Notes on scattering theory

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1 Introduction

Quite unsurprisingly, scattering theory aims at describing scattering experiments. These experiments consist, in a nutshell, in taking bunches of free particles, throw them at each other or at some fixed target, and observe what happens. If we wait long enough, what generally happens is that one sees again (possibly different) free particles coming out of the collision. Free particles thus label the possible setups of the experiments, i.e., their initial states, and their possible outcomes, i.e., their final states. It is thus worth spending a few words on this concept.

Free particles Free particles are first of all an experimental concept. A free particle is something well localised in space that moves on a straight-line trajectory at constant speed. Its energy, E, and momentum, $\vec{p}$, are constant in time, and are related as follows:

$$E = \frac{\vec{p}^{\,2}}{2m} \quad \text{(non-relativistic case)}\,, \qquad E = \sqrt{\vec{p}^{\,2} + m^2} \quad \text{(relativistic case)}\,, \tag{1.1}$$

where m is a constant called the mass of the particle. There are other measurable quantities, like, e.g., spin, electric charge,..., which are also constants of motion for a free particle, and fully characterise the particle state. In particular, mass, spin and electric charge essentially identify a particle species. A free multiparticle state is observed when there are several localised objects travelling independently on straight lines. Notice that all the quantities mentioned above have a well-defined experimental meaning.

The concept of free particles is actually an idealised concept: experimentalists are well aware that in order to observe a free particle they have to reduce any possible external disturbance, and the more they are able to do so the more they observe something which satisfies our definition of a free particle. In the case of multiparticle states, this means in particular that the particles have to be localised far away from each other, in order to make their mutual interaction negligible. Summarising: free particles are defined by their behaviour in an idealised situation, which can never really be achieved, but can be approximated arbitrarily well. As experimental accuracy is always limited, this is of no practical consequence: since beyond some point it is impossible to detect any deviation from the ideal behaviour, the state observed is indistinguishable from a free particle state for all practical purposes.

Scattering experiments As we have briefly explained above, in a scattering experiment we prepare the system in a free particle state, let it evolve and finally look at it after a while. The initial state typically consists of two beams of particles, initially far away and moving towards each other; or of one such beam and some fixed target. Beams and targets are usually prepared in such a way that the particles within them are practically free, i.e., interacting only weakly

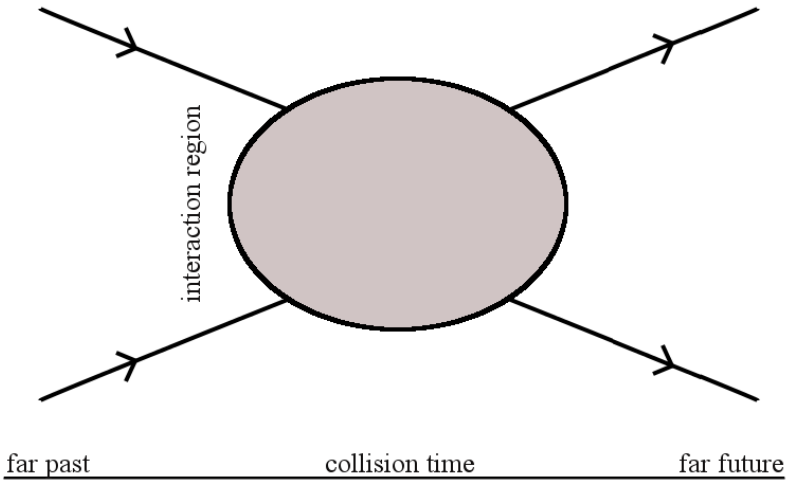

Figure 1: Schematic depiction of a scattering process.

with each other, due to the typically large inter-particle distance;[1] and that only one particle in one beam interacts with only one particle in the other beam or in the target. For practical purposes one can use a simplified description of the initial state, with two free particles initially far away and moving towards each other.

After having let evolve the system for some time, observations are made with detectors located sufficiently far away from the initial (classical) trajectories. What is observed is again a free particle state, different from the initial one.[2] Indeed, if detectors are placed sufficiently far away from the initial trajectories, then the particles in the final state are observed far apart from each other, and behave like free particles. How do we describe in words what has happened? Initially the system consists of two free particles, far enough not to feel each other: we say that they are outside of the interaction region, and the system evolves essentially freely. When we observe again the system after a sufficiently long time, we see it evolving freely but in a different state, and so something must have happened in the meantime, with interactions taking place and changing the state of the system. We can therefore define qualitatively three stages of the scattering process: an initial stage, usually called the "past", where the system is in a specified state and evolving freely; an intermediate stage, where the evolution is not free anymore due to the interactions between the two initial particles, which we call "collision time"; and a final stage, called the "future", where the system evolves freely again, albeit typically in a different state. The experiment is set up in the "far past", when one prepares two well-separated particle

[1] Taken at face value, this statement is obviously wrong for particles in the target, since this is usually a piece of some solid material. However, the typical crystal and electronic binding energies are much smaller than the typical energy of particles in the beam, and can therefore be neglected.

[2] The case of the final state being equal to the initial state is of course a possibility, but one that cannot be observed directly. Furthermore, one cannot of course distinguish the case of no scattering from that of scattering leading to the same state. To observe what is called forward elastic scattering one needs to extrapolate from the near-forward direction.

states; measurements are made in the "far future", when the system appears again as a collection of well-separated particles if we look at it. "Collision time" corresponds to the particles being in the interaction region, i.e., feeling the presence of each other: of course here we are speaking loosely, since we cannot even make sense of the concept of particles when they are interacting.

It is a fact that the time passing between the setup of the experiment and the moment when interactions cannot be neglected anymore, and similarly the time between the moment when interactions are negligible again and the measurements, are much larger than the duration of collision time.[3] There should therefore be no problem in considering the far past as $t = -\infty$, and the far future as $t = +\infty$.

Theoretical description of scattering The work of theorists (in between coffees) is to set up an appropriate mathematical description of the experimental findings. Since all we know about the scattering system are the free particle states corresponding to the initial and final states of the collision process, there is no point in trying to account for its detailed (and also experimentally inaccessible) time evolution. What we would rather do is to predict the probability that given a certain initial free-particle state, we will observe a prescribed final free-particle state.

The first step of our program consists in finding how to describe the states of a scattering system. In general, the states of a system are associated to vectors (or rather rays) in a Hilbert space. In quantum mechanics (QM), the appropriate Hilbert space is the tensor product of $L^2(\mathbb{R}^3)$ spaces, one for each particle involved, times possibly internal spaces to account for spin degrees of freedom.[4]

The second step consists in finding the appropriate dynamics governing the time evolution of the system. In both cases, this must be such that certain states of the system, when looked at in the far past or in the far future, look like free-particle states - as it happens in experiments. Of course, a description in terms of freely evolving states only would be insufficient, for there would be no scattering at all.

Finally, we need a way to relate the experimentally accessible information about the initial and final states, which is associated to freely evolving states, to the exact states of the system, i.e., those evolving according to the full (interacting) dynamics. This is accomplished by the so-called formal theory of scattering. Having done this, we can compute all the desired probabilities.

Outline of the course After this brief introduction, here is the outline of the course. We will mainly discuss the non-relativistic case, but the relativistic generalisation of certain results will also be presented. In Section 2 we describe in detail the most common types of scattering experiments, and we introduce the main observable, i.e., the cross section. In Section 3 we briefly review some useful results of Quantum Mechanics. In Section 4 we discuss the formal theory of scattering in the time-dependent formalism, introducing the S-matrix and relating it to the experimentally measurable cross sections. We also discuss the consequences of unitarity and of symmetries. In Section 5 we introduce the time-independent formalism, relating the scattering amplitudes to the asymptotic behaviour of the positive-energy solutions of the Schrödinger equation. In Section 6 we discuss in more detail the case of central potentials. Finally, in Section 7 we discuss the analiticity properties of the S-matrix.

[3] In the worst case collision time lasts around $10^{-10}s$, which is much less than the overall time scale of the typical experiment.

[4] In quantum field theory (QFT) the situation is more complicated; however, we know how to properly describe free particle states in terms of vectors in the so-called Fock space.

The main reference for the course is the excellent book by J. R. Taylor [Taylor], on which the course itself is based. Further references for some specific mathematical results are also included.

2 Scattering experiments and cross sections

Typical scattering experiments are of two types: fixed target experiments and collider experiments. In this section we describe them, and introduce the central observable quantity, i.e., the cross section. Before doing that, we briefly describe the classification of scattering processes.

Usually, the initial state of a scattering process consists of two particles directed towards each other. If an interaction takes place, changing the initial state, we say that the particles have been scattered. After the collision, one might observe that the final state contains the same two particles as the initial state, although moving now with different velocities. In this case one speaks of an elastic scattering process. Otherwise, the final state might consist of a (partially or totally) different set of particles: in this case one speaks of an inelastic scattering process. One can further refine the classification of inelastic scattering processes, and distinguish between particle production processes (the final state contains the same particles of the initial state and some more), ionisation processes, excitation processes, and so on. In general, a process is denoted as

$$a + b \longrightarrow c + d + \dots \,, \tag{2.1}$$

where a, b, etc., correspond to the various particles. For an elastic process we thus have

$$a + b \longrightarrow a + b \,, \tag{2.2}$$

while, for example, for a particle production process we have

$$a + b \longrightarrow a + b + X \,, \tag{2.3}$$

where X stands for all the remaining particles in the final state.

2.1 Fixed target experiments

In a fixed target experiment, a beam of particles (projectiles) is accelerated and directed to a sample of some material (the target) at rest in the laboratory. The target is usually a thin layer of material, in order to avoid multiple scatterings from its constituents (scatterers). The beam has to be sufficiently collimated, but not too much in order to avoid interactions among the particles. The target has usually a flat surface and the beam is directed onto it perpendicularly. Detectors are placed sufficiently far from the target to observe the final products of the process.

In a typical experiment the targets are "dilute", i.e., they have low surface density (number of scatterers in the target over the area of its surface): this requires that they be thin and with typical interatomic distance larger than the coherence length of the projectile (the size of the wave packet). In this setting, the projectile will then see at most one scatterer while traversing the target. In a typical experiment also the beams are "dilute", so that the projectiles do not interact with one another, and do not get close to the same scatterer at the same time. Under these conditions, scattering events will therefore be independent, involving only one particle from the target and one from the beam. The initial stage of the process can thus be described by a two-particle state. Moreover, the total number of events will be proportional to the number

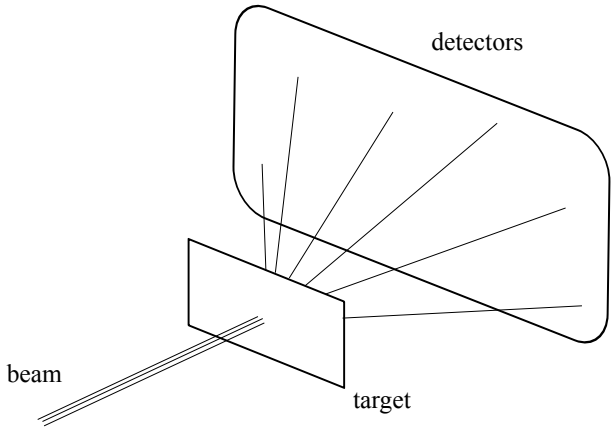

Figure 2: Setup of a fixed target experiment.

of particles in the beam, N_b, and to the number of scatterers in the target "under" the beam (in the full depth of the target), N_t.[5] For short-range interactions, a projectile from the beam will effectively "see" a scatterer from the target only if its trajectory happens to pass close enough to it. This identifies a small part of the surface of the target that the projectile has to "hit" in order to interact with the scatterer. The probability that a scattering event takes place involving a given projectile and a given scatterer will then be inversely proportional to the area of the cross-section of the beam, A, since $1/A$ is the probability density for that projectile to be near the point where that scatterer is.

We thus have that the number of scattering events, N_s, can be written as

$$N_s = \sigma \frac{N_b N_t}{A} \,, \tag{2.4}$$

with σ a proportionality constant with dimensions of an area. From the discussion above, it is clear that σ plays the role of the effective area of a scatterer as seen by the projectile. Indeed, classically, a particle in the beam is scattered if it hits that fraction of the surface of the target which is actually filled by the scatterers, so that $N_s = N_b \frac{A_{\rm eff}}{A}$. The area $A_{\rm eff}$ of this surface is N_t times that corresponding to a single scatterer, and rearranging Eq. (2.4) one easily identifies $A_{\rm eff} = \sigma N_t$, i.e., σ can be interpreted as the effective area of a scatterer. This quantity is called total cross section of the process. In general, it will depend not only on the type of scatterer, but also on the type of beam: it is an effective area which depends on the type of particles involved and on their mutual interaction. The commonly used unit for cross sections is the barn (b), which corresponds to $1\text{b} = 10^{-24}\text{cm}$. The phenomenological definition of total cross section given above can be equivalently recast as

$$\sigma = \frac{N_s}{N_b \frac{N_t}{A}} = \frac{N_s}{\Phi \Delta t N_t} \,, \tag{2.5}$$

where the flux $\Phi = N_b/(A\Delta t)$ is the number of particles in the beam impinging on the target per unit area and unit time. Thus, σ is the number of scattering events divided by the number

[5] The scatterers need not be on the surface, as the impinging particle might travel essentially undisturbed for some distance within the target before scoring a hit. One can then imagine the target as having effectively all its scatterers on the surface. N_t is thus the number of scatterers within the area illuminated by the beam and in the full depth of the target.

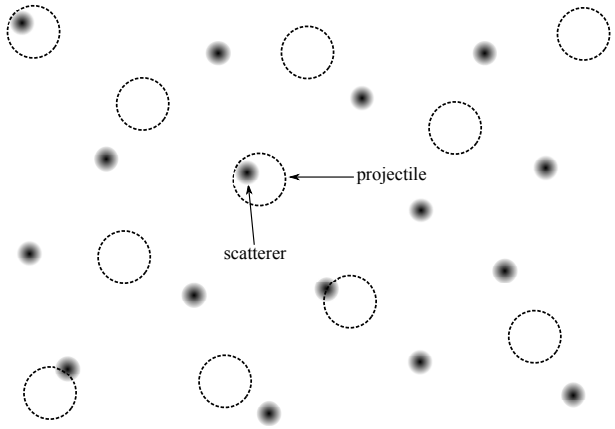

Figure 3: The target as seen from the beam.

of beam particles and by the surface density $\frac{N_t}{A}$ of the target, or equivalently the number of scattering events per unit flux, per unit time and per scatterer in the target. With one final rearrangement we write this as

$$\frac{N_s}{\Delta t} = \Phi N_t \sigma = \mathcal{L}\,\sigma\,, \tag{2.6}$$

so that the number of events per unit time is given by the cross section times the luminosity $\mathcal{L} = \Phi N_t$.

Usually, detectors are capable of more than just recording a scattering event, and they collect information about the energy, speed, direction, etc., of the outgoing particles. The scattering events can then be grouped into bins according to, e.g., the momenta of the final particles. The number of events corresponding to a prescribed choice of momenta will again be proportional to $\frac{N_b N_t}{A}$ since each scattering event is independent from the others. The proportionality constant is the differential cross section,

$$d\sigma = \frac{dN_s(\xi)}{\frac{N_b N_t}{A}} = \frac{dN_s}{d\xi\,\frac{N_b N_t}{A}} d\xi \Rightarrow \frac{d\sigma}{d\xi} = \frac{dN_s}{d\xi\,\frac{N_b N_t}{A}} = \frac{dN_s}{d\xi\,\Phi \Delta t N_t}\,. \tag{2.7}$$

Here ξ denotes collectively the momenta of the particles in the final state, and $dN_s(\xi) = \frac{dN_s}{d\xi} d\xi$ is the number of events with momenta in an infinitesimal range $d\xi$ about the desired value.

2.2 Collider experiments

In a collider experiment, two beams of particles are accelerated and directed against each other. If the beams are sufficiently diluted, both in the longitudinal and transverse directions (with respect to the beam trajectory), then interactions will involve at most one particle from each beam. Reasoning as in the case of a fixed target experiment, we see that the number of scattering events will be

$$N_s = \sigma \frac{N_{b_1} N_{b_2}}{A}\,, \tag{2.8}$$

where $N_{b1,2}$ are the number of particles in each beam and A the area of their cross sections (taken equal for simplicity). The proportionality constant is again the total cross section of the process.

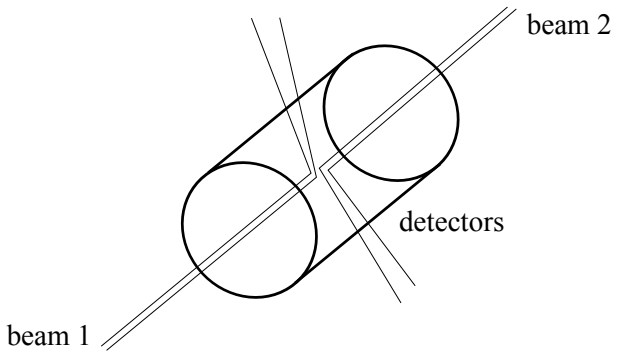

Figure 4: Setup of a collider experiment.

In a typical experiment at a circular collider, the beams are constituted by two groups of $N_{B1,2}$ bunches of $N_{b1,2}$ particles, respectively, travelling on a circular trajectory in opposite directions. Interactions take place at each bunch crossing; since two bunches cross twice as they complete an orbit in the period T, the number of events per second is given by

$$\frac{dN_s}{dt} = \frac{2N_{B1}N_{B2}}{T}\frac{N_{b_1}N_{b_2}}{A}\sigma = \mathcal{L}\sigma\,, \tag{2.9}$$

where we have not taken into account the loss of particles from the beams due to scattering. Here $\mathcal{L}$ is again the luminosity. More precisely, $\mathcal{L}$ is the istantaneous luminosity, while the integrated luminosity, as its name suggests, is the integral of $\mathcal{L}$ over time (this applies to fixed target experiments as well).

2.3 Cross section and boosts

One might wonder if the σ appearing in Eq. (2.4) and that in Eq. (2.8) are the same. To answer this question, notice that going over to the rest frame of, say, beam 2, the process looks exactly like a fixed target experiment, with beam 2 acting as the target. In doing so, the number of recorded events, as well as the number of particles in the beams, will obviously not change. As for the area of the cross-section of the beam, it will not change either, as it is orthogonal to the relative velocity of the two frames, and is therefore unaffected by the change of reference frame, both in the non-relativistic and in the relativistic cases.[6] As a consequence, σ is the same, independently of the type of experiment.

The reference frame in which one of the initial particles is at rest is called the laboratory (lab) frame, and is the most convenient for the description of fixed target experiments. The frame in which the total (spatial) momentum is zero is the center of mass (CM) frame, and collider experiments are usually carried in such a way that the center of mass frame coincides with the experimental facility.

Differently from total cross sections, differential cross sections will change when changing reference frame. Consider the same scattering experiment observed in the lab and in the CM frame. Let $dN_s^{\rm lab}(\xi^{\rm lab}, d\xi^{\rm lab})$ be the number of recorded events that in the lab frame have momenta in an interval $d\xi^{\rm lab}$ around $\xi^{\rm lab}$. In the CM frame, those same events will appear

[6] For more general reference frame transformations, σ will remain invariant provided A is taken to be the area of the cross section of the beams orthogonal to the relative direction of motion.

to have momenta in an interval $d\xi^{\rm CM}$ around $\xi^{\rm CM}$, related to that in the lab frame by known transformation laws. Therefore,

$$dN_s^{\rm lab}(\xi^{\rm lab}, d\xi^{\rm lab}) = dN_s^{\rm CM}(\xi^{\rm CM}, d\xi^{\rm CM}) \tag{2.10}$$

and one concludes

$$\left(\frac{d\sigma}{d\xi}\right)^{\rm lab} = \left(\frac{d\sigma}{d\xi}\right)^{\rm CM} \frac{d\xi^{\rm CM}}{d\xi^{\rm lab}}\,. \tag{2.11}$$

At high energy an accurate description of scattering processes requires the use of special relativity. It is therefore worth writing down the definition of cross section in a manifestly Lorentz-invariant way. To do so, consider the process in the lab frame and notice that the flux Φ of the beam can be written as $\Phi = \rho_1 v$ where ρ_1 is the (volume) density of the beam and v its velocity, and that $N_t = \rho_2 V$ with ρ_2 the density of the target or of the other beam, and V its volume.[7] We have therefore

$$\sigma = \frac{N_s}{\Phi \Delta t N_t} = \frac{N_s}{\Delta t\, V \rho_1 \rho_2 v}\,. \tag{2.12}$$

In this expression, N_s and $\Delta t\, V$ are relativistic invariants. As for ρ_i, they have to transform like an energy,[8] and therefore $\rho_i = \rho_i^0 \frac{p_i^0}{m_i}$, with ρ_i^0 being the density in the corresponding rest frame, p_i^0 the energy of a particle in the system (beam/target) labelled by i, and m_i the corresponding mass. Moreover, $v = \frac{|\vec{p}_1|}{p_1^0}$. In the lab frame $p_2^0 = m_2$, and so

$$\sigma = \frac{N_s}{\Delta t\, V \rho_1^0 \rho_2^0 \frac{|\vec{p}_1| m_2}{m_1 m_2}}\,. \tag{2.13}$$

The last step is finding the relativistically invariant expression for $I = |\vec{p}_1| m_2$. One can verify that in the lab frame, where $P_1 = (E^{\rm lab}, \vec{p}^{\,\rm lab})$ and $P_2 = (m_2, 0)$, one has

$$(P_1 \cdot P_2)^2 - P_1^2 P_2^2 = (E^{\rm lab} m_2)^2 - m_1^2 m_2^2 = I^2\,. \tag{2.14}$$

In the CM frame, where $P_1 = (E_1^{\rm CM}, \vec{p}^{\,\rm CM})$ and $P_2 = (E_2^{\rm CM}, -\vec{p}^{\,\rm CM})$ one thus finds (choosing for simplicity the momentum along direction 1)

$$\begin{aligned} I^2 &= \frac{1}{2}\varepsilon_{\mu\nu\alpha\beta}\varepsilon^{\mu\nu}{}_{\gamma\delta} P_1^\alpha P_2^\beta P_1^\gamma P_2^\delta = (\varepsilon_{23\alpha\beta} P_1^\alpha P_2^\beta)^2 = [(E_1^{\rm CM} + E_2^{\rm CM}) p^{\rm CM}]^2 \\ &= (E^{\rm CM} p^{\rm CM})^2\,. \end{aligned} \tag{2.15}$$

3 Review of Quantum Mechanics

Before embarking in the development of the formal theory of scattering in QM, it is worth collecting and reviewing a few useful results.

3.1 Abstract Hilbert spaces

In quantum mechanics the states of a system are associated with vectors $|\psi\rangle$ in an abstract separable Hilbert space $\mathcal{H}$, and observables with linear operators in $\mathcal{H}$. Here we review some general notions about Hilbert spaces.

[7] For a fixed target, the volume is of that part of the sample illuminated by the beam.

[8] This is because ρ_i times a volume is the number of particles within a certain region, which is a relativistically invariant quantity.

Hilbert spaces A Hilbert space is a complex linear space endowed with a positive-definite scalar product, which is furthermore complete, in the sense explained below. A vector is denoted by $|\psi\rangle$; we will sometimes use the unconventional notation $|\alpha\psi+\beta\phi\rangle = \alpha|\psi\rangle + \beta|\phi\rangle$. We denote the scalar product of two vectors $|\psi\rangle$ and $|\phi\rangle$ as $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$, and the norm of a vector as $\|\psi\| \equiv \sqrt{\langle\psi|\psi\rangle}$. Notice that every element of $\mathcal{H}$ has a finite norm. Positive-definiteness means that $\langle\psi|\psi\rangle > 0$ if $|\psi\rangle \neq 0$, so $\langle\psi|\psi\rangle = 0$ if and only if $|\psi\rangle = 0$. We note in passing the useful Schwartz inequality, $|\langle\phi|\psi\rangle| \leq \|\phi\|\|\psi\|$, valid for any pair of vectors. A separable Hilbert space is one that possesses a countable orthonormal basis, i.e., it is such that each vector can be written uniquely as $|\psi\rangle = \sum_n c_n|e_n\rangle$ with countably many basis elements $|e_n\rangle$ satisfying $\langle e_n|e_m\rangle = \delta_{nm}$. A sequence $\{|\psi_n\rangle\}$ of elements of $\mathcal{H}$ is said to be a Cauchy sequence if $\|\psi_n - \psi_m\| \to 0$ as $n, m \to \infty$. Completeness means that every Cauchy sequence $\{|\psi_n\rangle\}$ is convergent, i.e., $\lim_{n\to\infty}|\psi_n\rangle = |\psi\rangle$ for some $|\psi\rangle \in \mathcal{H}$. A Hilbert subspace $\mathcal{H}'$ is a subset $\mathcal{H}' \subseteq \mathcal{H}$ which is also a Hilbert space; in particular, completeness requires that any convergent sequence in $\mathcal{H}'$ must converge in $\mathcal{H}'$.

Linear operators Observables are associated with linear self-adjoint operators in $\mathcal{H}$. A linear operator A is such that for every $|\psi\rangle, |\phi\rangle \in \mathcal{D}(A) \subseteq \mathcal{H}$ and for every $\alpha, \beta \in \mathbb{C}$ one has $A(\alpha|\psi\rangle + \beta|\phi\rangle) = \alpha A|\psi\rangle + \beta A|\phi\rangle$. Also in this case we will sometimes use the unconventional notation $|A\psi\rangle = A|\psi\rangle$. The subset $\mathcal{D}(A)$ is called the domain of A, and need not coincide with the whole of $\mathcal{H}$, but we will always assume that it is a dense subset thereof, i.e., that for any $|\psi\rangle \in \mathcal{H}$ and any positive ϵ one can find $|\psi_\epsilon\rangle \in \mathcal{D}(A)$ so that $\|\psi - \psi_\epsilon\| < \epsilon$. The image of $\mathcal{D}(A)$ under A is called the range of A and is denoted as $\mathcal{R}(A)$. Let $\mathcal{D}^*(A)$ be the set of those $|\phi\rangle$ such that $\langle\phi|A\psi\rangle = \langle\eta_\phi|\psi\rangle$ for some $|\eta_\phi\rangle$ and for all $|\psi\rangle \in \mathcal{D}(A)$. The adjoint $A^\dagger$ of an operator is then defined on the domain $\mathcal{D}(A^\dagger) = \mathcal{D}^*(A)$ as $A^\dagger|\phi\rangle = |\eta_\phi\rangle$, and $\langle\phi|A\psi\rangle = \langle A^\dagger\phi|\psi\rangle = \langle\psi|A^\dagger\phi\rangle^*$. An operator is called Hermitian if $\langle\phi|A\psi\rangle = \langle A\phi|\psi\rangle$ for $|\psi\rangle, |\phi\rangle \in \mathcal{D}(A)$, and it is called self-adjoint if $\mathcal{D}(A) = \mathcal{D}(A^\dagger)$. For these operators we can use the notation $\langle\phi|A|\psi\rangle = \langle\phi|A\psi\rangle = \langle A\phi|\psi\rangle$ without any ambiguity. For general operators, we understand that $\langle\phi|A|\psi\rangle = \langle\phi|A\psi\rangle = \langle A^\dagger\phi|\psi\rangle$.

Self-adjoint operators admit a so-called spectral decomposition of the form

$$A = \sum_n a_n|a_n\rangle\langle a_n| + \int_{\sigma(A)} d\lambda\, \lambda\, |\lambda\rangle\langle\lambda|\,, \qquad a_n \in \mathbb{R}\,, \quad \sigma(A) \subseteq \mathbb{R}\,, \tag{3.1}$$

where $|a_n\rangle$ are the proper normalised eigenstates of A and a_n the corresponding (real) eigenvalues, $A|a_n\rangle = a_n|a_n\rangle$ with $\langle a_n|a_m\rangle = \delta_{nm}$, and $|\lambda\rangle$ are the improper eigenvectors of A, with $A|\lambda\rangle = \lambda|\lambda\rangle$ and $\langle\lambda'|\lambda\rangle = \delta(\lambda'-\lambda)$. The set $\{a_n\}$ forms the discrete spectrum of A, and the subset $\sigma(A)$ of the real line is the continuous spectrum of A. Moreover, the following completeness relation holds,

$$\mathbf{1} = \sum_n |a_n\rangle\langle a_n| + \int_{\sigma(A)} d\lambda\, |\lambda\rangle\langle\lambda|\,. \tag{3.2}$$

The improper eigenvectors $|\lambda\rangle$ are clearly not elements of $\mathcal{H}$, and their rigorous treatment is way beyond the scope of these lectures. For our purposes, it suffices to say that they are well-defined objects such that the "scalar product" (technically, the linear functional) $\langle\lambda|\psi\rangle$ is well defined in (a dense subset of) $\mathcal{H}$, yielding a well defined complex number, and such that $\langle\lambda|A|\psi\rangle = \lambda\langle\lambda|\psi\rangle$. One has also that $\langle\psi|\lambda\rangle = \langle\lambda|\psi\rangle^*$.

