \int_{\Delta E} \mathrm{d}E\ |\alpha, E\rangle\, \rho(E,\alpha)\, \langle\alpha, E| \tag{7.86}$$

where $\rho(E,\alpha)$ is the *density of states* with generalized eigenvalues α and E. Then the relevant transition probability is

$$\begin{aligned} w_{i\to[f]}(t) &= \int_{\Delta\nu} \mathrm{d}\nu\ \langle i|\, \widetilde{U}^\dagger(t)\, |\nu\rangle\langle\nu|\, \widetilde{U}(t)\, |i\rangle \\ &= \int_{\Delta\alpha} \mathrm{d}\alpha \int_{\Delta E} \mathrm{d}E\ \langle i|\, \widetilde{U}^\dagger(t)\, |\alpha, E\rangle\, \rho(E,\alpha)\, \langle\alpha, E|\, \widetilde{U}(t)\, |i\rangle \\ &\equiv \int_{\Delta\alpha} \mathrm{d}\alpha \int_{\Delta E} \mathrm{d}E\, w_{i\to\alpha,E}(t) \end{aligned} \tag{7.87}$$

where

$$w_{i\to\alpha,E}(t) = \rho(E,\alpha)\, |\, \langle\alpha, E|\, \widetilde{U}(t)\, |i\rangle\, |^2 \tag{7.88}$$

is a *probability density*.

Let us calculate it at first order after a long t:

$$\begin{aligned} w_{i\to\alpha,E}(t) &= \rho(E,\alpha) \lim_{t\to\infty} \frac{4|V_{\alpha,E\,i}|^2}{(\Delta E)^2} \sin^2\frac{\Delta E\, t}{2\hbar} = \rho(E,\alpha)\frac{|V_{\alpha,E\,i}|^2}{\hbar^2} \lim_{t\to\infty} \frac{\sin^2\dfrac{\Delta E\, t}{2\hbar}}{\left(\dfrac{\Delta E}{2\hbar}\right)^2} \\ &= \rho(E,\alpha)\frac{|V_{\alpha,E\,i}|^2}{\hbar^2}\pi t\, \delta\left(\frac{\Delta E}{2\hbar}\right) = \frac{2\pi}{\hbar}|V_{\alpha,E\,i}|^2\rho(E,\alpha)\delta(E - E_i)\, t \end{aligned} \tag{7.89}$$

where we have used the following representation of the Dirac delta:

$$\delta(x) = \lim_{t\to\infty} \frac{1}{\pi}\frac{\sin^2 xt}{x^2 t}. \tag{7.90}$$

We see that the total transition probability actually grows linearly with t for large times (it is proportional to the area of the curve in Fig. 7.2, that is proportional to height of the peak $\sim t^2$

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times the width $\sim t^{-1}$). We also confirm that after a "long" time there will only be transitions that preserve the energy.

It is therefore convenient to define the (differential) **transition rate** or transition probability per unit time for large times,

$$\Gamma(i \to \alpha, E) = \lim_{t\to\infty} \frac{w_{i\to\alpha,E}(t)}{t} \tag{7.91}$$

that results in the (second) **Fermi's golden rule** (actually due to Dirac):

$$\boxed{\Gamma(i \to \alpha, E) = \frac{2\pi}{\hbar}|V_{\alpha,E\,i}|^2 \rho(E,\alpha)\delta(E - E_i)} \tag{7.92}$$

Notice that the delta function selects final states with the same energy as the initial one. And, of course, this rule is only applicable for large times *and* within the range of validity of the Born approximation. Integrating now the set of final states $|f\rangle$ over $\Delta\alpha$ and ΔE:

$$\boxed{\Gamma(i \to [f]) = \frac{2\pi}{\hbar}|\overline{V}_{fi}|^2 \rho(E = E_i)} \tag{7.93}$$

where $|\overline{V}_{fi}|^2$ is the average of $|V_{\alpha,E\,i}|^2$ and $\rho(E)$ the number density of final states with $E \approx E_i$.

7.2.5 Harmonic perturbation

Consider now the following time-dependent perturbation

$$V(t) = \mathcal{V}\mathrm{e}^{\mathrm{i}\omega t} + \mathcal{V}^\dagger \mathrm{e}^{-\mathrm{i}\omega t} \tag{7.94}$$

where $\mathcal{V}$ is independent of t but may depend on $\vec{x}$, $\vec{p}$ and $\vec{s}$. Then at first order, for $i \neq f$,

$$\begin{aligned}
\langle f|\,\widetilde{U}(t)\,|i\rangle &= -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\ \langle f|\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t'} V(t') \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0 t'}\,|i\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_f - E_i)t}\,\langle f|\,V(t')\,|i\rangle \\
&= \frac{\mathcal{V}_{fi}}{E_f - E_i + \hbar\omega}\left(1 - \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_f - E_i + \hbar\omega)t}\right) + \frac{\mathcal{V}^\dagger_{fi}}{E_f - E_i - \hbar\omega}\left(1 - \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_f - E_i - \hbar\omega)t}\right)
\end{aligned} \tag{7.95}$$

with

$$\mathcal{V}_{fi} = \langle f|\,\mathcal{V}\,|i\rangle\,, \quad \mathcal{V}^\dagger_{fi} = \langle f|\,\mathcal{V}^\dagger\,|i\rangle\,. \tag{7.96}$$

This is similar to the constant perturbation case with the change

$$\Delta E \to E_f - E_i \pm \hbar\omega. \tag{7.97}$$

So as $t \to \infty$ the transition probability density is given by the Fermi's golden rule:

$$w_{i\to\alpha,E}(t) = \frac{2\pi}{\hbar}\rho(E,\alpha)\left[|\mathcal{V}_{fi}|^2\,\delta(E - E_i + \hbar\omega) + |\mathcal{V}_{if}|^2\,\delta(E - E_i - \hbar\omega)\right]\,t \tag{7.98}$$

and the transition rate is

$$\Gamma(i \to [f]) = \begin{cases} \dfrac{2\pi}{\hbar}|\overline{\mathcal{V}}_{fi}|^2 \rho(E = E_i - \hbar\omega) \\ \dfrac{2\pi}{\hbar}|\overline{\mathcal{V}}_{if}|^2 \rho(E = E_i + \hbar\omega) \end{cases} \tag{7.99}$$

where we have used that $|\mathcal{V}^\dagger_{fi}| = |\mathcal{V}^*_{if}| = |\mathcal{V}_{if}|$, that is different from zero only when the final energy $E = E_i - \hbar\omega$ (stimulated emission) or $E = E_i + \hbar\omega$ (absorption), as illustrated in Fig. 7.3. In the first case the system emits energy $\hbar\omega$, what is only possible when the initial state is excited. In the second case the system absorbs energy $\hbar\omega$ becoming an excited state (or ionizes).

To summarize:

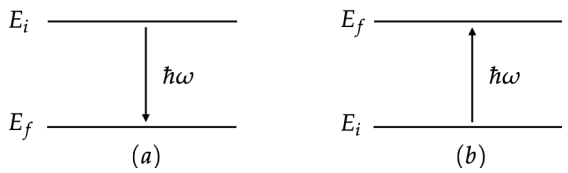


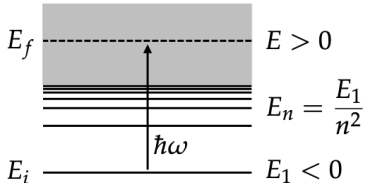
Figure 7.3: (a) Stimulated emission (possible only if initial state is excited). (b) Absorption.

- For a constant perturbation we obtain an appreciable transition probability for $|i\rangle \to |f\rangle$ when $E_f \approx E_i$.
- For a harmonic perturbation we obtain an appreciable transition probability for $|i\rangle \to |f\rangle$ when $E_f \approx E_i - \hbar\omega$ (stimulated emission) or $E_f \approx E_i + \hbar\omega$ (absorption).

Example: Consider a hydrogen atom in the ground state at $t = 0$. We then apply a uniform and periodic electric field $\vec{E} = \vec{E}_0 \sin\omega t$.

- Find the minimum frequency ω_0 of the field in order to ionize the atom.
- Determine to first order in perturbation theory the probability to ionize the atom per unit time.

The hydrogen atom has a discrete energy spectrum E_n of bound electrons plus a continuum of free electrons of momentum $\vec{p}$ and energy $E = \frac{p^2}{2m}$:



The energy and wave function of the ground state are:

$$E_1 = -\frac{\alpha^2 mc^2}{2} = -13.6 \text{ eV} \tag{7.100}$$

$$\psi_1(\vec{x}) = \psi_1(r) = \frac{1}{\sqrt{\pi a_0^3}} \mathrm{e}^{-\frac{r}{a_0}} \tag{7.101}$$

with $a_0 = \dfrac{\hbar}{mc\alpha} = 0.0529$ nm (Bohr radius) and $\alpha = \dfrac{e^2}{4\pi\epsilon_0\hbar c} \approx \dfrac{1}{137}$.

The periodic electric field is a harmonic perturbation:

$$\begin{aligned} &\nabla V = -e\,\vec{E}, \quad \vec{E} = \vec{E}_0 \sin\omega t \\ \Rightarrow \quad &V = -e\,\vec{E}_0 \cdot \vec{x}\, \frac{\mathrm{e}^{\mathrm{i}\omega t} - \mathrm{e}^{-\mathrm{i}\omega t}}{2\mathrm{i}} \\ \Rightarrow \quad &V = \mathcal{V}\mathrm{e}^{\mathrm{i}\omega t} + \mathcal{V}^\dagger \mathrm{e}^{-\mathrm{i}\omega t} \quad \text{with} \quad \mathcal{V}(\vec{x}) = \mathrm{i}\frac{e\vec{E}_0 \cdot \vec{x}}{2} \end{aligned} \tag{7.102}$$

From Fermi's golden rule, the transition rate to a free state with energy E_f is

$$\Gamma(i \to [f]) = \frac{2\pi}{\hbar} |\overline{\mathcal{V}}_{fi}|^2 \rho(E_f = E_i + \hbar\omega) \tag{7.103}$$

To get a free electron with energy E_f we need a frequency ω such that

$$E_i = E_1 \quad \Rightarrow \quad E_f = -\frac{\alpha^2 mc^2}{2} + \hbar\omega \tag{7.104}$$

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Hence the minimum frequency is $\omega_0 = \dfrac{\alpha^2 mc^2}{2\hbar}$.

To calculate the transition rate we need first:

- The density of final states $\rho(E)$.
- The matrix element $\mathcal{V}_{fi} = \langle\vec{p}|\,\mathcal{V}\,|i\rangle$ between the initial state $\langle\vec{x}|i\rangle = \psi_1(r)$ and a final state given by the plane wave $\langle\vec{x}|\vec{p}\rangle$ with $E = \frac{p^2}{2m}$.

Density of final states: Suppose the free electron of momentum $\vec{p}$ confined within a cube of size L (we will take $L \to \infty$ only at the end). Then inside the cube,

$$\langle\vec{x}|\vec{p}\rangle = \frac{1}{\sqrt{V}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}} \quad \text{with} \quad V = L^3 \quad \text{so that} \quad 1 = \langle\vec{p}|\vec{p}\rangle = \int_V \mathrm{d}^3x\ \langle\vec{p}|\vec{x}\rangle\,\langle\vec{x}|\vec{p}\rangle \tag{7.105}$$

and its momentum is quantized (periodic boundary conditions with period L):

$$\vec{p} = \frac{2\pi\hbar}{L}(n_x, n_y, n_z) \quad \Rightarrow \quad \mathrm{d}n = \frac{V}{(2\pi\hbar)^3}\,\mathrm{d}^3p = \frac{V}{(2\pi\hbar)^3}\,p^2\mathrm{d}p\,\mathrm{d}\Omega \tag{7.106}$$

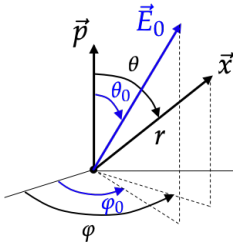
So the number of states per interval of momentum $[p, p+\mathrm{d}p]$ and solid angle is:

$$\rho(p,\Omega) = \frac{\mathrm{d}n}{\mathrm{d}p\,\mathrm{d}\Omega} = \frac{V}{(2\pi\hbar)^3}p^2, \quad E = \frac{p^2}{2m} \Rightarrow p = \sqrt{2mE} \tag{7.107}$$

and the number of states per interval of energy $[E, E+\mathrm{d}E]$ and solid angle is:

$$\mathrm{d}E = \frac{p}{m}\mathrm{d}p \Rightarrow \frac{\mathrm{d}n}{\mathrm{d}E\,\mathrm{d}\Omega} = \frac{m}{p}\frac{\mathrm{d}n}{\mathrm{d}p\,\mathrm{d}\Omega} = \boxed{\rho(E,\Omega) = \frac{V}{(2\pi\hbar)^3}\sqrt{2m^3E}} \tag{7.108}$$

Matrix element: In spherical coordinates: $\vec{E_0}\cdot\vec{x} = E_0 r\,[\sin\theta\sin\theta_0\cos(\varphi-\varphi_0) + \cos\theta\cos\theta_0]$ where the first terms vanishes after integration over φ and



$$\begin{aligned}
\mathcal{V}_{fi} &= \int \mathrm{d}^3x\ \langle\vec{p}|\vec{x}\rangle\,\mathcal{V}(\vec{x})\,\langle\vec{x}|i\rangle \\
&= \frac{1}{\sqrt{V}}\frac{1}{\sqrt{\pi a_0^3}}\mathrm{i}\frac{e}{2}\int \mathrm{d}^3x\,\vec{E}_0\cdot\vec{x}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}-\frac{r}{a_0}} \\
&= \frac{1}{\sqrt{V}}\frac{1}{\sqrt{\pi a_0^3}}\mathrm{i}\frac{e}{2}E_0\int_0^{2\pi}\mathrm{d}\varphi\int_{-1}^{1}\mathrm{d}\cos\theta\int_0^\infty \mathrm{d}r\,r^3\cos\theta\cos\theta_0\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}pr\cos\theta-\frac{r}{a_0}} \\
&= \frac{1}{\sqrt{V}}\frac{1}{\sqrt{\pi a_0^3}}\mathrm{i}\frac{e}{2}E_0\,2\pi\cos\theta_0\int_{-1}^{1}\mathrm{d}\cos\theta\,\cos\theta\int_0^\infty \mathrm{d}r\,r^3\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}pr\cos\theta-\frac{r}{a_0}} \\
&= \frac{1}{\sqrt{V}}\frac{1}{\sqrt{\pi a_0^3}}\mathrm{i}\frac{e}{2}E_0\,2\pi\cos\theta_0\,(-\mathrm{i})\frac{16a_0^5p}{\hbar\left(1+\frac{p^2a_0^2}{\hbar^2}\right)^3}
\end{aligned} \tag{7.109}$$

Transition rate:

$$\Gamma(i\to[f]) = \frac{2\pi}{\hbar}\int\mathrm{d}\Omega\int\mathrm{d}E_f\,\rho(E_f,\Omega)|\mathcal{V}_{fi}|^2\delta(E_f - E_i - \hbar\omega) \tag{7.110}$$

with $\displaystyle\int\mathrm{d}\Omega = 2\pi\int_{-1}^{1}\mathrm{d}\cos\theta_0$. Therefore the volume factors drop and

$$\Gamma(i\to[f]) = \frac{2\pi}{\hbar}2\pi\frac{2}{3}\frac{1}{\pi a_0^3}\frac{e^2}{4}E_0^2 4\pi^2\frac{(16a_0^5p)^2}{\hbar^2\left(1+\frac{p^2a_0^2}{\hbar^2}\right)^6}\frac{\sqrt{2m^3E}}{2\pi\hbar^3}\Bigg|_{E=\frac{p^2}{2m}=E_i+\hbar\omega}$$

$$= \frac{1024\pi^2}{3\hbar^6} \frac{e^2 E_0^2 a_0^7 m p^3}{\left(1+\frac{p^2 a_0^2}{\hbar^2}\right)^6}\Bigg|_{p^2=2m(E_i+\hbar\omega)} \tag{7.111}$$

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Chapter 8

Scattering theory

8.1 Scattering in Classical and Quantum Mechanics

Scattering theory is a complex subject that must be treated in more detail in a course on quantum field theory. Here we will describe just the main concepts, in a non relativistic framework.

In a first approximation, a collision or *scattering* is a process where two particles initially very far from each other (and hence *free*) approach, interact (exchanging energy and momentum) and finally move apart (becoming free again). We will discuss just *elastic* collisions, where the number and nature of initial and final particles is preserved. In contrast, energy can be converted into mass and viceversa in inelastic collisions, that can can only be studied in the context of a relativistic quantum field theory.

Usually we will consider the simpler case where one particle, the *target*, is fixed and does not move during the process, which is a good enough approximation if it is much heavier than the incoming particle, the *projectile*. Then we have the interaction of one particle with a *static potential* created by the target and the process is called *scattering* (Fig. 8.1). One can reduce the first to the second case going to the center of mass frame.

For the quantum treatment of the scattering process we will consider in more detail the *time-dependent formalism* where one finds the time evolution of the state $|\psi(t)\rangle$ of the projectile. This is conceptually closer to the description of the classical scattering and also to the formalism in quantum field theory. At the end of this chapter there will be a brief summary of the *time-independent formalism*.

Classically, the scattering of a particle by a fixed target could be divided in three phases depicted in Fig. 8.2 (left). In microscopical processes the interaction region (zone where the potential is relevant) is tiny, so is the interaction time for projectiles that travel usually at close to the speed

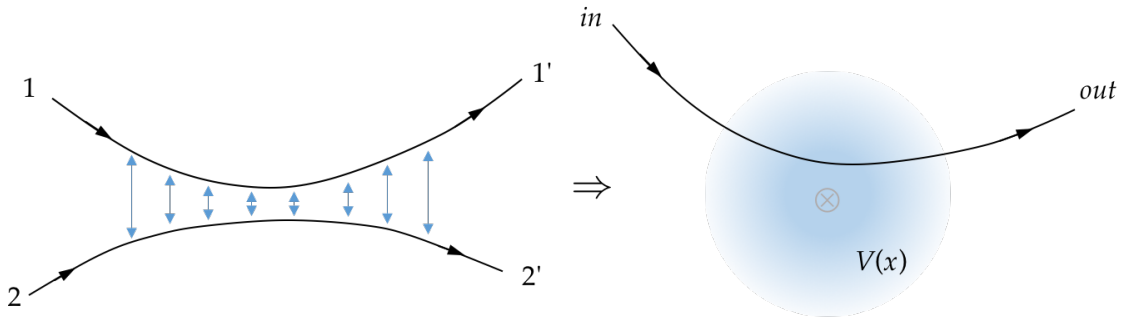

Figure 8.1: Collision of two particles viewed as a scattering by a potential.

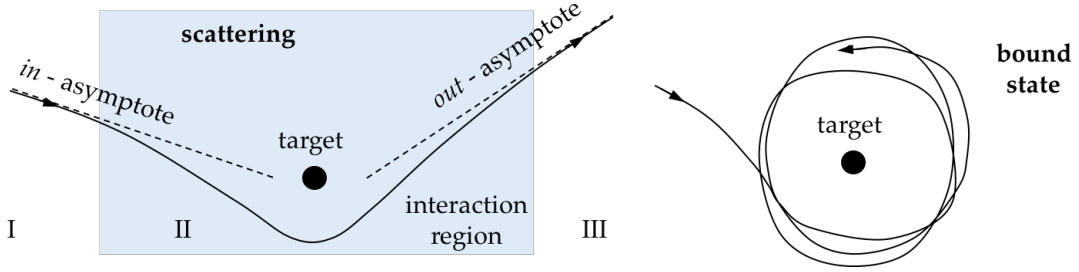

Figure 8.2: Sketch of a scattering process (left) and a bound state (right).

of light,

$$d \sim \text{Å} = 10^{-10}\ \text{m}, \quad v \sim c = 3 \times 10^8\ \text{m/s} \quad \Rightarrow \quad t \sim \frac{d}{v} \sim 10^{-18}\ \text{s}. \tag{8.1}$$

The classical trajectory is given by Newton's law,

$$m\ddot{\vec{x}} = -\vec{\nabla} V. \tag{8.2}$$

If the interaction takes place at $t \sim 0$, the trajectory $x(t)$ must be asymptotically a straight line for $t \to \mp\infty$ when the particle moves almost freely ($V \approx 0$),

$$\vec{x}_{\text{in}}(t) = \vec{a}_{\text{in}} + \vec{v}_{\text{in}} t \xleftarrow[t\to-\infty]{} \vec{x}(t) \xrightarrow[t\to+\infty]{} \vec{x}_{\text{out}}(t) = \vec{a}_{\text{out}} + \vec{v}_{\text{out}} t \tag{8.3}$$

where $\vec{x}_{\text{in}}(t)$ and $\vec{x}_{\text{out}}(t)$ are the *in* and *out asymptotes*. The real trajectory at $t \to \mp\infty$ coincides with the asymptotic one. If a particle approaches the target following an in-asymptote the classical scattering trajectory is completely determined. But not all trajectories define an out asymptote, because there are also bound states, whose trajectories are captured in the interaction region.

In **quantum mechanics** the scattering trajectory is replaced by a ket $|\psi(t)\rangle$ that evolves according to the Schrödinger equation,

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle = H |\psi(t)\rangle . \tag{8.4}$$

We will assume a time-independent Hamiltonian,

$$H = \frac{p^2}{2m} + V(\vec{x}) = H^0 + V(\vec{x}). \tag{8.5}$$

Then, taking $|\psi\rangle = |\psi(t=0)\rangle$, we can write

$$|\psi(t)\rangle = U(t) |\psi\rangle , \quad U(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} Ht}. \tag{8.6}$$

Suppose that the interaction takes place at $t \sim 0$. Then at $t \to \mp\infty$ the state $|\psi(t)\rangle$ must correspond to a free particle if it represents a scattering state,

$$|\psi_{\text{in}}(t)\rangle \xleftarrow[t\to-\infty]{} |\psi(t)\rangle \xrightarrow[t\to+\infty]{} |\psi_{\text{out}}(t)\rangle \tag{8.7}$$

where the asymptotic in and out states evolve like a free particle,

$$|\psi_{\text{in}}(t)\rangle = U^0(t) |\psi_{\text{in}}\rangle , \quad |\psi_{\text{out}}(t)\rangle = U^0(t) |\psi_{\text{out}}\rangle , \quad U^0(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H^0 t}. \tag{8.8}$$

The kets $|\psi_{\text{in}}\rangle$ ($|\psi_{\text{out}}\rangle$) are *asymptotic states* at $t = 0$ that evolve freely to $t \to -\infty$ ($t \to +\infty$) when they coincide with the *scattering state* $|\psi(t)\rangle$ (see Fig. 8.3).

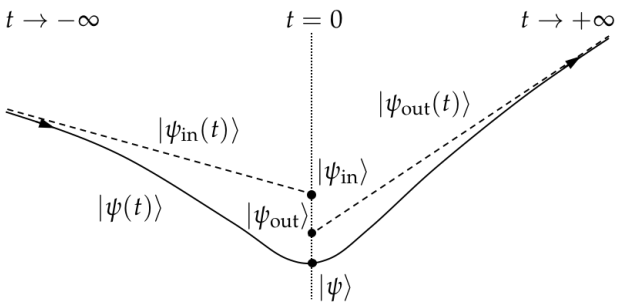

Figure 8.3: Sketch of the scattering and asymptotic states.

8.2 Asymptotic conditions. The scattering operator or *S*-matrix

To have a well defined scattering theory the potential must satisfy some *asymptotic conditions*, that are difficult to prove and are not known with full generality. In the simpler case of a spherical potential, $V(r)$, the following three conditions must be satisfied:[a]

1. The potential must go to zero faster than r^{-3} at large r, or otherwise the particle would never approach an asymptote (that would result in infinite total cross sections as we will see),

$$\frac{V(r)}{\frac{1}{r^3}} \xrightarrow[r\to\infty]{} 0. \tag{8.9}$$

2. The potential must diverge slower than $r^{-3/2}$ at $r \to 0$, or otherwise the particle will be captured,

$$\frac{V(r)}{\frac{1}{r^{3/2}}} \xrightarrow[r\to 0]{} 0. \tag{8.10}$$

3. The potential must be continuous at $0 < r < \infty$, except perhaps at a finite number of finite discontinuities.

Under these conditions, for every $|\psi_{\rm in}\rangle$ there is a *unique* scattering state $|\psi\rangle$ such that

$$\begin{aligned} &|\psi(t)\rangle - |\psi_{\rm in}(t)\rangle = U(t)\,|\psi\rangle - U^0(t)\,|\psi_{\rm in}\rangle \xrightarrow[t\to-\infty]{} 0 \\ \text{or}\quad &|\psi\rangle = \lim_{t\to-\infty} U^\dagger(t)U^0(t)\,|\psi_{\rm in}\rangle \equiv \Omega_+\,|\psi_{\rm in}\rangle\,. \end{aligned} \tag{8.11}$$

And analogously, for every $|\psi_{\rm out}\rangle$ there is a *unique* scattering state $|\psi\rangle$ such that

$$\begin{aligned} &|\psi(t)\rangle - |\psi_{\rm out}(t)\rangle = U(t)\,|\psi\rangle - U^0(t)\,|\psi_{\rm out}\rangle \xrightarrow[t\to+\infty]{} 0 \\ \text{or}\quad &|\psi\rangle = \lim_{t\to+\infty} U^\dagger(t)U^0(t)\,|\psi_{\rm out}\rangle \equiv \Omega_-\,|\psi_{\rm out}\rangle\,. \end{aligned} \tag{8.12}$$

The $\Omega_\pm$ are called *Møller operators*, that relate the in and out asymptotic states at $t = 0$ with the scattering state also at $t = 0$ (see Fig 8.3):

$$\boxed{|\psi\rangle = \Omega_+\,|\psi_{\rm in}\rangle = \Omega_-\,|\psi_{\rm out}\rangle} \tag{8.13}$$

Notice that *any state* of the Hilbert space *can represent an in (or out) asymptote*. Hence the domain of the operator Ω_+ is the whole Hilbert space $\mathcal{H}$. However, not all the states have an

[a] The Coulomb potential $V(r) \sim r^{-1}$ does not fulfill the first condition, but this is not a problem because a target generating such a potential is always screened at large distance in physical situations.

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in-asymptote, i.e. not all are scattering states. The rest are the bound states.[b] Therefore, the scattering states belong to $\mathcal{R}_+ = \mathcal{R}(\Omega_+)$, the *range* or image of Ω_+,

$$\forall\, |\psi_{\rm in}\rangle \in \mathcal{H}, \quad \Omega_+ \,|\psi_{\rm in}\rangle \in \mathcal{R}_+ \tag{8.14}$$

and $\mathcal{B}$ contains the bound states of $\mathcal{H}$. One can see that

$$\mathcal{H} = \mathcal{R}_+ \oplus \mathcal{B}. \tag{8.15}$$

And the same with the asymptotic states $|\psi_{\rm out}\rangle$. The domain of Ω_- is $\mathcal{H}$ and its range $\mathcal{R}_- = \mathcal{R}(\Omega_-)$ is also orthogonal to the subspace of bound states,

$$\forall\, |\psi_{\rm out}\rangle \in \mathcal{H}, \quad \Omega_- \,|\psi_{\rm out}\rangle \in \mathcal{R}_- \quad \Rightarrow \quad \mathcal{H} = \mathcal{R}_- \oplus \mathcal{B}. \tag{8.16}$$

In fact, one can prove that $\mathcal{R}_+ = \mathcal{R}_- \equiv \mathcal{R}$. The Møller operators

$$\Omega_\pm = \lim_{t\to\mp\infty} U^\dagger(t) U^0(t) \tag{8.17}$$

are *isometric* (not unitary) because $\Omega_\pm^{-1} = \Omega_\pm^\dagger$ but the domain of $\Omega_\pm^\dagger$ is not $\mathcal{H}$ but $\mathcal{R}$:

$$\Omega_+^\dagger \underbrace{(\Omega_+ \,|\psi_{\rm in}\rangle)}_{\in\mathcal{R}} = |\psi_{\rm in}\rangle\,, \quad \Omega_-^\dagger \underbrace{(\Omega_- \,|\psi_{\rm out}\rangle)}_{\in\mathcal{R}} = |\psi_{\rm out}\rangle\,. \tag{8.18}$$

Therefore, we can write

$$|\psi\rangle = \Omega_- \,|\psi_{\rm out}\rangle \quad \Rightarrow \quad |\psi_{\rm out}\rangle = \Omega_-^\dagger \,|\psi\rangle = \Omega_-^\dagger \Omega_+ \,|\psi_{\rm in}\rangle \tag{8.19}$$

which defines the *scattering operator* or *S-matrix*,

$$\boxed{S = \Omega_-^\dagger \Omega_+} \quad \text{with} \quad \boxed{|\psi_{\rm out}\rangle = S\,|\psi_{\rm in}\rangle} \tag{8.20}$$

The operator S establishes a one-to-one correspondence between the in and the out asymptotic states. For every $|\psi_{\rm in}\rangle$ there is a $|\psi_{\rm out}\rangle$ and viceversa. The operator S is unitary and it is all we need to know to describe a scattering process: we send a state $|\psi_{\rm in}\rangle$ and after the collision we have a state $|\psi_{\rm out}\rangle = S\,|\psi_{\rm in}\rangle$. The probability that the state $|\psi_{\rm in}\rangle$ becomes whatever state $|\phi_{\rm out}\rangle$ is

$$w(\psi_{\rm in} \to \phi_{\rm out}) = |\,\langle\phi_{\rm out}|\psi_{\rm out}\rangle\,|^2 = |\,\langle\phi_{\rm out}|\,S\,|\psi_{\rm in}\rangle\,|^2. \tag{8.21}$$

8.3 Energy conservation

The Hamiltonian $H = H^0 + V(\vec{x})$ is time-independent. Therefore the expectation value of the energy in a scattering state $|\psi(t)\rangle$ is constant,

$$\frac{\rm d}{{\rm d}t}\,\langle\psi(t)|\,H\,|\psi(t)\rangle = \langle\psi(t)|\,[H,H]\,|\psi(t)\rangle = 0, \tag{8.22}$$

and hence the energy of the in and out states must be the same,

$$\begin{aligned} E_{\rm in} &= \langle\psi_{\rm in}|\,H^0\,|\psi_{\rm in}\rangle \\ = E_{\rm out} &= \langle\psi_{\rm out}|\,H^0\,|\psi_{\rm out}\rangle = \langle\psi_{\rm in}|\,S^\dagger H^0 S\,|\psi_{\rm in}\rangle \\ &\Rightarrow \quad S^\dagger H^0 S = H^0 \quad \Rightarrow \quad [S,H^0] = 0. \end{aligned} \tag{8.23}$$

In the momentum representation,

$$\psi_{\rm out}(\vec{p}\,') = \langle\vec{p}\,'|\psi_{\rm out}\rangle = \langle\vec{p}\,'|\,S\,|\psi_{\rm in}\rangle = \int {\rm d}^3p\; \langle\vec{p}\,'|\,S\,|\vec{p}\rangle\,\langle\vec{p}|\psi_{\rm in}\rangle$$

[b] For instance, the harmonic oscillator potential has no scattering states, it has only bound states.

$$= \int \mathrm{d}^3p \; \langle \vec{p}' | \, S \, | \vec{p} \rangle \, \psi_{\mathrm{in}}(\vec{p}). \tag{8.24}$$

The *S-matrix element* $\langle \vec{p}' | \, S \, | \vec{p} \rangle$ is the probability amplitude to have an out-state with momentum $\vec{p}'$ if the in-state has momentum $\vec{p}$,

$$|\psi_{\mathrm{in}}\rangle = |\vec{p}\rangle \quad \Rightarrow \quad \psi_{\mathrm{out}}(\vec{p}') = \langle \vec{p}' | \, S \, | \vec{p} \rangle \, . \tag{8.25}$$

Note: Remember that states with well defined momentum cannot represent scattering states because they are stationary (they do not evolve with time). In fact, they are unphysical (not normalizable). Consequently, in physical situations, this matrix element between states with well defined momenta will always appear within an integral (see above). We will come back to this discussion at the beginning of the Section on the time-independent formalism.