There are other important classes of operators. An operator $A : \mathcal{D}(A) \to \mathcal{S} \subseteq \mathcal{H}$ is said to be onto $\mathcal{S}$ if every element of $\mathcal{S}$ is the image of an element of $\mathcal{D}(A)$. In particular, A is onto its image

$\mathcal{R}(A)$. An operator A is said to be one-to-one if $|\psi\rangle \neq |\phi\rangle \Rightarrow A|\psi\rangle \neq A|\phi\rangle$. Since A is linear, this is equivalent to $A|\psi\rangle = 0 \Leftrightarrow |\psi\rangle = 0$. In this case every element $|\chi\rangle \in \mathcal{R}(A)$ is associated to a unique element $|\psi_\chi\rangle \in \mathcal{D}(A)$, and so we can define the inverse operator $A^{-1} : \mathcal{R}(A) \to \mathcal{D}(A)$, which is onto $\mathcal{D}(A)$ and satisfies $A^{-1}A = \mathbf{1}_{\mathcal{D}(A)}$ and $AA^{-1} = \mathbf{1}_{\mathcal{R}(A)}$. Finally, a norm-preserving operator is one satisfying $\|A\psi\| = \|\psi\|$. A norm-preserving operator is automatically one-to-one, thus invertible on its range. We can now define two important classes of operators:

- a linear operator Ω is isometric if it is norm-preserving and defined on the whole of $\mathcal{H}$, i.e., $\mathcal{D}(\Omega) = \mathcal{H}$ and $\|\Omega\psi\| = \|\psi\|$;
- a linear operator U is unitary if it is norm-preserving, defined on the whole of $\mathcal{H}$, and onto $\mathcal{H}$.

A unitary operator is obviously isometric, but in general the converse is not true.[9] We will return on these kinds of operators as they play an immportant role in the formal theory of scattering.

Temporal evolution The temporal evolution of the system (in the Schrödinger representation) is described by assigning the state vector $|\psi(t)\rangle$ to the system at time t, and treating the observables as time-independent. The dynamics governing the evolution of the system is determined by the Schrödinger equation,

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle\,, \tag{3.3}$$

where $\hat{H}$ is the Hamiltonian of the system. This is a self-adjoint operator in $\mathcal{H}$. The formal solution of Eq. (3.3) is

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle\,, \qquad U(t) \equiv e^{-i\hat{H}t}\,. \tag{3.4}$$

A theorem in functional analysis (Stone's theorem) guarantees that the exponential of a self-adjoint operator is unitary (see [Reed & Simon], vol. 1, §VIII.4), and so the temporal evolution $U(t)$ is unitary.

3.2 Systems of free particles

For practical calculations one needs a concrete (as opposed to abstract) realisation of the Hilbert space of the states of the system. These realisations constitute the representations of the abstract Hilbert space associated to the system, and of course they depend on which physical system is under consideration. For a single (spinless) free particle, the state of the system in the so-called coordinate representation is described by a wavefunction $\psi(\vec{x}) \in L^2(\mathbb{R}^3)$, assigned at some definite time, which we take to be $t = 0$. The space $L^2(\mathbb{R}^3)$ is the complex linear space formed by (Lebesgue) square-integrable functions $\psi(\vec{x})$, i.e., $\int d^3x\,|\psi(\vec{x})|^2 < \infty$.[10] Endowing it with the scalar product $(\phi, \psi) = \int d^3x\,\phi^*(\vec{x})\psi(\vec{x})$ makes it into a separable Hilbert space (Riesz-Fischer theorem, see [Reed & Simon], vol. 1, chapter II, or [Riesz & Nagy], pag. 59). In this space of functions one can construct a concrete representation of the algebra of canonical

[9] It is true for finite-dimensional spaces.

[10] Elements of L^2 are actually equivalence classes of functions differing only on a set of zero measure, but our sloppier definition will suffice for our purposes.

commutation relations $[\hat{q}_j, \hat{p}_k] = i\delta_{jk}$, $[\hat{q}_j, \hat{q}_k] = [\hat{p}_j, \hat{p}_k] = 0$, where $\hat{q}_j$ and $\hat{p}_k$ are the (abstract) position and momentum operators, respectively. This representation is obtained through

$$\begin{aligned} (\hat{q}_j\psi)(\vec{x}) &= x_j\psi(\vec{x})\,, \\ (\hat{p}_k\psi)(\vec{x}) &= -i\frac{\partial}{\partial x_k}\psi(\vec{x})\,, \end{aligned} \tag{3.5}$$

i.e., $\hat{q}_j = x_j$ and $\hat{p}_k = -i\frac{\partial}{\partial x_j}$ in this representation. The temporal evolution of the wavefunction is governed by the free Schrödinger equation, which reads $i\partial_t|\psi(t)\rangle = \hat{H}_0|\psi(t)\rangle$ in abstract notation, with $\hat{H}_0$ the free Hamiltonian,

$$\hat{H}_0 = \frac{\vec{\hat{p}}^{\,2}}{2m}\,, \tag{3.6}$$

where m is the mass of the particle. The formal solution of the free Schrödinger equation is

$$|\psi(t)\rangle = U_0(t)|\psi\rangle\,, \quad U_0(t) \equiv e^{-i\hat{H}_0 t}\,, \tag{3.7}$$

where $|\psi\rangle = |\psi(0)\rangle$, and $U_0(t)$ is unitary. In the coordinate representation

$$i\frac{\partial}{\partial t}\psi(t,\vec{x}) = -\frac{\Delta}{2m}\psi(t,\vec{x})\,, \tag{3.8}$$

with $\psi(0,\vec{x}) = \psi(\vec{x})$ corresponding to the state at time $t = 0$. Wavefunctions are usually normalised to 1, $\int d^3x\,|\psi(\vec{x})|^2 = 1$, and the normalisation is preserved by the unitary temporal evolution. The physical interpretation of the wavefunction is that $dp(t,\vec{x}) = |\psi(t,\vec{x})|^2 d^3x$ is the probability of observing the particle at time t in an infinitesimal neighbourhood of $\vec{x}$; the normalisation guarantees that the probability to find the particle anywhere is just 1.

Analogously, one can construct the momentum representation, where the state of the particle (at $t = 0$) is described by the function $\tilde{\psi}(\vec{k}) \in L^2(\mathbb{R}^3)$. In this representation the momentum operators act multiplicatively and the position operators act as derivatives,

$$\begin{aligned} (\hat{p}_j\tilde{\psi})(\vec{k}) &= k_j\tilde{\psi}(\vec{k})\,, \\ (\hat{q}_k\tilde{\psi})(\vec{k}) &= i\frac{\partial}{\partial k_k}\tilde{\psi}(\vec{k})\,; \end{aligned} \tag{3.9}$$

the free Hamiltonian is therefore diagonal and $\tilde{\psi}(t,\vec{k}) = (e^{-i\hat{H}_0 t}\tilde{\psi})(\vec{k}) = e^{-iE_k t}\tilde{\psi}(\vec{k})$, where $E_k = \frac{\vec{k}^{\,2}}{2m}$. The momentum wavefunction is usually normalised as $\int d_3k\,|\tilde{\psi}(\vec{k})|^2 = 1$, where we have introduced the notation $d_3k = \frac{d^3k}{(2\pi)^3}$. The probability $d\tilde{p}(t,\vec{k}) = |\tilde{\psi}(t,\vec{k})|^2 d_3k = |\tilde{\psi}(\vec{k})|^2 d_3k$ to find the particle in the interval d^3k around momentum $\vec{k}$ is independent of time.

An easy way to connect the abstract and the concrete Hilbert space, and to connect the coordinate and the momentum representations, is provided by the (improper) eigenstates of the position and momentum operators, $\vec{\hat{q}}\,|\vec{x}\rangle = \vec{x}|\vec{x}\rangle$ and $\vec{\hat{p}}\,|\vec{k}\,\rangle = \vec{k}\,|\vec{k}\,\rangle$. These states satisfy the normalisation conditions

$$\langle\vec{x}\,'|\vec{x}\rangle = \delta^{(3)}(\vec{x}\,' - \vec{x})\,, \qquad \langle\vec{k}\,'|\vec{k}\,\rangle = (2\pi)^3\delta^{(3)}(\vec{k}\,' - \vec{k}\,)\,, \tag{3.10}$$

and the completeness relations

$$\mathbf{1} = \int d^3x\,|\vec{x}\rangle\langle\vec{x}| = \int d_3k\,|\vec{k}\,\rangle\langle\vec{k}\,|\,. \tag{3.11}$$

The coordinate representation of the state $|\psi\rangle$ is obtained by projecting it on the coordinate eigenstates,

$$\psi(\vec{x}) = \langle \vec{x}|\psi\rangle \,. \tag{3.12}$$

Analogously, the momentum representation of the state $|\psi\rangle$ is obtained by projecting it on the momentum eigenstates,

$$\tilde{\psi}(\vec{k}) = \langle \vec{k}\,|\psi\rangle \,. \tag{3.13}$$

With our choice of normalisation, the momentum eigenstates in the coordinate basis read

$$\langle \vec{x}|\vec{k}\,\rangle = e^{i\vec{k}\cdot\vec{x}} \,. \tag{3.14}$$

This expression allows to connect the coordinate and momentum representations, the link being simply the Fourier transform:

$$\psi(\vec{x}) = \langle \vec{x}|\psi\rangle = \int d_3k\, \langle \vec{x}|\vec{k}\,\rangle\langle \vec{k}\,|\psi\rangle = \int d_3k\, e^{i\vec{k}\cdot\vec{x}}\, \tilde{\psi}(\vec{k}) \,. \tag{3.15}$$

As already mentioned in our general discussion, it is evident from Eq. (3.10) that the improper vectors $|\vec{x}\rangle$ and $|\vec{k}\,\rangle$ are not elements of $\mathcal{H}$, and a rigorous treatment of these objects would lead us too far. For practical purposes, they are just objects whose (formal) scalar product with a proper abstract vector yields the corresponding representative in the desired representation.

The generalisation to several free particles is immediate. Denoting with $\mathcal{H}_a$ the one-particle Hilbert space of particle a, we have that the full Hilbert space is simply the tensor product $\mathcal{H} = \otimes_{a=1}^{N}\mathcal{H}_a$, and the N-particle free Hamiltonian is just

$$H_0^{(N)} = \sum_{a=1}^{N} \frac{\vec{\hat{p}}^{\,2}_{(a)}}{2m_a} \,, \tag{3.16}$$

with $\vec{\hat{p}}_{(a)}$ the momentum operator of particle a and m_a its mass. Coordinate operators $\vec{\hat{q}}_{(a)}$ are also defined, and the canonical commutation relations are extended to $[\hat{q}_{(a)\,j}, \hat{p}_{(b)\,k}] = i\delta_{ab}\delta_{jk}$ (all other commutators being zero). The concrete representation of the system (for spinless particles) is provided by the space[11] $L^2_N = \otimes_{a=1}^{N} L^2(\mathbb{R}^3_a)$, with $L^2(\mathbb{R}^3_a)$ corresponding to particle a. Elements of L^2_N are the functions $\psi(\vec{x}_1, \ldots, \vec{x}_N)$ generated by the basis $\{\prod_{a=1}^{N} \psi_n^{(a)}(\vec{x}_i)\}$, with $\{\psi_n^{(a)}(\vec{x})\}$ a basis of $L^2(\mathbb{R}^3_a)$. In L^2_N, the coordinate operators and the momentum operators are represented as $\vec{\hat{q}}_{(a)} = \vec{x}_{(a)}$ and $\vec{\hat{p}}_{(a)} = -i\vec{\nabla}_{(a)}$, respectively.

The inclusion of spin is also straightforward. For a particle of spin s, i.e., such that $\vec{s}^{\,2} = s(s+1)$ on its states, bases of (improper) vectors of the Hilbert space are now $|\vec{x}, s_3\rangle$ and $|\vec{p}, s_3\rangle$, where $s_3 = -s, \ldots, s$ is the third component of the spin. The coordinate and the momentum representation are realised in the Hilbert space $L^2(\mathbb{R}^3)\otimes\mathbb{R}^{2s+1}$, and instead of a single wavefunction one has $2s+1$ wavefunctions $\langle \vec{x}, s_3|\psi\rangle = \psi_{s_3}(\vec{x})$, and momentum wavefunctions $\langle \vec{p}, s_3|\psi\rangle = \tilde{\psi}_{s_3}(\vec{p})$. For factorised states we will write the wavefunction as $\psi(\vec{x})\chi_{s_3}$, with $\vec{x}$-independent $(2s+1)$-dimensional spinor χ. The generalisation to N particles with possibly different spins is immediate.

[11] The notation L^2_N for the N-particle space has just been made up.

3.3 Free-particle wave packets

As a first application of the formalism described in the previous subsection, we will review in some detail the temporal evolution of general one-particle states.

The general solution of the time-dependent Schrödinger equation Eq. (3.8) is most easily obtained starting from the eigenvalue equation (time-independent Schrödinger equation)

$$\hat{H}_0|\psi\rangle = \frac{\vec{\hat{p}}^2}{2m}|\psi\rangle = E|\psi\rangle\,. \tag{3.17}$$

The solutions of this equation are simply the momentum eigenstates $|\vec{p}\rangle$, which satisfy it with energy $E = E_p \equiv \frac{\vec{p}^2}{2m}$. Using the formal solution in terms of $U_0(t) = e^{-i\hat{H}_0 t}$ and $|\psi(0)\rangle = |\psi\rangle$, and expanding the latter in the momentum basis $|\psi\rangle = \int d_3p\,|\vec{p}\rangle\langle\vec{p}|\psi\rangle$, we find

$$|\psi(t)\rangle = \int d_3p\, e^{-i\hat{H}_0 t}|\vec{p}\rangle\langle\vec{p}|\psi\rangle = \int d_3p\, e^{-iE_p t}|\vec{p}\rangle\langle\vec{p}|\psi\rangle\,. \tag{3.18}$$

For a momentum eigenstate the temporal evolution corresponds to multiplication by an appropriate phase, so its wavefunction at any time will be that of a plane wave. A general vector $|\psi\rangle$ contains various momentum eigenstates, and it represents therefore not a plane wave, but rather a wave packet.

It is instructive to study how the wave packet evolves over time. Obviously the expectation values of $\vec{\hat{p}}$ and $\vec{\hat{p}}^2$ are time-independent. One can show that

$$[\hat{q}_i, f(\vec{\hat{p}})] = i\frac{\partial f}{\partial p_i}(\vec{\hat{p}})\,, \tag{3.19}$$

starting with polynomials and using induction, and then extending the result to analytic functions. From this one proves that

$$U_0(t)^\dagger \hat{q} U_0(t) = \hat{q} + U_0(t)^\dagger[\hat{q}, U_0(t)] = \hat{q} + t\frac{\hat{p}}{m}\,, \qquad U_0(t)^\dagger \hat{q}^n U_0(t) = \left(\hat{q} + t\frac{\hat{p}}{m}\right)^n\,. \tag{3.20}$$

Using these results we obtain

$$\begin{aligned}
\langle q\rangle_t =& \langle\psi(t)|q|\psi(t)\rangle = \langle q\rangle_0 + \frac{t}{m}\langle p\rangle_0 \\
\Delta_\psi q^2(t) \equiv& \langle\psi(t)|q^2|\psi(t)\rangle - \langle\psi(t)|q|\psi(t)\rangle^2 \\
=& \Delta_\psi q^2(0) + \left(\frac{t}{m}\right)^2 \Delta_\psi p^2(0) + \frac{t}{m}\left[\langle\psi|\{q,p\}|\psi\rangle - 2\langle\psi|q|\psi\rangle\langle\psi|p|\psi\rangle\right]\,,
\end{aligned} \tag{3.21}$$

which shows that the center of the packet moves along a straight line with constant velocity $\langle p\rangle_0/m$, and that the wave packet inevitably spreads out as time passes.

The abstract result Eq. (3.18) can be projected on the desired basis. Let us look at the wavefunction in the coordinate basis,

$$\begin{aligned}
\psi(t,\vec{x}) = \langle\vec{x}|\psi(t)\rangle =& \int d_3p\, e^{-iE_p t}\langle\vec{x}|\vec{p}\rangle\langle\vec{p}|\psi\rangle = \int d_3p\, e^{-iE_p t} e^{i\vec{p}\cdot\vec{x}} \int d^3x'\langle\vec{p}|\vec{x}'\rangle\langle\vec{x}'|\psi\rangle \\
=& \int d^3x'\langle\vec{x}'|\psi\rangle \int d_3p\, e^{-iE_p t} e^{i\vec{p}\cdot(\vec{x}-\vec{x}')} = \int d^3x' \mathcal{K}_t(\vec{x}-\vec{x}')\psi(\vec{x}')\,,
\end{aligned} \tag{3.22}$$

where

$$\mathcal{K}_t(\vec{x}-\vec{x}') \equiv \int d_3p\, e^{-iE_pt} e^{i\vec{p}\cdot(\vec{x}-\vec{x}')}\,. \tag{3.23}$$

To carry out this integral, notice that

$$-E_pt + \vec{p}\cdot(\vec{x}-\vec{x}') = -\frac{t}{2m}\left[\vec{p} - \frac{m}{t}(\vec{x}-\vec{x}')\right]^2 + \frac{m}{2t}(\vec{x}-\vec{x}')^2\,. \tag{3.24}$$

A simple change of variables thus yields

$$\begin{aligned}\mathcal{K}_t(\vec{x}-\vec{x}') &= e^{i\frac{m}{2t}(\vec{x}-\vec{x}')^2}\int d_3p\, e^{-i\frac{t}{2m}\vec{p}^2} = \left(\frac{2m}{|t|}\right)^{\frac{3}{2}} e^{i\frac{m}{2t}(\vec{x}-\vec{x}')^2}\int d_3p\, e^{-i\mathrm{sgn}\,(t)\vec{p}^2} \\ &= \left(\frac{m}{2\pi t i}\right)^{\frac{3}{2}} e^{i\frac{m}{2t}(\vec{x}-\vec{x}')^2}\,,\end{aligned} \tag{3.25}$$

where in the last step we have applied Cauchy theorem for the integral of analytic functions to obtain

$$\int d_3p\, e^{\mp i\vec{p}^2} = \left(\frac{1}{2}\sqrt{\frac{1}{\pm i\pi}}\right)^3\,.$$

In conclusion,

$$\psi(t,\vec{x}) = \left(\frac{m}{2\pi t i}\right)^{\frac{3}{2}}\int d^3x' e^{i\frac{m}{2t}(\vec{x}-\vec{x}')^2}\psi(\vec{x}') = \left(\frac{m}{2\pi t i}\right)^{\frac{3}{2}} e^{i\frac{m}{2t}\vec{x}^2}\int d^3x' e^{-i\frac{m}{t}\vec{x}\cdot\vec{x}'} e^{i\frac{m}{2t}\vec{x}'^2}\psi(\vec{x}')\,. \tag{3.26}$$

A few comments are now in order.

1. The integral Eq. (3.26) certainly exists if $\psi(\vec{x})$ is a smooth (infinitely differentiable) rapidly vanishing function, i.e., such that it and all its derivatives vanish at infinity faster than any polynomial. The set of such functions is usually denoted by $\mathscr{S}$. In this case

$$|\psi(t,\vec{x})| \le \left(\frac{m}{2\pi|t|}\right)^{\frac{3}{2}}\int d^3x'|\psi(\vec{x}')| < \infty\,. \tag{3.27}$$

   Since $\mathscr{S}$ is dense in $L^2(\mathbb{R}^3)$, we have thus found the action of $U_0(t)$ on a dense subset of the Hilbert space.[12] Moreover, if we have a convergent, or equivalently (due to completeness) Cauchy sequence $|\psi_n\rangle \to |\psi\rangle$, then $\|\psi_n(t)-\psi_m(t)\| = \|\psi_n-\psi_m\| \to 0$ due to the fact that $U_0(t)$ is norm-preserving, and completeness implies that $|\psi_n(t)\rangle \to |\psi(t)\rangle$ for some $|\psi(t)\rangle \in L^2(\mathbb{R}^3)$. This limit is independent of the sequence: given two convergent sequences $|\psi_n\rangle, |\psi'_n\rangle \to |\psi\rangle$ with $|\psi_n(t)\rangle \to |\psi(t)\rangle$ and $|\psi'_n(t)\rangle \to |\psi'(t)\rangle$, then $0 = \lim_{n\to\infty}\|\psi_n - \psi'_n\| = \lim_{n\to\infty}\|U_0(t)\psi_n - U_0(t)\psi'_n\| = \lim_{n\to\infty}\|\psi_n(t)-\psi'_n(t)\| = \|\psi(t)-\psi'(t)\|$. We can thus extend the action of $U_0(t)$ to the whole Hilbert space by continuity.

2. If $\psi(\vec{x}) \in \mathscr{S}$, then from Eq. (3.26) we see that $\psi(t,\vec{x}) \in \mathscr{S}$: clearly $e^{i\frac{m}{2t}\vec{x}'^2}\psi(\vec{x}') \in \mathscr{S}$; the ensuing Fourier transform leaves $\mathscr{S}$ invariant; and for the remaining phase factor the same applies as above.

[12] It would actually suffice to consider the dense subset $L^1(\mathbb{R}^3)\cap L^2(\mathbb{R}^3)$, for which the bound Eq. (3.27) holds, but $\mathscr{S}$ is a "nicer" set.

3. Given two arbitrary convergent sequences $|\chi_n\rangle \to |\chi\rangle$ and $|\psi_n\rangle \to |\psi\rangle$ (including the identical ones) of elements of $\mathscr{S}$, then

$$\begin{aligned}\left|\langle\chi|\psi(t)\rangle\right| &= \left|\langle\chi-\chi_n|\psi(t)-\psi_n(t)\rangle + \langle\chi-\chi_n|\psi_n(t)\rangle + \langle\chi_n|\psi(t)-\psi_n(t)\rangle + \langle\chi_n|\psi_n(t)\rangle\right| \\ &\leq \|\chi-\chi_n\|\|\psi-\psi_n\| + \|\chi-\chi_n\|\|\psi_n\| + \|\chi_n\|\|\psi-\psi_n\| + \left|\langle\chi_n|\psi_n(t)\rangle\right|.\end{aligned} \tag{3.28}$$

The first three terms can be taken arbitrarily small, and add up to some arbitrarily small $\epsilon > 0$. Therefore

$$\begin{aligned}|\langle\chi|\psi(t)\rangle| &< \epsilon + \left(\frac{m}{2\pi|t|}\right)^{\frac{3}{2}} \left|\int d^3x \chi_n^*(\vec{x}) \int d^3x' e^{i\frac{m}{2t}(\vec{x}-\vec{x}')^2}\psi_n(\vec{x}')\right| \\ &\leq \epsilon + \left(\frac{m}{2\pi|t|}\right)^{\frac{3}{2}} \int d^3x |\chi_n(\vec{x})| \int d^3x' |\psi_n(\vec{x}')|\,.\end{aligned} \tag{3.29}$$

The integrals certainly exist, and so as $t \to \infty$ one finds $\lim_{t\to\infty}|\langle\chi|\psi(t)\rangle| \leq \epsilon$ for arbitrarily small ϵ, i.e., $\lim_{t\to\infty}\langle\chi|\psi(t)\rangle = 0$ for any $|\chi\rangle, |\psi\rangle$. In particular, for elements of $\mathscr{S}$, $\langle\chi|\psi(t)\rangle$ vanishes at least as $|t|^{-\frac{3}{2}}$. Both results will be useful later.

4. The inclusion of spin does not involve any additional difficulty: since H_0 commutes with $\vec{s}$, one can treat the wavefunction components independently, and for each of them the results obtained above apply.

3.4 Interacting systems: the two-particle Hamiltonian

In order to describe real physical systems, for which we observe that the time evolution cannot be (always) described as a free evolution, we have to somehow modify the mathematical description. The space of possible states has to include the free states, since these are (approximately) observed in Nature. If we furthermore want this space to be a separable Hilbert space, then the essential uniqueness of the spaces $L^2(\mathbb{R}^n)$ implies that the appropriate setting for interacting systems will be the same as that of free systems, i.e., a space of square-integrable functions.

To change the dynamics of the system we have then to change the Hamiltonian. For clarity we discuss this issue in the case of a system of two spinless particles. The simplest possible modification of the free two-particle Hamiltonian consists in adding to $\hat{H}_0$ a function of the coordinates of the two particles, i.e., a potential. If the system is translation-invariant, then the potential has to depend only on the relative position of the particles; if the system is also rotation invariant, then the potential must depend only on their relative distance. Another sensible physical requirement is that the potential becomes constant at large distance; this constant can be freely chosen to be zero. The Hamiltonian of our system therefore reads

$$\hat{H} = \frac{\vec{\hat{p}}_1^{\,2}}{2m_1} + \frac{\vec{\hat{p}}_2^{\,2}}{2m_2} + V(|\vec{\hat{q}}_1 - \vec{\hat{q}}_2|)\,, \tag{3.30}$$

and the temporal evolution of a state described by $|\Psi\rangle$ at $t = 0$ is

$$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi\rangle\,. \tag{3.31}$$

A canonical transformation to the center of mass and relative coordinates,

$$\begin{aligned} \hat{Q} &= \frac{m_1\hat{q}_1 + m_2\hat{q}_2}{m_1+m_2}\,, \qquad & \hat{q} &= \hat{q}_1 - \hat{q}_2\,, \\ \hat{P} &= \hat{p}_1 + \hat{p}_2 & \hat{p} &= \frac{m_2\hat{p}_1 - m_1\hat{p}_2}{m_1+m_2}\,, \end{aligned} \tag{3.32}$$

allows to rewrite H as follows,

$$\hat{H} = \frac{\vec{\hat{P}}^{\,2}}{2M} + \frac{\vec{\hat{p}}^{\,2}}{2m} + V(|\vec{\hat{q}}|)\,, \tag{3.33}$$

where $M = m_1 + m_2$, and $m = \frac{m_1 m_2}{m_1+m_2}$ is the reduced mass of the system. Since $[\vec{\hat{P}}, \hat{H}] = 0$, the total momentum is a constant of motion. The dynamics factors exactly into a free center-of-mass part, and an interacting relative part, i.e.,

$$e^{-i\hat{H}t} = e^{-i\frac{\vec{\hat{P}}^{\,2}}{2M}t} e^{-i\hat{H}_{\rm rel}t}\,, \tag{3.34}$$

with $\hat{H}_{\rm rel} = \frac{\vec{\hat{p}}^{\,2}}{2m} + V(|\vec{\hat{q}}|)$ being the Hamiltonian of one particle in a potential. Since $V \to 0$ at large distance, bound states of $\hat{H}_{\rm rel}$ have negative energy.

The case of two particles with spin is not very much different, besides the fact that now the potential can be spin dependent. If we denote with $\vec{s}_{1,2}$ the spin operators associated with the two particles, and still assume rotational invariance, then possible extra terms in the Hamiltonian are for example $\vec{s}_1 \cdot \vec{s}_2 V_{ss}(|\vec{\hat{q}}|)$ and $\vec{L}\cdot\vec{S}V_{LS}(|\vec{\hat{q}}|)$, where $\vec{L} = \vec{q}\wedge\vec{p}$ is the orbital angular momentum and $\vec{S} = \vec{s}_1 + \vec{s}_2$ is the total spin, and V_{ss} and V_{LS} are scalars.

In the discussion above we have used the expression "two-particle Hamiltonian", but as we have repeatedly pointed out in the introduction the concept of particle is well-defined when the particle is free. What has been understood in the previous discussion is that the temporal evolution generated by the Hamiltonian Eq. (3.30) is expected to lead, in the appropriate situation, to states evolving like freely evolving two-particle states. Showing that this is actually the case is the subject of the next section.

4 The formal theory of scattering

This section is devoted to the formal theory of scattering. Our purpose is to lay the foundations for any practical calculation related to a physical scattering process. We adopt here the so-called time-dependent approach, which provides a description of the scattering process as it develops through time.

From now on, except when explicitly stated otherwise, our discussion of scattering processes will focus on systems described by a Hamiltonian of the form Eq. (3.33). Since particles cannot be created or destroyed in quantum mechanics, the scope of our discussion will therefore be limited to two-body elastic scattering processes. This will be sufficient to introduce the main ideas, which can then be generalised to more complicated systems. A brief comment on this will be made at the end of this section.

Before starting, a comment about notation is in order: from now on we will omit the "hat" on top of operators, as it will always be clear whether the object under consideration is an operator or a c-number.

4.1 Asymptotic condition

As we have repeatedly said, in a scattering experiment the system is initially prepared in a free particle state, or more accurately, in a state whose evolution is indistinguishable from the free evolution; and that after a long time it is observed again behaving like a free particle state. We know that these statements have to be approximate, because the particles are never really free due to interactions. We also know that the farther apart the particles, the more accurate the description as a freely evolving state is. Let us now express these ideas in mathematical form.