8.4 On-shell *T*-matrix and scattering amplitude

The states with well defined momentum are energy eigenstates of the free Hamiltonian:

$$H^0 \, |\vec{p}\rangle = E_{\vec{p}} \, |\vec{p}\rangle \, , \quad E_{\vec{p}} = \frac{p^2}{2m}. \tag{8.26}$$

Since S and H^0 commute, the energy is conserved in the collision:

$$0 = \langle \vec{p}' | \, [H^0, S] \, | \vec{p} \rangle = \langle \vec{p}' | \, (H^0 S - S H^0) \, | \vec{p} \rangle = (E_{\vec{p}'} - E_{\vec{p}}) \, \langle \vec{p}' | \, S \, | \vec{p} \rangle \tag{8.27}$$

and therefore

$$\langle \vec{p}' | \, S \, | \vec{p} \rangle = 0 \quad \text{if} \quad E_{\vec{p}} \neq E_{\vec{p}'} . \tag{8.28}$$

This means that $\vec{p}$ may go to $\vec{p}' \neq \vec{p}$ but $|\vec{p}| = |\vec{p}'|$. We can redefine the S matrix as follows:

$$S \equiv I + R \tag{8.29}$$

where $S = I$ would correspond to $\vec{p} = \vec{p}'$, the case when $V = 0$ (absence of interactions) and R is the remainder. Then the S-matrix elements read

$$\langle \vec{p}' | \, S \, | \vec{p} \rangle \equiv \delta^3(\vec{p}' - \vec{p}) - 2\pi \mathrm{i} \, \delta(E_{\vec{p}'} - E_{\vec{p}}) \, t(\vec{p}' \leftarrow \vec{p}) \tag{8.30}$$

where we have introduced the *on-shell T-matrix* element $t(\vec{p'} \leftarrow \vec{p})$ that really contains the effect of the collision.

Notice that the on-shell T-matrix is only defined "on the energy-shell", that is for $E_{\vec{p}} = E_{\vec{p}'}$ or $|\vec{p}| = |\vec{p}'|$. The off-shell T-matrix, whose elements would be $\langle \vec{p}' | \, T \, | \vec{p} \rangle$ for arbitrary $\vec{p}$ and $\vec{p}'$, coincides with $t(\vec{p'} \leftarrow \vec{p})$ when $|\vec{p}| = |\vec{p}'|$. Although only the on-shell T-matrix elements are relevant for the observations related to scattering processes, we will see that the off-shell T-matrix is a useful tool in calculations (in particular, it satisfies the Lippmann-Schwinger equation).

In addition, we define the *scattering amplitude* $f(\vec{p}' \leftarrow \vec{p})$ from the on-shell T-matrix element as

$$f(\vec{p}' \leftarrow \vec{p}) \equiv -(2\pi)^2 \, \hbar m \, t(\vec{p}' \leftarrow \vec{p}). \tag{8.31}$$

It has dimensions of a length. We will see next that the (differential) cross section of a scattering process is just $|f(\vec{p}' \leftarrow \vec{p})|^2$. In terms of the scattering amplitude we have:

$$\langle \vec{p}' | \, S \, | \vec{p} \rangle = \delta^3(\vec{p}' - \vec{p}) + \frac{\mathrm{i}}{2\pi\hbar m} \delta(E_{\vec{p}'} - E_{\vec{p}}) f(\vec{p}' \leftarrow \vec{p}) \tag{8.32}$$

and

$$\begin{aligned} \psi_{\mathrm{out}}(\vec{p}') &= \int \mathrm{d}^3p \; \langle \vec{p}' | \, S \, | \vec{p} \rangle \, \psi_{\mathrm{in}}(\vec{p}) \\ &= \psi_{\mathrm{in}}(\vec{p}') + \frac{\mathrm{i}}{2\pi\hbar m} \int \mathrm{d}^3p \, \delta(E_{\vec{p}'} - E_{\vec{p}}) f(\vec{p}' \leftarrow \vec{p}) \, \psi_{\mathrm{in}}(\vec{p}). \end{aligned} \tag{8.33}$$

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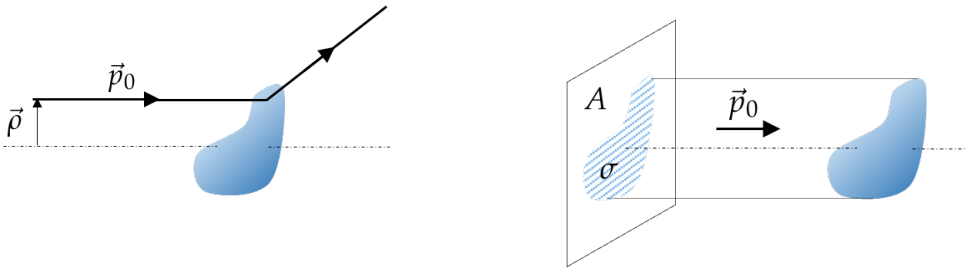

Figure 8.4: Classical scattering of a pointlike particle by a fixed rigid body. The cross section σ is the projection of the rigid body on the plane normal to $\vec{p}_0$.

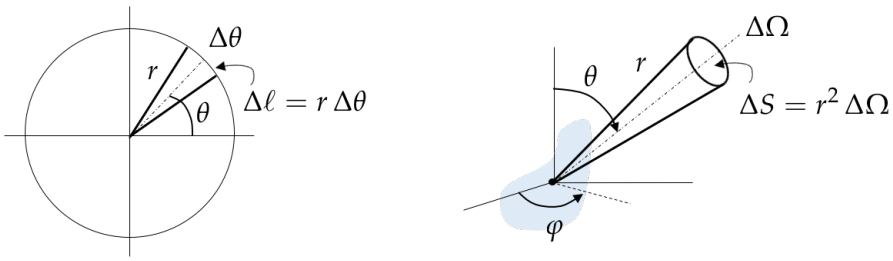

Figure 8.5: A solid angle Ω in steradians (sr) is the area of a patch of a unit sphere ($r = 1$), in the same way a planar angle θ in radians (rad) is the length of an arc of a unit circle.

8.5 Cross section

8.5.1 The classical cross section

Suppose the scattering of a pointlike particle by a *fixed rigid body* (Fig. 8.4). Assume we know the momentum $\vec{p}_0$ of the projectile but we ignore its impact parameter $\vec{\rho}$, defined as the distance (vector) between a chosen axis and the incident trajectory.

We would learn very little about the target from a single passage of the projectile: if it emerges with a momentum different from $\vec{p}_0$ we know that it must have "hit" the target; otherwise, it must have "missed" it. We rather repeat the experiment many times with the same incoming momentum but with random impact parameters. If we send $n_{\text{inc}} = N_{\text{inc}}/A$ particles per unit area (normal to $\vec{p}_0$) then N_{sc} will scatter with

$$\frac{N_{\text{sc}}}{N_{\text{inc}}} = \frac{\sigma}{A} \quad \Rightarrow \quad N_{\text{sc}} = n_{\text{inc}}\,\sigma \tag{8.34}$$

where σ is the cross-sectional area of the target, the scattering *cross section*.

And we can get even more information if we count the number of scattered particles in a given direction. Let us denote by ΔN_{sc} the number of particles scattered into the solid angle $\Delta\Omega$ (Fig. 8.5). Then

$$\Delta N_{\text{sc}} = n_{\text{inc}}\,\Delta\sigma. \tag{8.35}$$

Dividing by $\Delta\Omega$ and taking the limit $\Delta\Omega \to 0$,

$$\frac{\mathrm{d}N_{\text{sc}}}{\mathrm{d}\Omega} = n_{\text{inc}}\,\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}, \quad \mathrm{d}\Omega = \mathrm{d}\cos\theta\mathrm{d}\varphi. \tag{8.36}$$

The *differential cross section* $\mathrm{d}\sigma/\mathrm{d}\Omega$ is the cross section of the part of the target that scatters into $\mathrm{d}\Omega$. Integrating over all directions one gets the total cross section σ:

$$\sigma = \int \mathrm{d}\Omega\,\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \int_{-1}^{1} \mathrm{d}\cos\theta \int_0^{2\pi} \mathrm{d}\varphi\,\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(\theta,\varphi). \tag{8.37}$$

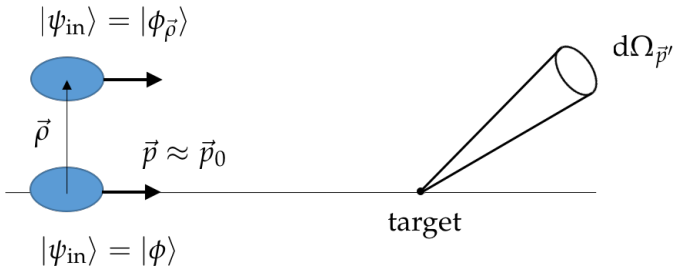

Figure 8.6: Two incoming wave packets with $\vec p \approx \vec p_0$ differing by an impact parameter $\vec\rho$ perpendicular to $\vec p_0$.

If instead of a fixed rigid body the particle is scattered by the potential created by a target, the cross section is a measure of the *effective area* of the target as seen by the projectile.

8.5.2 The quantum cross section

In QM we have an in asymptotic state $|\psi_{\rm in}\rangle$ going against the target with wave function

$$\psi_{\rm in}(\vec p) = \langle \vec p|\psi_{\rm in}\rangle\,. \tag{8.38}$$

After the interaction we have the state $|\psi_{\rm out}\rangle$ with wave function

$$\psi_{\rm out}(\vec p') = \langle \vec p'|\psi_{\rm out}\rangle\,. \tag{8.39}$$

The probability to find the out state within a cone of directions $d\Omega_{\vec p'}$ is:

$$w(\psi_{\rm in} \to d\Omega_{\vec p'}) = d\Omega_{\vec p'} \int_0^\infty p'^2 dp'\, |\psi_{\rm out}(\vec p')|^2. \tag{8.40}$$

Suppose you send a *beam* of particles, that is, many particles with wave functions of momentum $\vec p \approx \vec p_0$ and random impact parameters $\vec\rho$, such that we have $n_{\rm inc}$ particles per unit area normal to $\vec p_0$. We must assume that the interaction among the particles in the beam is negligible. Then, we define the differential cross section from

$$\frac{dN_{\rm sc}}{d\Omega_{\vec p'}} = n_{\rm inc}\frac{d\sigma}{d\Omega_{\vec p'}}. \tag{8.41}$$

On the other hand, the *number of interactions* is the number of incoming particles per unit area times the probability of an interaction integrated over all the impact parameters:

$$dN_{\rm sc} = \int d^2\rho\, n_{\rm inc}\, \widetilde w(\phi_{\vec\rho} \to d\Omega_{\vec p'}), \tag{8.42}$$

where in $\widetilde w$ we must restrict ourselves to the *scattered* wave function $\widetilde\psi_{\rm out}(\vec p')$, subtracting from the *outgoing* wave function $\psi_{\rm out}(\vec p')$ the contribution from the incoming (*unscattered*) part $\psi_{\rm in}(\vec p)$, that has not interacted,

$$\widetilde\psi_{\rm out}(\vec p') = \int d^3p\ \langle \vec p'|\, R\, |\vec p\rangle\, \psi_{\rm in}(\vec p) \tag{8.43}$$

and $\phi_{\vec\rho}(\vec p)$ is a wave packet traveling along the axis, that is obtained by a translation $\vec\rho$ of the $\phi(\vec p)$ (see Fig. 8.6):

$$|\phi_{\vec\rho}\rangle = T(\vec\rho)\,|\phi\rangle = e^{-\frac{i}{\hbar}\vec P\cdot\vec\rho}\,|\phi\rangle \tag{8.44}$$

$$\phi(\vec p) = \langle \vec p|\phi\rangle\,, \quad \phi_{\vec\rho}(\vec p) = \langle \vec p|\phi_{\vec\rho}\rangle = e^{-\frac{i}{\hbar}\vec p\cdot\vec\rho}\phi(\vec p). \tag{8.45}$$

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Therefore, from (8.36), (8.40) and (8.42),

$$\mathrm{d}\sigma = \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega_{\vec{p}'}}\mathrm{d}\Omega_{\vec{p}'} = \int \mathrm{d}^2\rho\, \widetilde{w}(\phi_{\vec{\rho}} \to \mathrm{d}\Omega_{\vec{p}'}) = \int \mathrm{d}^2\rho\, \mathrm{d}\Omega_{\vec{p}'} \int_0^\infty p'^2 \mathrm{d}p'\, |\widetilde{\psi}_{\mathrm{out}}(\vec{p}')|^2. \tag{8.46}$$

Remember that outgoing is not the same as scattered. Therefore in $\widetilde{\psi}_{\mathrm{out}}(\vec{p}')$ we have subtracted from the *outgoing* wave function the contribution from the unscattered part $\psi_{\mathrm{in}}(\vec{p}) = \phi_{\vec{\rho}}(\vec{p})$, that is unrelated to the collision:

$$\widetilde{\psi}_{\mathrm{out}}(\vec{p}') = \int \mathrm{d}^3p\, \langle \vec{p}'|\, R\, |\vec{p}\rangle\, \psi_{\mathrm{in}}(\vec{p}) = \frac{\mathrm{i}}{2\pi\hbar m} \int \mathrm{d}^3p\, \delta(E_{\vec{p}'} - E_{\vec{p}}) f(\vec{p}' \leftarrow \vec{p})\, \phi_{\vec{\rho}}(\vec{p}). \tag{8.47}$$

In this way, the cross section $\sigma = 0$ if $|\psi_{\mathrm{out}}\rangle = |\psi_{\mathrm{in}}\rangle$. Substituting (8.47) in (8.46):

$$\begin{aligned}\mathrm{d}\sigma = \frac{\mathrm{d}\Omega_{\vec{p}'}}{(2\pi\hbar m)^2} \int \mathrm{d}^2\rho \int_0^\infty p'^2 \mathrm{d}p' \int \mathrm{d}^3p_1\, \delta(E_{\vec{p}'} - E_{\vec{p}_1}) f(\vec{p}' \leftarrow \vec{p}_1)\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\vec{p}_1\cdot\vec{\rho}} \phi(\vec{p}_1) \\ \times \int \mathrm{d}^3p_2\, \delta(E_{\vec{p}'} - E_{\vec{p}_2}) f^*(\vec{p}' \leftarrow \vec{p}_2)\, \mathrm{e}^{+\frac{\mathrm{i}}{\hbar}\vec{p}_2\cdot\vec{\rho}} \phi^*(\vec{p}_2).\end{aligned} \tag{8.48}$$

Since $E_{\vec{p}'} = E_{\vec{p}_1}$ and $E_{\vec{p}'} = E_{\vec{p}_2}$ we have $E_{\vec{p}_1} = E_{\vec{p}_2}$, and we can replace $\delta(E_{\vec{p}'} - E_{\vec{p}_2})$ by $\delta(E_{\vec{p}_1} - E_{\vec{p}_2})$. Besides,

$$\int \mathrm{d}^2\rho\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(\vec{p}_1 - \vec{p}_2)\cdot\vec{\rho}} = (2\pi\hbar)^2 \delta^2(\vec{p}_{1\perp} - \vec{p}_{2\perp}). \tag{8.49}$$

And because $0 = E_{\vec{p}_1} - E_{\vec{p}_2} = (p_1^2 - p_2^2)/(2m)$ we have $p_{1\parallel} = \pm p_{2\parallel}$ but $p_{1\parallel} = -p_{2\parallel}$ does not contribute to the integral for sufficiently narrow wave functions: $\phi(\vec{p}_1)$ and $\phi(\vec{p}_2)$ would not overlap. Hence

$$\delta^2(\vec{p}_{1\perp} - \vec{p}_{2\perp})\delta(E_{\vec{p}_1} - E_{\vec{p}_2}) = \frac{m}{p_{1\parallel}} \delta^3(\vec{p}_1 - \vec{p}_2). \tag{8.50}$$

Collecting terms and reintroducing the dummy variable $\vec{p} = \vec{p}_1$:

$$\mathrm{d}\sigma = \frac{\mathrm{d}\Omega_{\vec{p}'}}{m} \int_0^\infty p'^2 \mathrm{d}p' \int \mathrm{d}^3p\, \frac{1}{p_\parallel} \delta(E_{\vec{p}'} - E_{\vec{p}}) |f(\vec{p}' \leftarrow \vec{p}) \phi(\vec{p})|^2. \tag{8.51}$$

Finally, since $\phi(\vec{p}) \neq 0$ only at $\vec{p} \approx \vec{p}_0$ we have:

$$f(\vec{p}' \leftarrow \vec{p}) \approx f(\vec{p}' \leftarrow \vec{p}_0) \tag{8.52}$$

$$\left.\begin{aligned} E_{\vec{p}'} - E_{\vec{p}} \approx E_{\vec{p}'} - E_{\vec{p}_0} = (p'^2 - p_0^2)/(2m) \\ p_\parallel \approx p_0 \end{aligned}\right\} \Rightarrow \delta(E_{\vec{p}'} - E_{\vec{p}}) = \frac{m}{p_0} \delta(p' - p_0) \tag{8.53}$$

$$\int \mathrm{d}^3p\, |\phi(\vec{p})|^2 = 1. \tag{8.54}$$

Therefore the *differential cross section* is

$$\mathrm{d}\sigma = \frac{\mathrm{d}\Omega_{\vec{p}'}}{m} p_0^2 \frac{1}{p_0} \frac{m}{p_0} |f(\vec{p}' \leftarrow \vec{p}_0)|^2 \quad \Rightarrow \quad \boxed{\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega_{\vec{p}'}} = |f(\vec{p}' \leftarrow \vec{p}_0)|^2} \tag{8.55}$$

and the *total cross section* is

$$\boxed{\sigma(\vec{p}_0) = \int \mathrm{d}\Omega_{\vec{p}'}\, |f(\vec{p}' \leftarrow \vec{p}_0)|^2} \tag{8.56}$$

So, the scattering amplitude is all we need to know to calculate the cross section of a scattering process.

8.6 Optical theorem

The optical theorem is a consequence of the unitarity of the S matrix:

$$S^\dagger S = I; \tag{8.57}$$

$$(I+R)^\dagger (I+R) = I; \tag{8.58}$$

$$R + R^\dagger = -R^\dagger R; \tag{8.59}$$

$$\langle \vec{p}\,'| R |\vec{p}\rangle + \langle \vec{p}\,'| R^\dagger |\vec{p}\rangle = -\int \mathrm{d}^3p''\ \langle \vec{p}\,'| R^\dagger |\vec{p}\,''\rangle\langle \vec{p}\,''| R |\vec{p}\rangle\,; \tag{8.60}$$

$$\langle \vec{p}\,'| R |\vec{p}\rangle + \langle \vec{p}| R |\vec{p}\,'\rangle^* = -\int \mathrm{d}^3p''\ \langle \vec{p}\,''| R |\vec{p}\,'\rangle^* \langle \vec{p}\,''| R |\vec{p}\rangle\,. \tag{8.61}$$

Then

$$\begin{aligned} &\cancel{\frac{\mathrm{i}}{2\pi\hbar m}}\cancel{\delta(E_{\vec{p}\,'} - E_{\vec{p}})}\,[f(\vec{p}\,' \leftarrow \vec{p}) - f^*(\vec{p} \leftarrow \vec{p}\,')] \\ &\quad = \left(\frac{\mathrm{i}}{2\pi\hbar m}\right)^{\cancel{2}} \int \mathrm{d}^3p''\,\cancel{\delta(E_{\vec{p}\,'} - E_{\vec{p}})}\delta(E_{\vec{p}\,''} - E_{\vec{p}}) f^*(\vec{p}\,'' \leftarrow \vec{p}\,') f(\vec{p}\,'' \leftarrow \vec{p}) \end{aligned} \tag{8.62}$$

where we have used $\delta(E_{\vec{p}\,''} - E_{\vec{p}\,'})\delta(E_{\vec{p}\,''} - E_{\vec{p}}) = \delta(E_{\vec{p}\,'} - E_{\vec{p}})\delta(E_{\vec{p}\,''} - E_{\vec{p}})$ and hence

$$f(\vec{p}\,' \leftarrow \vec{p}) - f^*(\vec{p} \leftarrow \vec{p}\,') = \frac{\mathrm{i}}{2\pi\hbar m} \int p''^2\, \mathrm{d}p''\, \mathrm{d}\Omega_{\vec{p}\,''}\, \delta(E_{\vec{p}\,''} - E_{\vec{p}}) f^*(\vec{p}\,'' \leftarrow \vec{p}\,') f(\vec{p}\,'' \leftarrow \vec{p}). \tag{8.63}$$

Finally, doing the integral over p''

$$\int \mathrm{d}p''\, \delta(E_{\vec{p}\,''} - E_{\vec{p}}) g(p'') = \left|\frac{\mathrm{d}E_{\mathrm{p}''}}{\mathrm{d}p''}\right|^{-1}_{p''=p} g(p) = \frac{m}{p} g(p), \tag{8.64}$$

we have

$$f(\vec{p}\,' \leftarrow \vec{p}) - f^*(\vec{p} \leftarrow \vec{p}\,') = \frac{\mathrm{i}}{2\pi\hbar} p \int \mathrm{d}\Omega_{\vec{p}\,''}\, f^*(\vec{p}\,'' \leftarrow \vec{p}\,') f(\vec{p}\,'' \leftarrow \vec{p}) \tag{8.65}$$

with $p = |\vec{p}| = |\vec{p}\,'| = |\vec{p}\,''|$. And taking $\vec{p}\,' = \vec{p}$:

$$\mathrm{Im}\, f(\vec{p} \leftarrow \vec{p}) = \frac{p}{4\pi\hbar} \int \mathrm{d}\Omega_{\vec{p}\,''}\, |f(\vec{p}\,'' \leftarrow \vec{p})|^2. \tag{8.66}$$

Recalling the definition of total cross section (8.56),

$$\sigma(\vec{p}) = \int \mathrm{d}\Omega_{\vec{p}\,''}\, |f(\vec{p}\,'' \leftarrow \vec{p})|^2, \tag{8.67}$$

the previous expression can be written as

$$\boxed{\mathrm{Im}\, f(\vec{p} \leftarrow \vec{p}) = \frac{p}{4\pi\hbar}\, \sigma(\vec{p})} \tag{8.68}$$

This is the **optical theorem**: the imaginary part of the *forward* scattering amplitude $f(\vec{p} \leftarrow \vec{p})$ is proportional to the total cross section. It is remarkable that unitarity forces the scattering amplitude to be complex in the forward direction ($\vec{p}\,' = \vec{p}$) and the size of its imaginary part fixes the total cross section, that comes from integrating over all $\vec{p}\,'$ with $|\vec{p}\,'| = |\vec{p}|$.

Next we will find the expression of the scattering amplitude for a given potential. But first, we need to introduce the Green's operator G and the T operator.

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8.7 The Green's operator G

The Green's operator of the Hamiltonians $H^0 = \dfrac{p^2}{2m}$ and $H = H^0 + V$ is defined, respectively, as:

$$G^0(z) \equiv \frac{1}{z - H^0} \tag{8.69}$$

$$G(z) \equiv \frac{1}{z - H} \qquad \text{with } z \in \mathbb{C}. \tag{8.70}$$

Then

$$(z - H^0)\, G^0(z) = I \quad \Rightarrow \quad \langle \vec{x}| \,(z - H^0)\, G^0(z)\, |\vec{x}'\rangle = \delta^3(\vec{x} - \vec{x}'). \tag{8.71}$$

The left hand side can be written as

$$\begin{aligned}
\langle \vec{x}| \,(z - H^0)\, G^0(z)\, |\vec{x}'\rangle &= \int \mathrm{d}^3x''\ \langle \vec{x}| \,(z - H^0)\, |\vec{x}''\rangle \,\langle \vec{x}''|\, G^0(z)\, |\vec{x}'\rangle \\
&= \int \mathrm{d}^3x''\, \delta^3(\vec{x} - \vec{x}'') \left(\frac{\hbar^2\nabla^2}{2m} + z\right) \langle \vec{x}''|\, G^0(z)\, |\vec{x}'\rangle \\
&= \left(\frac{\hbar^2\nabla^2}{2m} + z\right) \langle \vec{x}|\, G^0(z)\, |\vec{x}'\rangle\,.
\end{aligned} \tag{8.72}$$

Therefore $\langle \vec{x}|\, G^0(z)\, |\vec{x}'\rangle$ is the *Green's function* of the differential operator $\dfrac{\hbar^2\nabla^2}{2m} + z$:

$$\left(\frac{\hbar^2\nabla^2}{2m} + z\right) \langle \vec{x}|\, G^0(z)\, |\vec{x}'\rangle = \delta^3(\vec{x} - \vec{x}'). \tag{8.73}$$

Analogously $\langle \vec{x}|\, G(z)\, |\vec{x}'\rangle$ is the Green's function of $\dfrac{\hbar^2\nabla^2}{2m} - V(\vec{x}) + z$:

$$\left(\frac{\hbar^2\nabla^2}{2m} - V(\vec{x}) + z\right) \langle \vec{x}|\, G(z)\, |\vec{x}'\rangle = \delta^3(\vec{x} - \vec{x}'). \tag{8.74}$$

Notice that the Green's operator is not defined for $z = E_n$ (energy eigenvalues), since

$$H\,|n\rangle = E_n\,|n\rangle \quad \Rightarrow \quad \frac{1}{z - H}\,|n\rangle = \frac{1}{z - E_n}\,|n\rangle \quad \text{diverges for } z = E_n. \tag{8.75}$$

In the basis of energy eigenvectors we have:

$$G(z) = \frac{1}{z - H} \sum_n |n\rangle\langle n| = \sum_n \frac{|n\rangle\langle n|}{z - E_n} \tag{8.76}$$

or for a continuous energy spectrum:

$$G(z) = \int \mathrm{d}E\, \frac{|E\rangle\langle E|}{z - E}. \tag{8.77}$$

In particular, the *free* Green's operator in the momentum representation is

$$G^0(z)\,|\vec{p}\rangle = (z - H^0)^{-1}\,|\vec{p}\rangle = \frac{1}{z - E_{\vec{p}}}\,|\vec{p}\rangle \quad \Rightarrow \quad G^0(z) \doteq \frac{1}{z - E_{\vec{p}}}. \tag{8.78}$$

We can relate $G(z)$ and $G^0(z)$ using the simple expression:

$$A^{-1} = B^{-1} + B^{-1}(B - A)A^{-1}. \tag{8.79}$$

Taking $A = z - H$ and $B = z - H^0$, where $B - A = V$, we have

$$\boxed{G(z) = G^0(z) + G^0(z)VG(z)} \tag{8.80}$$

Or, exchanging B and A:

$$\boxed{G(z) = G^0(z) + G(z)VG^0(z)} \tag{8.81}$$

These are the *Lippmann-Schwinger equations for the operator* $G(z)$.

8.8 The T operator

The T operator is defined from the Green's operator as

$$T(z) \equiv V + VG(z)V. \tag{8.82}$$

It is analytic in the complex plane except in the energy eigenvalues ($z = E_n$).

Multiplying the definition of T by $G^0(z)$ and applying the LS equations above we find:

$$G^0(z)T(z) = G^0(z)V + G^0(z)VG(z)V \quad \Rightarrow \quad \boxed{G^0(z)T(z) = G(z)V} \tag{8.83}$$

$$T(z)G^0(z) = VG^0(z) + VG(z)VG^0(z) \quad \Rightarrow \quad \boxed{T(z)G^0(z) = VG(z)} \tag{8.84}$$

Multiplying now the first one by V on the left and using the definition of T:

$$VG^0(z)T(z) = VG(z)V = -V + V + VG(z)V = -V + T(z) \tag{8.85}$$

we get

$$\boxed{T(z) = V + VG^0(z)T(z)} \tag{8.86}$$

This is the *Lippmann-Schwinger equation for the operator* $T(z)$, the starting point for the calculation of the scattering amplitudes applying perturbative methods as we will see.

8.9 The S operator in terms of T and G

Remember that the Møller operators relate the asymptotic in and out states with the scattering state at $t = 0$,

$$|\psi\rangle = \Omega_- |\psi_{\text{out}}\rangle = \Omega_+ |\psi_{\text{in}}\rangle \tag{8.87}$$

with

$$\Omega_\mp = \lim_{t\to\pm\infty} U^\dagger(t)U^0(t). \tag{8.88}$$

The time evolution operators satisfy the following relation that we will use afterwards:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}U^\dagger(t)U^0(t) &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0t}\right) \\ &= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}(H - H^0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0t} \\ &= \frac{\mathrm{i}}{\hbar}U^\dagger(t)VU^0(t). \end{aligned} \tag{8.89}$$

Now use the following trick. Write $f(t) = U^\dagger(t)U^0(t)$ as the integral of its derivative:

$$\int_0^t \mathrm{d}\tau \, \frac{\mathrm{d}f(\tau)}{\mathrm{d}\tau} = f(t) - f(0) \quad \Rightarrow \quad f(t) = f(0) + \int_0^t \mathrm{d}\tau \, \frac{\mathrm{d}f(\tau)}{\mathrm{d}\tau}. \tag{8.90}$$

Then

$$U^\dagger(t)U^0(t) = I + \frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}\tau \, U^\dagger(\tau)VU^0(\tau) \tag{8.91}$$

and

$$|\psi\rangle = \Omega_- |\psi_{\text{out}}\rangle = \lim_{t\to\infty} U^\dagger(t)U^0(t) |\psi_{\text{out}}\rangle$$

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$$= |\psi_{\rm out}\rangle + \frac{\rm i}{\hbar}\int_0^\infty {\rm d}t\, U^\dagger(t) V U^0(t)\, |\psi_{\rm out}\rangle\,. \tag{8.92}$$

Analogously,

$$\begin{aligned} |\psi\rangle = \Omega_+ |\psi_{\rm in}\rangle &= \lim_{t\to-\infty} U^\dagger(t) U^0(t)\, |\psi_{\rm in}\rangle \\ &= |\psi_{\rm in}\rangle + \frac{\rm i}{\hbar}\int_0^{-\infty} {\rm d}t\, U^\dagger(t) V U^0(t)\, |\psi_{\rm in}\rangle\,. \end{aligned} \tag{8.93}$$

Both integrals must be convergent if the potential satisfies the asymptotic conditions. Next we use another trick:

$$\int_0^\infty {\rm d}t\, g(t) \;\text{ convergent} \quad\Rightarrow\quad \int_0^\infty {\rm d}t\, g(t) = \lim_{\epsilon\to 0^+}\int_0^\infty {\rm d}t\, {\rm e}^{-\frac{\epsilon t}{\hbar}}\, g(t). \tag{8.94}$$

The damping factor ${\rm e}^{-\frac{\epsilon t}{\hbar}} \approx 1$ for small t, and it is < 1 for $t\to\infty$, in the region where V must be irrelevant. For $t\to-\infty$ the appropriate damping factor is ${\rm e}^{+\frac{\epsilon t}{\hbar}}$. The fact that we can do scattering theory replacing V by $V{\rm e}^{-\epsilon|t|/hbar}$ is known as the *adiabatic theorem*. Therefore we may write:

$$|\psi\rangle = |\psi_{\rm out}\rangle + \frac{\rm i}{\hbar}\lim_{\epsilon\to 0^+}\int_0^\infty {\rm d}t\, {\rm e}^{-\frac{\epsilon t}{\hbar}}\, U^\dagger(t) V U^0(t)\, |\psi_{\rm out}\rangle \tag{8.95}$$

$$|\psi\rangle = |\psi_{\rm in}\rangle + \frac{\rm i}{\hbar}\lim_{\epsilon\to 0^+}\int_0^{-\infty} {\rm d}t\, {\rm e}^{+\frac{\epsilon t}{\hbar}}\, U^\dagger(t) V U^0(t)\, |\psi_{\rm in}\rangle\,. \tag{8.96}$$

In the momentum representation:

$$\begin{aligned} &\frac{\rm i}{\hbar}\lim_{\epsilon\to 0^+}\int {\rm d}^3p \int_0^\infty {\rm d}t\, {\rm e}^{-\frac{\epsilon t}{\hbar}}\, U^\dagger(t) V U^0(t)\, |\vec p\rangle\, \langle\vec p|\psi_{\rm out}\rangle \\ &= \frac{\rm i}{\hbar}\lim_{\epsilon\to 0^+}\int {\rm d}^3p \int_0^\infty {\rm d}t\, {\rm e}^{-\frac{\rm i}{\hbar}(E_{\vec p}-{\rm i}\epsilon-H)t} V\, |\vec p\rangle\, \langle\vec p|\psi_{\rm out}\rangle \\ &= -\lim_{\epsilon\to 0^+}\int {\rm d}^3p \left[\frac{{\rm e}^{-\frac{\rm i}{\hbar}(E_{\vec p}-{\rm i}\epsilon-H)t}}{E_{\vec p}-{\rm i}\epsilon-H}\right]_0^\infty V\, |\vec p\rangle\, \langle\vec p|\psi_{\rm out}\rangle \\ &= \lim_{\epsilon\to 0^+}\int {\rm d}^3p\, \frac{1}{E_{\vec p}-{\rm i}\epsilon-H} V\, |\vec p\rangle\, \langle\vec p|\psi_{\rm out}\rangle \\ &= \lim_{\epsilon\to 0^+}\int {\rm d}^3p\, G(E_{\vec p}-{\rm i}\epsilon) V\, |\vec p\rangle\, \langle\vec p|\psi_{\rm out}\rangle \end{aligned} \tag{8.97}$$

where the integral over t is convergent thanks to the damping factor. Hence

$$|\psi\rangle = \Omega_-\, |\psi_{\rm out}\rangle = |\psi_{\rm out}\rangle + \lim_{\epsilon\to 0^+}\int {\rm d}^3p\, G(E_{\vec p}-{\rm i}\epsilon) V\, |\vec p\rangle\, \langle\vec p|\psi_{\rm out}\rangle \tag{8.98}$$

and analogously,

$$|\psi\rangle = \Omega_+\, |\psi_{\rm in}\rangle = |\psi_{\rm in}\rangle + \lim_{\epsilon\to 0^+}\int {\rm d}^3p\, G(E_{\vec p}+{\rm i}\epsilon) V\, |\vec p\rangle\, \langle\vec p|\psi_{\rm in}\rangle\,. \tag{8.99}$$

This gives us the relation between the Møller operators and the Green's operator:

$$\Omega_\pm = I + \lim_{\epsilon\to 0^+}\int {\rm d}^3p\, G(E_{\vec p}\pm{\rm i}\epsilon) V\, |\vec p\rangle\langle\vec p|\,. \tag{8.100}$$

Now we understand the reason for the choice of the subscripts: the $\pm{\rm i}\epsilon$ in $G(E_{\vec p}\pm{\rm i}\epsilon)$ are the same as the $\pm$ in $\Omega_\pm$. And from $G(z)V = G^0(z)T(z)$ we also have the relation between the Møller operators and the T operator.