It is convenient to use center-of-mass and relative coordinates, which for a two-particle system have been defined in Eq. (3.32). Without loss of generality we can assume that the system is in a factorised state $|\Psi\rangle = |\bar{\psi}\rangle_{\rm CM} \otimes |\psi\rangle_{\rm rel}$ at $t = 0$, with $|\bar{\psi}\rangle_{\rm CM} \in L^2(\mathbb{R}^3_{\rm CM})$ and $|\psi\rangle_{\rm rel} \in L^2(\mathbb{R}^3_{\rm rel})$. Since the time evolution of $|\bar{\psi}\rangle_{\rm CM}$ is trivial [see Eq. (3.34)], we can just focus on the relative part, drop the subscripts for notational simplicity and denote $\mathcal{H} = L^2(\mathbb{R}^3_{\rm rel})$. The problem is thus reduced to the study of scattering of one particle in a potential. The exact time evolution of $|\psi\rangle$ is governed by the full relative Hamiltonian $H = H_0 + V$, and reads $|\psi(t)\rangle = U(t)|\psi\rangle$ with $U(t) \equiv e^{-iHt}$. A freely evolving state reads instead $U_0(t)|\phi\rangle$, for some $|\phi\rangle \in \mathcal{H}$ and with $U_0(t) \equiv e^{-iH_0 t}$. Indistinguishability of two states $|\psi_{1,2}\rangle$ means that they yield indistinguishable results for any measurement. Since these can be expressed in terms of projectors $|\chi\rangle\langle\chi|$, indistinguishability of any expectation value entails that $|\langle\chi|\psi_1\rangle|^2 = |\langle\chi|\psi_2\rangle|^2$, $\forall|\chi\rangle \in \mathcal{H}$. This in turn implies that $|\psi_1\rangle$ and $|\psi_2\rangle$ are equal up to a phase.[13] In our case we have practical indistinguishability, which means that there are some $|\phi_i\rangle$ and $|\phi_f\rangle$ such that $\|U(t)\psi - U_0(t)\phi_{i,f}\| < \epsilon$, for some small ϵ, when $t \to -\infty$ and $t \to +\infty$, respectively. There is no need for $|\phi_i\rangle$ to be the same as $|\phi_f\rangle$. As the indistinguishability improves as $|t|$ becomes larger, we eventually expect that it becomes exact in the far past $t = -\infty$ and in the far future $t = +\infty$:

$$\begin{aligned} \lim_{t\to-\infty} \|U(t)\psi - U_0(t)\phi_i\| = 0\,, \\ \lim_{t\to+\infty} \|U(t)\psi - U_0(t)\phi_f\| = 0\,. \end{aligned} \tag{4.1}$$

These relations are called the asymptotic conditions, and ϕ_i and ϕ_f are the past and future asymptotes, respectively.

So far we have just argued that the asymptotic conditions should hold for states describing a scattering process, and before trying to prove them, two questions are in order. Do we expect the conditions Eq. (4.1) to hold, with appropriate $|\phi_{i,f}\rangle$, for any state $|\psi\rangle$? Conversely, what kind of states $|\phi_{i,f}\rangle$ do we expect to describe the asymptotic, free-like behaviour of states at large times?

The first question amounts to asking if we expect any possible state of the system to look asymptotically like a freely-evolving state, and stated in this way it is obvious that in general the answer is no: we know of the possible existence of bound states, in which the two particles can never escape to infinity, and which therefore will never look like a system of two free particles. There might be also other states which do not satisfy Eq. (4.1): to prove that this is not the case is a very hard task, and will be discussed at the qualitative level in subsection 4.3.

As for the second question, since we are free to prepare the initial state that we want, we expect no limitation on $|\phi_i\rangle$; since the final state of a scattering process can be used as the initial

[13] Using as $|\chi\rangle$ the elements of a complete basis and finite linear combinations thereof, one can prove equality of the modulus of the expansion coefficients and of their relative phases.

state of another one, the same expectation holds for $|\phi_f\rangle$. For a wide class of potentials, this can be proved rather easily as we now show.

The central result of this section is the proof of the validity of the asymptotic conditions:

> **(asymptotic condition)** for any $|\phi\rangle \in \mathcal{H}$, there exist vectors $|\psi_\pm\rangle$ such that the following relations hold,
>
> $$\lim_{t\to\mp\infty} \|U(t)\psi_\pm - U_0(t)\phi\| = 0\,. \tag{4.2}$$

The apparently bizarre choice of signs $|\psi_\pm\rangle$ in Eq. (4.2) is of historical origin, and we will keep it not as a homage to tradition, but as a torment for students.

Proof. Since $U(t)$ is unitary, proving Eq. (4.2) is equivalent to prove

$$\lim_{t\to\mp\infty} \|\psi_\pm - W(t)\phi\| = 0\,, \qquad W(t) \equiv U(t)^\dagger U_0(t)\,. \tag{4.3}$$

The existence of $|\psi_\pm\rangle$ is guaranteed by the completeness of the Hilbert space, if we are able to prove that $W(t)|\phi\rangle$ is Cauchy, i.e., if $\Delta(t_1,t_2) = \|W(t_2)\phi - W(t_1)\phi\| \to 0$ as $t_{1,2} \to \pm\infty$. To do this we write[14]

$$W(t_2)|\phi\rangle - W(t_1)|\phi\rangle = \int_{t_1}^{t_2} dt\, \frac{d}{dt} W(t)|\phi\rangle = i\int_{t_1}^{t_2} dt\, U(t)^\dagger V U_0(t)|\phi\rangle\,. \tag{4.4}$$

Using the properties of the norm and of the integral, and the unitarity of $U(t)$, we have

$$\Delta(t_1,t_2) \le \int_{t_1}^{t_2} dt\, \|V U_0(t)\phi\|\,. \tag{4.5}$$

In the coordinate representation

$$\|V U_0(t)\phi\|^2 = \int d^3x V(\vec{x})^2 |\phi(t,\vec{x})|^2\,, \tag{4.6}$$

where $\phi(t,\vec{x}) = \langle \vec{x}\,|U_0(t)|\phi\rangle$. We now take $|\phi\rangle$ such that $\phi(\vec{x}) = \langle \vec{x}\,|\phi\rangle \in \mathscr{S}$. For such functions the bound Eq. (3.27) applies, and $\phi(t,\vec{x})$ vanishes at least like $|t|^{-\frac{3}{2}}$ as $t \to \pm\infty$.[15] Moreover, $\mathscr{S}$ is dense in $L^2(\mathbb{R}^3)$, and this will allow us to extend easily our result to the whole space. Furthermore, we assume that the potential is square-integrable. With these assumptions, it is easy to show that

$$\|V U_0(t)\phi\|^2 \le \left(\frac{m}{2\pi|t|}\right)^3 \int d^3x V(\vec{x})^2 \left(\int d^3x' |\phi(\vec{x}')|\right)^2 = \frac{C}{|t|^3}\,, \tag{4.7}$$

[14] We ignore for the moment whether we are allowed to take the derivative of $W(t)$. If you care, then look at footnote 15.

[15] Since also Eq. (3.26) applies, one has that also $\psi(t,\vec{x}) \in \mathscr{S}\ \forall t$. Functions in $\mathscr{S}$ are in the domain of both the free and the interacting Hamiltonian (at least for potentials which are not too singular). Stone's theorem (see [Reed & Simon], vol. 1, §VIII.4) guarantees that given some self-adjoint operator A, then $U(t) = e^{iAt}$ is a one-parameter group of unitary operators, and moreover if $|\psi\rangle \in \mathcal{D}(A)$ then $\lim_{\epsilon\to 0} \frac{1}{\epsilon}[U(t+\epsilon) - U(t)]|\psi\rangle = iA|\psi\rangle$. Taking the derivative of $W(t)$ is thus justified for our choice of $\psi(\vec{x})$.

with some positive constant C. We finally conclude that, taking $t_2 \geq t_1 > 0$ or $0 > t_1 \geq t_2$ without loss of generality.

$$\Delta(t_1, t_2) \leq \int_{t_1}^{t_2} dt \, \frac{C^{\frac{1}{2}}}{|t|^{\frac{3}{2}}} = 2C^{\frac{1}{2}} \left(\frac{1}{|t_1|^{\frac{1}{2}}} - \frac{1}{|t_2|^{\frac{1}{2}}} \right) \underset{t_1, t_2 \to \infty}{\to} 0 \,. \tag{4.8}$$

This concludes the proof for $\phi(\vec{x}) \in \mathscr{S}$. Since $\mathscr{S}$ is dense in $L^2(\mathbb{R}^3)$, for a generic vector $|\phi\rangle$ we can find $|\phi_\epsilon\rangle$ with $\phi_\epsilon(\vec{x}) \in \mathscr{S}$ and $\|\phi - \phi_\epsilon\| < \epsilon/2$. Then

$$\begin{aligned} \Delta(t_1, t_2) &= \|[W(t_2) - W(t_1)][(\phi - \phi_\epsilon) + \phi_\epsilon]\| \\ &\leq \|[W(t_2) - W(t_1)](\phi - \phi_\epsilon)\| + \|[W(t_2) - W(t_1)]\phi_\epsilon\| \\ &\leq \epsilon + \|[W(t_2) - W(t_1)]\phi_\epsilon\| \,, \end{aligned} \tag{4.9}$$

from which it follows that $\lim_{t_1, t_2 \to \infty} \Delta(t_1, t_2) \leq \epsilon$ for arbitrarily small ϵ, i.e., that this limit vanishes. □

In conclusion, the limits

$$\lim_{t \to \mp\infty} W(t)|\phi\rangle = \lim_{t \to \mp\infty} U(t)^\dagger U_0(t)|\phi\rangle = |\psi_\pm\rangle \tag{4.10}$$

exist $\forall |\phi\rangle \in \mathcal{H}$ if the potential V is sufficiently well-behaved. We give here a list of conditions for which the above derivation holds, and for which all the results that we will further discuss in this section also hold, in the case of a spherical potential, i.e., $V = V(r)$, $r = |\vec{x}|$ (see [Taylor], pag. 27):

1. $V(r) = \mathcal{O}(r^{-3-\epsilon})$ as $r \to \infty$, for some $\epsilon > 0$;
2. $V(r) = \mathcal{O}(r^{-\frac{3}{2}+\epsilon})$ as $r \to 0$, for some $\epsilon > 0$;
3. $V(r)$ is continuous for $r \in (0, \infty)$, with at most a finite number of finite discontinuities.

These conditions on V can actually be relaxed, and it is possible to show (Kupsch-Sandhas theorem) that the limit exists as long as $V(\vec{x}) \sim |\vec{x}|^{-1-\epsilon}$ as $|\vec{x}| \to \infty$ (and as long as it is not too singular anywhere else).

The inclusion of spin presents no particular difficulty. The proof given above remains unchanged until Eq. (4.6), which now reads

$$\|VU_0(t)\phi\|^2 = \int d^3x \phi(t, \vec{x})^\dagger V(\vec{x})^2 \phi(t, \vec{x}) \,, \tag{4.11}$$

where now $\phi(t, \vec{x})$ is a spinor collecting the $(2s_1+1)(2s_2+1)$ components $\phi_{s_3^{(1)} s_3^{(2)}}(t, \vec{x})$ of the wave function, where $s_3^{(1,2)}$ denote the third components of the spin of the two particles. Similarly, $V(\vec{x})$ is now a Hermitian matrix with entries $V_{s_3^{(1)\prime} s_3^{(2)\prime}, s_3^{(1)} s_3^{(2)}}(\vec{x})$. The bound Eq. (4.7) is changed into

$$\begin{aligned} \|VU_0(t)\phi\|^2 &\leq \int d^3x \|V(\vec{x})\|^2_{\text{spin}} \|\phi(t, \vec{x})\|_{\text{spin}} \\ &\leq \left(\frac{m}{2\pi|t|} \right)^3 \int d^3x \|V(\vec{x})\|^2_{\text{spin}} \sum_{s_3^{(1)} s_3^{(2)}} \left(\int d^3x' |\phi_{s_3^{(1)} s_3^{(2)}}(\vec{x}')| \right)^2 = \frac{C}{|t|^3} \,, \end{aligned} \tag{4.12}$$

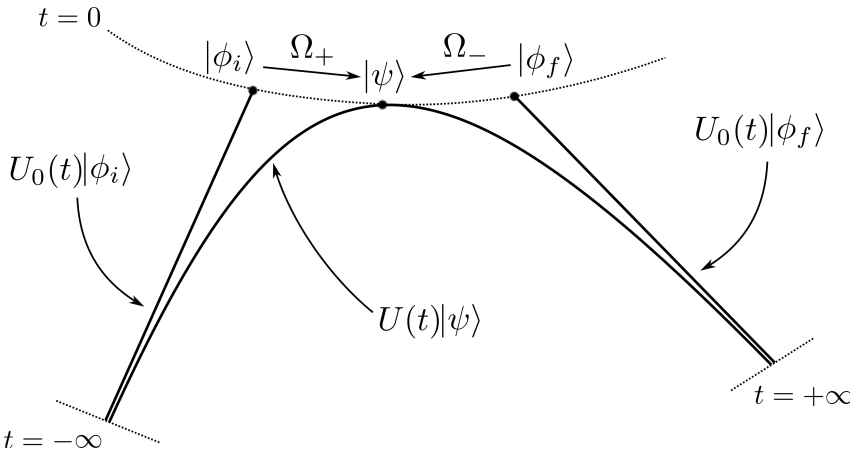

Figure 5: Relation between exact and asymptotic trajectories.

with some new constant C. Here $\|\phi(t,\vec{x})\|_{\text{spin}}$ denotes the norm of the spinor $\phi(t,\vec{x})$ in the spin Hilbert space, $\|\phi(t,\vec{x})\|^2_{\text{spin}} = \sum_{s_3^{(1)} s_3^{(2)}} |\phi_{s_3^{(1)} s_3^{(2)}}(t,\vec{x})|^2$, and $\|V(\vec{x})\|_{\text{spin}}$ is the norm of the matrix $V(\vec{x})$ in the same space, which coincides with the magnitude of its largest eigenvector. The rest of the proof remains the same.

4.2 Scattering operators

The result above shows that given $|\phi\rangle$, we can assign a unique $|\psi_\pm\rangle$ to it: this defines two operators $\Omega_\pm$ on the whole of $\mathcal{H}$,

$$|\psi_\pm\rangle = \Omega_\pm |\phi\rangle \,. \tag{4.13}$$

The $\Omega_\pm$ are called scattering (or Møller) operators, and map the vectors that describe the free evolution at asymptotic times to the vectors that describe the exact evolution. In practical terms, they map our physical knowledge about the system at asymptotic times to the exact state vector. The situation is illustrated in Fig. 5. We now prove two important properties of these operators.

The first property is that scattering operators are isometric. Since they are defined on the whole of $\mathcal{H}$, to prove this it is enough to show that they are norm-preserving, and this follows at once from the fact that they are the limits (in the strong sense) for $t \to \pm\infty$ of the unitary operator $W(t) = U(t)^\dagger U_0(t)$. Indeed,

$$\begin{aligned} \|\psi_\pm\| &= \|\psi_\pm - W(\mp T)\phi + W(\mp T)\phi\| \leq \|\phi\| + \|\psi_\pm - W(\mp T)\phi\| \,, \\ \|\phi\| &= \|W(\mp T)\phi\| = \|\psi_\pm + W(\mp T)\phi - \psi_\pm\| \leq \|\psi_\pm\| + \|W(\mp T)\phi - \psi_\pm\| \,, \end{aligned} \tag{4.14}$$

and since the last term in both inequalities can be made arbitrarily small by choosing T sufficiently large, we conclude that $\|\psi_\pm\| = \|\phi\|$.

Isometric operators can be inverted on their range, so we can define $\Omega_\pm^{-1} : \mathcal{R}(\Omega_\pm) \to \mathcal{H}$ (which is onto $\mathcal{H}$). We can now easily construct the adjoint operators $\Omega_\pm^\dagger$, which by definition are such that $\langle \Omega_\pm^\dagger \chi | \phi \rangle = \langle \chi | \Omega \phi \rangle$ on the whole domain of $\Omega_\pm$, which is $\mathcal{H}$. Let first $|\chi\rangle \in \mathcal{R}(\Omega_\pm)$.

Then $|\chi\rangle = \Omega_\pm|\phi'\rangle$ for some $|\phi'\rangle$, and so[16]

$$\langle\chi|\Omega_\pm\phi\rangle = \langle\Omega_\pm\phi'|\Omega_\pm\phi\rangle = \langle\phi'|\phi\rangle = \langle\Omega_\pm^{-1}\chi|\phi\rangle = \langle\Omega_\pm^\dagger\chi|\phi\rangle\,. \tag{4.15}$$

For $|\chi\rangle \in \mathcal{R}(\Omega_\pm)^\perp$, i.e., in the orthogonal complement of the range, we simply have $\langle\chi|\Omega_\pm\phi\rangle = 0 = \langle\Omega_\pm^\dagger\chi|\phi\rangle$, and in conclusion

$$\Omega_\pm^\dagger = \begin{cases} \Omega_\pm^{-1} & \text{on } \mathcal{R}(\Omega_\pm)\,, \\ 0 & \text{on } \mathcal{R}(\Omega_\pm)^\perp\,. \end{cases} \tag{4.16}$$

It then follows

$$\Omega_\pm^\dagger\Omega_\pm = \mathbf{1}\,, \qquad \Omega_\pm\Omega_\pm^\dagger = P_{\mathcal{R}(\Omega_\pm)}\,, \tag{4.17}$$

where $P_\mathcal{S}$ is the orthogonal projector on subspace $\mathcal{S}$. The first relation can also be seen to follow directly from the fact that $\Omega_\pm$ are isometries.

The second important result is the intertwining relation

$$H\Omega_\pm = \Omega_\pm H_0\,. \tag{4.18}$$

To prove this, notice that[17]

$$\begin{aligned} U(s)\Omega_\pm|\phi\rangle &= U(s)\lim_{t\to\mp\infty} W(t)|\phi\rangle = \lim_{t\to\mp\infty} U(s)W(t)|\phi\rangle \\ &= \lim_{t\to\mp\infty} W(t-s)U_0(s)|\phi\rangle = \Omega_\pm U_0(s)|\phi\rangle\,, \end{aligned} \tag{4.19}$$

for any $|\phi\rangle \in \mathcal{H}$, so that $U(s)\Omega_\pm = \Omega_\pm U_0(s)$. Taking the derivative with respect to s and then setting $s = 0$, Eq. (4.18) follows.

The intertwining relation expresses conservation of energy in a scattering process. To see this, recall that the experimentalists make measurements on the particles in the initial and final state by observing their temporal evolution, which is that of free particles. The information so collected enters the state vectors $|\phi_{i,f}\rangle$, which allow to describe the (asymptotic) temporal evolution through the action of the free Hamiltonian. Measurements of energy correspond therefore to the determination of the expectation values $E_{i,f} = \langle\phi_{i,f}|H_0|\phi_{i,f}\rangle$. Suppose that the exact state vector of the system is $|\psi\rangle$, and that it possesses asymptotes $|\phi_{i,f}\rangle$ at $t \to \mp\infty$, i.e., $|\psi\rangle = \Omega_-|\phi_f\rangle = \Omega_+|\phi_i\rangle$. From Eq. (4.18) we thus find

$$E_{i,f} = \langle\phi_{i,f}|H_0|\phi_{i,f}\rangle = \langle\phi_{i,f}|\Omega_\pm^\dagger\Omega_\pm H_0|\phi_{i,f}\rangle = \langle\phi_{i,f}|\Omega_\pm^\dagger H\Omega_\pm|\phi_{i,f}\rangle = \langle\psi|H|\psi\rangle\,, \tag{4.20}$$

i.e., E_i and E_f are equal, and both are equal to the expectation value of the exact Hamitonian on the exact state vector.

To conclude this section, we now derive an expression for $\Omega_\pm$ which will be useful later. Recalling that $\Omega_+ = \lim_{t\to-\infty} W(t)$, and taking the derivative of $W(t)$ and integrating between $-\infty$ and 0 we find

$$\begin{aligned} W(0) - \lim_{t\to-\infty} W(t) &= \int_{-\infty}^0 dt\,\frac{d}{dt}W(t) = i\int_{-\infty}^0 dt\,(HW(t) - W(t)H_0) \\ &= i\int_{-\infty}^0 dt\,U(t)^\dagger V U_0(t)\,, \end{aligned} \tag{4.21}$$

[16] We use here the fact that $\langle\Omega_\pm\phi'|\Omega_\pm\phi\rangle = \langle\phi'|\phi\rangle$ for arbitrary $|\phi\rangle, |\phi'\rangle$. This is proved by using norm preservation for the vectors $|\phi\rangle + |\phi'\rangle$ and $|\phi\rangle + i|\phi'\rangle$.

[17] The second equality follows from the relation $\|B\chi_t - B\chi\| \le \|B\|\|\chi_t - \chi\| \to 0$ as $t \to \pm\infty$, valid for any bounded operator B and any convergent sequence $|\chi_t\rangle \to |\chi\rangle$ as $t \to \pm\infty$.

from which it follows at once that (since $W(0) = \mathbf{1}$)

$$\Omega_+ = \mathbf{1} - i\int_{-\infty}^{0} dt\, U(t)^\dagger V U_0(t) = \mathbf{1} - i\int_{-\infty}^{0} dt\, e^{iHt} V e^{-iH_0 t}\,. \tag{4.22}$$

A similar calculation yields

$$\Omega_- = \mathbf{1} + i\int_{0}^{+\infty} dt\, U(t)^\dagger V U_0(t) = \mathbf{1} + i\int_{0}^{+\infty} dt\, e^{iHt} V e^{-iH_0 t}\,. \tag{4.23}$$

4.3 Orthogonality and asymptotic completeness

In the introductory discussion at the beginning of section 4.1 we asked ourselves if there are states which do not satisfy the asymptotic conditions Eq. (4.1), and we argued that bound states should not. We now prove this assertion.

States which satisfy the asymptotic condition lie in the range $\mathcal{R}(\Omega_\pm)$ of $\Omega_\pm$. It then follows that states which lie in the orthogonal complements $\mathcal{R}(\Omega_\pm)^\perp$ do not satisfy it.[18] We now prove that for the subspace of bound states, $\mathcal{B}$, one has $\mathcal{B} \subseteq \mathcal{R}(\Omega_\pm)^\perp$. The subspace $\mathcal{B}$ is the subspace spanned by the (proper) eigenvectors $|E_n\rangle$ of H, i.e., $H|E_n\rangle = E_n|E_n\rangle$ with $\langle E_n|E_n\rangle < \infty$, and so to check $\mathcal{B} \subseteq \mathcal{R}(\Omega_\pm)^\perp$ it suffices to check that $|E_n\rangle \in \mathcal{R}(\Omega_\pm)^\perp$. For $|\psi_\pm\rangle = \Omega_\pm|\phi\rangle \in \mathcal{R}(\Omega_\pm)$ we have

$$\langle E_n|\psi_\pm\rangle = \langle E_n|\Omega_\pm|\phi\rangle = \lim_{t\to\mp\infty}\langle E_n|U(t)^\dagger U_0(t)|\phi\rangle = \lim_{t\to\mp\infty} e^{iE_n t}\langle E_n|U_0(t)|\phi\rangle\,. \tag{4.24}$$

From subsection 3.3 [see Eq. (3.29)] we know that $|\langle E_n|U_0(t)|\phi\rangle| \to 0$ as $t \to \pm\infty$, so we conclude that $\langle E_n|\psi_\pm\rangle = 0$.

Having shown that $\mathcal{B} \subseteq \mathcal{R}(\Omega_\pm)^\perp$ is not sufficient to characterise completely the states for which the asymptotic conditions do not hold, for there might be other states in $\mathcal{R}(\Omega_\pm)^\perp$. One might also wonder if it is possible that $\mathcal{R}(\Omega_+) \neq \mathcal{R}(\Omega_-)$, i.e., that the sets of states with a past or future asymptote do not match exactly. According to experience, we expect that if $|\psi\rangle = \Omega_+|\phi_i\rangle$ is the vector corresponding to some initial state of free particles $|\phi_i\rangle$, then the time evolution of $|\psi\rangle$ at large positive times will also look like a free particle state, so that $|\psi\rangle = \Omega_-|\phi_f\rangle$ for some $|\phi_f\rangle$, i.e, $\mathcal{R}(\Omega_+) \subseteq \mathcal{R}(\Omega_-)$. In fact, for a wide class of potentials, including those satisfying the conditions listed on pag. 20, one can actually prove (after a lot of work) the following result:

(asymptotic completeness)

1. $\mathcal{R}(\Omega_+) = \mathcal{R}(\Omega_-) \equiv \mathcal{R}$;
2. $\mathcal{B} \oplus \mathcal{R} = \mathcal{H}$.

The subspace $\mathcal{R}$ is called the subspace of scattering states. The result above is called asymptotic completeness, and a theory for which it holds is called asymptotically complete. In such a theory, besides the bound states, there are only scattering states which possess both a past and a future asymptote, i.e., for all $|\psi\rangle \in \mathcal{R}$ one has $|\psi\rangle = \Omega_\pm|\phi_\pm\rangle$ for some $|\phi_\pm\rangle$, and so $|\phi_\pm\rangle = \Omega_\pm^\dagger|\psi\rangle$.

[18] The most general state not satisfying the asymptotic condition has a nonvanishing projection on $\mathcal{R}(\Omega_\pm)^\perp$.

4.4 The S matrix

We finally have all the tools to (formally) predict all the transition probabilities in a scattering experiment. More precisely, we want to predict the probability of observing a certain final state given the knowledge of the initial free-particle state.

Scattering experiments are set up by preparing an initial, "accelerator" state $|\mathrm{acc}(-T_i)\rangle$ at some early time $t = -T_i$ ($T_i > 0$). After letting the system evolve, at some late time $t = T_f$ ($T_f > 0$) we use detectors to make measurements on the system. This can be expressed mathematically as projecting the state of the system on a prescribed "detector" state $|\mathrm{det}(T_f)\rangle$. Here T_i and T_f are taken large enough so that the evolution of the system is indistinguishable from the free evolution. The probability that at time $t = T_f$ we activate our detector is given by the expectation value

$$P_{i\to f} = \langle \mathrm{acc}(T_f)|\mathrm{det}(T_f)\rangle\langle \mathrm{det}(T_f)|\mathrm{acc}(T_f)\rangle = |\langle \mathrm{det}(T_f)|U(T_i+T_f)|\mathrm{acc}(-T_i)\rangle|^2 = |\langle\psi_-|\psi_+\rangle|^2\,, \tag{4.25}$$

where $|\psi_+\rangle = |\mathrm{acc}(0)\rangle$ and $|\psi_-\rangle = |\mathrm{det}(0)\rangle$. The states $|\psi_+\rangle$ and $|\psi_-\rangle$ are called the <u>in</u> and the <u>out</u> state of the process, and label the exact trajectories of the states of the system as functions of time.[19] Now, $|\psi_+\rangle = \Omega_+|\phi_i\rangle$ for the appropriate incoming asymptote $|\phi_i\rangle$, and similarly $|\psi_-\rangle = \Omega_-|\phi_f\rangle$ for the appropriate outgoing asymptote $|\phi_f\rangle$. Therefore

$$P_{i\to f} = |\langle\psi_-|\psi_+\rangle|^2 = |\langle\phi_f|\Omega_-^\dagger\Omega_+|\phi_i\rangle|^2 = |\langle\phi_f|S|\phi_i\rangle|^2\,, \tag{4.26}$$

where we have introduced the operator

$$S \equiv \Omega_-^\dagger\Omega_+\,.$$

The matrix elements $S_{fi} = \langle\phi_f|S|\phi_i\rangle$ are the <u>scattering amplitudes</u>, which taken together form the so-called <u>S-matrix</u>. The S-matrix encodes all the relevant information as far as the prediction of the outcome of a scattering experiment is concerned, which is now possible once the experimentally available information on the initial and final state is given.

Before turning to the study of the properties of S, we want to make a brief remark about the experimental accessibility of the asymptotes. Knowledge of $|\mathrm{acc}(-T_i)\rangle$ is equivalent to knowledge of

$$|\phi_{i,\,\mathrm{exp},T_i}\rangle = U_0(T_i)|\mathrm{acc}(-T_i)\rangle = U_0(T_i)U(-T_i)|\psi_+\rangle = W(-T_i)^\dagger|\psi_+\rangle\,.$$

This vector is experimentally accessible, since we know $|\mathrm{acc}(-T_i)\rangle$ and we know how to compute the free evolution, but it differs from the exact asymptote $|\phi_i\rangle$. Nevertheless, by construction $0 = W(-T_i)|\phi_{i,\,\mathrm{exp},T_i}\rangle - \Omega_+|\phi_i\rangle$ and so $0 = \|W(-T_i)\phi_{i,\,\mathrm{exp},T_i} - \Omega_+\phi_i\| = \|\phi_{i,\,\mathrm{exp},T_i} - W(-T_i)^\dagger\Omega_+\phi_i\|$. For a vector $|\psi\rangle \in \mathcal{R}$ such that $|\psi\rangle = \Omega_+|\chi\rangle$ one has

$$0 = \lim_{t\to-\infty}\|\psi - W(t)\chi\| = \lim_{t\to-\infty}\|W(t)^\dagger\psi - \chi\| = \lim_{t\to-\infty}\|W(t)^\dagger\psi - \Omega_+^\dagger\psi\|\,,$$

i.e., $W(t)^\dagger \to \Omega^\dagger$ in $\mathcal{R}$. Therefore,

$$0 = \lim_{T_i\to\infty}\|\phi_{i,\,\mathrm{exp},T_i} - W(-T_i)^\dagger\Omega_+\phi_i\| = \|\lim_{T_i\to\infty}\phi_{i,\,\mathrm{exp},T_i} - \Omega_+^\dagger\Omega_+\phi_i\| = \|\phi_{i,\,\mathrm{exp},\infty} - \phi_i\|\,, \tag{4.27}$$

[19] The usage of this nomenclature in the literature is of course not consistent: some authors reserve the qualification of in and out states for the initial and final asymptotes $|\phi_i\rangle$ and $|\phi_f\rangle$.

and so taking T_i sufficiently large we can approximate $|\phi_i\rangle$ arbitrarily well. Similarly, we can approximate $|\phi_f\rangle$ arbitrarily well by taking T_f sufficiently large.[20]

The most important property of S is that it is a unitary operator. This is equivalent to the operator relations

$$S^\dagger S = S S^\dagger = \mathbf{1}\,. \tag{4.28}$$

Indeed, since a unitary operator U is necessarily isometric, the relation $U^\dagger U = \mathbf{1}$ follows at once [see the first relation in Eq. (4.17)], and it shows that $U^\dagger = U^{-1}$ on the range of U, which is the whole of $\mathcal{H}$. Multiplying the relation above by U on both sides, we find $U(U^\dagger U) = U = (UU^\dagger)U$ using associativity, which implies $UU^\dagger = \mathbf{1}$ on $\mathcal{R}(U) = \mathcal{H}$. Conversely, an operator S defined on the whole Hilbert space and satisfying Eq. (4.28) is such that $S^\dagger = S^{-1}$ on $\mathcal{R}(S)$. Since in $\mathcal{R}(S)^\perp$ one has $S^\dagger = 0$, the second relation can hold only if $\mathcal{R}(S)^\perp = \{0\}$, i.e., $\mathcal{R}(S) = \mathcal{H}$.

To prove unitarity of S, notice first that the adjoint $S^\dagger = \Omega_+^\dagger \Omega_-$ is defined on the whole of $\mathcal{H}$. We can now write, using both relations in Eq. (4.17) and asymptotic completeness

$$\begin{aligned} S^\dagger S &= \Omega_+^\dagger \Omega_- \Omega_-^\dagger \Omega_+ = \Omega_+^\dagger P_{\mathcal{R}} \Omega_+ = \Omega_+^\dagger \Omega_+ = \mathbf{1}\,, \\ S S^\dagger &= \Omega_-^\dagger \Omega_+ \Omega_+^\dagger \Omega_- = \Omega_-^\dagger P_{\mathcal{R}} \Omega_- = \Omega_-^\dagger \Omega_- = \mathbf{1}\,, \end{aligned} \tag{4.29}$$

where we have also used the obvious fact that $P_{\mathcal{R}}\Omega_\pm = \Omega_\pm$.

Another important property of S is that it commutes with the free Hamiltonian. Indeed, using the intertwining relations, Eq. (4.18), we see at once that

$$S H_0 = \Omega_-^\dagger \Omega_+ H_0 = \Omega_-^\dagger H \Omega_+ = H_0 \Omega_-^\dagger \Omega_+ = H_0 S \Rightarrow [H_0, S] = 0\,. \tag{4.30}$$

This expresses again conservation of energy in a scattering process: if $|E_{i,f}\rangle$ denote eigenstates of H_0, then

$$0 = \langle E_f | [H_0, S] | E_i \rangle = (E_f - E_i) \langle E_f | S | E_i \rangle\,, \tag{4.31}$$

i.e., $\langle E_f | S | E_i \rangle$ can be nonzero only if $E_f = E_i$.

More generally, any symmetry generator M commuting both with H_0 and H will commute with S. Indeed, such a M will commute with $W(t)$ for all times, and so also with $\Omega_\pm$. The physically relevant symmetries in QM are spatial translations, rotations, (non-relativistic) boosts, parity and time reversal. We will discuss their consequences in detail in due time. Here we briefly mention that translation and rotation invariance imply conservation of the total momentum, $\vec{P}$ and of the total angular momentum, $\vec{J}$: the proof is as in Eq. (4.31). Invariance under boosts implies that the scattering amplitude between two given states is independent of the reference

[20] Neglecting these small errors, we could have taken the limit of a scattering process taking place from minus to plus temporal infinity, defining

$$P_{i\to f} = \lim_{T_i, T_f \to \infty} |\langle \det(T_f) | U(T_f + T_i) | \mathrm{acc}(-T_i) \rangle|^2 = |\langle \psi_- | \psi_+ \rangle|^2\,,$$

which would have led to the alternative derivation

$$\begin{aligned} P_{i\to f} = |\langle \psi_- | \psi_+ \rangle|^2 &= \lim_{T_i, T_f \to \infty} |\langle \psi_- | U(T_f)^\dagger U(T_f + T_i) U(T_i)^\dagger | \psi_+ \rangle|^2 \\ &= \lim_{T_i, T_f \to \infty} |\langle \phi_f | U_0(T_f)^\dagger U(T_f) U(T_i) U_0(T_i)^\dagger | \phi_i \rangle|^2 \\ &= \lim_{T_i, T_f \to \infty} |\langle \phi_f | W(T_f)^\dagger W(-T_i) | \phi_i \rangle|^2 = \lim_{T_i, T_f \to \infty} |\langle \phi_f | \Omega_-^\dagger \Omega_+ | \phi_i \rangle|^2\,. \end{aligned}$$

frame that one uses.[21] These symmetries, together with parity and time reversal, also imply useful relations between different S-matrix elements.

We conclude this section by restoring the full description of the two-body system in terms of CM and relative coordinates. A general state of the system is a superposition of factorised states $|\Phi\rangle = \sum_i c_i |\bar{\phi}_i\rangle_{\rm CM} \otimes |\phi_i\rangle_{\rm rel}$, and one can immediately show that

$$\begin{aligned}\lim_{t\to\pm\infty} U(t)^\dagger U_0(t)|\Phi\rangle &= \sum_i c_i \lim_{t\to\pm\infty} [U_{0\,\rm CM}(t)U_{\rm rel}(t)]^\dagger U_{0\,\rm CM}(t)U_{0\,\rm rel}(t)|\bar{\phi}_i\rangle_{\rm CM}\otimes|\phi_i\rangle_{\rm rel} \\ &= \sum_i c_i \lim_{t\to\pm\infty} |\bar{\phi}_i\rangle_{\rm CM}\otimes U_{\rm rel}(t)]^\dagger U_{0\,\rm rel}(t)|\phi_i\rangle_{\rm rel} \\ &= \sum_i c_i |\bar{\phi}_i\rangle_{\rm CM}\otimes \Omega_{\pm\,\rm rel}|\phi_i\rangle_{\rm rel} = \mathbf{1}_{\rm CM}\Omega_{\pm\,\rm rel}|\Phi\rangle = \Omega_\pm|\Phi\rangle\,,\end{aligned} \tag{4.32}$$

i.e., there is an isometry $\Omega_\pm$ that maps $\Omega_\pm|\Phi\rangle = |\Psi_\pm\rangle$ with $\|e^{-iHt}\Psi_\pm - e^{-iH_0t}\Phi\| \to 0$ as $t\to\mp\infty$, which acts trivially on the CM quantities. Similarly, $S = \mathbf{1}_{\rm CM}S_{\rm rel}$.

As we have already remarked, elastic two-body scattering is mathematically equivalent to scattering of a single particle with mass given by the reduced mass of the system in an external potential. Before studying this problem in detail in the next section, we want to spend a few words on more general scattering processes and the relative required generalisations of the formalism.

4.5 Multichannel scattering

The results discussed so far can be quite readily extended to describe elastic processes involving more than two particles. In this case, what one looks for are mappings between N-particle states obeying the free evolution, determined by the free N-particle Hamiltonian $H_0^{(N)}$, and states obeying the exact evolution determined by the interacting N-particle Hamiltonian $H^{(N)}$. The interacting Hamiltonian is usually of the form $H^{(N)} = H_0^{(N)} + \sum_{i<j} V_{ij}$, with V_{ij} the two-body interaction between particles i and j. These mappings are defined by the requirement that $e^{-iH^{(N)}t}|\Psi_\pm\rangle \sim e^{-iH_0^{(N)}t}|\Phi\rangle$ at large negative or positive times.

However, for such systems there are also new kinds of processes that can take place. Consider for example an idealised system of three particles, a, b, c, in which only a single bound state bc can form. For such a system, besides elastic scattering $a+b+c \to a+b+c$, one can consider the disintegration process $a+bc \to a+b+c$. Configurations of type $a+b+c$ and of type $a+bc$ are said to correspond to two different scattering channels of the system.

Let us focus on the disintegration process. The Hamiltonian reads $H^{a,b,c} = H_0^{a,b,c} + V_{ab} + V_{bc} + V_{ca}$. While the free asymptotic evolution of the final state is determined by the free three-particle Hamiltonian $H_0^{a,b,c}$, to describe the initial state we have to take into account also the interaction V_{bc} between b and c which keeps the state bc bound. This yields the channel Hamiltonian $H^{a,bc} = H_0^{a,b,c} + V_{bc}$, which, separating the motion of b and c into the corresponding center of mass and relative part, can be written as $H^{a,bc} = H_0^{a,bc} + H_{{\rm rel}\,bc}$. Here

[21] Here one should be careful in distinguishing the physical state and the state vector: observers in different frames will assign different state vectors to the same physical state, as they measure different values for the observables. Still, the transition probability between given physical states should not depend on the reference frame, and this is certainly the case if the amplitudes do not depend on which particular choice is made for the state vectors between the various equivalent possibilities (i.e., the various frames of reference).

$H_0^{a,bc}$ is the free two-body Hamiltonian for a and the center of mass of the bc system, and $H_{\mathrm{rel}\,bc}$ is the interacting Hamiltonian which describes the internal motion of the bound state. Moreover, the part of the asymptotic wave function of the system that depends on the relative coordinates must be precisely the eigenfunction of $H_{\mathrm{rel}\,bc}$ corresponding to the bc bound state. A state corresponding to this early-time behaviour must therefore evolve asymptotically like $e^{-iH^{a,b,c}t}|\psi\rangle \to e^{-iH_0^{a,bc}t}e^{-iE_{bc}t}|\phi_{bc}\rangle$ with $|\phi_{bc}\rangle$ of the type discussed above, for $t \to -\infty$. A similar reasoning can be made in the case when the final state is of type $a + bc$. States of the type $|\phi_{bc}\rangle$ form the channel subspace $\mathcal{S}_{a,bc} = \mathcal{S}_1$. For states which asymptotically look like a free three-particle state one has instead $e^{-iH^{a,b,c}t}|\psi\rangle \to e^{-iH_0^{a,b,c}t}|\phi\rangle$, with any $|\phi\rangle \in \mathcal{H}$. For uniformity of notation, we say that they form the channel subspace $\mathcal{S}_{a,b,c} = \mathcal{S}_0$, with channel Hamiltonian $H^{a,b,c}$.

The construction above can be easily generalised to any number of channels, with corresponding channel subspaces $\mathcal{S}_\alpha$ containing the possible corresponding asymptotes. One can then proceed and show the existence of isometric operators $\Omega_\pm^\alpha$, one for each channel, which map the asymptotes to the corresponding exact state. It is possible to show that $\mathcal{R}(\Omega_+^\alpha) \perp \mathcal{R}(\Omega_+^{\alpha'})$ for $\alpha \neq \alpha'$ and $\mathcal{R}(\Omega_+^\alpha) \perp \mathcal{B}$, and similarly for $\mathcal{R}(\Omega_-^\alpha)$: this is expected since states with asymptotes in different channels should be clearly different. For suitable potentials, one has furthermore that $\mathcal{H} = \oplus_\alpha \mathcal{R}(\Omega_+^\alpha) \oplus \mathcal{B} = \oplus_\alpha \mathcal{R}(\Omega_-^\alpha) \oplus \mathcal{B}$. One can now construct the channel S-matrix $S_{\alpha'\alpha} = \Omega_-^{\alpha'\dagger}\Omega_+^\alpha$, and express the scattering amplitudes as $S_{i,\alpha\to f,\alpha'} = \langle f, \alpha'|S_{\alpha'\alpha}|i, \alpha\rangle$. The final step is to define the space of asymptotic states $\mathcal{H}_{\mathrm{as}} = \oplus_\alpha \mathcal{S}_\alpha$ as the direct sum of the channel subspaces: an element $|\phi\rangle\!\rangle \in \mathcal{H}_{\mathrm{as}}$ is specified by a sequence $|\phi\rangle\!\rangle = \{|\phi, \alpha\rangle\}$, with $|\phi, \alpha\rangle \in \mathcal{S}_\alpha$. Correspondingly, one defines the operator $S : \mathcal{H}_{\mathrm{as}} \to \mathcal{H}_{\mathrm{as}}$ as

$$\langle\!\langle f|S|i\rangle\!\rangle \equiv \sum_{\alpha\alpha'} \langle f, \alpha'|S_{\alpha'\alpha}|i, \alpha\rangle \,, \tag{4.33}$$

and one finally shows that S is a unitary operator.

Except for this brief discussion, we will not be dealing with multichannel scattering in QM in these lectures, and we will focus on single-channel elastic scattering only. Although this is certainly far from covering all the possible experimental outcomes, nevertheless it allows to introduce all the main ideas. Besides this, it is not only of academic interest, since it can be consistently applied in low energy non-relativistic processes, when the energy is so low that it does not allow the breakup of bound states or the creation of new particles. Most of the results that we will derive are valid also in multichannel scattering after the appropriate generalisation, but deriving them in that case would cost a lot more in terms of fine details, and this is outside the purpose of these introductory lectures.

4.6 Cross section from the S-matrix

The last step we need to take before turning to the development of tools for the actual computation of scattering amplitudes is to establish the relation between the S-matrix elements and the experimentally observable cross sections. We will be dealing only with the most common experimental setup, namely two-particle scattering processes, but the results obtained here are valid for any kind of final state, i.e., both for single-channel and multi-channel scattering. Moreover, the derivation given below applies essentially unchanged to the relativistic case, with minor modifications due to the different normalisation usually chosen for the momentum eigenstates, and to the different relation between energy and momentum.

As we have already repeated *ad nauseam*, in a typical scattering experiment one fires a beam of particles against a fixed target or against another beam of particles. If the beams and the targets involved are sufficiently dilute, then only two particles at a time (if any) can effectively interact. The initial state of the relevant part of the system is thus a two-particle state $|\phi_1\,\phi_2\rangle$, which we take normalised to 1, $\langle\phi_1\,\phi_2|\phi_1\,\phi_2\rangle = 1$. The final state, corresponding to the information accessed through a detector, will be denoted by $|\Phi_f\rangle$, again with $\langle\Phi_f|\Phi_f\rangle = 1$. The transition probability corresponding to the activation of our detector reads therefore[22]

$$P_{i\to f} = |S_{fi}|^2 = |\langle\Phi_f|S|\phi_1\phi_2\rangle|^2\,. \tag{4.34}$$

Let us now go over to the momentum representation. For the initial state we have

$$|\phi_1\,\phi_2\rangle = \int d_3k_1 \int d_3k_2\,\phi_1(\vec{k}_1)\phi_2(\vec{k}_2)|\vec{k}_1\,\vec{k}_2\rangle\,, \qquad \int d_3k\,|\phi_i(\vec{k})|^2 = 1\,. \tag{4.35}$$

In a typical experiment, the wavefunctions $\phi_i(\vec{k})$ describe wave packets peaked with some small width Δp around some values $\vec{p}_i$ of the momenta, corresponding to the average (nominal) momenta of the particles produced by the accelerator. For a fixed target one obviously has $\vec{p}_{\rm target} = 0$. The uncertainty principle implies that these wave packets will be localised in space with typical length scale of the order of $\Delta x \sim 1/\Delta p$.[23] Detectors are usually devised to measure precisely the momenta of the outgoing products, so the corresponding state will be strongly peaked in momentum. We can therefore replace $|\Phi_f\rangle$ with a momentum eigenstate, provided we take into account the appropriate normalisation. It is a simple exercise to show that for a factorised state $|\Phi_f\rangle = \prod_n |\phi_f^{(n)}\rangle$, with $|\phi_f^{(n)}\rangle = \int d_3k\,\phi^{(n)}(\vec{k})|\vec{k}\rangle$ and wavefunctions of the form

$$\phi^{(n)}(\vec{k}) = \prod_{j=1}^{3}\left(\frac{2\pi}{\Delta_j^{(n)}}\right)^{\frac{1}{2}} \chi_{\left[p_j^{(n)}-\frac{\Delta_j^{(n)}}{2},p_j^{(n)}+\frac{\Delta_j^{(n)}}{2}\right]}(k_j)\,, \tag{4.36}$$

we obtain for the projector on $|\phi_f^{(n)}\rangle$ in the limit $\Delta_j^{(n)} \to 0$

$$\begin{aligned} |\phi_f^{(n)}\rangle\langle\phi_f^{(n)}| &= \left[\prod_{j=1}^{3}\left(\frac{\Delta_j^{(n)}}{2\pi}\right)\int_{-\frac{1}{2}}^{+\frac{1}{2}} d\kappa_j \int_{-\frac{1}{2}}^{+\frac{1}{2}} d\kappa'_j\right]\, |\vec{p}^{(n)} + \overrightarrow{(\Delta^{(n)}\kappa)}\rangle\langle\vec{p}^{(n)} + \overrightarrow{(\Delta^{(n)}\kappa')}| \\ &\to \left[\prod_{j=1}^{3}\left(\frac{\Delta_j^{(n)}}{2\pi}\right)\right]|\vec{p}^{(n)}\rangle\langle\vec{p}^{(n)}| = \frac{d^3p^{(n)}}{(2\pi)^3}|\vec{p}^{(n)}\rangle\langle\vec{p}^{(n)}|\,, \end{aligned} \tag{4.37}$$

where $(\Delta^{(n)}\kappa)_j = \Delta_j^{(n)}\kappa_j$, and in the last step we made $\Delta_j^{(n)}$ infinitesimal. Therefore

$$|\Phi_f\rangle\langle\Phi_f| \to \left[\prod_n \frac{d^3p^{(n)}}{(2\pi)^3}\right]\left(\otimes_n|\vec{p}^{(n)}\rangle\langle\vec{p}^{(n)}|\right) = dp_f|\vec{p}_f\rangle\langle\vec{p}_f|\,, \tag{4.38}$$

[22] At the present stage we have to *assume* that also in the relativistic case there esists a unitary operator S, whose matrix elements $\langle\Phi_f|S|\phi_1\phi_2\rangle$ determine the scattering amplitude for the transition between the given initial and final states.

[23] This need not be a large scale, since putting back factors of $\hbar$ one has $\Delta x \sim \hbar/\Delta p$.

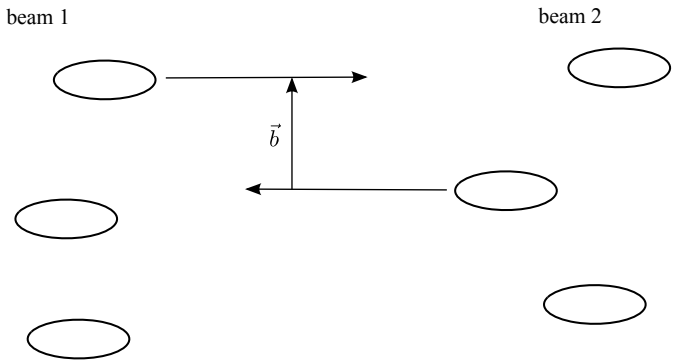

Figure 6: Schematic representation of the collision of two beams, showing the relative transverse displacement of wave packets.

where $\vec{p}_f$ denotes collectively the momenta of all the particles in the final state, and

$$dp_f \equiv \prod_n \frac{d^3p_n}{(2\pi)^3}\,, \qquad |\vec{p}_f\rangle \equiv \left(\otimes_n |\vec{p}^{\,(n)}\rangle\langle\vec{p}^{\,(n)}|\right)\,, \tag{4.39}$$

with products running over the particles in the final state. Finally, denoting with $\langle\vec{p}_f|S|\vec{k}_1\,\vec{k}_2\rangle$ the S operator in the momentum representation, we can write for the infinitesimal transition probability $dP_{i\to f}$

$$\begin{aligned} dP_{i\to f} = dp_f \int d_3k_1 \int d_3k_2 \int d_3k_1' \int d_3k_2'\ \phi_1(\vec{k}_1)\phi_2(\vec{k}_2)\phi_1(\vec{k}_1')^*\phi_2(\vec{k}_2')^* \\ \times \langle\vec{p}_f|S|\vec{k}_1\,\vec{k}_2\rangle\langle\vec{p}_f|S|\vec{k}_1'\,\vec{k}_2'\rangle^*\,. \end{aligned} \tag{4.40}$$

In principle, in order to compute any scattering amplitude it would now suffice to compute the matrix elements $\langle\vec{p}_f|S|\vec{k}_1\,\vec{k}_2\rangle$.[24] Unfortunately, the state of the system cannot be known with infinite precision, i.e., $\phi_i(\vec{k})$ are not known exactly: accelerators produce wave packets with reasonably well known average momenta and positions, but the details of the wave packets are unknown, and moreover fluctuate from packet to packet. The calculation of Eq. (4.40) is therefore out of reach. In any case, however, Eq. (4.40) does not really describe the probability that we can measure in an experiment, for we should actually average over the details of the wave packets. This seems to complicate things to a hopeless level, but in fact simplifies them quite a lot.

Among the properties of the wave packets, the one which is expected to affect the most the way the process develops is how they are displaced in the direction transverse to the beam velocity (their displacement along the beam is irrelevant), while their precise size and shape should not be as important. Let us therefore study in detail what are the consequences of averaging over the transverse displacement, which we denote by the vector $\vec{b}_i$. For this purpose we make explicit the dependence of the wave packets on $\vec{b}_i$, replacing $\phi_i(\vec{k}_i) \to \phi_i^{b_i}(\vec{k}_i) = e^{-i\vec{k}_i\cdot\vec{b}_i}\phi_i(\vec{k}_i)$.

[24] Although the terminology "matrix elements" is common, strictly speaking, and as we said above, this notation represents the S operator in the momentum representation, and not the matrix element of S corresponding to the given momentum (improper) eigenstate. If you do not appreciate the difference, then forgetting about this footnote will do you no harm - for the time being.

Denoting the distribution of the packets in the transverse plane as $n_i(\vec{b}_i)$ we have for the relevant probability

$$\begin{aligned} dP_{i\to f} = dp_f \int d^2b_1\, n_1(\vec{b}_1) \int d^2b_2\, n_2(\vec{b}_2) \int d_3k_1 \int d_3k_2 \int d_3k_1' \int d_3k_2' \\ \times\ \phi_1^{b_1}(\vec{k}_1)\phi_2^{b_2}(\vec{k}_2)\phi_1^{b_1}(\vec{k}_1')^*\phi_2^{b_2}(\vec{k}_2')^* \langle \vec{p}_f|S|\vec{k}_1\,\vec{k}_2\rangle\langle\vec{p}_f|S|\vec{k}_1'\,\vec{k}_2'\rangle^* \,. \end{aligned} \tag{4.41}$$

Exploiting translation invariance (and the fact that $|\vec{p}_f\rangle$ is a momentum eigenstate) we can also write ($\vec{b} = \vec{b}_1 - \vec{b}_2$)

$$\begin{aligned} dP_{i\to f} = dp_f \int d^2b_2\, n_2(\vec{b}_2) \int d^2b\, n_1(\vec{b}+\vec{b}_2) \int d_3k_1 \int d_3k_2 \int d_3k_1' \int d_3k_2' \\ \times\ \phi_1^{b}(\vec{k}_1)\phi_2(\vec{k}_2)\phi_1^{b}(\vec{k}_1')^*\phi_2(\vec{k}_2')^* \langle \vec{p}_f|S|\vec{k}_1\,\vec{k}_2\rangle\langle\vec{p}_f|S|\vec{k}_1'\,\vec{k}_2'\rangle^* \,. \end{aligned} \tag{4.42}$$

Particles in the beam and in the target are usually distributed uniformly within some area A, where therefore $n_i = \frac{N_i}{A}$. Furthermore, since the wave packets are spatially localised, there will be no overlap between ϕ_1^b and ϕ_2 when $|\vec{b}|$ is much larger than the interaction range and than the packet size, and the transverse size of the beam is typically much larger than this. This means that we can extend the integration over $\vec{b}$ to the whole transverse plane without appreciably changing the result. This yields at once

$$\begin{aligned} dP_{i\to f} &= dp_f \frac{N_1N_2}{A} \int d^2b \int d_3k_1 \int d_3k_2 \int d_3k_1' \int d_3k_2'\, e^{-i(\vec{k}_1-\vec{k}_1')\cdot\vec{b}} \\ &\quad\times\ \phi_1(\vec{k}_1)\phi_2(\vec{k}_2)\phi_1(\vec{k}_1')^*\phi_2(\vec{k}_2')^* \langle \vec{p}_f|S|\vec{k}_1\,\vec{k}_2\rangle\langle\vec{p}_f|S|\vec{k}_1'\,\vec{k}_2'\rangle^* \\ &= dp_f \frac{N_1N_2}{A} \int d_3k_1 \int d_3k_2 \int d_3k_1' \int d_3k_2'\, (2\pi)^2\delta_\perp^{(2)}(\vec{k}_1-\vec{k}_1') \\ &\quad\times\ \phi_1(\vec{k}_1)\phi_2(\vec{k}_2)\phi_1(\vec{k}_1')^*\phi_2(\vec{k}_2')^* \langle \vec{p}_f|S|\vec{k}_1\,\vec{k}_2\rangle\langle\vec{p}_f|S|\vec{k}_1'\,\vec{k}_2'\rangle^* \,. \end{aligned} \tag{4.43}$$

We now restrict our attention to (physically accessible) non-forward processes, i.e., to $|\vec{p}_f\rangle \neq |\vec{k}_1\,\vec{k}_2\rangle$. For our purposes it is convenient to set $S = \mathbf{1} + R$: since $S = \mathbf{1}$ in the absence of interactions, the first term corresponds to the amplitude for no scattering, while R accounts for the consequences of the interactions, and thus gives the amplitude for the particles being actually scattered. Clearly, for non-forward processes $S = R$. Recall now that S commutes with the Hamiltonian and with the total momentum, and therefore so does R. We account for this fact by writing

$$\langle \vec{p}_f|R|\vec{k}_1\,\vec{k}_2\rangle = i(2\pi)^4\delta(E_f - E)\delta^{(3)}(\vec{P}_f - \vec{K})M(\vec{k}_1,\vec{k}_2\to\vec{p}_f)\,. \tag{4.44}$$

where E_f and $\vec{P}_f$ are the final energy and total momentum, $\vec{K} = \vec{k}_1 + \vec{k}_2$ and $E = \frac{\vec{k}_1^{\,2}}{2m_1} + \frac{\vec{k}_2^{\,2}}{2m_2}$, and $M(\vec{k}_1,\vec{k}_2\to\vec{p}_f)$, is the "reduced" matrix element, which is expected to be some reasonable function, and to not contain any other delta function. The factor of i is chosen for future convenience. Taking this into account, we see that in Eq. (4.43) we have the product of delta functions

$$\begin{aligned} &(2\pi)^2\delta_\perp^{(2)}(\vec{k}_1-\vec{k}_1')(2\pi)^4\delta(E_f-E)\delta^{(3)}(\vec{P}_f-\vec{K})(2\pi)^4\delta(E_f-E')\delta^{(3)}(\vec{P}_f-\vec{K}\,') \\ &= (2\pi)^2\delta_\perp^{(2)}(\vec{k}_1-\vec{k}_1')(2\pi)^2\delta_\perp^{(2)}(\vec{k}_2-\vec{k}_2')2\pi\delta(E-E')2\pi\delta_\parallel(\vec{K}-\vec{K}\,') \\ &\quad\times (2\pi)^4\delta(E_f-\tfrac{E+E'}{2})\delta^{(3)}(\vec{P}_f-\tfrac{\vec{K}+\vec{K}\,'}{2})\,. \end{aligned} \tag{4.45}$$

Moreover,

$$E - E' = \frac{\vec{K}^{\,2}}{2M} - \frac{\vec{K}^{\,\prime 2}}{2M} + \frac{\vec{k}^{\,2}}{2m} - \frac{\vec{k}^{\,\prime 2}}{2m}\,, \tag{4.46}$$

where $\vec{k} = \frac{m_2\vec{k}_1 - m_1\vec{k}_2}{m_1 m_2}$ is the relative momentum (and similarly for $\vec{k}\,'$), M the total mass and m the reduced mass. The other delta functions impose that $\vec{K} = \vec{K}\,'$, and similarly for the transverse part of the relative momentum, so only the longitudinal reduced part remains. We then have to consider

$$\delta\left(\frac{k_\parallel^2}{2m} - \frac{k_\parallel^{\prime 2}}{2m}\right) = \frac{m}{k_\parallel}\left[\delta\left(k_\parallel - k_\parallel'\right) + \delta\left(k_\parallel + k_\parallel'\right)\right]\,. \tag{4.47}$$

We now recall that the wave functions are peaked around the average momenta of the particles. We can therefore drop the second term in Eq. (4.47), and get finally

$$\begin{aligned}\text{Eq. (4.45)} \to\ & (2\pi)^3\delta^{(3)}(\vec{k}_1 - \vec{k}_1')(2\pi)^3\delta^{(3)}(\vec{k}_2 - \vec{k}_2')(2\pi)^4\delta(E_f - \tfrac{E+E'}{2})\delta^{(3)}(\vec{P}_f - \tfrac{\vec{K}+\vec{K}\,'}{2}) \\ &= \frac{m}{k_\parallel}(2\pi)^3\delta^{(3)}(\vec{k}_1 - \vec{k}_1')(2\pi)^3\delta^{(3)}(\vec{k}_2 - \vec{k}_2')(2\pi)^4\delta(E_f - E)\delta^{(3)}(\vec{P}_f - \vec{K})\,.\end{aligned} \tag{4.48}$$

We can now carry out trivially the integration over the primed variables, and recalling that

$$dP_{i\to f} = d\sigma_{i\to f}\frac{N_1 N_2}{A} \tag{4.49}$$

we obtain

$$\begin{aligned}d\sigma_{i\to f} = dp_f \int d_3k_1 \int d_3k_2\,(2\pi)^4\delta(E_f - E)\delta^{(3)}(\vec{P}_f - \vec{K}) \\ \times\,|\phi_1(\vec{k}_1)|^2|\phi_2(\vec{k}_2)|^2\,\frac{m}{k_\parallel}|M(\vec{k}_1,\vec{k}_2 \to \vec{p}_f)|^2\,.\end{aligned} \tag{4.50}$$

The expression for $d\sigma_{i\to f}$ has simplified a lot, but we still need the details of the wave packets. However, recalling again that the wave functions are peaked around $\vec{p}_{1,2}$, we can approximate $\vec{K} \simeq \vec{P}_i = \vec{p}_1 + \vec{p}_2$ and $E \simeq \frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} = E_i$, and similarly $k_\parallel \simeq p_{i\parallel}$ for the relative momentum, where $\vec{p} = \frac{m_2\vec{p}_1 - m_1\vec{p}_2}{m_1 m_2}$. Moreover, if the matrix element near $\vec{p}_{1,2}$ varies slowly (on the scale set by the width of the packets), we can take it out of the integral and obtain

$$d\sigma_{i\to f} = d\Phi^{(f)}\,\frac{m}{p_i}|M(\vec{p}_1,\vec{p}_2 \to \vec{p}_f)|^2 \int d_3k_1\,|\phi_1(\vec{k}_1)|^2 \int d_3k_2\,|\phi_2(\vec{k}_2)|^2\,, \tag{4.51}$$

where we have used $p_{i\parallel} = p_i \equiv |\vec{p}_i|$, and we have defined the <u>phase space element</u>

$$d\Phi^{(f)} = \prod_{j=1}^{3}\frac{d^3p_j}{(2\pi)^3}(2\pi)^4\delta(E_f - E_i)\delta^{(3)}(\vec{P}_f - \vec{P}_i)\,. \tag{4.52}$$

The integration is now trivial and we finally get

$$\frac{d\sigma_{i\to f}}{d\Phi^{(f)}} = \frac{m}{p_i}|M(\vec{p}_1,\vec{p}_2 \to \vec{p}_f)|^2\,. \tag{4.53}$$

We thus see that if the wave packets are sufficiently peaked, their details actually drop out of the calculation, and averaging over shape and size becomes trivial. By sufficiently peaked we mean

that Δp is much smaller than the scale over which the matrix element varies appreciably. Going over to coordinate space and using the uncertainty principle, we therefore need that the size Δx be larger than the length scale over which the interaction changes appreciably; for short-range interactions this is usually the case.