But we are mostly interested in the relation between S and T. We start by

$$\langle\vec p\,'|\, S\, |\vec p\rangle = \langle\vec p\,'|\, \Omega_-^\dagger \Omega_+\, |\vec p\rangle = \lim_{\substack{t\,\to\,+\infty \\ t'\,\to\,-\infty}} \langle\vec p\,'|\left({\rm e}^{\frac{\rm i}{\hbar}H^0 t}{\rm e}^{-\frac{\rm i}{\hbar}Ht}\right)\left({\rm e}^{\frac{\rm i}{\hbar}Ht'}{\rm e}^{-\frac{\rm i}{\hbar}H^0 t'}\right)|\vec p\rangle$$

$$= \lim_{t\to\infty} \langle\vec{p}'| \left(\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}\right)\left(\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t}\right)|\vec{p}\rangle\,, \tag{8.101}$$

where we have taken the limit with $t' = -t$. Now write the operator $f(t)$ in the braket as the derivative of its integral:

$$\begin{aligned}\frac{\mathrm{d}f(t)}{\mathrm{d}t} &= \frac{\mathrm{i}}{\hbar}\left\{\left(\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t}(H^0-H)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}\right)\left(\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t}\right) - \left(\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}\right)\left(\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}(H-H^0)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t}\right)\right\} \\ &= -\frac{\mathrm{i}}{\hbar}\left\{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t}V\mathrm{e}^{-2\frac{\mathrm{i}}{\hbar}Ht}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t} + \mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t}\mathrm{e}^{-2\frac{\mathrm{i}}{\hbar}Ht}V\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0 t}\right\}\end{aligned} \tag{8.102}$$

and

$$\begin{aligned}\lim_{t\to\infty} f(t) &= f(0) + \int_0^\infty \mathrm{d}t \frac{\mathrm{d}f(t)}{\mathrm{d}t} \\ &= f(0) + \lim_{\epsilon\to 0^+}\int_0^\infty \mathrm{d}t\,\mathrm{e}^{-\frac{\epsilon t}{\hbar}}\,\frac{\mathrm{d}f(t)}{\mathrm{d}t},\end{aligned} \tag{8.103}$$

where in the last line we have introduced a damping factor as we did before. Then

$$\begin{aligned}\langle\vec{p}'|\,S\,|\vec{p}\rangle &= \langle\vec{p}'|\vec{p}\rangle - \frac{\mathrm{i}}{\hbar}\lim_{\epsilon\to 0^+}\int_0^\infty \mathrm{d}t\,\langle\vec{p}'|\left\{V\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_{\vec{p}'}+E_{\vec{p}}+\mathrm{i}\epsilon-2H)t} + \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_{\vec{p}'}+E_{\vec{p}}+\mathrm{i}\epsilon-2H)t}V\right\}|\vec{p}\rangle \\ &= \delta^3(\vec{p}'-\vec{p}) + \lim_{\epsilon\to 0^+}\langle\vec{p}'|\left\{V\frac{1}{E_{\vec{p}'}+E_{\vec{p}}+\mathrm{i}\epsilon-2H} + \frac{1}{E_{\vec{p}'}+E_{\vec{p}}+\mathrm{i}\epsilon-2H}V\right\}|\vec{p}\rangle \\ &= \delta^3(\vec{p}'-\vec{p}) + \frac{1}{2}\lim_{\epsilon\to 0^+}\langle\vec{p}'|\left\{VG\left(\frac{E_{\vec{p}'}+E_{\vec{p}}+\mathrm{i}\epsilon}{2}\right) + G\left(\frac{E_{\vec{p}'}+E_{\vec{p}}+\mathrm{i}\epsilon}{2}\right)V\right\}|\vec{p}\rangle \\ &= \delta^3(\vec{p}'-\vec{p}) + \frac{1}{2}\lim_{\epsilon\to 0^+}\left(\frac{2}{E_{\vec{p}'}-E_{\vec{p}}+\mathrm{i}\epsilon} + \frac{2}{E_{\vec{p}}-E_{\vec{p}'}+\mathrm{i}\epsilon}\right)\langle\vec{p}'|\,T\left(\frac{E_{\vec{p}'}+E_{\vec{p}}+\mathrm{i}\epsilon}{2}\right)|\vec{p}\rangle \\ &= \delta^3(\vec{p}'-\vec{p}) - 2\mathrm{i}\lim_{\epsilon\to 0^+}\frac{\epsilon}{(E_{\vec{p}'}-E_{\vec{p}'})^2+\epsilon^2}\,\langle\vec{p}'|\,T\left(\frac{E_{\vec{p}'}+E_{\vec{p}}+\mathrm{i}\epsilon}{2}\right)|\vec{p}\rangle\end{aligned} \tag{8.104}$$

where we have performed the integral over t, introduced the definition of $G(z)$, replaced

$$VG(z) = T(z)G^0(z), \quad G(z)V = G^0(z)T(z) \tag{8.105}$$

and substituted

$$G^0(z)\,|\vec{p}\rangle = \frac{1}{z-E_{\vec{p}}}\,|\vec{p}\rangle, \quad \langle\vec{p}'|\,G^0(z) = \frac{1}{z-E_{\vec{p}'}}\,\langle\vec{p}'| \tag{8.106}$$

$$\frac{E_{\vec{p}'}+E_{\vec{p}}}{2} - E_{\vec{p}} = \frac{E_{\vec{p}'}-E_{\vec{p}}}{2} \tag{8.107}$$

$$\frac{E_{\vec{p}'}+E_{\vec{p}}}{2} - E_{\vec{p}'} = \frac{E_{\vec{p}}-E_{\vec{p}'}}{2}. \tag{8.108}$$

We recognize the prefactor of the T-matrix element as one of the representations of the Dirac delta,

$$\delta(x) = \lim_{\epsilon\to 0+}\frac{\epsilon/\pi}{x^2+\epsilon^2}. \tag{8.109}$$

So (redefining ϵ to 2ϵ, a small positive parameter anyway) we have:

$$\boxed{\langle\vec{p}'|\,S\,|\vec{p}\rangle = \delta^3(\vec{p}'-\vec{p}) - 2\pi\mathrm{i}\,\delta(E_{\vec{p}'}-E_{\vec{p}})\,\langle\vec{p}'|\,T\,(E_{\vec{p}}+\mathrm{i}\epsilon)\,|\vec{p}\rangle} \tag{8.110}$$

[From here on, $T(E_{\vec{p}}+\mathrm{i}\epsilon)$ means *take the limit* $\epsilon\to 0^+$ *to the matrix element.*] The expression above implies, from the definitions of the on-shell T-matix t and the scattering amplitude f, that *on the energy-shell* ($E_{\vec{p}'} = E_{\vec{p}}$):

$$\boxed{t(\vec{p}'\leftarrow\vec{p}) = \langle\vec{p}'|\,T\,(E_{\vec{p}}+\mathrm{i}\epsilon)\,|\vec{p}\rangle = -\frac{1}{(2\pi)^2\hbar m}f(\vec{p}'\leftarrow\vec{p})} \tag{8.111}$$

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8.10 The Born series

We want to find $\langle\vec{p}'|\, T(E_{\vec{p}}+\mathrm{i}\epsilon)\,|\vec{p}\rangle$ solving the Lippmann-Schwinger equation for $T(z)$,

$$T(z) = V + VG^0(z)T(z), \quad z = E_{\vec{p}} + \mathrm{i}\epsilon. \tag{8.112}$$

This is a transcendental equation (of a similar type as $e^x = x$) whose solution can only be obtained by numerical methods or perturbatively. To understand the perturbative solution, let us rescale the potential V by a dimensionless factor λ, that can be taken as a "coupling constant". If $\lambda = 0$ we have the free theory (no collisions), and if λ is small the interaction is weak. We can organize the different contributions to $T(z)$ as an expansion in powers of λ:

$$T = \sum_{n=0}^{\infty} \lambda^n T^{(n)} = T^{(0)} + \lambda T^{(1)} + \lambda^2 T^{(2)} + \dots \tag{8.113}$$

Then the Lippmann-Schwinger equation for $T(z)$ reads:

$$T = \lambda V + \lambda V G^0 T \tag{8.114}$$

$$T^{(0)} + \lambda T^{(1)} + \lambda^2 T^{(2)} + \dots = \lambda V + \lambda V G^0 (T^{(0)} + \lambda T^{(1)} + \lambda^2 T^{(2)} + \dots) \tag{8.115}$$

Solving for each power of λ we obtain:

$$T^{(0)} = 0 \tag{8.116}$$

$$T^{(1)} = V + VG^0T^{(0)} = V \tag{8.117}$$

$$T^{(2)} = VG^0T^{(1)} = VG^0V \tag{8.118}$$

$$T^{(3)} = VG^0T^{(2)} = (VG^0)^2V \tag{8.119}$$

$$\vdots$$

$$T^{(n)} = (VG^0)^{n-1}V. \tag{8.120}$$

And inserting the coupling constant in the potential ($\lambda V \to V$) we get:

$$\boxed{T(z) = V + VG^0(z)V + VG^0(z)VG^0(z)V + \dots} \tag{8.121}$$

This is the *Born series*, an expansion in powers of $\dfrac{V}{z - H^0}$ with $z = E_{\vec{p}} + \mathrm{i}\epsilon$.

The first order approximation is the so called *Born approximation*:

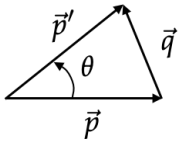
$$T = V. \tag{8.122}$$

This is a good approximation when *(i)* the coupling λ is small (weak interaction) or *(ii)* the kinetic energy is large ($E_{\vec{p}} \gg V$). In this domain,

$$\begin{aligned} f(\vec{p}' \leftarrow \vec{p}) \approx f^{(1)}(\vec{p}' \leftarrow \vec{p}) &= -(2\pi)^2\hbar m\, \langle\vec{p}'|\, V\,|\vec{p}\rangle \\ &= -(2\pi)^2\hbar m \int \mathrm{d}^3x'\mathrm{d}^3x\, \langle\vec{p}'|\vec{x}'\rangle \langle\vec{x}'|\vec{x}\rangle\, V(\vec{x})\, \langle\vec{p}|\vec{x}\rangle^* \\ &= -\frac{(2\pi)^2\hbar m}{(2\pi\hbar)^3} \int \mathrm{d}^3x\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\vec{p}'\cdot\vec{x}} V(\vec{x}) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}} \end{aligned} \tag{8.123}$$

$$\Rightarrow \quad \boxed{f^{(1)}(\vec{p}' \leftarrow \vec{p}) = -\frac{m}{2\pi\hbar^2} \int \mathrm{d}^3x\, V(\vec{x}) \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\vec{q}\cdot\vec{x}}} \tag{8.124}$$

where $\vec{q} = \vec{p}' - \vec{p}$ is the *momentum transfer* in the collision with



$$\vec{q} = \vec{p}' - \vec{p} \qquad q = |\vec{p}' - \vec{p}| = \sqrt{2p^2(1-\cos\theta)} = 2p\sin\frac{\theta}{2} \tag{8.125}$$

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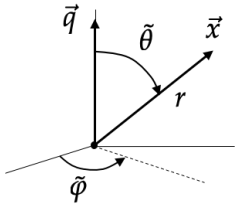
and θ is the *scattering angle*.

For a central potential (spherically symmetric) $V(\vec{x}) = V(r)$,

$$\begin{aligned} f(\vec{p}' \leftarrow \vec{p}) \approx f^{(1)}(\vec{p}' \leftarrow \vec{p}) &= f(p,\theta) \\ &= -\frac{m}{2\pi\hbar^2}\int_0^\infty \mathrm{d}r\, r^2 V(r) \int_0^{2\pi} \mathrm{d}\tilde{\varphi} \int_{-1}^{1} \mathrm{d}\cos\tilde{\theta}\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} qr\cos\tilde{\theta}} \\ &= -\frac{2m}{\hbar^2}\int_0^\infty \mathrm{d}r\, r^2 V(r)\, \frac{\sin\frac{qr}{\hbar}}{\frac{qr}{\hbar}} \\ &= -\frac{2m}{q\hbar}\int_0^\infty \mathrm{d}r\, rV(r)\, \sin\frac{qr}{\hbar} \qquad \text{with} \quad q = 2p\sin\frac{\theta}{2}. \end{aligned} \tag{8.126}$$



Notice that:

- If $\vec{p}' = \vec{p}$, that is $q = 0$ (*forward* scattering) we have:

$$f^{(1)}(\vec{p} \leftarrow \vec{p}) = -\frac{2m}{\hbar^2}\int_0^\infty \mathrm{d}r\, r^2\, V(r). \tag{8.127}$$

  Thus, the Born forward amplitude is *energy-independent*, it does not depend on p.

- At high energy (large p) the Born amplitude goes to zero like p^{-1}, except forward, since at fixed $\theta \neq 0$ we have $q \propto p$.

- The Born approximation violates the optical theorem since the forward amplitude is real but the total cross section does not vanish:

$$\mathrm{Im}\, f(\vec{p} \leftarrow \vec{p}) = 0 \tag{8.128}$$

$$\frac{p}{4\pi\hbar}\sigma(p) = \frac{p}{4\pi\hbar}\int \mathrm{d}\Omega\, |f(p,\theta)|^2 = \frac{p}{2\hbar}\int_{-1}^{1} \mathrm{d}\cos\theta\, |f(p,\theta)|^2 \neq 0. \tag{8.129}$$

  This is because the imaginary part of f is of order λ while σ is of order λ^2.

8.11 Plane waves and spherical waves

We have just studied the effect of the scattering potential on states with well defined momenta (plane waves). When the potential is $V(\vec{x}) = V(r)$ the effect on spherical waves is simpler. A plane wave of momentum $\vec{p}$ is an eigenfunction of the free Hamiltonian $H^0 = \dfrac{P^2}{2m}$:

$$|\vec{p}\rangle \quad \text{(plane wave)}. \tag{8.130}$$

In the position representation:

$$\boxed{\langle \vec{x}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}}} \quad \text{(plane wave function)}. \tag{8.131}$$

However, H^0 (not $\vec{P}$) also commutes with L^2 and L_z. Hence we can define a basis of common eigenstates of H^0, L^2 and L_z (not a basis of $\vec{P}$):

$$|E\ell m\rangle \quad \text{(spherical wave)} \qquad [\text{this } m \text{ should not be confused with the mass } m] \tag{8.132}$$

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Spherical waves are an othonormal basis of $\mathcal{H}$:

$$\langle E'\ell'm'|E\ell m\rangle = \delta(E'-E)\,\delta_{\ell'\ell}\,\delta_{m'm}. \tag{8.133}$$

The spherical waves do not have a well defined momentum $\vec{p}$. In fact, they are a linear combination of all momentum eigenstates:

$$\boxed{|E\ell m\rangle = \int \mathrm{d}^3p\ |\vec{p}\rangle\,\frac{1}{\sqrt{mp}}\delta\left(\frac{p^2}{2m}-E\right)Y_\ell^m(\hat{p})} \tag{8.134}$$

because

$$\begin{aligned}
\langle E'\ell'm'|E\ell m\rangle &= \int \mathrm{d}^3p''\ \langle E'\ell'm'|\vec{p}''\rangle\,\langle\vec{p}''|E\ell m\rangle \\
&= \int \mathrm{d}^3p''\,\frac{1}{\sqrt{mp''}}\delta\left(\frac{p''^2}{2m}-E'\right)Y_{\ell'}^{m'*}(\hat{p}'')\frac{1}{\sqrt{mp''}}\delta\left(\frac{p''^2}{2m}-E\right)Y_\ell^m(\hat{p}'') \\
&= \delta(E'-E)\int_0^\infty \mathrm{d}p''\,p''^2\frac{1}{mp''}\delta\left(\frac{p''^2}{2m}-E\right) \\
&\qquad\qquad \times\int_{-1}^1 \mathrm{d}\cos\theta\int_0^{2\pi}\mathrm{d}\varphi\,Y_{\ell'}^{m'*}(\theta,\varphi)Y_\ell^m(\theta,\varphi) \\
&= \delta(E'-E)\delta_{\ell'\ell}\delta_{m'm}\int_0^\infty \mathrm{d}p''p''^2\frac{1}{mp''}\frac{m}{p''}\delta\left(p''-p=\sqrt{2mE}\right) \\
&= \delta(E'-E)\,\delta_{\ell'\ell}\,\delta_{m'm}.
\end{aligned} \tag{8.135}$$

Then,

$$\langle\vec{p}|E\ell m\rangle = \frac{1}{\sqrt{mp}}\delta\left(\frac{p^2}{2m}-E\right)Y_\ell^m(\hat{p}) \tag{8.136}$$

and the plane wave $|\vec{p}\rangle$ is the following linear combination of spherical waves (a plane wave contains all angular momenta):

$$|\vec{p}\rangle = \int \mathrm{d}E\sum_{\ell=0}^\infty\sum_{m=-\ell}^\ell |E\ell m\rangle\,\langle E\ell m|\vec{p}\rangle = \int \mathrm{d}E\sum_{\ell=0}^\infty\sum_{m=-\ell}^\ell |E\ell m\rangle\,\frac{1}{\sqrt{mp}}\delta\left(\frac{p^2}{2m}-E\right)Y_\ell^{m*}(\hat{p})$$

$$\boxed{|\vec{p}\rangle = \sum_{\ell=0}^\infty\sum_{m=-\ell}^\ell |E\ell m\rangle\Big|_{E=\frac{p^2}{2m}}\frac{1}{\sqrt{mp}}Y_\ell^{m*}(\hat{p})} \tag{8.137}$$

In order to find the spherical waves in the position representation (spherical wave functions) $\langle\vec{x}|E\ell m\rangle$, we will use

$$\begin{aligned}
\langle\vec{x}|\,P^2\,|E\ell m\rangle &= -\hbar^2\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{\ell(\ell+1)}{r^2}\right]\langle\vec{x}|E\ell m\rangle \\
&= p^2\,\langle\vec{x}|E\ell m\rangle \quad \text{with} \quad E=\frac{p^2}{2m}.
\end{aligned} \tag{8.138}$$

This implies that the radial part of $\langle\vec{x}|E\ell m\rangle$ defined by

$$\langle\vec{x}|E\ell m\rangle \equiv \frac{1}{r}y_\ell(r)Y_\ell^m(\hat{x}), \quad \vec{x}=r\hat{x}, \tag{8.139}$$

verifies the following differential equation:

$$-\hbar^2\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r}-\frac{\ell(\ell+1)}{r^2}\right]\frac{1}{r}y_\ell(r) = \frac{p^2}{r}y_\ell(r) \tag{8.140}$$

or

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\ell(\ell+1)}{r^2} + \frac{p^2}{\hbar^2}\right] y_\ell(r) = 0. \tag{8.141}$$

The solutions of the standard differential equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{\ell(\ell+1)}{x^2} + 1\right] y_\ell(x) = 0 \quad \left(x = \frac{pr}{\hbar}\right) \tag{8.142}$$

are linear combinations of

$$\tilde{j}_\ell(x) = x j_\ell(x) \quad \text{(Ricati-Bessel functions)} \tag{8.143}$$
$$\tilde{n}_\ell(x) = x n_\ell(x) \quad \text{(Ricati-Neumann functions)} \tag{8.144}$$

where $j_\ell(x)$ and $n_\ell(x)$ are, respectively, the spherical Bessel and Neumann functions of order ℓ. But only $\tilde{j}_\ell(x)$ is regular at the origin, because

$$j_\ell(x) \xrightarrow[x\to 0]{} \frac{x^\ell}{(2\ell+1)!!} \tag{8.145}$$
$$n_\ell(x) \xrightarrow[x\to 0]{} -\frac{(2\ell-1)!!}{x^{\ell+1}} \tag{8.146}$$

with the double factorial defined as

$$n!! = \prod_{k=0}^{[\frac{n}{2}]-1} (n-2k) = n(n-2)(n-4)\cdots, \qquad [x] = \text{integer part of } x. \tag{8.147}$$

Since $\langle \vec{x}|E\ell m\rangle \propto y_\ell(r)/r$ must be well defined at the origin, the function $y_\ell(r)$ must go to zero at $r \to 0$ and hence

$$y_\ell(r) = C\, \tilde{j}_\ell(\tfrac{pr}{\hbar}) \tag{8.148}$$

where the normalization constant C is fixed by

$$\langle \vec{x}|E\ell m\rangle = \frac{C}{r}\tilde{j}_\ell(\tfrac{pr}{\hbar}) Y_\ell^m(\hat{x}) \tag{8.149}$$

$$\begin{aligned}\delta(E'-E)\,\delta_{\ell'\ell}\,\delta_{m'm} &= \int \mathrm{d}^3x\ \langle E'\ell'm'|\vec{x}\rangle\,\langle \vec{x}|E\ell m\rangle \\ &= |C|^2 \int_0^\infty \mathrm{d}r\, r^2 \frac{1}{r^2}\tilde{j}_\ell(\tfrac{p'r}{\hbar})\tilde{j}_\ell(\tfrac{pr}{\hbar}) \int \mathrm{d}\Omega\, Y_{\ell'}^{m'*}(\hat{x}) Y_\ell^m(\hat{x}) \\ &= \delta_{\ell'\ell}\,\delta_{m'm}|C|^2 \int_0^\infty \mathrm{d}r\, \tilde{j}_\ell(\tfrac{p'r}{\hbar})\tilde{j}_\ell(\tfrac{pr}{\hbar})\end{aligned} \tag{8.150}$$

using that

$$\int_0^\infty \mathrm{d}r\, \tilde{j}_\ell(\tfrac{p'r}{\hbar})\tilde{j}_\ell(\tfrac{pr}{\hbar}) = \frac{\pi\hbar}{2}\delta(p'-p) = \frac{\pi\hbar p}{2m}\delta(E'-E). \tag{8.151}$$

Therefore

$$|C|^2 = \frac{2m}{\pi\hbar p} \quad \Rightarrow \quad C \equiv \mathrm{i}^\ell \sqrt{\frac{2m}{\pi\hbar p}} \tag{8.152}$$

where a conventional phase i^ℓ has been introduced. Then

$$\boxed{\langle \vec{x}|E\ell m\rangle = \frac{\mathrm{i}^\ell}{\hbar}\sqrt{\frac{2mp}{\pi\hbar}} j_\ell(\tfrac{pr}{\hbar}) Y_\ell^m(\hat{x})} \quad \text{(spherical wave function).} \tag{8.153}$$

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Finally, from (8.137) we can write the plane wave functions in terms of spherical waves:

$$\begin{aligned}\langle\vec{x}|\vec{p}\rangle &= \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\langle\vec{x}|E\ell m\rangle\,\frac{1}{\sqrt{mp}}Y_\ell^{m*}(\hat{p})\\ &= \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{\mathrm{i}^\ell}{\hbar}\sqrt{\frac{2}{\pi\hbar}}j_\ell(\tfrac{pr}{\hbar})Y_\ell^m(\hat{x})Y_\ell^{m*}(\hat{p}).\end{aligned}\tag{8.154}$$

Using the following relation between spherical harmonics and Legendre polynomials:

$$\sum_{m=-\ell}^{\ell}Y_\ell^m(\hat{x})Y_\ell^{m*}(\hat{p}) = \frac{2\ell+1}{4\pi}P_\ell(\hat{p}\cdot\hat{x})\tag{8.155}$$

we have

$$\boxed{\frac{1}{(2\pi\hbar)^{3/2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}} = \frac{1}{(2\pi\hbar)^{3/2}}\sum_{\ell=0}^{\infty}(2\ell+1)\mathrm{i}^\ell j_\ell(\tfrac{pr}{\hbar})P_\ell(\hat{p}\cdot\hat{x})}\tag{8.156}$$

In the limit of large distances, appropriate for asymptotic states, we can use

$$j_\ell(x) \xrightarrow[x\to\infty]{} \frac{1}{x}\sin\left(x-\ell\frac{\pi}{2}\right)\tag{8.157}$$

$$\Rightarrow\quad \mathrm{i}^\ell j_\ell(\tfrac{pr}{\hbar}) \xrightarrow[r\to\infty]{} \frac{1}{2}\left[\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr}+(-1)^{\ell+1}\frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr}\right]\tag{8.158}$$

(that justifies the introduction of $\mathrm{i}^\ell = \mathrm{e}^{\mathrm{i}\ell\frac{\pi}{2}}$ before) and write the plane wave as the following combination of spherical waves

$$\frac{1}{(2\pi\hbar)^{3/2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}} \xrightarrow[r\to\infty]{} \frac{1}{(2\pi\hbar)^{3/2}}\sum_{\ell=0}^{\infty}(\ell+\tfrac{1}{2})\left[\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr}+(-1)^{\ell+1}\frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr}\right]P_\ell(\hat{p}\cdot\hat{x}).\tag{8.159}$$

8.12 Partial-wave *S*-matrix

Isolated systems are invariant under rotations, $[H,\vec{J}]=0$. Therefore the Møller operators and the scattering operator S must be rotationally invariant, $[S,\vec{J}]=0$. For the scattering of spinless particles, $\vec{J}=\vec{L}$, we have $[S,\vec{L}]=0$. And remember that $[S,H^0]=0$. Then $|E\ell m\rangle$ is an eigenstate of S:

$$\langle E'\ell'm'|\,S\,|E\ell m\rangle = \delta(E'-E)\delta_{\ell'\ell}\delta_{m'm}s_\ell(E).\tag{8.160}$$

That the number $s_\ell(E)$ is actually independent of m is a consequence of the Wigner-Eckart theorem (because S is a scalar operator) but it can also be checked explicitly:

$$\begin{aligned}L_\pm\,|\ell\,m\rangle &= \hbar\sqrt{\ell(\ell+1)-m(m\pm1)}\,|\ell\,m\pm1\rangle\,;\\ L_\mp L_\pm\,|\ell\,m\rangle &= \hbar^2[\ell(\ell+1)-m(m\pm1)]\,|\ell\,m\rangle\,;\\ [S,L_\pm]=0 \quad&\Rightarrow\quad SL_\pm L_\mp = L_\pm SL_\mp\\ &\Rightarrow\quad \langle\ell\,m|\,SL_\pm L_\mp\,|\ell\,m\rangle = \langle\ell\,m|\,L_\pm SL_\mp\,|\ell\,m\rangle\\ &\Rightarrow\quad \langle\ell\,m|\,S\,|\ell\,m\rangle = \langle\ell\,m\mp1|\,S\,|\ell\,m\mp1\rangle\,.\end{aligned}\tag{8.161}$$

Since S is unitary, its eigenvalues must have modulus 1 and can be written as

$$S\,|E\ell m\rangle = s_\ell(E)\,|E\ell m\rangle \equiv \mathrm{e}^{2\mathrm{i}\delta_\ell(E)}\,|E\ell m\rangle\,,\tag{8.162}$$

where $\delta_\ell(E)$ is called the *phase shift* (defined modulo π).

Remember that

$$\langle\vec{p}'|\,(S-I)\,|\vec{p}\rangle = \frac{\mathrm{i}}{2\pi\hbar m}\delta(E_{\vec{p}'}-E_{\vec{p}})f(\vec{p}'-\vec{p}) \tag{8.163}$$

that can be now written as follows:

$$\begin{aligned}
\langle\vec{p}'|\,(S-I)\,|\vec{p}\rangle &= \langle\vec{p}'|\,(S-I)\sum_{\ell m}\int \mathrm{d}E\;|E\ell m\rangle\,\langle E\ell m|\vec{p}\rangle \\
&= \sum_{\ell m}\int \mathrm{d}E\;\langle\vec{p}'|E\ell m\rangle\,[s_\ell(E)-1]\,\langle E\ell m|\vec{p}\rangle \\
&= \sum_{\ell m}\int \mathrm{d}E\,\frac{1}{\sqrt{mp'}}\delta(E_{\vec{p}'}-E)Y_\ell^m(\hat{p}')[s_\ell(E)-1]\frac{1}{\sqrt{mp}}\delta(E_{\vec{p}}-E)Y_\ell^{m*}(\hat{p}) \\
&= \frac{\delta(E_{\vec{p}'}-E_{\vec{p}})}{mp}\sum_{\ell m}Y_\ell^m(\hat{p}')Y_\ell^{m*}(\hat{p})\int \mathrm{d}E\,\delta(E_{\vec{p}}-E)[s_\ell(E)-1] \\
&= \frac{\delta(E_{\vec{p}'}-E_{\vec{p}})}{mp}\sum_{\ell=0}^{\infty}[s_\ell(E_{\vec{p}})-1]\sum_{m=-\ell}^{\ell}Y_\ell^m(\hat{p}')Y_\ell^{m*}(\hat{p}) \\
&= \frac{\delta(E_{\vec{p}'}-E_{\vec{p}})}{mp}\sum_{\ell=0}^{\infty}[s_\ell(E_{\vec{p}})-1]\frac{2\ell+1}{4\pi}P_\ell(\cos\theta) \\
&= \delta(E_{\vec{p}'}-E_{\vec{p}})\frac{1}{4\pi mp}\sum_{\ell=0}^{\infty}(2\ell+1)[\mathrm{e}^{2\mathrm{i}\delta_\ell(E_{\vec{p}})}-1]P_\ell(\cos\theta)
\end{aligned} \tag{8.164}$$

where we have introduced the definition of the phase shift δ_ℓ, the relation between spherical harmonics and Legendre polynomials, and the scattering angle in $\hat{p}\cdot\hat{p}'=\cos\theta$. Hence,

$$f(E_{\vec{p}},\theta)\equiv f(\vec{p}'\leftarrow\vec{p}) = \frac{\hbar}{2\mathrm{i}p}\sum_{\ell=0}^{\infty}(2\ell+1)[\mathrm{e}^{2\mathrm{i}\delta_\ell(E_{\vec{p}})}-1]P_\ell(\cos\theta). \tag{8.165}$$

It is useful to define the *scattering amplitude in the partial wave* ℓ:

$$\boxed{f_\ell(E)\equiv\frac{\hbar}{p}\frac{\mathrm{e}^{2\mathrm{i}\delta_\ell(E)}-1}{2\mathrm{i}} = \frac{\hbar}{p}\mathrm{e}^{\mathrm{i}\delta_\ell(E)}\sin\delta_\ell(E)\quad\text{with } p=\sqrt{2mE}} \tag{8.166}$$

so that we can write the *partial-wave expansion* of the scattering amplitude as:

$$\boxed{f(E,\theta)=\sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(E)P_\ell(\cos\theta)} \tag{8.167}$$

Using the orthogonality of the Legendre polynomials,

$$\int_{-1}^{1}\mathrm{d}x\,P_m(x)P_n(x)=\frac{2}{2n+1}\delta_{mn} \tag{8.168}$$

we can obtain, in turn, every partial wave from the scattering amplitude by

$$f_\ell(E)=\frac{1}{2}\int_{-1}^{1}\mathrm{d}\cos\theta\,f(E,\theta)P_\ell(\cos\theta). \tag{8.169}$$

The *total cross section* can also be expanded in terms of partial-wave contributions:

$$\sigma(E)=\int_0^{2\pi}\mathrm{d}\varphi\int_{-1}^{1}\mathrm{d}\cos\theta\,|f(E,\theta)|^2$$

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$$
\begin{aligned}
&= 2\pi \sum_{\ell=0}^{\infty}\sum_{\ell'=0}^{\infty}(2\ell+1)(2\ell'+1) f_\ell(E) f^*_{\ell'}(E) \int_{-1}^{1} \mathrm{d}\cos\theta\, P_\ell(\cos\theta) P_{\ell'}(\cos\theta) \\
&= 4\pi \sum_{\ell=0}^{\infty}(2\ell+1)|f_\ell(E)|^2 \\
\Rightarrow \quad & \boxed{\sigma(E) = \sum_\ell \sigma_\ell(E) \quad \text{with } \sigma_\ell(E) = 4\pi(2\ell+1)|f_\ell(E)|^2}
\end{aligned}
\tag{8.170}
$$

or, in terms of the phase shifts,

$$
\boxed{\sigma_\ell(E) = \frac{4\pi\hbar^2}{p^2}(2\ell+1)\sin^2\delta_\ell(E)}
\tag{8.171}
$$

Since $|\sin\delta_\ell| \leq 1$, the contribution of each partial wave to the total cross section cannot exceed the so called *unitarity bound* (because it has to do with the unitarity of S):

$$
\sigma_\ell \leq \frac{4\pi\hbar^2}{p^2}(2\ell+1).
\tag{8.172}
$$

Note that partial waves fulfill the optical theorem:

$$
\left.
\begin{aligned}
f(p,\theta) &= \sum_{\ell=0}^{\infty}(2\ell+1)\frac{\hbar}{p}\mathrm{e}^{\mathrm{i}\delta_\ell}\sin\delta_\ell P_\ell(\cos\theta) \\
\sigma &= \sum_{\ell=0}^{\infty}(2\ell+1)\frac{4\pi\hbar^2}{p^2}\sin^2\delta_\ell
\end{aligned}
\right\} \Rightarrow \mathrm{Im} f(p,0) = \frac{p}{4\pi\hbar}\sigma = \sum_{\ell=0}^{\infty}(2\ell+1)\frac{\hbar}{p}\sin^2\delta_\ell
\tag{8.173}
$$

where we have used that $P_\ell(1) = 1$.