Spin The are only little modifications required in the case of particles with spin being involved in the scattering process. For incoming particles in a definite spin state (i.e., with definite component of the spin in some direction) the momentum wavefunction spinor has the factorised form $\phi_{1,2}(\vec{k})\chi_{1,2\,s_{3\,1,2}}$. If we measure the spin of the final products of the process, the corresponding state contains the collective spinor $\xi_{f\,s_{3\,f}}$, where $s_{3\,f}$ denotes the third component of the spin of the final particles. The relevant transition probability reads

$$\begin{aligned} dP_{i\to f} = dp_f \int d^2b_1\, n_1(\vec{b}_1) \int d^2b_2\, n_2(\vec{b}_2) \int d_3k_1 \int d_3k_2 \int d_3k_1' \int d_3k_2' \\ \times\ \phi_1^{b_1}(\vec{k}_1)\phi_2^{b_2}(\vec{k}_2)\phi_1^{b_1}(\vec{k}_1')^*\phi_2^{b_2}(\vec{k}_2')^*\chi_{1\,s_{3\,1}}\chi_{2\,s_{3\,2}}\chi^*_{1\,s'_{3\,1}}\chi^*_{2\,s'_{3\,2}}\xi^*_{f\,s_{3\,f}}\xi_{f\,s'_{3\,f}} \\ \times\ \langle \vec{p}_f\, s_{3\,f}|S|\vec{k}_1\, s_{3\,1}\, \vec{k}_2\, s_{3\,2}\rangle\langle \vec{p}_f\, s'_{3\,f}|S|\vec{k}_1'\, s'_{3\,1}\, \vec{k}_2'\, s'_{3\,2}\rangle^* \,. \end{aligned} \tag{4.54}$$

Exactly the same line of reasoning allows to simplify the expression above in the case of peaked wave packets, and denoting the relevant S matrix elements as

$$\begin{aligned} \langle \vec{p}_f\, s_{3\,f}|S-\mathbf{1}|\vec{p}_1\, s_{3\,1}\vec{p}_2\, s_{3\,2}\rangle &= \langle \vec{p}_f\, s_{3\,f}|R|\vec{p}_1\, s_{3\,1}\vec{p}_2\, s_{3\,2}\rangle \\ &= i(2\pi)^4\delta(E_f-E_i)\delta^{(3)}(\vec{P}_f-\vec{P}_i)M(\vec{p}_1,s_{3\,1},\vec{p}_2,s_{3\,2}\to\vec{p}_f,s_{3\,f})\,, \end{aligned} \tag{4.55}$$

we find in this case that

$$\frac{d\sigma_{i\to f}}{d\Phi^{(f)}} = \frac{m}{p_i}\left|\sum_{s_{3\,1},s_{3\,2},s_{3\,f}} \chi_{1\,s_{3\,1}}\chi_{2\,s_{3\,2}}\xi^*_{f\,s'_{3\,f}} M(\vec{p}_1,s_{3\,1},\vec{p}_2,s_{3\,2}\to\vec{p}_f,s_{3\,f})\right|^2 . \tag{4.56}$$

This expression can be written more compactly using the formalism of the density matrix. Let ξ_i denote collectively the spin state of the initial set of particles, and let $\xi_{s_{3_f}}$ be the spin state corresponding to final particles with third components of the spin s_{3_f}. Let furthermore use matrix notation for M in spin space. Eq. (4.56) then becomes

$$\frac{d\sigma_{i\to f}}{d\Phi^{(f)}} = \frac{m}{p_i}|\xi^\dagger_{s_{3_f}} M\xi_i|^2 = \mathrm{tr}_{\,\mathrm{spin}}\,\xi_{s_{3_f}}\otimes\xi^\dagger_{s_{3_f}} M\xi_i\otimes\xi_i^\dagger M^\dagger\,. \tag{4.57}$$

For an incoherent superposition of spin states, the initial state is described by a density matrix $\rho_i=\sum_n w_n^i\xi_n\otimes\xi_n^\dagger$. One then has

$$\frac{d\sigma_{i\to f}}{d\Phi^{(f)}} = \frac{m}{p_i}\mathrm{tr}_{\,\mathrm{spin}}\,\xi_{s_{3_f}}\otimes\xi^\dagger_{s_{3_f}} M\rho_i M^\dagger = \frac{m}{p_i}\mathrm{tr}_{\,\mathrm{spin}}\,\xi_{s_{3_f}}\otimes\xi^\dagger_{s_{3_f}}\rho_f\,, \tag{4.58}$$

where $\rho_f\equiv M\rho_i M^\dagger$. It often happens in experiments that the spins of the particles in the final state are not observed. In this case one has to sum the expression above over such spins, and since $\sum_{s_{3\,f}}\xi_{s_{3_f}}\otimes\xi^\dagger_{s_{3_f}}=\mathbf{1}$, one finds

$$\left.\frac{d\sigma_{i\to f}}{d\Phi^{(f)}}\right|_{\text{sum over final spins}} = \frac{m}{p_i}\mathrm{tr}_{\,\mathrm{spin}}\,\rho_f\,. \tag{4.59}$$

In the case of unpolarised beams, the initial density matrix is proportional to the identity, $\rho_i = \frac{1}{(2s_1+1)(2s_2+1)}\mathbf{1}$, and the cross section further simplifies to

$$\left.\frac{d\sigma_{i\to f}}{d\Phi^{(f)}}\right|_{\substack{\text{sum over final spins}\\ \text{unpolarised beams}}} = \frac{1}{(2s_1+1)(2s_2+1)}\frac{m}{p_i}\mathrm{tr}_{\text{ spin}}\, MM^\dagger\,. \tag{4.60}$$

Relativistic case Eq. (4.53), together with the definition of phase space in Eq. (4.52), provide the desired relation between theoretically and experimentally accessible quantities in the non-relativistic case. The generalisation to the relativistic case is quite straightforward, and for this reason we discuss it now although we will not use it until much later. The first difference with the non-relativistic case is that in the relativistic theory, momentum eigenstates are usually chosen to satisfy the relativistic invariant normalisation

$$\text{(relativistic normalisation)} \qquad \langle\vec{p}\,'|\vec{p}\rangle = (2\pi)^3 2p^0\delta^{(3)}(\vec{p}\,'-\vec{p})\,. \tag{4.61}$$

With this choice one has to modify the completeness relations, substituting

$$d_3p \longrightarrow \frac{d^3p}{(2\pi)^3 2p^0} = \frac{d_3p}{2p^0}\,. \tag{4.62}$$

Finally, in Eq. (4.46) and (4.47) we have to use the relativistic expression for the energy, which leads to

$$E-E' = \sqrt{\vec{k}_1^{\,2}+m_1^2}+\sqrt{\vec{k}_2^{\,2}+m_2^2}-\sqrt{\vec{k}_1^{\,\prime 2}+m_1^2}-\sqrt{\vec{k}_2^{\,\prime 2}+m_2^2}\,. \tag{4.63}$$

The energy and longitudinal-momentum delta functions can be recast as

$$\delta(E-E')\delta(K_\parallel-K'_\parallel) = \left|\det\frac{\partial(E',K'_\parallel)}{\partial(k'_{1\parallel},k'_{2\parallel})}\right|^{-1}\delta(k'_{1\parallel}-\bar{k}_{1\parallel})\delta(k'_{2\parallel}-\bar{k}_{2\parallel})\,, \tag{4.64}$$

where $\bar{k}_{1,2\parallel}$ denote the solutions of the system of equations $E=E'$, $K_\parallel = K'_\parallel$. The delta functions of Eq. (4.45) force $K_\mu = K'_\mu = P_{f\mu}$, and so in the center-of-mass frame ($\vec{P}_f = 0$)

$$P_f = k_1+k_2 \Rightarrow (P_f-k_1)^2 = k_2^2 = m_2^2 \Rightarrow P_f^2+m_1^2-2E_fE_1 = m_2^2\,, \tag{4.65}$$

and since the same relation holds for E'_1,

$$E_1 = E'_1 = \frac{E_f^2+m_1^2-m_2^2}{2E_f}\,. \tag{4.66}$$

Since the transverse component of primed and unprimed momenta are equal, we find that $|k_{1\parallel}| = |k'_{1\parallel}|$ and $|k_{2\parallel}| = |k'_{2\parallel}|$ in the center-of-mass frame, and since the wave functions are peaked, only the case $k_{1\parallel} = k'_{1\parallel}$, $k_{2\parallel} = k'_{2\parallel}$ is relevant. We thus have $k_{1,2\mu} = k'_{1,2\mu}$ in the CM frame, and since the equation is covariant, this actually holds in any frame. After computing the Jacobian we can therefore replace Eq. (4.64) with

$$\delta(E-E')\delta(K_\parallel-K'_\parallel) \longrightarrow \left|\frac{k_{1\parallel}}{E_1}-\frac{k_{2\parallel}}{E_2}\right|^{-1}\delta(k'_{1\parallel}-k_{1\parallel})\delta(k'_{2\parallel}-k_{2\parallel})\,, \tag{4.67}$$

and thus obtain after carrying out the trivial integration over primed momenta

$$d\sigma_{i\to f} = dp_f \int d_3k_1 \int d_3k_2\, (2\pi)^4\delta^{(4)}(P_f - K)\, |4(k_{1\|}E_2 - k_{2\|}E_1)|^{-1} \\ \times |\phi_1(\vec{k}_1)|^2|\phi_2(\vec{k}_2)|^2|M(\vec{k}_1,\vec{k}_2 \to \vec{p}_f)|^2\,. \tag{4.68}$$

The rest of the calculation proceeds as before and yields

$$\frac{d\sigma_{i\to f}}{d\Phi^{(f)}_{\rm rel}} = \frac{1}{4I}|M(\vec{p}_1,\vec{p}_2 \to \vec{p}_f)|^2\,, \tag{4.69}$$

where $d\Phi^{(f)}_{\rm rel}$ is the element of relativistic phase space,

$$d\Phi^{(f)}_{\rm rel} = \prod_{j=1}^{3} \frac{d^3p_j}{(2\pi)^3 2p_j^0}(2\pi)^4\delta^{(4)}(P_f - P_i)\,, \tag{4.70}$$

and

$$I = E_1E_2v = |p_{1\|}E_2 - p_{2\|}E_1| = |\epsilon_{23\alpha\beta}p_1^\alpha p_2^\beta|\,, \tag{4.71}$$

where v is called the relative velocity, and it is indeed the velocity of one of the particles in the rest frame of the other [see Eqs. (2.14) and (2.15)]. The inclusion of spin is straightforward. By construction, $d\Phi^{(f)}_{\rm rel}$ and the matrix element are relativistically invariant (since S commutes with boosts). To make Eq. (4.69) manifestly invariant we notice that in the lab frame, since $E_2 = m_2$ and $\vec{p}_2 = 0$, we have

$$(P_1\cdot P_2)^2 - P_1^2P_2^2 = (E_1^2 - m_1^2)m_2^2 = \vec{p}_1^{\,2}m_2^2 = I^2\,, \tag{4.72}$$

see Eq. (2.15).

Two-body phase space To conclude this section, we now derive the explicit expression for the phase space element $d\Phi^{(2)}$ for a two-body state. In the non-relativistic case,

$$\begin{aligned} d\Phi^{(2)} &= d_3p_1d_3p_2(2\pi)^4\delta(\tfrac{\vec{p}_1^{\,2}}{2m_1} + \tfrac{\vec{p}_2^{\,2}}{2m_2} - E_i)\delta^{(3)}(\vec{p}_1 + \vec{p}_2 - \vec{P}_i) \\ &= d_3P_fd_3p_f(2\pi)^4\delta(\tfrac{\vec{p}_f^{\,2}}{2m_f} - \tfrac{\vec{p}_i^{\,2}}{2m_i})\delta^{(3)}(\vec{P}_f - \vec{P}_i) \\ &= d_3p_f\frac{2\pi m_f}{p_f}\delta(p_f - p_i\sqrt{\tfrac{m_f}{m_i}}) = \frac{d\Omega}{(2\pi)^2}m_fp_i\sqrt{\tfrac{m_f}{m_i}}\,, \end{aligned} \tag{4.73}$$

with $d\Omega$ the solid angle element $d\Omega = d\cos\theta d\phi$. For two-body$\to$ two-body processes we thus have

$$\frac{d\sigma_{2\to2}}{d\Omega} = \frac{m_im_f}{(2\pi)^2}\frac{p_f}{p_i}|M(\vec{p}_1,\vec{p}_2 \to \vec{p}_1',\vec{p}_2')|^2\,, \qquad p_f = \sqrt{\tfrac{m_f}{m_i}}p_i\,. \tag{4.74}$$

In the relativistic case

$$d\Phi^{(2)}_{\rm rel} = \frac{d_3p_1}{2p_1^0}\frac{d_3p_2}{2p_2^0}(2\pi)^4\delta^{(4)}(P_f - P_i)\,, \tag{4.75}$$

and we can perform the calculation in any reference frame thanks to Lorentz invariance. Things are especially simple in the CM frame, where $\vec{p}_1 + \vec{p}_2 = 0$. Integrating out $\vec{p}_2$ and setting $\vec{p}_{\rm CM} = \vec{p}_1$ and $p_{\rm CM} = |\vec{p}_{\rm CM}|$, we find

$$d\Phi^{(2)}_{\rm rel} = d_3p_{CM}\frac{1}{2p_1^02p_2^0}2\pi\delta(E_f - E_i) = \frac{d\Omega_{\rm CM}}{(2\pi)^2}\frac{p_{\rm CM}^2}{2p_1^02p_2^0}\left|\frac{\partial(p_1^0 + p_2^0)}{\partial p_{\rm CM}}\right|^{-1} = \frac{d\Omega_{\rm CM}}{16\pi^2}\frac{p_{\rm CM}}{E_{\rm CM}}\,. \tag{4.76}$$

For two-body→ two-body processes we thus have (recall that $I = E_{\rm CM} p_{\rm CM}$)

$$\frac{d\sigma_{2\to 2}}{d\Omega} = \frac{1}{64\pi^2 E_{\rm CM}^2} \frac{p'_{\rm CM}}{p_{\rm CM}} |M(\vec{p}_1, \vec{p}_2 \to \vec{p}_1', \vec{p}_2')|^2 \,. \tag{4.77}$$

4.7 The optical theorem

In this subsection we discuss an important consequence of the unitarity of S. As we did in the previous subsection, we show explicitly in S the "no scattering" term, i.e., the identity, by writing $S = \mathbf{1} + R$. The matrix element of S for forward scattering, i.e., for identical initial and final state, will receive contributions both from the case of no scattering, and from the case in which the particles actually interact but end up being in the same state. The two cases are experimentally indistinguishable, but nevertheless the forward matrix element of R can be obtained through extrapolation from the near-forward case. In the previous subsection we also conveniently used the momentum representation, and isolated an energy-conserving delta function and total-momentum-conserving delta functions from R, writing

$$S_{fi} = \delta_{fi} + i(2\pi)^4 \delta(E_f - E_i) \delta^{(3)}(\vec{P}_f - \vec{P}_i) M_{fi} \,, \tag{4.78}$$

where the numerical factor is chosen for convenience, and $E_{i,f}$ are the total energies in the initial and final state. Here we are using the shorthand notations $\delta_{fi} = \langle \{\vec{p}_f\} | \{\vec{p}_i\} \rangle$ and $S_{fi} = \langle \{\vec{p}_f\} | S | \{\vec{p}_i\} \rangle$, with $\{\vec{p}_{i,f}\}$ sets of momenta corresponding to the initial and final particles, and similarly $M_{fi} = M(\{\vec{p}_i\} \to \{\vec{p}_f\})$. From $S^\dagger S = \mathbf{1}$, and inserting a complete set of states, we find

$$\begin{aligned} \sum_n S^*_{nf} S_{ni} = \sum_n & [\delta_{fn} - i(2\pi)^4 \delta(E_f - E_n) \delta^{(3)}(\vec{P}_f - \vec{P}_n) M^*_{nf}] \\ & \times [\delta_{ni} + i(2\pi)^4 \delta(E_n - E_i) \delta^{(3)}(\vec{P}_n - \vec{P}_i) M_{ni}] = \delta_{fi} \,, \end{aligned} \tag{4.79}$$

and through simple manipulations

$$\begin{aligned} & (2\pi)^4 \delta(E_f - E_i) \delta^{(3)}(\vec{P}_f - \vec{P}_i) \\ & \qquad \times \left\{ i(M_{fi} - M^*_{if}) + \sum_n (2\pi)^4 \delta(E_n - E_i) \delta^{(3)}(\vec{P}_n - \vec{P}_i) M^*_{nf} M_{ni} \right\} = 0 \,. \end{aligned} \tag{4.80}$$

Focusing now on the term in braces and specialising to forward scattering $f = i$ we obtain

$$2 \,\mathrm{Im}\, M_{ii} = \sum_n (2\pi)^4 \delta(E_n - E_i) \delta^{(3)}(\vec{P}_n - \vec{P}_i) |M_{ni}|^2 \,. \tag{4.81}$$

The right-hand side is easily recognised to be proportional to the sum of the differential cross sections $\frac{d\sigma}{d\Phi^{(n)}}$ over the accessible final states n. More precisely, we find in the non-relativistic case

$$\mathrm{Im}\, M_{ii} = \frac{p_i}{2m} \sigma_i \,, \qquad \sigma_i = \frac{2m}{p_i} \mathrm{Im}\, M_{ii} \,. \tag{4.82}$$

In the relativistic case we have instead[25]

$$\mathrm{Im}\, M_{ii} = 2I\sigma_i = 2E_{\rm CM} p_{\rm CM} \sigma_i \,, \qquad \sigma_i = \frac{1}{2E_{\rm CM} p_{\rm CM}} \mathrm{Im}\, M_{ii} \,. \tag{4.83}$$

[25]The different mass dimension of the prefactor reflects the different dimensions of the matrix element when the non-relativistic or the relativistic normalisation is used for the momentum eigenstates.

The equations Eq. (4.81), (4.82) and (4.83) express the optical theorem.

An obvious consequence of the optical theorem is that, since $\sigma \geq 0$, the imaginary part of the forward amplitude M_{ii} must be positive.

4.8 Symmetries of the S-matrix

We now discuss in some details the consequences of symmetry for the S-matrix.

Rotations For a spinless particle, the effect of a proper rotation $R \in SO(3)$ on a momentum eigenstate is $U(R)|\vec{p}\rangle = |R\vec{p}\rangle$, where $U(R)$ is the unitary operator representing R on the Hilbert space $\mathcal{H}$. If R is a rotation of angle θ around the direction $\hat{\theta}$, then $U(R) = e^{i\vec{\theta}.\vec{J}}$ with $\vec{J}$ the total angular momentum operator and $\vec{\theta} = \theta\hat{\theta}$.[26] Denoting collectively with $\vec{p}_{i,f}$ the momenta in the initial and final states, for a system of spinless particles

$$\langle \vec{p}_f|S|\vec{p}_i\rangle = \langle \vec{p}_f|U(R)^\dagger S U(R)|\vec{p}_i\rangle = \langle R\vec{p}_f|S|R\vec{p}_i\rangle\,, \tag{4.84}$$

so that $\langle \vec{p}_f|S|\vec{p}_i\rangle$ must be a scalar function of the scalar combinations of the initial and final momenta. To make further progress, notice that S acts trivially on the CM part of the state, so that only the relative momenta have to be considered. For two-particle elastic scattering one is thus left only with the initial and final relative momenta, which moreover have the same magnitude due to conservation of energy. Rotation invariance implies then that the S-matrix element depends only on the magnitude p and on the relative angle $\theta \in [0, \pi]$ between the initial and final momenta. Since exchanging the initial and final relative momenta does not change neither p nor $\cos\theta$, one has that in this case $S_{fi} = \langle \vec{p}_f|S|\vec{p}_i\rangle = \langle \vec{p}_i|S|\vec{p}_f\rangle = S_{if}$. This can be seen also more directly by noticing that in the center of mass one can transform the sets $\vec{p}_i$ and $\vec{p}_f$ into each other by means of a rotation.

The situation is more complicated in the case of particles with spin. In this case the effect of a rotation on a momentum eigenstate is

$$U(R)|\vec{p}\, s_3\rangle = \mathscr{D}^{(s)}_{s_3' s_3}(R)|R\vec{p}\, s_3'\rangle \tag{4.85}$$

where $\mathscr{D}^{(s)}_{s_3' s_3}(R)$ is a unitary matrix, more precisely the representative of R in the spin-s representation of the rotation group. In general it has a complicated expression, but for a rotation of φ around the $\hat{3}$ direction one finds simply

$$U(R)|\vec{p}\, s_3\rangle = e^{i\varphi s_3}|R\vec{p}\, s_3\rangle\,. \tag{4.86}$$

The most important consequence of rotation invariance is that since the S-matrix commutes with energy and angular momentum, it will be diagonal in a basis where the energy and the angular momentum are diagonal. Considering for generality the multichannel case, we have[27]

$$\langle E'\, j'\, j_z'\,, \alpha'|S|E\, j\, j_z\,, \alpha\rangle = \delta_{j'j}\delta_{j_z' j_z} N(E)\delta(E' - E) S^j_{\alpha'\alpha}(E) \tag{4.87}$$

[26] We are using here the so-called *active* point of view on symmetry transformations: here $R\vec{p}$ is the result of an anticlockwise rotation of angle θ around $\hat{\theta}$ applied on the vector $\vec{p}$. In the *passive* point of view it is the reference frame to be rotated, and one can be easily convinced that $R_{\text{passive}}(\theta) = R_{\text{active}}(\theta)^{-1} = R_{\text{active}}(-\theta)$, so that the effect of the transformation on the states is implemented instead by $U(R)_{\text{passive}} = e^{-i\vec{\theta}.\vec{J}}$.

[27] For notational simplicity we drop the subscript α', α from the S operator.

where $N(E) = \frac{(2\pi)^3}{mp}$ has been factored out for convenience. As the notation indicates, $S^j_{\alpha'\alpha}(E)$ is independent of j_z: this is a consequence of the Wigner-Eckart theorem, and can also be verified explicitly using the fact that $[\vec{J}, S] = 0$. As a consequence of unitarity, the matrix $S^j(E)$ with entries $S^j_{\alpha'\alpha}(E)$ is a unitary matrix:

$$\begin{aligned}
\delta_{j'j}\delta_{j'_z j_z} N(E)\delta(E'-E)\delta_{\alpha'\alpha} &= \sum_{\bar{j}\,\bar{j}_z\,\bar{\alpha}} \int \frac{d\bar{E}}{N(\bar{E})} \langle E'\, j'\, j'_z\,, \alpha' | S^\dagger | \bar{E}\,\bar{j}\,\bar{j}_z\,, \bar{\alpha}\rangle \langle \bar{E}\,\bar{j}\,\bar{j}_z\,, \bar{\alpha} | S | E\, j\, j_z\,, \alpha\rangle \\
&= \sum_{\bar{j}\,\bar{j}_z} \int \frac{d\bar{E}}{N(\bar{E})} \delta_{j'\bar{j}}\delta_{j'_z\bar{j}_z} N(E')\delta(E'-\bar{E})\delta_{\bar{j}j}\delta_{\bar{j}_z j_z} N(E)\delta(E'-\bar{E}) S^{j'}_{\bar{\alpha}\alpha'}(E')^* S^j_{\bar{\alpha}\alpha}(E) \\
&= \delta_{j'j}\delta_{j'_z j_z} N(E)[\delta(E'-E) S^j(E)^\dagger S^j(E)]_{\alpha'\alpha}\,.
\end{aligned} \tag{4.88}$$

Parity The effect of parity, P, is to change momenta into $\vec{p} \to -\vec{p}$, and to leave the spin unchanged. Then

$$P|\vec{p}\, s_3\rangle = \eta | -\vec{p}\, s_3\rangle\,. \tag{4.89}$$

The phase is spin-independent, since $[P, \vec{S}] = 0$.[28] One then has

$$\langle \vec{p}_f\, s_{3\,f} | S | \vec{p}_i\, s_{3\,i}\rangle = \langle \vec{p}_f\, s_{3\,f} | P^\dagger S P | \vec{p}_i\, s_{3\,i}\rangle = \eta_i \eta_f^* \langle -\vec{p}_f\, s_{3\,f} | S | -\vec{p}_i\, s_{3\,i}\rangle\,. \tag{4.90}$$

Suppose we are interested in the average of some observable over the final state $|f\rangle$. An observable will be in general of the form $\mathcal{O} = \sum_m \mathcal{O}_m |m\rangle\langle m|$, where $\mathcal{O}$ are the eigenvalues of $\mathcal{O}$ and $|m\rangle$ are the corresponding eigenstates. The average $\langle\mathcal{O}\rangle_f$ we are interested in is then given by

$$\langle\mathcal{O}\rangle_f = \frac{\sum_m \mathcal{O}_m P_{i\to m}}{\sum_m P_{i\to m}\,,}\,, \tag{4.91}$$

where $P_{i\to m}$ is the transition probability from the initial state i to $|m\rangle$. If the initial state is an incoherent superposition of states $|n\rangle$ with weights w_n, then it is described by the density matrix $\rho_i = \sum_n w_n |n\rangle\langle n|$, and

$$P_{i\to m} = \sum_n w_n |\langle m|S|n\rangle|^2 = \mathrm{tr}\,|m\rangle\langle m| S\rho_i S^\dagger = \mathrm{tr}\,|m\rangle\langle m|\rho_f\,, \tag{4.92}$$

where $\rho_f \equiv S\rho_i S^\dagger$. We then find

$$\begin{aligned}
\langle\mathcal{O}\rangle_f &= \sum_m \mathcal{O}_m \sum_n w_n \langle m|S|n\rangle\langle n|S^\dagger|m\rangle = \sum_m \sum_n w_n \langle m|\mathcal{O}S|n\rangle\langle n|S^\dagger|m\rangle \\
&= \sum_m \langle m|\mathcal{O}S \left(\sum_n w_n |n\rangle\langle n|\right) S^\dagger|m\rangle = \mathrm{tr}\,\mathcal{O}S\rho_i S^\dagger = \mathrm{tr}\,\mathcal{O}\rho_f\,.
\end{aligned} \tag{4.93}$$

From this result we can costruct other kind of averages. For example we might be interested in averaging only over part of the possible momenta and spins. Denoting with $\Pi_f = \sum_m \pi_m |m\rangle\langle m|$ with $\pi_m = 0, 1$ the appropriate projector, the relevant average will read

$$\langle\langle\mathcal{O}\rangle\rangle_f = \frac{\mathrm{tr}\,\Pi_f \mathcal{O}\rho_f}{\mathrm{tr}\,\Pi_f \rho_f}\,. \tag{4.94}$$

[28] It is also p-independent since we are using momentum states for which $|\vec{p}\rangle = e^{-i\vec{q}\cdot\vec{p}}|\vec{0}\rangle$, and $P^\dagger \vec{q} P = -\vec{q}$. In the relativistic case the same holds, provided one uses the appropriate boost generator instead of the position operator $\vec{q}$.