8.13 Time-independent formalism: stationary states

An asymptotic state of *well-defined momentum* $|\vec{p}\rangle$ is actually *unphysical*, since it is not normalized. In addition, it does not make much sense to say that in a collision a momentum eigenstate approaches or leaves the target, because it is *stationary*: it does not evolve with time (it has always been there). We can call $|\vec{p}\rangle$ an *improper* state.

However, by *combining* states $|\vec{p}\rangle$ with well-defined momentum (plane waves) one can build *physical* states (**wave packets**) with momentum around (but not exactly) $\vec{p}_0$, that are not stationary but evolve and can therefore approach and leave the target in a scattering process:

$$
|\phi\rangle = \int \mathrm{d}^3p\, \phi(\vec{p})\,|\vec{p}\rangle\,, \quad \langle\phi|\phi\rangle = \int \mathrm{d}^3p\,|\phi(\vec{p})|^2 = 1.
\tag{8.174}
$$

It is *only in this context* that *plane waves are related to asymptotic states*. Let us see this.

Consider the scattering state $|\psi\rangle \equiv |\vec{p}+\rangle$ "associated" to an in-state $|\psi_{\mathrm{in}}\rangle \equiv |\vec{p}\rangle$:

$$
|\vec{p}+\rangle = \Omega_+\,|\vec{p}\rangle
\tag{8.175}
$$

The state $|\vec{p}+\rangle$ is not a physical state either, but it is a basis vector of the physical stattering states $|\phi+\rangle$:

$$
|\phi+\rangle = \Omega_+\,|\phi\rangle = \int \mathrm{d}^3p\,\phi(\vec{p})\,\Omega_+\,|\vec{p}\rangle = \int \mathrm{d}^3p\,\phi(\vec{p})\,|\vec{p}+\rangle\,.
\tag{8.176}
$$

We see that the scattering state $|\phi+\rangle$ has the same expansion in the basis $\{|\vec{p}+\rangle\}$ as its asymptotic state $|\phi\rangle$ in the basis $\{|\vec{p}\rangle\}$.

We expect that the states $|\vec{p}\rangle$ and $|\vec{p}+\rangle$ have the same energy $E_{\vec{p}} = \frac{p^2}{2m}$ since

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}\Omega_+ = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}\lim_{t'\to-\infty}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht'}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0t'} = \lim_{t'\to-\infty}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H(t+t')}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H^0(t+t')}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0t} = \Omega_+\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H^0t} \tag{8.177}$$

and taking an infinitesimal time δt:

$$(I + \frac{\mathrm{i}}{\hbar}H\delta t)\,\Omega_+ = \Omega_+\,(I + \frac{\mathrm{i}}{\hbar}H^0\delta t) \quad \Rightarrow \quad H\Omega_+ = \Omega_+H^0 \tag{8.178}$$

$$\Rightarrow \quad H\,|\vec{p}+\rangle = H\Omega_+\,|\vec{p}\rangle = \Omega_+H^0\,|\vec{p}\rangle = \frac{p^2}{2m}\Omega_+\,|\vec{p}\rangle = \frac{p^2}{2m}\,|\vec{p}+\rangle = E_{\vec{p}}\,|\vec{p}+\rangle\,. \tag{8.179}$$

Therefore:

$\boxed{|\vec{p}+\rangle \text{ is an eigenvector of } H \text{ with same eigenvalue } E_{\vec{p}} \text{ as that of } H^0 \text{ acting on } |\vec{p}\rangle}$

This means that $|\vec{p}\rangle$ and $|\vec{p}+\rangle$ are stationary states, not evolving with time:

$$U(t)\,|\vec{p}+\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_{\vec{p}}t}\,|\vec{p}+\rangle \tag{8.180}$$

$$U^0(t)\,|\vec{p}\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_{\vec{p}}t}\,|\vec{p}\rangle\,. \tag{8.181}$$

Hence it is *impossible* to satisfy $U(t)\,|\vec{p}+\rangle - U^0(t)\,|\vec{p}\rangle \xrightarrow[t\to-\infty]{} 0$. This is not surprising since, as mentioned before, none of these states are physical.

But if we slightly *localize* in space the initial position of the particle by *smearing* $\vec{p}$, we obtain physical states that *do evolve* with time (they are no longer stationary) and may satisfy the asymptotic condition:

$$U(t)\,|\phi+\rangle = \int \mathrm{d}^3p\,\phi(\vec{p})[U(t)\,|\vec{p}+\rangle] \tag{8.182}$$

$$U^0(t)\,|\phi\rangle = \int \mathrm{d}^3p\,\phi(\vec{p})[U^0(t)\,|\vec{p}\rangle] \tag{8.183}$$

$$U(t)\,|\phi+\rangle - U^0(t)\,|\phi\rangle \xrightarrow[t\to-\infty]{} 0 \quad \Rightarrow \quad |\phi+\rangle = \lim_{t\to-\infty}U^\dagger(t)U^0(t)\,|\phi\rangle \equiv \Omega_+\,|\phi\rangle\,. \tag{8.184}$$

The same applies to the scattering states $|\phi-\rangle = \Omega_-\,|\phi\rangle = \int \mathrm{d}^3p\,\phi(\vec{p})\,|\vec{p}-\rangle$.

We see that plane waves $\{|\vec{p}\rangle\}$ form an orthonormal basis of our Hilbert space $\mathcal{H}$, made of eigenvectors of H^0. Since $\Omega_\pm$ map $\mathcal{H}$ onto the subspace $\mathcal{R}$ of scattering states, we expect that $\{|\vec{p}+\rangle\}$ (or $\{|\vec{p}-\rangle\}$) should span $\mathcal{R}$. In fact, from

$$|\phi+\rangle = \int \mathrm{d}^3p\,\phi(\vec{p})\,|\vec{p}+\rangle \tag{8.185}$$

$$\Rightarrow \quad \langle\vec{p}\,'+|\vec{p}+\rangle = \langle\vec{p}\,'|\,\Omega_+^\dagger\Omega_+\,|\vec{p}\rangle = \langle\vec{p}\,'|\vec{p}\rangle = \delta^3(\vec{p}\,'-\vec{p}) \tag{8.186}$$

that is, the vectors $\{|\vec{p}+\rangle\}$ are an orthonormal basis of $\mathcal{R}$. The same holds for $\{|\vec{p}-\rangle\}$. Remember that

$$\mathcal{H} = \mathcal{R}\oplus\mathcal{B} \tag{8.187}$$

where the subspace $\mathcal{B}$ of bound states is spanned by $\{|n\rangle\}$, say. Therefore we have

$$I = \int \mathrm{d}^3p\;|\vec{p}\rangle\langle\vec{p}| \tag{8.188}$$

$$= \int \mathrm{d}^3p\;|\vec{p}+\rangle\langle\vec{p}+| + \sum_n |n\rangle\langle n| \tag{8.189}$$

$$= \int \mathrm{d}^3p\;|\vec{p}-\rangle\langle\vec{p}-| + \sum_n |n\rangle\langle n|\,. \tag{8.190}$$

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We know that given a proper (physical) asymptotic state $|\phi\rangle$ one can find the scattering state $|\phi_\pm\rangle = \Omega_\pm |\phi\rangle$ in terms of the Green's operator as:

$$|\phi_\pm\rangle = |\phi\rangle + \int \mathrm{d}^3p'\, G(E_{\vec{p}'} \pm \mathrm{i}\epsilon) V |\vec{p}'\rangle \langle \vec{p}'|\phi\rangle \,. \tag{8.191}$$

Then, in terms of improper states (understood as the basis on which $|\phi_\pm\rangle$ and $|\phi\rangle$ can be expanded):

$$\begin{aligned} |\vec{p}\pm\rangle &= |\vec{p}\rangle + \int \mathrm{d}^3p'\, G(E_{\vec{p}'} \pm \mathrm{i}\epsilon) V |\vec{p}'\rangle \langle \vec{p}'|\vec{p}\rangle \\ &= [I + G(E_{\vec{p}} \pm \mathrm{i}\epsilon)V] |\vec{p}\rangle \,. \end{aligned} \tag{8.192}$$

Since the T operator was defined as $T(z) = V + VG(z)V$ the expression above implies:

$$T(E_{\vec{p}} \pm \mathrm{i}\epsilon) |\vec{p}\rangle = V [I + G(E_{\vec{p}} \pm \mathrm{i}\epsilon)V] |\vec{p}\rangle = V |\vec{p}\pm\rangle \,. \tag{8.193}$$

From $G(z)V = G^0(z)T(z)$ we obtain the *Lippmann-Schwinger equation* for $|\vec{p}\pm\rangle$:

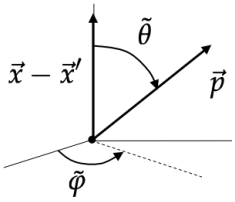
$$\left.\begin{aligned} |\vec{p}\pm\rangle &= |\vec{p}\rangle + G(E_{\vec{p}} \pm \mathrm{i}\epsilon)V |\vec{p}\rangle \\ G(E_{\vec{p}} \pm \mathrm{i}\epsilon)V |\vec{p}\rangle &= G^0(E_{\vec{p}} \pm \mathrm{i}\epsilon)T(E_{\vec{p}} \pm \mathrm{i}\epsilon) |\vec{p}\rangle \\ T(E_{\vec{p}} \pm \mathrm{i}\epsilon) |\vec{p}\rangle &= V |\vec{p}\pm\rangle \end{aligned}\right\} \Rightarrow \boxed{|\vec{p}\pm\rangle = |\vec{p}\rangle + G^0(E_{\vec{p}} \pm \mathrm{i}\epsilon)V |\vec{p}\pm\rangle} \tag{8.194}$$

And from this equation it follows that the *stationary wave functions* $\langle \vec{x}|\vec{p}\pm\rangle$ are the solutions of the integral equation:

$$\langle \vec{x}|\vec{p}\pm\rangle = \langle \vec{x}|\vec{p}\rangle + \int \mathrm{d}^3x'\ \langle \vec{x}| G^0(E_{\vec{p}} \pm \mathrm{i}\epsilon) |\vec{x}'\rangle V(\vec{x}') \langle \vec{x}'|\vec{p}\pm\rangle \,. \tag{8.195}$$

Before solving it, we have to calculate the Green's function $\langle \vec{x}| G^0(E_{\vec{p}} \pm \mathrm{i}\epsilon) |\vec{x}'\rangle$:

$$\begin{aligned} \langle \vec{x}| G^0(z) |\vec{x}'\rangle &= \int \mathrm{d}^3p\ \langle \vec{x}| G^0(z) |\vec{p}\rangle \langle \vec{p}|\vec{x}'\rangle \\ &= \int \mathrm{d}^3p\ \langle \vec{x}|\vec{p}\rangle \frac{1}{z - E_{\vec{p}}} \langle \vec{p}|\vec{x}'\rangle \\ &= \frac{1}{(2\pi\hbar)^3} \int \mathrm{d}^3p\, \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot(\vec{x}-\vec{x}')}}{z - E_{\vec{p}}} \\ &= \frac{1}{(2\pi\hbar)^3} \int_0^\infty \mathrm{d}p\, p^2 \int_0^{2\pi} \mathrm{d}\tilde{\varphi} \int_{-1}^{1} \mathrm{d}\cos\tilde{\theta}\, \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|\cos\tilde{\theta}}}{z - E_{\vec{p}}} \\ &= \frac{2\pi}{(2\pi\hbar)^3} \int_0^\infty \mathrm{d}p\, p^2 \frac{1}{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|} \left(\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|} - \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{z - E_{\vec{p}}} \right) \\ &= \frac{\mathrm{i}2m}{(2\pi\hbar)^2} \frac{1}{|\vec{x}-\vec{x}'|} \int_0^\infty \mathrm{d}p\, p \left(\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|} - \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{p^2 - 2mz} \right) \\ &= \frac{\mathrm{i}m}{2\pi^2\hbar^2} \frac{1}{|\vec{x}-\vec{x}'|} \int_{-\infty}^\infty \mathrm{d}p\, p\, \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{p^2 - 2mz} \end{aligned} \tag{8.196}$$

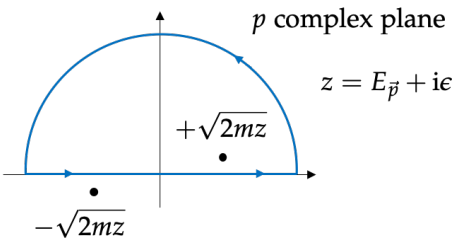


where in the last step we have changed $p' = -p$ in the second term:

$$-\int_0^{-\infty} \mathrm{d}p'\, p' \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p'|\vec{x}-\vec{x}'|}}{p'^2 - 2mz} = \int_{-\infty}^0 \mathrm{d}p\, p \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{p^2 - 2mz}. \tag{8.197}$$

Now we can calculate the integral (suppose the case of $z = E_{\vec{p}} + \mathrm{i}\epsilon$):

$$\int_{-\infty}^\infty \mathrm{d}p\, p \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{p^2 - 2mz} = \oint \mathrm{d}p\, p \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{p^2 - 2mz} \tag{8.198}$$



in the p complex plane by choosing the closed contour in the figure with $|p| \to \infty$ that contains one pole at $p = +\sqrt{2mz}$ (remember that $\epsilon \to 0^+$). Then, applying Cauchy's residue theorem:

$$\oint \mathrm{d}p\, p\, \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{p^2-2mz} = 2\pi\mathrm{i}\mathrm{Res}(\sqrt{2mz}) = 2\pi\mathrm{i}\lim_{p\to\sqrt{2mz}}\left(p-\sqrt{2mz}\right)\frac{p\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{p^2-2mz}$$
$$= \pi\mathrm{i}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|} \text{ with } p=\sqrt{2mE}. \tag{8.199}$$

Therefore,

$$\langle\vec{x}|\, G^0(E_{\vec{p}}+\mathrm{i}\epsilon)\,|\vec{x}'\rangle = \frac{\mathrm{i}m}{2\pi^2\hbar^2}\frac{1}{|\vec{x}-\vec{x}|}\pi\mathrm{i}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|} = -\frac{m}{2\pi\hbar^2|\vec{x}-\vec{x}'|}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}. \tag{8.200}$$

Analogously, for $z = E_{\vec{p}} - \mathrm{i}\epsilon$ one finds

$$\langle\vec{x}|\, G^0(E_{\vec{p}}-\mathrm{i}\epsilon)\,|\vec{x}'\rangle = -\frac{m}{2\pi\hbar^2|\vec{x}-\vec{x}'|}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}. \tag{8.201}$$

Hence, the stationary wave functions satisfy the equation

$$\langle\vec{x}|\vec{p}\pm\rangle = \langle\vec{x}|\vec{p}\rangle - \frac{m}{2\pi\hbar^2}\int \mathrm{d}^3x'\,\frac{\mathrm{e}^{\pm\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}V(\vec{x}')\,\langle\vec{x}'|\vec{p}\pm\rangle\,. \tag{8.202}$$

We will focus in the solutions for $\langle\vec{x}|\vec{p}+\rangle$.