Notice that if the subspace corresponding to Π_f is orthogonal to the subspace spanned by $\{|n\rangle\}$, then in Eq. (4.94) we can replace S with $S-1$ in the explicit expression for ρ_f. In the limit where the initial states are well-peaked wave packets in momentum space times some spin state, and the weights w_n correspond to a uniform beam of cross section A containing N_b particles, times the weights for the different spin components, one can carry on the derivation of section 4.6 and obtain

$$\mathrm{tr}\,\Pi_f\rho_f = \sum_m \pi_m d\Phi^{(f)} \frac{d\sigma_{i\to m}}{d\Phi^{(f)}} \Phi\Delta t N_t\,, \tag{4.95}$$

where $\frac{d\sigma_{i\to m}}{d\Phi^{(f)}}$ is the one of Eq. (4.56). From Eq. (4.91)

$$\langle\langle\mathcal{O}\rangle\rangle_f = \frac{\sum_m \mathcal{O}_m \pi_m d\Phi^{(f)} \frac{d\sigma_{i\to m}}{d\Phi^{(f)}} \Phi\Delta t N_t}{\sum_m \pi_m d\Phi^{(f)} \frac{d\sigma_{i\to m}}{d\Phi^{(f)}} \Phi\Delta t N_t} = \frac{\sum_m \mathcal{O}_m \pi_m \frac{d\sigma_{i\to m}}{d\Phi^{(f)}}}{\sum_m \pi_m \frac{d\sigma_{i\to m}}{d\Phi^{(f)}}}\,, \tag{4.96}$$

as it should be intuitively.[29]

Let us now consider a symmetry transformation U that leaves ρ_i invariant (it leaves S invariant as well since it is a symmetry). Then

$$\langle U^\dagger\mathcal{O}U\rangle_f = \mathrm{tr}\,U^\dagger\mathcal{O}U\rho_f = \mathrm{tr}\,\mathcal{O}U\rho_f U^\dagger = \mathrm{tr}\,\mathcal{O}\rho_f = \langle\mathcal{O}\rangle_f\,, \tag{4.97}$$

since

$$U\rho_f U^\dagger = US\rho_i S^\dagger U^\dagger = \rho_f\,. \tag{4.98}$$

The symmetry transformation we want to use is the composition of parity, P, and a rotation R_π of π around an axis orthogonal to the initial momentum $\vec{p}_i$ (we work in the CM or in the lab frame, where there is only one relevant direction for the initial momentum). Such a transformation leaves $\vec{p}_i$ invariant. If the cross section of the beams is symmetric under rotation around the beam directions, which we take along $\hat{3}$, and made of wave packets which are similarly symmetric under rotations around $\hat{3}$, then one sees that the momentum part of the initial density matrix is invariant under $U = R_\pi P$. In order to make the spin part invariant as well, we take the initial beams to be unpolarised: in this case the spin density matrix is a multiple of the identity, and so unaffected by rotations (it is not affected by parity at all).

Consider now the following observables,

$$\mathcal{O}_1 = |\vec{p}_f\rangle\langle\vec{p}_f|\vec{\mathbf{s}}_f\cdot\vec{p}_i\,,\qquad \mathcal{O}_2 = |\vec{p}_f\rangle\langle\vec{p}_f|\vec{\mathbf{s}}_f\cdot\vec{p}_f\,,\qquad \mathcal{O}_3 = |\vec{p}_f\rangle\langle\vec{p}_f|\vec{\mathbf{s}}_f\cdot\vec{p}_i\wedge\vec{p}_f\,, \tag{4.99}$$

where $|\vec{p}_f\rangle\langle\vec{p}_f|$ selects the momentum of one of the final particles to be equal to $\vec{p}_f$, $\vec{\mathbf{s}}_f$ is the spin operator for this particle, and $\vec{p}_i$ is the momentum of one of the two initial particles involved in the process. Let R_π be the rotation of π around the axis determined by $\vec{p}_i\wedge\vec{p}_f$. Then for $U = U(R_\pi)P$ we have that $R_\pi P\vec{p}_{i,f} = \vec{p}_{i,f}$, and so

$$U^\dagger\mathcal{O}_1 U = |R_\pi P\vec{p}_f\rangle\langle R_\pi P\vec{p}_f|(R_\pi P\vec{\mathbf{s}}_f)\cdot\vec{p}_i = |\vec{p}_f\rangle\langle\vec{p}_f|(-\vec{\mathbf{s}}_f\cdot\vec{p}_i) = -\mathcal{O}_1\,. \tag{4.100}$$

Similarly,

$$U^\dagger\mathcal{O}_2 U = -\mathcal{O}_2\,. \tag{4.101}$$

[29] We assumed here that $[\mathcal{O},\Pi_f]=0$. If not, then in Eq. (4.94) one should replace $\Pi_f\mathcal{O}\to\Pi_f\mathcal{O}\Pi_f$ in the numerator, and in Eq. (4.96) one has to replace $\mathcal{O}_m\to\overline{\mathcal{O}}_m\equiv\langle m|\mathcal{O}|m\rangle$.

On the other hand,

$$U^\dagger \mathcal{O}_3 U = |R_\pi P \vec{p}_f\rangle\langle R_\pi P \vec{p}_f|(R_\pi P \vec{\mathbf{s}}_f)\cdot \vec{p}_i \wedge \vec{p}_f = |\vec{p}_f\rangle\langle \vec{p}_f|\vec{\mathbf{s}}_f \cdot \vec{p}_i \wedge \vec{p}_f = \mathcal{O}_3\,. \tag{4.102}$$

From Eq. (4.97), we have therefore that for unpolarised beams $\langle \mathcal{O}_{1,2}\rangle_f = 0$, while $\langle \mathcal{O}_3\rangle_f$ can be nonzero: in other words, the polarisation of a particle in the final state can only be orthogonal to the scattering plane, i.e., the one spanned by $\vec{p}_i$ and $\vec{p}_f$ (Adair's argument).

Time reversal Time reversal is a particularly annoying symmetry, in that it is realised in the Hilbert space by an antiunitary operator rather than a unitary one. An antiunitary operator A is defined as follows. Recall that an antilinear operator is defined through the following relation,

$$A(\alpha|\psi\rangle + \beta|\phi\rangle) = \alpha^* A|\psi\rangle + \beta^*|\phi\rangle\,. \tag{4.103}$$

For an antilinear operator, the adjoint is defined via the relation

$$\langle \psi|A\phi\rangle = \langle A^\dagger \psi|\phi\rangle^*\,. \tag{4.104}$$

An antiunitary operator W is a norm-preserving antilinear operator which is onto $\mathcal{H}$. Norm-preservation together with Eq. (4.104) implies that W satisfies the identity

$$\langle W\psi|W\phi\rangle = \langle\psi|\phi\rangle^*\,. \tag{4.105}$$

This can be seen rewriting the scalar product $\langle\psi|\phi\rangle$ as a linear combination of the norms of appropriate vectors. In turn, Eq. (4.104) implies $W^\dagger W = \mathbf{1}$. Being onto, W satisfies also $WW^\dagger = \mathbf{1}$.

The time reversal operator T is defined as the antilinear operator realising

$$T|\vec{p}\, s_3\rangle = \eta_{s_3}|-\vec{p}\,-s_3\rangle\,, \tag{4.106}$$

so that $T^\dagger \vec{\mathbf{p}} T = -\vec{\mathbf{p}}$ and $T^\dagger \vec{\mathbf{s}} T = -\vec{\mathbf{s}}$. This time the phase η_{s_3} is spin dependent,[30] and a simple calculation shows that

$$\begin{aligned} T|\vec{p}\, s_3\rangle &= C^+_{s_3} T S^{s-s_3}_- |\vec{p}\, s\rangle = C^+_{s_3}(-1)^{s-s_3} S^{s-s_3}_+ T|\vec{p}\, s\rangle = \eta_s C^+_{s_3}(-1)^{s-s_3} S^{s-s_3}_+ |-\vec{p}\,-s\rangle \\ &= \eta_s (-1)^{s-s_3}\frac{C^+_{s_3}}{C^-_{-s_3}}|-\vec{p}\,-s_3\rangle = \eta_s(-1)^{s-s_3}|-\vec{p}\,-s_3\rangle\,, \end{aligned} \tag{4.107}$$

where $C^\pm_{s_3}$ are real positive constants satisfying

$$C^{\pm\,2}_{s_3} = \langle s_3|S^{s-s_3}_\pm S^{s-s_3}_\mp|s_3\rangle\,. \tag{4.108}$$

Since a rotation $R_\pi = e^{i\pi \mathbf{s}_2}$ gives $R_\pi|s_3\rangle = \zeta|-s_3\rangle$ for some phase factor ζ, then

$$\begin{aligned} {C^-_{-s_3}}^2 &= \langle -s_3|S^{s-s_3}_- S^{s-s_3}_+|-s_3\rangle = \langle s_3|R^\dagger_\pi S^{s-s_3}_- S^{s-s_3}_+ R_\pi|s_3\rangle \\ &= \langle s_3|(-S_+)^{s-s_3}(-S_-)^{s-s_3}|s_3\rangle = C^{+\,2}_{s_3}\,. \end{aligned} \tag{4.109}$$

[30] It still is p-independent: since we are using momentum states for which $T|\vec{p}\, s_3\rangle = Te^{-i\vec{q}\cdot\vec{p}}|\vec{0}\, s_3\rangle = e^{+i\vec{q}\cdot\vec{p}}T|\vec{0}\, s_3\rangle = e^{+i\vec{q}\cdot\vec{p}}\eta_{0,s_3}|\vec{0}\,-s_3\rangle$, since $T^\dagger \vec{q} T = \vec{q}$. In the relativistic case one has to use the transformation properties of the appropriate boost generator.

In conclusion,

$$\eta_{s_3} = \eta_s (-1)^{s-s_3} \,. \tag{4.110}$$

The remaining phase factor η_s is physically irrelevant, and can be redefined away: setting $|\vec{p}\, s_3\rangle = \zeta |\vec{p}\, s_3\,, \text{new}\rangle$, then

$$T|\vec{p}\, s_3\,, \text{new}\rangle = \zeta^* \eta_s (-1)^{s-s_3} |\vec{p}\, s_3\rangle = (\zeta^*)^2 \eta_s (-1)^{s-s_3} |\vec{p}\, s_3\,, \text{new}\rangle \,, \tag{4.111}$$

and we can choose $(\zeta^*)^2 \eta_s = 1$ so that η_s disappears.

If we ask our Hamiltonian to be invariant under time reversal, then since $T^\dagger U(t) T = U(-t)$ and $T^\dagger U_0(t) T = U_0(-t)$, one finds that

$$T^\dagger \Omega_\pm T = \Omega_\mp \Longrightarrow T^\dagger S T = T^\dagger \Omega_-^\dagger \Omega_+ T = T^\dagger \Omega_+^\dagger \Omega_- = S^\dagger \,. \tag{4.112}$$

It follows that the matrix elements obey

$$\begin{aligned} \langle T(\vec{p}_f\, s_{3\,f}) | S | T(\vec{p}_i\, s_{3\,i}) \rangle &= c_{s_{3\,f}, s_{3\,i}} \langle -\vec{p}_f\ - s_{3\,f} | S | -\vec{p}_i\ - s_{3\,i} \rangle = \langle \vec{p}_f\, s_{3\,f} | T^\dagger S T | \vec{p}_i\, s_{3\,i} \rangle^* \\ &= \langle \vec{p}_f\, s_{3\,f} | S^\dagger | \vec{p}_i\, s_{3\,i} \rangle^* = \langle \vec{p}_i\, s_{3\,i} | S | \vec{p}_f\, s_{3\,f} \rangle \,. \end{aligned} \tag{4.113}$$

In compact form $S_{Tf\,Ti} = S_{if}$, or equivalently $S_{fi} = S_{Ti\,Tf}$. This is sometimes referred to as the principle of detailed balance. Consider now a $2 \to 2$ scattering process. Since it is the absolute value square of the matrix elements that enters the cross section, one has from Eq. (4.74)

$$\frac{d\sigma_{fi}}{d\Omega} = \frac{m_i m_f}{(2\pi)^2} \frac{p_f}{p_i} |M_{fi}|^2 = \frac{m_i m_f}{(2\pi)^2} \left(\frac{p_f}{p_i}\right)^2 \frac{p_i}{p_f} |M_{Ti\,Tf}|^2 = \left(\frac{p_f}{p_i}\right)^2 \frac{d\sigma_{Ti\,Tf}}{d\Omega} \,. \tag{4.114}$$

If we sum over final spins and average over initial spins, then denoting with $\frac{d\bar{\sigma}}{d\Omega}$ the corresponding cross section and using Eq. (4.60) and Eq. (4.114) we find

$$(2s_{i\,1}+1)(2s_{i\,2}+1) \frac{d\bar{\sigma}_{fi}}{d\Omega} = (2s_{f\,1}+1)(2s_{f\,2}+1) \left(\frac{p_f}{p_i}\right)^2 \frac{d\sigma_{Ti\,Tf}}{d\Omega} \,, \tag{4.115}$$

i.e., from the ratio of the cross sections of the direct ($i \to f$) and inverse ($Tf \to Ti$) processes one obtains information on the spin of the particles involved:

$$\left(\frac{p_i}{p_f}\right)^2 \frac{\frac{d\bar{\sigma}_{fi}}{d\Omega}}{\frac{d\sigma_{Ti\,Tf}}{d\Omega}} = \frac{(2s_{f\,1}+1)(2s_{f\,2}+1)}{(2s_{i\,1}+1)(2s_{i\,2}+1)} \,. \tag{4.116}$$

This formula has been used to determine experimentally the spin of the pion: studying the processes $\pi^+ d \to p\,p$ and its inverse $p\,p \to \pi^+ d$, and knowing the spins of the proton and of the deuteron, the spin of the pion can be determined via Eq. (4.116).

5 The time-independent formalism

The time-dependent formalism developed in the previous section, based on the temporal evolution of physical states, has allowed a physically clear derivation of the S-matrix, the central quantity in scattering theory. However, it has not provided us with a practical recipe for calculating the S-matrix elements. This is provided instead by the time-independent approach, which

is based on the study of the positive-energy stationary solutions of the Schrödinger equation. These solutions are not normalisable, and therefore they do not represent physical states. In practice, however, they can be consistently treated in the same way as the momentum eigenfunctions, i.e., as a convenient basis for the representation of the physical (scattering) states.

As we will see, from a logical point of view the time-independent approach is not alternative to the time-dependent one, but it represents its natural development. As is often the case, this was not the way in which things developed historically.

5.1 In and out momentum states

The basis of the time-independent formalism is the construction of in and out states corresponding to the momentum eigenstates. One might immediately object that this is an ill-advised program. First of all, momentum eigenstates are not possible states of a physical system. Secondly, even if they were, they would yield in and out states that are stationary states of the full interacting Hamiltonian (as it follows from the intertwining relations, and as we will see below), and as such they could never develop into freely evolving states, since they do not develop at all. These objections are actually correct, but they should not intimidate you: although our derivation will be heuristic, we will be able to fully make sense of our results. Indeed, a rigorous formulation of the problem is possible, which shows that the results that we will obtain have a well-defined mathematical meaning: we will briefly comment on this point later. In any case, one has to keep in mind that the in and out momentum eigenstates are not really states of the system evolving asymptotically into (free) momentum eigenstates.

Consider as usual a system of two particles of masses m_1 and m_2, undergoing elastic scattering processes of the type $\vec{p}_1 + \vec{p}_2 \to \vec{p}_1' + \vec{p}_2'$, where the notation indicates explicitly the momenta of the particles. We can describe the process using center-of-mass and relative coordinates $\vec{P} = (\vec{p}_1 + \vec{p}_2)/M$ and $\vec{p} = (m_2\vec{p}_1 - m_1\vec{p}_2)/M$, where $M = m_1 + m_2$, and $m = m_1 m_2/M$ will denote the reduced mass of the system. As before, we assume that the system is in a factorised state $|\vec{P}\rangle_{\rm CM} \otimes |\phi\rangle_{\rm rel}$, and we ignore the trivial evolution of the CM part, focussing on the relative part only and dropping all subscripts for clarity.

We now proceed with the derivation. Recall that [see Eq. (4.22) and Eq. (4.23)]

$$\Omega_+ = \mathbf{1} - i\int_{-\infty}^{0} dt\, e^{iHt} V e^{-iH_0 t}\,, \qquad \Omega_- = \mathbf{1} + i\int_{0}^{+\infty} dt\, e^{iHt} V e^{-iH_0 t}\,. \tag{5.1}$$

Applying both sides of the equations on a state $|\phi\rangle$, and expanding in the momentum basis, we obtain

$$\Omega_\pm|\phi\rangle = \int d_3p\, |\vec{p}\rangle\langle\vec{p}|\phi\rangle + i\int_0^{\mp\infty} dt \int d_3p\, e^{iHt} V e^{-iH_0 t}|\vec{p}\rangle\langle\vec{p}|\phi\rangle\,. \tag{5.2}$$

For $|\phi\rangle$ with smooth and rapidly decreasing eigenfunction $\phi(\vec{x}) \in \mathscr{S}$, the integral over t is nicely convergent and does not change if we add a damping factor, i.e., for well-behaved functions $f(t)$

$$\int dt\, f(t) = \lim_{\epsilon\to 0}\int dt\, e^{-\epsilon|t|} f(t)\,. \tag{5.3}$$

Exchanging now the order of integration we find

$$\Omega_\pm|\phi\rangle = \int d_3p\, \left[\mathbf{1} + \lim_{\epsilon\to 0}\, i\int_0^{\mp\infty} dt\, e^{iHt} V e^{-iE_p t} e^{-\epsilon|t|}\right] |\vec{p}\rangle\langle\vec{p}|\phi\rangle\,, \tag{5.4}$$

with $E_p = \frac{\vec{p}^2}{2m}$. We now set

$$\begin{aligned} |\vec{p}\pm\rangle &\equiv |\vec{p}\rangle + \lim_{\epsilon\to 0} i\int_0^{\mp\infty} dt\, e^{iHt} V e^{-iE_p t} e^{-i(\pm i\epsilon)t} |\vec{p}\rangle \equiv \Omega_\pm(E_p)|\vec{p}\rangle \\ &= |\vec{p}\rangle + \lim_{\epsilon\to 0} \frac{1}{E_p - H \pm i\epsilon} V|\vec{p}\rangle = \lim_{\epsilon\to 0} \pm i\epsilon \frac{1}{E_p - H \pm i\epsilon}|\vec{p}\rangle\,, \end{aligned} \tag{5.5}$$

where we have defined the operators $\Omega_\pm(E_p)$, which depend explicitly on energy, and we have carried out the integration explicitly. Notice that $\Omega_\pm(E_p)$ involves operators that can be meaningfully applied on the momentum eigenfunctions. We see from Eq. (5.4) that

$$\Omega_\pm|\phi\rangle = \int d_3p\, \Omega_\pm(E_p)|\vec{p}\rangle\langle\vec{p}\,|\phi\rangle = \int d_3p\, |\vec{p}\pm\rangle\langle\vec{p}\,|\phi\rangle\,. \tag{5.6}$$

The states $|\vec{p}\pm\rangle$ are the in and out states corresponding to momentum eigenstates that we were looking for. For those who were still wondering about it, the signs of the $\pm i\epsilon$ term in Eq. (5.5) is the origin of the sign convention for $\Omega_\pm$. One mistery solved, now to explaining why neighbours like the sound of power drills in the morning.

We now discuss the properties of the states $|\vec{p}\pm\rangle$. First of all we show that they are normalised like momentum eigenstates. Indeed, since $\Omega_\pm$ are isometric, one has

$$0 = \langle\phi_1|\phi_2\rangle - \langle\phi_1\pm|\phi_2\pm\rangle = \int d_3p_1 \int d_3p_2\, \phi_1^*(\vec{p}_1)\phi_2(\vec{p}_2)\left[\langle\vec{p}_1|\vec{p}_2\rangle - \langle\vec{p}_1\pm|\vec{p}_2\pm\rangle\right]\,, \tag{5.7}$$

for any $\phi_{1,2}(\vec{p})$, and so

$$\langle\vec{p}_1\pm|\vec{p}_2\pm\rangle = \langle\vec{p}_1|\vec{p}_2\rangle = (2\pi)^3\delta^{(3)}(\vec{p}_1 - \vec{p}_2)\,. \tag{5.8}$$

This implies the formal relation

$$\Omega_\pm(E_{p'})^\dagger\Omega_\pm(E_p) = (2\pi)^3\delta^{(3)}(\vec{p}' - \vec{p})\,, \tag{5.9}$$

which is valid when sandwiched between the momentum states $|\vec{p}'\rangle$ and $|\vec{p}\rangle$. A similar reasoning leads to the following completeness relation for the states $|\vec{p}\pm\rangle$ in the scattering subspace $\mathcal{R}$:

$$\mathbf{1} = \int d_3p\, |\vec{p}\rangle\langle\vec{p}\,| \Longrightarrow \Omega_\pm\Omega_\pm^\dagger = \Pi_{\mathcal{R}} = \int d_3p\, \Omega_\pm(E_p)|\vec{p}\rangle\langle\vec{p}\,|\Omega_\pm(E_p)^\dagger = \int d_3p\, |\vec{p}\pm\rangle\langle\vec{p}\pm|\,. \tag{5.10}$$

We next show that the states $|\vec{p}\pm\rangle$ are stationary, i.e., eigenstates of the time-independent Schrödinger equation, with eigenvalue E_p, i.e., with the same energy as their asymptotes:[31] for this reason, we will refer to them as the in and out stationary states. The shortest proof would be based on the intertwining relations and goes $H|\vec{p}\pm\rangle = H\Omega_\pm(E_p)|\vec{p}\rangle = \Omega_\pm(E_p)H_0|\vec{p}\rangle = E_p|\vec{p}\pm\rangle$. However it is not clear if these relations hold, so it is better to proceed as above, applying the intertwining relation on a proper vector and expanding in the momentum basis:

$$H|\phi\pm\rangle = \int d_3p\, \phi(\vec{p})H|\vec{p}\pm\rangle = \Omega_\pm H_0|\phi\rangle = \Omega_\pm \int d_3p\, \phi(\vec{p})E_p|\vec{p}\rangle = \int d_3p\, \phi(\vec{p})E_p|\vec{p}\pm\rangle\,. \tag{5.11}$$

[31] Notice that "energy" corresponds to different Hamiltonians in the two cases.

This shows that the intertwining relations indeed hold also for $\Omega_\pm(E_p)$, $H\Omega_\pm(E_p) = \Omega_\pm(E_p)H_0$. A more direct proof is obtained from Eq. (5.5):

$$(H - E_p)|\vec{p}\pm\rangle = \lim_{\epsilon\to 0} \pm i\epsilon \left(-1 \pm i\epsilon \frac{1}{E_p - H \pm i\epsilon}\right)|\vec{p}\rangle = (\lim_{\epsilon\to 0} \pm i\epsilon)\,(|\vec{p}\pm\rangle - |\vec{p}\rangle) = 0\,. \tag{5.12}$$

Now the announced comment about rigour. The rigorous way to proceed would have been backwards: one should have shown that the states $|\vec{p}\pm\rangle$, as defined in the first line of Eq. (5.5), exist, satisfy the time-independent Schrödinger equation with energy E_p, and are properly normalised; that they can be used to expand any scattering (in or out) state $|\psi_\pm\rangle = \Omega_\pm|\phi\rangle$, in the same sense in which a function in L^2 is represented by its Fourier transform; and finally that the coefficients of the expansion of $|\psi_\pm\rangle$ in the basis $|\vec{p}\pm\rangle$ are the same as those of $|\phi\rangle$ in the basis $|\vec{p}\rangle$. All these things can actually be proved, and this justifies *a posteriori* our heuristic derivation (see [Reed & Simon], vol. 3, chapter XI).

The important point to retain from the discussion above is that the in and out momentum states make physical sense when (and only when) smeared by some momentum wavefunction $\phi(\vec{p})$: in that case they describe the scattering state of the system that evolves asymptotically in the wave packets of momentum eigenstates described by the same $\phi(\vec{p})$. Conversely, given the knowledge of the momentum eigenfunctions of the initial and final states of a scattering process, we can readily construct the relevant in and out states in terms of $|\vec{p}\pm\rangle$. Setting $\phi_{i,f}(\vec{p}) = \langle\vec{p}|\phi_{i,f}\rangle$ we can thus write for the S-matrix element[32]

$$\begin{aligned} S_{fi} = \langle\phi_f|S|\phi_i\rangle &= \int d_3p \int d_3p'\, \phi_i(\vec{p})\phi_f(\vec{p}')^*\langle\vec{p}'|S|\vec{p}\rangle \\ &= \int d_3p \int d_3p'\, \phi_i(\vec{p})\phi_f(\vec{p}')^*\langle\vec{p}'|\Omega_-^\dagger(E_{p'})\Omega_+(E_p)|\vec{p}\rangle \\ &= \int d_3p \int d_3p'\, \phi_i(\vec{p})\phi_f(\vec{p}')^*\langle\vec{p}'-|\vec{p}+\rangle\,. \end{aligned} \tag{5.13}$$

We conclude that formally one can write the suggestive relation

$$\langle\vec{p}'|S|\vec{p}\rangle = \langle\vec{p}'-|\vec{p}+\rangle\,. \tag{5.14}$$

Knowledge of the in and out stationary states thus guarantees the full knowledge of the S-matrix. In the remainder of this section we will see how one can actually compute the right-hand side of Eq. (5.14). In doing this one has to keep in mind that this quantity is not really a scalar product in our Hilbert space. Nevertheless, to obtain physical quantities this object is integrated over with suitable wave functions, and remembering this one can proceed with formal manipulations. In this sense, one has from Eq. (5.9)

$$\langle\vec{p}'|S|\vec{p}\rangle = \langle\vec{p}'|\mathbf{1} + [\Omega_-(E_{p'}) - \Omega_+(E_{p'})]^\dagger\Omega_+(E_p)|\vec{p}\rangle = \langle\vec{p}'|\mathbf{1} + [\Omega_-(E_{p'}) - \Omega_+(E_{p'})]^\dagger|\vec{p}+\rangle\,. \tag{5.15}$$

5.2 Green's operators, T-operator, and Lippmann-Schwinger equations

The study of Eq. (5.14) is made simpler by the introduction of certain energy-dependent operators. We begin by writing Eq. (5.5) as follows,

$$|\vec{p}\pm\rangle = \Omega_\pm(E_p)|\vec{p}\rangle = |\vec{p}\rangle + \lim_{\epsilon\to 0} G(E_p \pm i\epsilon)V|\vec{p}\rangle\,, \tag{5.16}$$

[32]Remember that we are considering here only the relative part of the S-matrix: a delta function conserving the total momentum of the system should multiply the expression below.

where $G(z)$ is the resolvent or Green's operator,

$$G(z) \equiv (z - H)^{-1}\,, \tag{5.17}$$

defined in general for complex $z \in \mathbb{C}$. For a generic operator O, the inverse $(z - O)^{-1}$ exists for those z not in the operator's spectrum. Since H is self-adjoint, its spectrum is real, and so $G(z)$ is certainly defined for all z such that $\mathrm{Im}\, z \neq 0$. In fact, in this case it is also analytic in z. The equation Eq. (5.16) is known as the Low equation, but it is of limited practical utility due to the appearance of the exact Green's operator $G(z)$, which is as difficult to compute as the spectrum of the full Hamiltonian.

In full analogy with Eq. (5.17), one can define the free Green's operator $G_0(z)$,

$$G_0(z) \equiv (z - H_0)^{-1}\,. \tag{5.18}$$

Since $H = H_0 + V$, one shows immediately that $G_0^{-1} - G^{-1} = V$, where we have dropped the dependence on z. Multiplying with G on the left and with G_0 on the right, and viceversa, one finds (Hilbert identity)

$$G - G_0 = GVG_0 = G_0VG\,. \tag{5.19}$$

Using this relation one can show that

$$(\mathbf{1} - G_0V)(\mathbf{1} + GV) = \mathbf{1} + (G - G_0)V - G_0VGV = \mathbf{1}\,. \tag{5.20}$$

We can thus recast the Low equation into the following alternative form,

$$|\vec{p}\pm\rangle = |\vec{p}\rangle + G_0(E_p \pm i\epsilon)V|\vec{p}\pm\rangle\,. \tag{5.21}$$

From now on the limit $\epsilon \to 0$ at the end of the calculation will be understood. This is the Lippmann-Schwinger equation for the stationary states. Since it is the free Green's operator appearing this time, one can use this equation to compute $|\vec{p}\pm\rangle$ iteratively:

$$|\vec{p}\pm\rangle = |\vec{p}\rangle + G_0(E_p \pm i\epsilon)V|\vec{p}\rangle + G_0(E_p \pm i\epsilon)VG_0(E_p \pm i\epsilon)V|\vec{p}\pm\rangle = \dots\,. \tag{5.22}$$

Similarly, from Eq. (5.19) we find the analogous equation

$$G = G_0 + G_0VG\,, \tag{5.23}$$

known as the Lippmann-Schwinger equation for G, which also allows a straightforward iterative approach to its solution.

We now use Eq. (5.16) to find a convenient expression for the matrix elements $\langle\vec{p}\,'|S|\vec{p}\rangle$ of Eq. (5.14). We have from Eq. (5.15)

$$\langle\vec{p}\,'|S|\vec{p}\rangle = \langle\vec{p}\,'|\vec{p}\rangle + \langle\vec{p}\,'|[\Omega_-(E_{p'}) - \Omega_+(E_{p'})]^\dagger\Omega_+(E_p)|\vec{p}\rangle\,, \tag{5.24}$$

and from Eq. (5.16)

$$\begin{aligned}[\Omega_-(E_{p'}) - \Omega_+(E_{p'})]|\vec{p}\rangle = [G(E_p - i\epsilon) - G(E_p + i\epsilon)]V|\vec{p}\rangle &= \frac{2i\epsilon}{(H - E_p)^2 + \epsilon^2}V|\vec{p}\rangle \\ &\equiv 2\pi i\delta_\epsilon(H - E_p)V|\vec{p}\rangle\,.\end{aligned} \tag{5.25}$$

We then find

$$\begin{aligned}\langle\vec{p}\,'|S|\vec{p}\rangle &= (2\pi)^3\delta^{(3)}(\vec{p}\,'-\vec{p}) - 2\pi i\langle\vec{p}\,'|V\delta_\epsilon(H-E_{p'})\Omega_+(E_p)|\vec{p}\rangle \\ &= (2\pi)^3\delta^{(3)}(\vec{p}\,'-\vec{p}) - 2\pi i\langle\vec{p}\,'|V\Omega_+(E_p)\delta_\epsilon(H_0-E_{p'})|\vec{p}\rangle \\ &= (2\pi)^3\delta^{(3)}(\vec{p}\,'-\vec{p}) - 2\pi i\delta_\epsilon(E_p-E_{p'})\langle\vec{p}\,'|V\Omega_+(E_p)|\vec{p}\rangle\,.\end{aligned} \tag{5.26}$$

In the last line the arguments of δ_ϵ are now c-numbers, and there is no problem in sending ϵ to zero, obtaining the usual Dirac delta. Using again Eq. (5.16), we see that $V\Omega_+(E_p) = V + VG(E_p+i\epsilon)V$, and if we now define the T-operator

$$T(z) = V + VG(z)V\,, \tag{5.27}$$

we conclude that

$$\langle\vec{p}\,'|S|\vec{p}\rangle = (2\pi)^3\delta^{(3)}(\vec{p}\,'-\vec{p}) - 2\pi i\delta(E_p-E_{p'})\langle\vec{p}\,'|T(E_p+i\epsilon)|\vec{p}\rangle\,. \tag{5.28}$$

It is straightforward to see that the T-matrix elements appearing in Eq. (5.28) are minus the "reduced" R-matrix elements of Eq. (4.78) in the case of two-body elastic scattering, i.e.,

$$M(\vec{p}\to\vec{p}\,') = -\lim_{\epsilon\to0}\langle\vec{p}\,'|T(E_p+i\epsilon)|\vec{p}\rangle = -\lim_{\epsilon\to0}\langle\vec{p}\,'|V|\vec{p}\pm\rangle\,. \tag{5.29}$$

The scattering amplitudes $M(\vec{p}\to\vec{p}\,')$ are thus the boundary values on the real axis of the matrix elements of the bounded analytic operator $T(z)$. We mention in passing that a straightforward application of Eq. (5.19) shows that T satisfies the equation

$$T(z) = V + VG_0(z)T(z)\,, \tag{5.30}$$

known as (guess what?) the Lippmann-Schwinger equation for T, which can be used to solve for T iteratively (you don't say?).

5.3 Asymptotic behaviour of the in states

We now make the decisive step in relating the scattering amplitudes with the positive-energy solutions of the Schrödinger equation. Expressing Eq. (5.21) in the coordinate representation, we find[33]

$$\psi_{p\pm}(\vec{x}) \equiv \langle\vec{x}\,|\vec{p}\pm\rangle = e^{i\vec{p}\cdot\vec{x}} + \int d^3x'\,\langle\vec{x}\,|\frac{1}{E_p-H_0\pm i\epsilon}|\vec{x}\,'\rangle V(\vec{x}\,')\psi_{p\pm}(\vec{x}\,')\,. \tag{5.31}$$

Expanding in the momentum basis, the matrix element of the Green's operator can be recast as

$$\begin{aligned}\langle\vec{x}\,|\frac{1}{E_p-H_0\pm i\epsilon}|\vec{x}\,'\rangle &= \int d_3p'\langle\vec{x}\,|\vec{p}\,'\rangle\langle\vec{p}\,'|\frac{1}{E_p-H_0\pm i\epsilon}|\vec{x}\,'\rangle \\ &= \int d_3p' e^{i\vec{p}\,'\cdot(\vec{x}-\vec{x}\,')}\frac{2m}{\vec{p}^{\,2}-\vec{p}\,'^2\pm i\epsilon} = \int d_3p' e^{i|\vec{p}\,'||\vec{x}-\vec{x}\,'|\cos\theta}\frac{2m}{\vec{p}^{\,2}-\vec{p}\,'^2\pm i\epsilon}\,.\end{aligned} \tag{5.32}$$

[33] Instead of $\psi_{p\pm}(\vec{x}\,')$, we should write $\langle\vec{x}\,'|\vec{p}\pm\rangle_\epsilon$ in the right-hand side, since the limit $\epsilon\to0$ has to be taken at the end of the calculation. However, since this limit exists for $\langle\vec{x}\,'|\vec{p}\pm\rangle_\epsilon$, we can replace this quantity with its limit $\psi_{p\pm}(\vec{x}\,')$.

Going over to polar coordinates and integrating over the angular variables we find

$$\begin{aligned}\langle\vec{x}\,|\frac{1}{E_p - H_0 \pm i\epsilon}|\vec{x}\,'\rangle &= \frac{2m}{(2\pi)^2 i}\frac{1}{|\vec{x}-\vec{x}\,'|}\int_0^\infty dp'\left(e^{ip'|\vec{x}-\vec{x}\,'|} - e^{-ip'|\vec{x}-\vec{x}\,'|}\right)\frac{p'}{p^2 - p'^2 \pm i\epsilon} \\ &= \frac{m}{2\pi^2 i}\frac{1}{|\vec{x}-\vec{x}\,'|}\int_{-\infty}^{+\infty} dp'\, e^{ip'|\vec{x}-\vec{x}\,'|}\frac{p'}{(p-p'\pm i\epsilon)(p+p'\pm i\epsilon)}\,.\end{aligned} \tag{5.33}$$

This integral can be computed using the residue theorem. Since $|\vec{x}-\vec{x}\,'|$ is positive, we can close the contour of integration in the upper half plane, thus picking the pole with positive imaginary part, i.e., $p' = \pm p + i\epsilon$. This finally yields

$$\langle\vec{x}\,|\frac{1}{E_p - H_0 \pm i\epsilon}|\vec{x}\,'\rangle = \frac{m}{2\pi^2 i}\frac{1}{|\vec{x}-\vec{x}\,'|}2\pi i e^{\pm ip|\vec{x}-\vec{x}\,'|}\frac{\mp p}{2p} = \mp\frac{m}{2\pi}\frac{1}{|\vec{x}-\vec{x}\,'|}e^{\pm ip|\vec{x}-\vec{x}\,'|}\,. \tag{5.34}$$

Plugging this into Eq. (5.31) we find

$$\psi_{p\pm}(\vec{x}) = e^{i\vec{p}\cdot\vec{x}} \mp \frac{m}{2\pi}\int d^3x'\,\frac{1}{|\vec{x}-\vec{x}\,'|}e^{\pm ip|\vec{x}-\vec{x}\,'|}V(\vec{x}\,')\psi_{p\pm}(\vec{x}\,')\,. \tag{5.35}$$

Let us focus now on $\psi_{p+}(\vec{x})$, and consider the limit of large $r \equiv |\vec{x}|$. For potentials with finite range (compact support, exponentials,...) this amounts to consider r much larger than such a range. Using

$$|\vec{x}-\vec{x}\,'| \simeq r - \hat{x}\cdot\vec{x}\,'\,, \tag{5.36}$$

where $\hat{x} = \vec{x}/r$, we obtain from Eq. (5.35)

$$\psi_{p+}(\vec{x}) = e^{i\vec{p}\cdot\vec{x}} - \frac{m}{2\pi}\frac{e^{ipr}}{r}\int d^3x'\,e^{-i\vec{p}\,'\hat{x}\cdot\vec{x}\,'}V(\vec{x}\,')\psi_{p+}(\vec{x}\,')\,, \tag{5.37}$$

where we have set $\vec{p}\,' = p\hat{x}$. But from Eqs. (5.26), (5.27) and (5.29) we know that

$$M(\vec{p}\to\vec{p}\,') = -\langle\vec{p}\,'|V|\vec{p}+\rangle = -\int d^3x'\,\langle\vec{p}\,'|\vec{x}\,'\rangle V(\vec{x}\,')\langle\vec{x}\,'|\vec{p}+\rangle = -\int d^3x'\,e^{-i\vec{p}\,'\cdot\vec{x}\,'}V(\vec{x}\,')\psi_{p+}(\vec{x}\,')\,, \tag{5.38}$$

and so comparing the two equations we see that

$$\psi_{p+}(\vec{x}) = e^{i\vec{p}\cdot\vec{x}} + \frac{m}{2\pi}\frac{e^{ipr}}{r}M(\vec{p}\to\vec{p}\,') = e^{i\vec{p}\cdot\vec{x}} + \frac{e^{ipr}}{r}f(p,\theta,\varphi)\,, \tag{5.39}$$

where

$$f(p,\theta,\varphi) \equiv \frac{m}{2\pi}M(\vec{p}\to\vec{p}\,') = -\frac{m}{2\pi}\langle\vec{p}\,'|T(E_p+i\epsilon)|\vec{p}\,\rangle\,. \tag{5.40}$$

We can now write down the final expression for the differential cross section in two-body elastic scattering. From Eq. (4.74) (using $p_f = \sqrt{\frac{m_f}{m_i}}p_i$ and $m_f = m_i$)

$$\frac{d\sigma_{2\to2}}{d\Omega} = \frac{m^2}{(2\pi)^2}|M(\vec{p}\to\vec{p}\,')|^2 = |f(p,\theta,\varphi)|^2\,. \tag{5.41}$$

The main conclusion is that the scattering amplitude, and therefore the differential cross section, are determined by the asymptotic, large-distance behaviour of the solution of the Schrödinger equation satisfying the following boundary condition: at large distances it looks like the sum

of a plane wave, corresponding to the incoming particle, and an outgoing spherical wave. The relative weight of the two terms determines the probability of detecting the particle scattered in a given direction.

This conclusion is actually not so surprising, as we now show, and in fact it would be the basis for the definition of cross section if the time-independent approach were taken as the fundamental one. This was the point of view when scattering theory was originally developed, with the time-dependent approach appearing later. Recall that a solution $\psi(t,\vec{x})$ of the time-dependent Schrödinger equation obeys the continuity equation

$$\frac{\partial}{\partial t}\rho(t,\vec{x}) + \vec{\partial}\cdot\vec{\jmath}(t,\vec{x}) = 0\,, \tag{5.42}$$

where

$$\rho(t,\vec{x}) = |\psi(t,\vec{x})|^2\,, \qquad \vec{\jmath}(t,\vec{x}) = \frac{1}{m}\mathrm{Im}\left[\psi(t,\vec{x})^*\vec{\partial}\psi(t,\vec{x})\right]. \tag{5.43}$$

This equation expresses the conservation of probability: if the probability to find the particle in an infinitesimal volume changes over time, then there must be a flux of probability crossing its surface. Therefore, as ρ gives the probability density, $\vec{\jmath}$ represents a probability current. Let us compute $\vec{\jmath}$ for a solution of the form Eq. (5.39). We have

$$\begin{aligned} m\vec{\jmath} &= \mathrm{Im}\,\psi^*\vec{\partial}\psi = \mathrm{Im}\left\{\left[e^{-i\vec{p}\cdot\vec{x}} + \frac{e^{-ipr}}{r}f^*\right]\left[i\vec{p}\,e^{i\vec{p}\cdot\vec{x}} + f\frac{e^{ipr}}{r}\left(ip-\frac{1}{r}\right)\frac{\vec{x}}{r} + \frac{e^{ipr}}{r}\vec{\partial}f\right]\right\} \\ &= \mathrm{Im}\left\{i\vec{p} + |f|^2\frac{1}{r^2}\left(ip-\frac{1}{r}\right)\frac{\vec{x}}{r} + e^{-i\vec{p}\cdot\vec{x}}f\frac{e^{ipr}}{r}\left(ip-\frac{1}{r}\right)\frac{\vec{x}}{r} + i\vec{p}\,e^{i\vec{p}\cdot\vec{x}}f^*\frac{e^{-ipr}}{r} + \right. \\ &\qquad\qquad \left. + e^{-i\vec{p}\cdot\vec{x}}\frac{e^{ipr}}{r}\vec{\partial}f + \frac{1}{r^2}f^*\vec{\partial}f\right\} \\ &= \vec{p} + |f|^2\frac{p}{r^2}\frac{\vec{x}}{r} + \mathrm{Im}\left\{e^{ipr(1-\cos\theta)}\left[\frac{f}{r}\left(ip-\frac{1}{r}\right)\frac{\vec{x}}{r} + i\vec{p}\,\frac{f^*}{r} + \frac{\vec{\partial}f}{r}\right] + \frac{1}{r^2}f^*\vec{\partial}f\right\}. \end{aligned} \tag{5.44}$$

The first term clearly represents the current corresponding to the incoming packet, which might also go unscattered. The flux of incoming particles is therefore $\vec{\jmath}_{\mathrm{in}} = \frac{\vec{p}}{m}$ (i.e., the velocity of the incoming particle).[34] The remainder $\vec{\jmath} - \vec{\jmath}_{\mathrm{in}}$ is made of two terms, namely

$$\vec{\jmath}_{\mathrm{scat}} = \frac{p}{m}\frac{|f|^2}{r^2}\hat{x}\,, \tag{5.45}$$

which represents a radially expanding wave, and an interference term $\vec{\jmath}_{\mathrm{int}} = \vec{\jmath} - \vec{\jmath}_{\mathrm{in}} - \vec{\jmath}_{\mathrm{scat}}$. We now show that this last term can be neglected. If we look at the system from a large distance R in direction $\hat{x}$ over a small solid angle $\Delta\Omega$, the flux of $\vec{\jmath}_{\mathrm{scat}}$ is R-independent and given by

$$\int_{\Delta\Omega} d\Omega\, R^2\vec{\jmath}_{\mathrm{scat}}\cdot\hat{x} = \int_{\Delta\Omega} d\Omega\frac{p}{m}|f|^2 \simeq \Delta\Omega\frac{p}{m}|f|^2\,. \tag{5.46}$$

[34] Since ψ is not normalisable, we cannot interpret the flux as given here as the probability that the particle crosses a unit area in a unit of time. In the real world the incoming particle is localised within some spatial region, so one could as well impose a spatial cutoff and substitute $\mathbb{R}^3$ with a finite cubic box of volume V. Momentum eigenfunctions would still look exactly the same (besides constraints on the allowed values of the momenta), but could be normalised to 1 simply by multiplying them by the factor $V^{-\frac{1}{2}}$. The current $\vec{\jmath}_{\mathrm{in}}$ would therefore be multiplied by V^{-1}, thus fully recovering its meaning of incoming flux of particles.

The flux of $\vec{\jmath}_{\rm int}$ that we observe is given instead by

$$\begin{aligned}
&\int_{\Delta\Omega} d\Omega\, R^2 m\vec{\jmath}_{\rm int}\cdot\hat{x}\\
&= mR\int_{\Delta\Omega} d\Omega\,{\rm Im}\left\{e^{ipR(1-\cos\theta)}\left[f\left(ip-\tfrac{1}{R}\right)+ip\cos\theta\, f+\frac{\partial f}{\partial r}\right]+\frac{1}{R}f^*\frac{\partial}{\partial r}f\right\} \qquad (5.47)\\
&\simeq mR\int_{\Delta\Omega} d\Omega\,{\rm Im}\left\{ipe^{ipR(1-\cos\theta)}f(1+\cos\theta)\right\},
\end{aligned}$$

where we used $\frac{\partial f}{\partial r}=0$, and we neglected a subleading term. For small $\Delta\Omega=\delta\varphi\delta\cos\theta$ we can bring f outside of the integral (assuming it is slowly varying), and get

$$\int_{\Delta\Omega} d\Omega\, R^2 m\vec{\jmath}_{\rm int}\cdot\hat{x}\simeq R\,{\rm Im}\left\{fe^{ipR}\left(ip-\frac{\partial}{\partial R}\right)\int_{\Delta\Omega} d\Omega\, e^{-ipR\cos\theta}\right\}. \qquad (5.48)$$

An integration by parts gives to leading order in R[35]

$$\begin{aligned}
&\int_{\Delta\Omega} d\Omega\, R^2 m\vec{\jmath}_{\rm int}\cdot\hat{x}\simeq -R\,{\rm Im}\left\{fe^{ipR}\left(ip-\frac{\partial}{\partial R}\right)\frac{\delta\varphi}{-ipR}e^{-ipR\cos\theta}\left(e^{-ipR\delta\cos\theta}-1\right)\right\}\\
&\simeq -{\rm Re}\left\{fe^{ipR}\frac{\delta\varphi}{p}\left(ip-\frac{\partial}{\partial R}\right)e^{-ipR\cos\theta}\left(e^{-ipR\delta\cos\theta}-1\right)\right\} \qquad (5.49)\\
&= -{\rm Re}\left\{ife^{ipR}\delta\varphi\left[(1+\cos\theta+\delta\cos\theta)e^{-ipR(\cos\theta+\delta\cos\theta)}-(1+\cos\theta)e^{-ipR\cos\theta}\right]\right\}.
\end{aligned}$$

Now we take into account that scattering processes actually involve wave packets, so that the current is obtain by folding Eq. (5.44) with some peaked wave function. In practice, this corresponds to integrating Eq. (5.44) over a small shell of momenta with $|\vec{p}|\in[p-\frac{\delta p}{2},p+\frac{\delta p}{2}]$. The contribution from Eq. (5.49) is

$$\begin{aligned}
&4\pi\int_{p-\frac{\delta p}{2}}^{p+\frac{\delta p}{2}} dp'\,p'^2\int_{\Delta\Omega} d\Omega\, R^2 m\vec{\jmath}_{\rm int}\cdot\hat{x}\\
&\simeq -4\pi{\rm Re}\left\{if\delta\varphi\int_{p-\frac{\delta p}{2}}^{p+\frac{\delta p}{2}} dp'\,p'^2\,\left[(2-A(\theta))e^{ip'RA(\theta)}-(2-B(\theta))e^{ip'RB(\theta)}\right]\right\} \qquad (5.50)\\
&= 4\pi\frac{\partial^2}{\partial R^2}{\rm Re}\left\{if\delta\varphi\int_{p-\frac{\delta p}{2}}^{p+\frac{\delta p}{2}} dp'\,\left[\frac{2-A(\theta)}{A(\theta)^2}e^{ip'RA(\theta)}-\frac{2-B(\theta)}{B(\theta)^2}e^{ip'RB(\theta)}\right]\right\}
\end{aligned}$$

where $A(\theta)=1-\cos\theta-\delta\cos\theta$ and $B(\theta)=1-\cos\theta$. Performing the integration, we have to leading order

$$\begin{aligned}
&\int_{p-\frac{\delta p}{2}}^{p+\frac{\delta p}{2}} dp'\,p'^2\int_{\Delta\Omega} d\Omega\, R^2 m\vec{\jmath}_{\rm int}\cdot\hat{x}\\
&\simeq \frac{1}{R}{\rm Re}\left\{f\delta\varphi\frac{\partial^2}{\partial R^2}\left[\frac{2-A(\theta)}{A(\theta)^3}\left(e^{iRA(\theta)(p+\frac{\delta p}{2})}-e^{iRA(\theta)(p-\frac{\delta p}{2})}\right)\right.\right. \qquad (5.51)\\
&\qquad\left.\left.-\frac{2-B(\theta)}{B(\theta)^3}\left(e^{iRB(\theta)(p+\frac{\delta p}{2})}-e^{iRB(\theta)(p-\frac{\delta p}{2})}\right)\right]\right\}.
\end{aligned}$$

[35]Notice that the integral in θ reads $\int_{\cos\theta-\delta\cos\theta}^{\cos\theta} d(\cos\theta)'$.

After this long and undeservedly detailed calculation we finally get to the main point: the contribution of the interference term to physical quantities vanishes like $1/R$ at large distance. This is true as long as we are not looking in the forward direction, for in that case the last line of Eq. (5.50) does not follow: in this case one gets instead

$$\begin{aligned}
&\int_{\Delta\Omega(\theta=0)} d\Omega\, R^2 m\vec{\jmath}_{\rm int}\cdot\hat{x} \simeq -{\rm Re}\left\{if\delta\varphi\left[(2+\delta\cos\theta)e^{-ipR\delta\cos\theta}-2\right]\right\}\,,\\
&4\pi\int_{p-\frac{\delta p}{2}}^{p+\frac{\delta p}{2}} dp'\,p'^2\int_{\Delta\Omega} d\Omega\, R^2 m\vec{\jmath}_{\rm int}\cdot\hat{x} \simeq -{\rm Re}\left\{-2if\delta\varphi\frac{4\pi\delta p^3}{3}\Big|_{p-\frac{\delta p}{2}}^{p+\frac{\delta p}{2}}\right\} = -2\delta\varphi{\rm Im}\, f\cdot 4\pi\delta p\,,
\end{aligned} \tag{5.52}$$

the only contribution in the large-R limit coming from the second term in square brackets in the first line. For this reason, this contribution is independent of $\delta\cos\theta$; moreover, since for any other θ one gets no contribution from the interference term, one can extend the integration over the whole polar angle without changing the result. If one extends the integration also to the whole range of the azimuthal angle, one gets for the first line above

$$\int d\Omega\, R^2\vec{\jmath}_{\rm int}\cdot\hat{x} \simeq -\frac{4\pi}{m}\,{\rm Im}\left\{f\left[1-(1+\tfrac{1}{2}\delta\cos\theta)e^{-ipR\delta\cos\theta}\right]\right\}\to -\frac{4\pi}{m}\,{\rm Im}\, f\,, \tag{5.53}$$

having dropped the oscillating term since it does not contribute after integrating over the momenta.

We thus have that at large distance the flux of scattered particles will be simply given by[36] $\vec{\jmath}_{\rm scat}$. Since we are dealing with a stationary solution, the physical situation that is being represented is that of a steady flux of incoming particles, plus a steady flux of scattered particles. Recalling Eq. (2.5), we see that their ratio (times the area of the detector) gives the number of events per unit time, unit flux and unit target, i.e., the cross section. For infinitesimal detectors we have

$$d\sigma = \frac{\vec{\jmath}_{\rm scat}\cdot\hat{x}R^2 d\Omega}{|\vec{\jmath}_{\rm in}|} = \frac{\frac{p}{m}|f|^2}{\frac{p}{m}}d\Omega = |f|^2 d\Omega\,, \tag{5.54}$$

i.e., $|f|^2$ is the differential cross section.

It is worth writing down explicitly the optical theorem in the case at hand. Recalling that $M=\frac{2\pi}{m}f$, we have from Eq. (4.82) (the choice $\varphi=0$ is of course arbitrary at $\theta=0$)

$${\rm Im}\, f(p,0,0) = \frac{p}{4\pi}\sigma\,,\qquad \sigma = \frac{4\pi}{p}{\rm Im}\, f(p,0,0)\,. \tag{5.55}$$

From Eq. (5.41) we then have

$${\rm Im}\, f(p,0,0) = \frac{p}{4\pi}\int d\Omega\,|f(p,\theta,\varphi)|^2\,. \tag{5.56}$$

This result can be rederived from Eqs. (5.45), (5.53) and (5.54), and from the fact that the probability current $\vec{\jmath}=\vec{\jmath}_{\rm in}+\vec{\jmath}_{\rm scat}+\vec{\jmath}_{\rm int}$ is conserved, $\nabla\cdot\vec{\jmath}=0$. Indeed, integrating the divergence of $\vec{\jmath}$ inside a sphere of (large) radius R we get

$$0 = \int_R d^3x\,\nabla\cdot\vec{\jmath} = \int d\Omega\, R^2\,\hat{x}\cdot(\vec{\jmath}_{\rm in}+\vec{\jmath}_{\rm scat}+\vec{\jmath}_{\rm int})\,. \tag{5.57}$$

[36] The same discussion made in footnote 34 applies also here: in a finite box $\vec{\jmath}_{\rm scat}$ would be multiplied by V^{-1}, recovering its usual meaning. Since the volume factors cancel out in the ratio, Eq. (5.54) below would not change.

Since the incoming flux gives no contribution (since $\int d\Omega \cos\theta = 0$), in the limit of large R one gets from the other two terms

$$0 = \int d\Omega \left[\frac{p}{m}|f|^2 - \frac{4\pi}{m}\,\mathrm{Im}\, f\right] = \frac{1}{m}\left\{p\int d\Omega \left[\frac{d\sigma}{d\Omega} - 4\pi\,\mathrm{Im}\, f\right]\right\} = \frac{1}{m}\left\{p\sigma_{\mathrm{tot}} - 4\pi\,\mathrm{Im}\, f\right\}\,, \quad (5.58)$$

which is again the optical theorem.

One last comment on the dependence of f on the direction of observation. When the potential is central, i.e., invariant under rotations, we have from the transformation law $U_R|\vec{p}\rangle = |\vec{p}_R\rangle$ and from the definition $|\vec{p}+\rangle = \Omega_+|\vec{p}\rangle$ that

$$U_R|\vec{p}+\rangle = U_R\Omega_+|\vec{p}\rangle = \Omega_+ U_R|\vec{p}\rangle = \Omega_+|\vec{p}_R\rangle = |\vec{p}_R+\rangle\,. \quad (5.59)$$

In the case of rotations around the direction of $\vec{p}$, i.e., $R\vec{p} = \vec{p}$, we thus find $|\vec{p}_R+\rangle = |\vec{p}+\rangle$, and therefore $\psi_{p+}(\vec{x}_R) = \psi_{p+}(\vec{x})$. It then follows that

$$\begin{aligned} f &= -\frac{m}{2\pi}\int d^3x'\, e^{-ip\hat{x}\cdot\vec{x}'} V(|\vec{x}'|)\psi_{p+}(\vec{x}') = -\frac{m}{2\pi}\int d^3x'\, e^{-ip\hat{x}_R\cdot\vec{x}'_R} V(|\vec{x}'|)\psi_{p+}(\vec{x}') \\ &= -\frac{m}{2\pi}\int d^3x'\, e^{-ip\hat{x}_R\cdot\vec{x}'} V(|\vec{x}'|)\psi_{p+}(\vec{x}')\,, \end{aligned} \quad (5.60)$$

i.e., $f = f(p,\theta)$.

5.4 The Born approximation

In the previous subsection we have seen how the calculation of scattering amplitudes reduces to solving the Schrödinger equation with a specific boundary conditions. This is no easy task, and solutions in closed form are known only for a limited number of potentials. In the general case we therefore have to rely on approximation techniques, a very common situation in physics. An obvious possibility is to solve the equations numerically, but it is nevertheless very useful to have also analytic approximation techniques.