At large distances $r = |\vec{x}|$, and with the integration variable within the range a of the potential, $r' = |\vec{x}'| \lesssim a \ll r$, we can approximate

$$|\vec{x}-\vec{x}'| = \sqrt{r^2+r'^2-2\vec{x}\cdot\vec{x}'} \approx r\left(1-\frac{\vec{x}\cdot\vec{x}'}{r^2}\right) \quad\Rightarrow\quad \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} \approx \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p\hat{x}\cdot\vec{x}'}}{r} \tag{8.203}$$

and we have

$$-\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3x'\,\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}V(\vec{x}')\,\langle\vec{x}'|\vec{p}+\rangle \xrightarrow[r\to\infty]{} -\frac{m}{2\pi\hbar^2}\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{r}\int \mathrm{d}^3x'\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p\hat{x}\cdot\vec{x}'}\,\langle\vec{x}'|\,V\,|\vec{p}+\rangle$$
$$= -\frac{m}{2\pi\hbar^2}(2\pi\hbar)^{3/2}\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{r}\,\langle p\hat{x}|\,V\,|\vec{p}+\rangle \tag{8.204}$$

because

$$|p\hat{x}\rangle = \int \mathrm{d}^3x'\;|\vec{x}'\rangle\,\langle\vec{x}'|p\hat{x}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\int \mathrm{d}^3x'\;|\vec{x}'\rangle\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p\hat{x}\cdot\vec{x}'}. \tag{8.205}$$

Now we will take the Born approximation, that is the first order approximation of the Born series obtained solving perturbatively the Lippmann-Schwinger equation for $|\vec{p}+\rangle$:

$$|\vec{p}+\rangle = |\vec{p}\rangle + G^0(z)V\,|\vec{p}+\rangle\,, \quad z = E_{\vec{p}}+\mathrm{i}\epsilon$$
$$= |\vec{p}\rangle + G^0(z)V\,|\vec{p}\rangle + G^0(z)VG^0(z)V\,|\vec{p}\rangle + \ldots \tag{8.206}$$

So, the Born approximation is just $|\vec{p}+\rangle = |\vec{p}\rangle$. Then,

$$-\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3x'\,\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}V(\vec{x}')\,\langle\vec{x}'|\vec{p}+\rangle \xrightarrow[r\to\infty]{} -\frac{m}{2\pi\hbar^2}(2\pi\hbar)^{3/2}\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{r}\,\langle p\hat{x}|\,V\,|\vec{p}\rangle$$
$$= \frac{1}{(2\pi\hbar)^{3/2}}\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{r}f(p\hat{x}\leftarrow\vec{p}) \tag{8.207}$$

where we have used the definition of the scattering amplitude in the Born approximation:

$$f(\vec{p}'\leftarrow\vec{p}) = -(2\pi)^2\hbar m\,\langle\vec{p}'|\,V\,|\vec{p}\rangle\,. \tag{8.208}$$

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Therefore, we conclude that

$$\langle \vec{x}|\vec{p}\pm\rangle = \langle \vec{x}|\vec{p}\rangle + \int \mathrm{d}x'\ \langle \vec{x}|\, G^0(E_{\vec{p}}\pm \mathrm{i}\epsilon)\,|\vec{x}'\rangle\, V(\vec{x}')\,\langle \vec{x}'|\vec{p}\pm\rangle$$
$$\xrightarrow[r\to\infty]{} \langle \vec{x}|\vec{p}\rangle + \frac{1}{(2\pi\hbar)^{3/2}}\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{r} f(p\hat{x}\leftarrow\vec{p}). \tag{8.209}$$

Namely:

$$\boxed{\langle \vec{x}|\vec{p}+\rangle \xrightarrow[r\to\infty]{} \frac{1}{(2\pi\hbar)^{3/2}}\left[\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}} + f(p\hat{x}\leftarrow\vec{p})\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{r}\right]} \tag{8.210}$$

This is an important result: the improper scattering state $|\vec{p}+\rangle$ includes the incident plane wave plus a spherical outgoing wave modulated by the scattering amplitude $f(p\hat{x}\leftarrow\vec{p})$.

The effect of the scattering is more transparent in terms of partial waves. Remember that in spherical coordinates:

$$f(\vec{p}'\leftarrow\vec{p}) = \frac{\hbar}{2\mathrm{i}p}\sum_{\ell=0}^{\infty}(2\ell+1)[\mathrm{e}^{2\mathrm{i}\delta_\ell(E_{\vec{p}})}-1]P_\ell(\cos\theta)$$
$$= \sum_{\ell=0}^{\infty}(\ell+\tfrac{1}{2})\frac{\mathrm{e}^{2\mathrm{i}\delta_\ell(E_{\vec{p}})}-1}{\frac{\mathrm{i}}{\hbar}p}P_\ell(\cos\theta) \tag{8.211}$$

and the expansion of the plane wave at large distances in spherical waves is:

$$\frac{1}{(2\pi\hbar)^{3/2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}} \xrightarrow[r\to\infty]{} \frac{1}{(2\pi\hbar)^{3/2}}\sum_{\ell=0}^{\infty}(\ell+\tfrac{1}{2})\left[\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr} + (-1)^{\ell+1}\frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr}\right]P_\ell(\hat{p}\cdot\hat{x}). \tag{8.212}$$

For $\vec{p}' = p\hat{x}$ we have $\cos\theta = \hat{p}\cdot\hat{p}' = \hat{p}\cdot\hat{x}$ and $\langle\vec{x}|\vec{p}+\rangle$ can be written as:

$$\boxed{\langle \vec{x}|\vec{p}+\rangle \xrightarrow[r\to\infty]{} \frac{1}{(2\pi\hbar)^{3/2}}\sum_{\ell=0}^{\infty}(\ell+\tfrac{1}{2})\left[\mathrm{e}^{2\mathrm{i}\delta_\ell(E_{\vec{p}})}\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr} + (-1)^{\ell+1}\frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr}\right]P_\ell(\cos\theta)} \tag{8.213}$$

So the scattering modifies each outgoing spherical wave by a phase-shift factor $\mathrm{e}^{2\mathrm{i}\delta_\ell}$.

Now we have the ingredients of the time-independent scattering theory. We need to find the stationary wave functions, eigenfunctions of $H = H^0 + V$ with eigenvalue $E_{\vec{p}} = \frac{p^2}{2m}$. They are the solutions of the Schrödinger equation for a given potential. Taking the appropriate asymptotic limits one can extract the phase shifts.

But before doing that, let us study the **validity of the Born approximation**. We have seen that it consists on replacing $\langle\vec{x}|\vec{p}+\rangle$ by $\langle\vec{x}|\vec{p}\rangle$ in the right hand side of

$$\langle \vec{x}|\vec{p}+\rangle = \langle \vec{x}|\vec{p}\rangle - \frac{m}{2\pi\hbar^2}\int \mathrm{d}^3x'\,\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}V(\vec{x}')\,\langle\vec{x}'|\vec{p}+\rangle\,. \tag{8.214}$$

The difference between these two wave functions will be larger within the interaction region, $|\vec{x}|\lesssim a$. Since usually the potential is largest at the origin, we can obtain a criterion for the goodness of the approximation by imposing that at $\vec{x}=0$ the second term is small with respect to the first one:

$$\frac{m}{2\pi\hbar^2}\left|\int \mathrm{d}^3x'\,\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr'}}{r'}V(\vec{x}')\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x}'}\right| \ll 1. \tag{8.215}$$

For a central potential, after doing the angular integration, the condition becomes:

$$\frac{m}{\hbar p}\left|\int_0^\infty \mathrm{d}r'\,V(r')\left(1-\mathrm{e}^{2\frac{\mathrm{i}}{\hbar}pr'}-1\right)\right| \ll 1. \tag{8.216}$$

Finally, let us calculate the **phase shifts from the Schrödinger equation** for a central potential by finding the (improper) stationary solutions of

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(\vec{x}) = E\psi(\vec{x}) \tag{8.217}$$

The solutions are spherical waves that can be written as

$$\langle \vec{x}|E\ell m+\rangle = A_\ell(r)Y_\ell^m(\hat{x}), \quad A_\ell(r) \equiv \frac{y_\ell(r)}{r} \tag{8.218}$$

where the radial part satisfies the differential equation:

$$\begin{aligned} -\frac{\hbar^2}{2m}\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\ell(\ell+1)}{r^2} - \frac{2m}{\hbar^2}V(r)\right]A_\ell(r) &= \frac{p^2}{2m}A_\ell(r) \\ \Rightarrow \quad \left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\ell(\ell+1)}{r^2} + \frac{p^2}{\hbar^2} - \frac{2m}{\hbar^2}V(r)\right]y_\ell(r) &= 0. \end{aligned} \tag{8.219}$$

We have seen that if there was no interaction, $V(r) = 0$, the general solution compatible with $A_\ell(r)$ being regular at the origin would be

$$V(r) = 0 \quad \forall r: \qquad A_\ell^0(r) = \frac{\mathrm{i}^\ell}{\hbar}\sqrt{\frac{2mp}{\pi\hbar}}\, j_\ell(\tfrac{pr}{\hbar}) \tag{8.220}$$

that gives the normalized state $\langle \vec{x}|E\ell m\rangle$.

If there is interaction by a potential with a finite range a, the general solution for $r > a$, where $V(r) = 0$, is

$$V(r) = 0 \quad \text{for } r > a: \qquad A_\ell(r) = \frac{y_\ell(r)}{r} = \frac{\mathrm{i}^\ell}{\hbar}\sqrt{\frac{2mp}{\pi\hbar}}\left[c_\ell^{(1)}h_\ell^{(1)}(\tfrac{pr}{\hbar}) + c_\ell^{(2)}h_\ell^{(2)}(\tfrac{pr}{\hbar})\right] \tag{8.221}$$

where $h^{(1)}(x)$ and $h^{(2)}(x)$ are the spherical Hanckel functions of the first and the second kind, respectively, that are combinations of the spherical Bessel and Neumann functions:

$$h_\ell^{(1)}(x) \equiv j_\ell(x) + \mathrm{i}n_\ell(x) \xrightarrow[x\to\infty]{} \frac{\mathrm{e}^{\mathrm{i}(x-\ell\frac{\pi}{2})}}{\mathrm{i}x} \tag{8.222}$$

$$h_\ell^{(2)}(x) \equiv j_\ell(x) - \mathrm{i}n_\ell(x) \xrightarrow[x\to\infty]{} -\frac{\mathrm{e}^{-\mathrm{i}(x-\ell\frac{\pi}{2})}}{\mathrm{i}x}. \tag{8.223}$$

It is convenient to introduce these combinations because then the coefficients are directly related to the phase shifts:

$$\begin{aligned} \langle \vec{x}|\vec{p}+\rangle &= \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\langle \vec{x}|E\ell m+\rangle\frac{1}{\sqrt{mp}}Y_\ell^{m*}(\hat{p}) \\ &= \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{\mathrm{i}^\ell}{\hbar}\sqrt{2}\pi\hbar\left[c_\ell^{(1)}h_\ell^{(1)}(\tfrac{pr}{\hbar}) + c_\ell^{(2)}h_\ell^{(2)}(\tfrac{pr}{\hbar})\right]Y_\ell^m(\hat{x})Y_\ell^{m*}(\hat{p}) \\ &= \frac{1}{(2\pi\hbar)^{3/2}}\sum_{\ell=0}^{\infty}(2\ell+1)\mathrm{i}^\ell\left[c_\ell^{(1)}h_\ell^{(1)}(\tfrac{pr}{\hbar}) + c_\ell^{(2)}h_\ell^{(2)}(\tfrac{pr}{\hbar})\right]P_\ell(\hat{p}\cdot\hat{x}) \\ &\xrightarrow[r\to\infty]{} \frac{1}{(2\pi\hbar)^{3/2}}\sum_{\ell=0}^{\infty}(2\ell+1)\left[c_\ell^{(1)}\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr} + (-1)^{\ell+1}c_\ell^{(2)}\frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr}\right]P_\ell(\cos\theta) \end{aligned} \tag{8.224}$$

to be compared with equation (8.213):

$$\langle \vec{x}|\vec{p}+\rangle \xrightarrow[r\to\infty]{} \frac{1}{(2\pi\hbar)^{3/2}}\sum_{\ell=0}^{\infty}(\ell+\tfrac{1}{2})\left[\mathrm{e}^{2\mathrm{i}\delta_\ell(E_{\vec{p}})}\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr} + (-1)^{\ell+1}\frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}pr}}{\frac{\mathrm{i}}{\hbar}pr}\right]P_\ell(\cos\theta). \tag{8.225}$$

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Therefore:

$$c_\ell^{(1)} = \tfrac{1}{2}\mathrm{e}^{2\mathrm{i}\delta_\ell}, \quad c_\ell^{(2)} = \tfrac{1}{2} \tag{8.226}$$

and hence

$$\begin{aligned} \text{for } r > a: \qquad A_\ell(r) = \frac{y_\ell(r)}{r} &= \frac{\mathrm{i}^\ell}{\hbar}\sqrt{\frac{2mp}{\pi\hbar}}\,\frac{1}{2}\left[\mathrm{e}^{2\mathrm{i}\delta_\ell} h_\ell^{(1)}(\tfrac{pr}{\hbar}) + h_\ell^{(2)}(\tfrac{pr}{\hbar})\right] \\ &= \frac{\mathrm{i}^\ell}{\hbar}\sqrt{\frac{2mp}{\pi\hbar}}\,\mathrm{e}^{\mathrm{i}\delta_\ell}\left[\frac{\mathrm{e}^{\mathrm{i}\delta_\ell}+\mathrm{e}^{-\mathrm{i}\delta_\ell}}{2} j_\ell(\tfrac{pr}{\hbar}) - \frac{\mathrm{e}^{\mathrm{i}\delta_\ell}-\mathrm{e}^{-\mathrm{i}\delta_\ell}}{2\mathrm{i}} n_\ell(\tfrac{pr}{\hbar})\right] \\ &= \frac{\mathrm{i}^\ell}{\hbar}\sqrt{\frac{2mp}{\pi\hbar}}\,\mathrm{e}^{\mathrm{i}\delta_\ell}[\cos\delta_\ell\, j_\ell(\tfrac{pr}{\hbar}) - \sin\delta_\ell\, n_\ell(\tfrac{pr}{\hbar})] \end{aligned} \tag{8.227}$$

and remember that

$$\text{for } r < a: \qquad y_\ell(r) \quad \text{satisfies} \quad \left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\ell(\ell+1)}{r^2} + \frac{p^2}{\hbar^2} - \frac{2m}{\hbar^2}V(r)\right] y_\ell(r) = 0. \tag{8.228}$$

Both radial functions must coincide at $r = a$. This way we have a **method to find the phase shifts**: match the solutions for $y(r)$ out and inside the range of the potential just at $r = a$. It is convenient to *equate the logarithmic derivatives* to avoid the normalization of the solutions:

$$\left.\frac{1}{y_\ell(r)}\frac{\mathrm{d}y_\ell(r)}{\mathrm{d}r}(r=a)\right|_{\text{outside}} = \left.\frac{1}{y_\ell(r)}\frac{\mathrm{d}y_\ell(r)}{\mathrm{d}r}(r=a)\right|_{\text{inside}} \tag{8.229}$$

And if the potential has *infinite range* then it will only vanish at $r \to \infty$ and one has to match the log of the solution of the Schrödinger equation in that limit with

$$\lim_{r\to\infty}\frac{1}{y_\ell(r)}\frac{\mathrm{d}y_\ell(r)}{\mathrm{d}r} = \frac{p}{\hbar}\cot\left(\tfrac{pr}{\hbar} - \ell\tfrac{\pi}{2} + \delta_\ell\right) \tag{8.230}$$

since

$$A_\ell(r) = \frac{y_\ell(r)}{r} \propto \frac{1}{2}\left[\mathrm{e}^{2\mathrm{i}\delta_\ell} h_\ell^{(1)}(\tfrac{pr}{\hbar}) + h_\ell^{(2)}(\tfrac{pr}{\hbar})\right] \xrightarrow[r\to\infty]{} \frac{\mathrm{e}^{\mathrm{i}\delta_\ell}}{\frac{\mathrm{i}}{\hbar}pr}\sin\left(\tfrac{pr}{\hbar} - \ell\tfrac{\pi}{2} + \delta_\ell\right). \tag{8.231}$$

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