The prototype of analytic approximations is the expansion of the quantities of interest in powers of some small numbers, most commonly the overall strength of the potential. In our case we want to solve the Lippmann-Schwinger equation Eq. (5.21), which can be written in compact form as

$$|\vec{p}+\rangle = (\mathbf{1} + G^+V)|\vec{p}\rangle\,, \quad (5.61)$$

where G^+ is a shorthand for $G(E_p + i\epsilon)$. Using equation Eq. (5.20) we can write this in terms of $G_0^+ = G_0(E_p + i\epsilon)$ as

$$|\vec{p}+\rangle = (\mathbf{1} - G_0^+V)^{-1}|\vec{p}\rangle\,. \quad (5.62)$$

If G_0^+V is suitably small, in a sense to be better specified below, we can expand this equation as

$$|\vec{p}+\rangle = \sum_{n=0}^{\infty}(G_0^+V)^n|\vec{p}\rangle\,. \quad (5.63)$$

This equation defines the Born series for the scattering states $|\vec{p}+\rangle$. In the same spirit, denoting $T = T(E_p + i\epsilon)$, we can rewrite Eq. (5.30) as

$$(\mathbf{1} - VG_0^+)T = V \Rightarrow T = (\mathbf{1} - VG_0^+)^{-1}V = \left(\sum_{n=0}^{\infty} VG_0^+\right)V\,. \quad (5.64)$$

This is the Born series for the T-matrix. To lowest orders we have

$$T = V + VG_0^+V + VG_0^+VG_0^+V + \dots ; \tag{5.65}$$

the first term $T \simeq V$ is the Born approximation for T. From Eq. (5.39) we thus have

$$\begin{aligned} f(p,\theta,\varphi) \simeq f_B(p,\theta,\varphi) &= -\frac{m}{2\pi}\langle p\hat{x}|V|\vec{p}\rangle = -\frac{m}{2\pi}\int d^3x' e^{i(\vec{p}-p\hat{x})\cdot\vec{x}'}V(\vec{x}') \\ &= -\frac{m}{2\pi}\int d^3x' e^{-i\vec{q}\cdot\vec{x}'}V(\vec{x}')\,, \end{aligned} \tag{5.66}$$

i.e., f_B is the Fourier transform of the potential at $-\vec{q}$, with $\vec{q} = \vec{p}' - \vec{p} = p\hat{x} - \vec{p}$ the transferred momentum. For central potentials

$$f(p,\theta) \simeq -m\int_0^\infty dr r^2 \int_{-1}^{+1} dz\, e^{-iqrz}V(r) = -\frac{2m}{q}\int_0^\infty dr\, r \sin qr\, V(r)\,. \tag{5.67}$$

One has for $q = |\vec{q}|$

$$q^2 = 2p^2(1-\cos\theta) = 4p^2\sin^2\tfrac{\theta}{2}\,, \tag{5.68}$$

where $\cos\theta = \hat{p}\cdot\hat{x}$ is the cosine of the angle between the beam velocity and the direction of observation. A few comments are in order.

1. The last integral in Eq. (5.67) is convergent for V decaying at least as $V \sim r^{-1-\epsilon}$ at large r, and V no more singular than $V \sim r^{-3+\epsilon}$ at the origin.

2. For small q,
$$\frac{1}{q}\int_0^\infty dr\, r \sin qr\, V(r) \to \int_0^\infty dr\, r^2 V(r)\,, \tag{5.69}$$
if the latter integral is convergent: this requires V to vanish at least as $V \sim r^{-(3+\epsilon)}$ at large r. In this case f_B becomes isotropic if p is small.

3. To study the large q behaviour, we write $[\tilde{V}(r) = rV(r)]$
$$\begin{aligned} \int_0^\infty dr\, \sin qr\, \tilde{V}(r) &= \int_0^\epsilon dr\, \sin qr\, \tilde{V}(r) + \int_\epsilon^\infty dr\, \sin qr\, \tilde{V}(r) \\ &= \int_0^\epsilon dr\, \sin qr\, \tilde{V}(r) + \frac{1}{q}\cos q\epsilon\, \tilde{V}(\epsilon) + \frac{1}{q}\int_\epsilon^\infty dr\, \cos qr\, \tilde{V}'(r)\,, \end{aligned} \tag{5.70}$$
with some small ϵ. Assuming that $\tilde{V}$ vanishes faster than $1/r$ at large r, we have
$$\left|\int_\epsilon^\infty dr\, \cos qr\, \tilde{V}'(r)\right| \le \int_\epsilon^\infty dr\, |\tilde{V}'(r)| < \infty\,, \tag{5.71}$$
so the last two terms in the second line of Eq. (5.70) are of order q^{-1}. If $\tilde{V}$ is regular at the origin we can set ϵ to 0, and find that $f_B \sim q^{-2}$ at large q. If it diverges like $r^{-\alpha}$ with $0 < \alpha < 2$, taking ϵ sufficiently small we can approximate the first term in the second line of Eq. (5.70) as
$$\begin{aligned} \int_0^\epsilon dr\, \sin qr\, \tilde{V}(r) \simeq C\int_0^\epsilon \frac{dr}{r^\alpha}\, \sin qr\, &= Cq^{\alpha-1}\int_0^{\epsilon q}\frac{dx}{x^\alpha}\sin x \\ &\underset{q\to\infty}{\to} Cq^{\alpha-1}\int_0^\infty \frac{dx}{x^\alpha}\sin x\,, \end{aligned} \tag{5.72}$$

the latter integral being convergent for $\alpha < 2$. We thus find $f_B \sim q^{\alpha-2}$. In general, at large energies we then find that the scattering amplitude is non negligible only within a cone of angular width $\theta \sim p^{-1}$ (forward cone).

We now briefly comment on when one can expect the Born approximation to work, and more generally the Born series to be convergent. Clearly, if V is weak enough we expect each new term appearing in Eq. (5.65) to be further suppressed. The discussion at point 3 above suggests that the insertion of a potential brings about a suppressing factor at large q, and so we expect the approximation to work at high energy (at least away from the forward cone). In fact, the two following results hold for potentials that vanish sufficiently fast at large r and are not too singular at $r = 0$:

- for potentials of the form $V = \lambda \bar{V}$ the Born series converges at all energies if λ is sufficiently small;
- the Born series converges for sufficiently large energies.

By taking a smaller λ, or a larger energy, the convergence is improved, and eventually the Born approximation will be accurate.

From Eq. (5.66) we see that if the potential is invariant under parity and/or under rotations, then f_B is real. In any case, f_B is real in the forward direction $\vec{q} = 0$. On the other hand, $\mathrm{Im}\, f(p, 0, 0) = 0$ is inconsistent with the optical theorem, see Eqs. (5.55) and (5.56). The Born approximation therefore violates unitarity. To understand more precisely how this happens, replace formally V with λV, so that the Born series becomes a power expansion in λ starting with the power λ^1. Since the right-hand side of Eq. (5.56) starts with λ^2, it is clear that the theorem will be satisfied to order λ^2 only if the first correction to the Born approximation is included. More generally, one can show that if the Born series is known only up to order λ^n, then the optical theorem (and so unitarity) will be violated to order λ^{n+1}.

6 Scattering in a central potential

As we have seen in the previous section, the problem of elastic two-body scattering is formally solved once we have determined the scattering amplitude $f(\theta, \varphi)$ which governs the large-distance behaviour of the positive-energy solutions of the (time-independent) Schrödinger equation. In this section we discuss this problem in detail in the case of a central potential.

6.1 Schrödinger equation in spherical coordinates

The time-independent Schrödinger equation,

$$\left(\frac{p^2}{2m} + V\right) |\psi\rangle = E|\psi\rangle \,, \tag{6.1}$$

reads in the coordinate representation

$$\left(-\frac{\Delta}{2m} + V(\vec{x})\right) \psi(\vec{x}) = E\psi(\vec{x}) \,, \tag{6.2}$$

where $\Delta = \vec{\nabla}^2$ is the Laplace operator. For central potentials $V = V(|\vec{x}|)$ it is convenient to work in spherical coordinates,

$$\begin{aligned} x &= r\sin\theta\cos\varphi\,, \\ y &= r\sin\theta\sin\varphi\,, \\ z &= r\cos\theta\,. \end{aligned} \tag{6.3}$$

The easiest way to proceed is to notice that in spherical coordinates the gradient reads

$$\vec{\nabla} = \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\,. \tag{6.4}$$

One thus has for the angular momentum operator

$$\vec{L} = \vec{x}\wedge\vec{p} = -i\vec{x}\wedge\vec{\nabla} = -i\left(\hat{r}\wedge\hat{\theta}\frac{\partial}{\partial\theta} + \hat{r}\wedge\hat{\varphi}\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}\right) = -i\left(\hat{\varphi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}\right)\,, \tag{6.5}$$

i.e., $\vec{L}$ acts only on the angular variables. Furthermore,

$$\begin{aligned} \vec{L}^{\,2} &= -\varepsilon_{ijk}\varepsilon_{ilm}x_j\partial_k x_l\partial_m = -(\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl})(x_j x_l\partial_k\partial_m + \delta_{kl}x_j\partial_m) \\ &= -r^2(\Delta - \hat{x}_i\hat{x}_j\partial_i\partial_j - 2r^{-1}\hat{x}_i\partial_i) = -r^2\left(\Delta - \frac{\partial^2}{\partial r^2} - 2\frac{1}{r}\frac{\partial}{\partial r}\right)\,, \end{aligned} \tag{6.6}$$

and so

$$\Delta = \frac{\partial^2}{\partial r^2} + 2\frac{1}{r}\frac{\partial}{\partial r} - \frac{1}{r^2}\vec{L}^{\,2} = \frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{1}{r^2}\vec{L}^{\,2}\,. \tag{6.7}$$

These results show explicitly something that we already knew, namely that the free Hamiltonian and the angular momentum commute.

We can now solve the Schrödinger equation by separation of variables. A complete set of angular momentum eigenfunctions is provided by the spherical harmonics $Y_{ll_z}(\hat{x})$, satisfying

$$\vec{L}^{\,2}Y_{ll_z}(\hat{x}) = l(l+1)Y_{ll_z}(\hat{x})\,, \quad L_zY_{ll_z}(\hat{x}) = l_zY_{ll_z}(\hat{x})\,, \qquad \int d\Omega\, Y^*_{l'l'_z}(\hat{x})Y_{ll_z}(\hat{x}) = \delta_{l'l}\delta_{l'_zl_z}\,. \tag{6.8}$$

We are interested in positive-energy solutions, so we set $E = \frac{p^2}{2m}$. The eigenfunctions of definite energy and angular momentum, $\psi_{Ell_z}(\vec{x})$, read therefore $\psi_{Ell_z}(\vec{x}) = Y_{ll_z}(\hat{x})R_{pl}(r)$ with $R_{pl}(r)$ satisfying

$$\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{l(l+1)}{r^2} - U(r) + p^2\right)R_{pl}(r) = 0\,, \tag{6.9}$$

where $U(r) = 2mV(r)$. It is convenient to factor out $1/r$, setting $R_{pl}(r) = 4\pi i^l\frac{u_{pl}(r)}{pr}$, where the numerical factor is chosen for future convenience. The function $u_{pl}(r)$ satisfies the equation,

$$\left(\frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2} - U(r) + p^2\right)u_{pl}(r) = 0\,, \tag{6.10}$$

known as the radial Schrödinger equation. Since we want $R_{pl}(r)$ to be sufficiently regular at $r = 0$, we need to impose the boundary condition $u_{pl}(0) = 0$.[37] Thanks to rotation invariance, we have reduced a three-dimensional problem to a one-dimensional one. This is the kind of simplifications that derive from symmetry.

[37] Actually, a solution of Eq. (6.10) *must* satisfy $u_{pl}(0) = 0$ in order to be a solution of the Schrödinger equation Eq. (6.2), so this boundary condition is more than just a regularity condition. The reason is that setting $R_{pl}(r) \propto u_{pl}(r)/r$ and substituting it in Eq. (6.2), one gets an extra singular term due to $\Delta\frac{1}{r} = -4\pi\delta^{(3)}(r)$. This therefore demands that u_{pl} vanish at the origin to have a solution (see [Shankar], §12.6).

6.2 The free case

We first study the radial Schrödinger equation Eq. (6.9) in the free case, $V = 0$. We will attach a superscript 0 to all functions to distinguish this case from the interacting one. By setting $z = pr$, we see from Eq. (6.10) that the solution depends only this combination of p and r,

$$\left(\frac{\partial^2}{\partial z^2} - \frac{l(l+1)}{z^2} + 1\right) v_l(z) = 0\,, \tag{6.11}$$

where we have temporarily set $u^0_{pl}(r) = v_l(z)$. The solutions of this equation are linear combinations of the Riccati-Bessel and Riccati-Neumann functions,

$$\begin{aligned} \hat{\jmath}_l(z) &= z j_l(z) = z\left(\frac{\pi}{2z}\right)^{\frac{1}{2}} J_{l+\frac{1}{2}}(z)\,, \\ \hat{n}_l(z) &= z n_l(z) = (-1)^l z\left(\frac{\pi}{2z}\right)^{\frac{1}{2}} J_{-l-\frac{1}{2}}(z)\,. \end{aligned} \tag{6.12}$$

Here $j_l(z)$ and $n_l(z)$ are respectively the spherical Bessel functions and the spherical Neumann functions, and $J_\alpha(z)$ are the Bessel functions of the first kind. For future utility we introduce also the Riccati-Hankel functions,

$$\hat{h}^\pm_l(z) = \hat{n}_l(z) \pm i\hat{\jmath}_l(z)\,. \tag{6.13}$$

The behaviour for small z of $\hat{\jmath}_l(z)$ and $\hat{n}_l(z)$ is[38]

$$\hat{\jmath}_l(z) \underset{z\to 0}{\simeq} \frac{z^{l+1}}{(2l+1)!!}\,, \qquad \hat{n}_l(z) \underset{z\to 0}{\simeq} \frac{(2l-1)!!}{z^l}\,, \tag{6.14}$$

and, except for the numerical factor, it can be derived directly from Eq. (6.11), since for small z the second term in brackets dominates over the constant term. One can similarly determine that the large-z behaviour must be a combination of $e^{\pm iz}$, by neglecting this time the second term. One has in fact

$$\hat{\jmath}_l(z) \underset{z\to\infty}{\simeq} \sin(z - \tfrac{\pi}{2}l)\,, \qquad \hat{n}_l(z) \underset{z\to\infty}{\simeq} \cos(z - \tfrac{\pi}{2}l)\,, \qquad \hat{h}^\pm_l(z) \underset{z\to\infty}{\simeq} e^{\pm i(z - \frac{\pi}{2}l)}\,. \tag{6.15}$$

The boundary condition $v_l(0) = 0$ forces us to choose the Riccati-Bessel functions, $v_l(z) = \hat{\jmath}_l(z)$. We are still free to choose the normalisation, and we fix it so that $u^0_{pl}(r) = \hat{\jmath}_l(pr)$, i.e., $R^0_{pl}(r) = 4\pi i^l j_l(pr)$. The reason for our choice of normalisation will soon become clear.

All in all, the solutions $\psi^0_{Ell_z}$ of the free Schrödinger equation with definite energy and angular momentum read

$$\psi^0_{Ell_z}(\vec{x}) = Y_{ll_z}(\hat{x}) 4\pi i^l j_l(pr)\,. \tag{6.16}$$

Since

$$\int dr\, r^2\, j_l(p'r) j_l(pr) = \frac{\pi}{2p^2}\delta(p'-p)\,, \qquad \int dr\, \hat{\jmath}_l(p'r)\hat{\jmath}_l(pr) = \frac{\pi}{2}\delta(p'-p)\,, \tag{6.17}$$

one has that $\psi^0_{Ell_z}$ are normalised according to

$$\int d^3x\, \psi^0_{E'l'l'_z}(\vec{x})^* \psi^0_{Ell_z}(\vec{x}) = \delta_{l'l}\delta_{l'_z l_z}\frac{\pi}{2p^2}\delta(p'-p)(4\pi)^2 = \delta_{l'l}\delta_{l'_z l_z} N(E)\delta(E'-E)\,, \tag{6.18}$$

[38] For odd $n > 0$, $(-n)!! = \frac{(-1)^{\frac{n-1}{2}} n}{n!!}$, so when $l = 0$, $(2l-1)!! = (-1)!! = 1$.

where we set $N(E) = \frac{(2\pi)^3}{mp}$. The $\psi^0_{Ell_z}$ form a complete set of solutions of the free Schrödinger equation, and so we have the following resolution of the identity,

$$\sum_{l=0}^{\infty}\sum_{l_z=-l}^{l}\int_0^\infty \frac{dE}{N(E)}\psi^0_{Ell_z}(\vec{x})\psi^0_{Ell_z}(\vec{y})^* = \delta^{(3)}(\vec{x}-\vec{y})\,. \tag{6.19}$$

Recall that we already knew another such complete set, namely the plane waves. It must therefore be possible to express a plane wave in terms of the solutions above. This corresponds to changing our basis from the momentum eigenbasis to the energy and angular momentum eigenbasis. To do this, we need the following two results:

$$e^{iz\cos\theta} = \sum_l (2l+1)P_l(\cos\theta)i^l j_l(z)\,, \qquad \sum_{l_z} Y_{ll_z}(\hat{p})^* Y_{ll_z}(\hat{x}) = \frac{2l+1}{4\pi}P_l(\hat{p}\cdot\hat{x})\,. \tag{6.20}$$

Here $P_l(x)$ are the Legendre polynomials. An important property of the Legendre polynomials is that they form a complete set of orthogonal functions in $L^2([-1,1])$, with normalisation

$$\int_{-1}^{1} dx\, P_{l'}(x)P_l(x) = \frac{2}{2l+1}\delta_{l'l}\,. \tag{6.21}$$

We then write

$$\begin{aligned} e^{i\vec{p}\cdot\vec{x}} = e^{ipx\cos\theta} &= \sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)i^l j_l(pr) = \sum_{l=0}^{\infty}\sum_{l_z=-l}^{l} Y_{ll_z}(\hat{p})^* Y_{ll_z}(\hat{x})4\pi i^l j_l(pr) \\ &= \sum_{l=0}^{\infty}\sum_{l_z=-l}^{l} Y_{ll_z}(\hat{p})^*\psi^0_{Ell_z}(\vec{x})\,. \end{aligned} \tag{6.22}$$

Using the abstract notation $|E\,l\,l_z\rangle$ for the energy and angular momentum eigenvectors, so that $\psi^0_{Ell_z}(\vec{x}) = \langle\vec{x}|E\,l\,l_z\rangle$, we can thus write

$$|\vec{p}\rangle = \sum_{l=0}^{\infty}\sum_{l_z=-l}^{l} Y_{ll_z}(\hat{p})^*|E\,l\,l_z\rangle\,. \tag{6.23}$$

Normalisation and completeness read in this notation

$$\langle E'\,l'\,l'_z|E\,l\,l_z\rangle = \delta_{l'l}\delta_{l'_z l_z}N(E)\delta(E'-E)\,, \qquad \sum_{l=0}^{\infty}\sum_{l_z=-l}^{l}\int_0^\infty \frac{dE}{N(E)}|E\,l\,l_z\rangle\langle E\,l\,l_z| = \mathbf{1}\,. \tag{6.24}$$

6.3 The partial-wave expansion

We have already commented on the fact that for central potentials one has independence of the azimuthal angle, $f = f(p,\theta)$. In general, for any square integrable function defined for $\theta \in [0,\pi]$ one can exploit the completeness of the Legendre polynomials to write

$$f(p,\theta) = \sum_l (2l+1)P_l(\cos\theta)f_l(E)\,. \tag{6.25}$$

Rotation invariance implies therefore that the scattering amplitude can always be written in the form Eq. (6.25). For such an expression to be of practical utility, one needs that only a few coefficients f_l be relevant: it turns out that at low energy this is actually the case.

We turn now to relating the coefficients f_l to theoretical computable quantities. The usefulness of the result Eq. (6.23) should be apparent once we recall that the S-matrix commutes with energy and angular momentum: this implies that it will be diagonal in the energy and angular momentum eigenbasis:

$$\langle E'\, l'\, l'_z|S|E\, l\, l_z\rangle = \delta_{l'l}\delta_{l'_z l_z} N(E)\delta(E'-E)s_l(E)\,, \tag{6.26}$$

where $N(E) = \frac{(2\pi)^3}{mp}$ has been factored out for convenience. We have already seen this result in the general case in section 4.8, here we focus on the case of spinless particles. In the case at hand there is only the orbital angular momentum $\vec{L}$, and $s_l(E)$ is independent of l_z, as a consequence of the Wigner-Eckart theorem. As a consequence of unitarity, $s_l(E)$ is a phase factor:

$$\begin{aligned}
\delta_{l'l}\delta_{l'_z l_z} N(E)\delta(E'-E) &= \sum_{\bar{l}\bar{l}_z}\int \frac{d\bar{E}}{N(\bar{E})}\langle E'\, l'\, l'_z|S^\dagger|\bar{E}\,\bar{l}\,\bar{l}_z\rangle\langle\bar{E}\,\bar{l}\,\bar{l}_z|S|E\, l\, l_z\rangle \\
&= \sum_{\bar{l}\bar{l}_z}\int \frac{d\bar{E}}{N(\bar{E})}\delta_{l'\bar{l}}\delta_{l'_z\bar{l}_z}N(E')\delta(E'-\bar{E})\delta_{\bar{l}l}\delta_{\bar{l}_z l_z}N(E)\delta(E'-\bar{E})s_{l'}(E')^* s_l(E) \\
&= \delta_{l'l}\delta_{l'_z l_z}N(E)\delta(E'-E)|s_l(E)|^2\,.
\end{aligned} \tag{6.27}$$

We thus write $s_l(E) = e^{2i\delta_l(E)}$, where the factor of 2 is again conventional. The quantities $\delta_l(E)$ are called phase shifts, and determine entirely the S-matrix in the case at hand (single-channel scattering). The phase shifts are affected by an inherent ambiguity modulo π: we will see below how this can be conveniently resolved.

We now make use of Eq. (6.23) to write for the usual matrix elements in the momentum basis

$$\begin{aligned}
\langle\vec{p}'|S|\vec{p}\rangle &= \sum_{l',l}\sum_{l'_z,l_z} Y_{l'l'_z}(\hat{p}')Y_{ll_z}(\hat{p})^*\langle E'\, l'\, l'_z|S|E\, l\, l_z\rangle \\
&= \sum_{l',l}\sum_{l'_z,l_z} Y_{l'l'_z}(\hat{p}')Y_{ll_z}(\hat{p})^*\delta_{l'l}\delta_{l'_z l_z}N(E)\delta(E'-E)s_l(E) \\
&= N(E)\delta(E'-E)\sum_l \frac{2l+1}{4\pi}P_l(\cos\theta)s_l(E)\,,
\end{aligned} \tag{6.28}$$

where we used Eq. (6.20), and we have set $\cos\theta = \hat{p}'\cdot\hat{p}$. Similarly,

$$\langle\vec{p}'|\vec{p}\rangle = N(E)\delta(E'-E)\sum_l \frac{2l+1}{4\pi}P_l(\cos\theta)\,. \tag{6.29}$$

Recalling

$$\langle\vec{p}'|S|\vec{p}\rangle - \langle\vec{p}'|\vec{p}\rangle = i\frac{(2\pi)^2}{m}\delta(E'-E)f(p,\theta)\,, \tag{6.30}$$

we find

$$i\frac{(2\pi)^2}{m}f(p,\theta) = \frac{(2\pi)^3}{mp}\sum_l \frac{2l+1}{4\pi}P_l(\cos\theta)(s_l(E)-1)\,, \tag{6.31}$$

i.e.,

$$f(p,\theta) = \sum_l (2l+1) P_l(\cos\theta) \frac{s_l(E)-1}{2ip} = \sum_l (2l+1) P_l(\cos\theta) f_l(E)\,. \tag{6.32}$$

This is the partial-wave expansion of the scattering amplitude. The nontrivial content of this calculation is the relation between the partial-wave coefficients f_l and the phase shifts,

$$f_l(E) = \frac{s_l(E)-1}{2ip} = \frac{e^{i\delta_l(E)}}{p} \sin\delta_l(E)\,. \tag{6.33}$$

As we mentioned above, Eq. (6.32) provides a good parameterisation of the low-energy scattering amplitude, in the sense that at low energies only a few coefficients are required to satisfactorily describe a scattering process.

It is instructive to check how the optical theorem is satisfied by the partial-wave expansion. To this end, we need the following properties of the Legendre polynomials [recall Eq. (6.21)]:

$$\int d\Omega\, P_{l'}(\cos\theta) P_l(\cos\theta) = \frac{4\pi}{2l+1}\delta_{l'l}\,, \qquad P_l(1) = 1\,. \tag{6.34}$$

We thus find

$$\begin{aligned} \mathrm{Im}\, f(0) &= \sum_l (2l+1) \frac{1-\cos 2\delta_l(E)}{2p} = \sum_l (2l+1) \frac{\sin^2\delta_l(E)}{p}\,, \\ \int d\Omega\, |f(\theta)|^2 &= \frac{4\pi}{p^2} \sum_l (2l+1) \sin^2\delta_l(E)\,, \end{aligned} \tag{6.35}$$

and the optical theorem is satisfied.

6.4 Interacting case

We now turn to the interacting case. In analogy with the free case, we set $R_{pl}(r) = 4\pi i^l \frac{u_{pl}(r)}{pr}$. Also in this case we need $u_{pl}(0) = 0$ (see footnote 37). If the potential is less singular than r^{-2}, the behaviour of the solutions of the radial Schrödinger equation, Eq. (6.10), for small r is the same as in the free case. For the regular solution we thus have

$$u_{pl}(r) \simeq r^{l+1}\,. \tag{6.36}$$

For large r, on the other hand, $u_{pl}(r)$ will be a linear combination of spherical waves, $e^{\pm ipr}$. The kind of solutions we are interested in are those representing in and out states, in the same sense in which the states $|\vec{p}\pm\rangle$ do. Since all we used in the construction of $|\vec{p}\pm\rangle$ was that the momentum eigenstates $|\vec{p}\rangle$ are energy eigenstates, the same construction works here, and we can define

$$|E\,l\,l_z\pm\rangle = \Omega_\pm(E)|E\,l\,l_z\rangle\,, \qquad \langle\vec{x}|E\,l\,l_z\pm\rangle = Y_{ll_z}(\hat{x}) 4\pi i^l \frac{u_{pl}(r)}{pr}\,. \tag{6.37}$$

The states $|E\,l\,l_z\pm\rangle$ are clearly normalised like the free states $|E\,l\,l_z\rangle$. From the intertwining relations it follows that they are eigenstates of H; from the fact that the scattering operators commute with angular momentum due to rotation invariance of the Hamiltonian, it follows that they are also eigenstates of $\vec{L}^{\,2}$ and L_z. Using now Eq. (6.23) we obtain

$$|\vec{p}\pm\rangle = \sum_{l,l_z} Y_{ll_z}(\hat{p})^* |E\,l\,l_z\pm\rangle\,. \tag{6.38}$$

In the coordinate representation

$$\psi_{p+}(\vec{x}) = \sum_{l,l_z} Y_{ll_z}(\hat{p})^* Y_{ll_z}(\hat{x}) 4\pi i^l \frac{u_{pl}(r)}{pr} = \sum_l (2l+1) P_l(\cos\theta) i^l \frac{u_{pl}(r)}{pr} \,. \tag{6.39}$$

For large r, $\psi_{p+}(\vec{x}) \simeq e^{i\vec{p}\cdot\vec{x}} + f(\theta)\frac{e^{ipr}}{r}$. Using the expansions Eqs. (6.22) and (6.32), and matching the coefficients of the Legendre polynomials we obtain

$$i^l j_l(pr) + f_l \frac{e^{ipr}}{r} = \frac{i^l}{pr}\left(\hat{\jmath}_l(pr) + p f_l e^{i(pr-\frac{\pi}{2}l)}\right) \simeq i^l \frac{u_{pl}(r)}{pr} \,, \tag{6.40}$$

i.e.,

$$u_{pl}(r) \simeq \hat{\jmath}_l(pr) + p f_l e^{i(pr - l\frac{\pi}{2})} \,. \tag{6.41}$$

Using the asymptotic behaviour of the Riccati-Bessel functions,

$$\hat{\jmath}_l(pr) \simeq \sin\left(pr - \frac{\pi}{2}l\right) \,, \tag{6.42}$$

we finally get

$$\begin{aligned} u_{pl}(r) &\simeq \frac{1}{2i}\left[(1+2ipf_l)\, e^{i(pr-\frac{\pi}{2}l)} - e^{-i(pr-\frac{\pi}{2}l)}\right] = \frac{1}{2i}\left[e^{i(pr-\frac{\pi}{2}l+2\delta_l(E))} - e^{-i(pr-\frac{\pi}{2}l)}\right] \\ &= e^{i\delta_l(E)}\frac{1}{2i}\left[e^{i(pr-\frac{\pi}{2}l+\delta_l(E))} - e^{-i(pr-\frac{\pi}{2}l+\delta_l(E))}\right] = e^{i\delta_l(E)}\sin\left(pr - \frac{\pi}{2}l + \delta_l(E)\right) \,. \end{aligned} \tag{6.43}$$

This relation explains the origin of the name "phase shift": δ_l is precisely the difference between the phases of the solutions of the Schrödinger equation in the interacting and in the free case at asymptotically large distances.

In order to determine the phase shifts one has therefore to solve the radial Schrödinger equation with boundary condition $u_{pl}(r) = 0$ and look at the large-r asymptotic behaviour. By construction, $u_{pl}(r)$ are normalised like Riccati-Bessel functions,

$$\int dr\, u_{p'l}(r) u_{pl}(r) = \frac{\pi}{2}\delta(p'-p) \,. \tag{6.44}$$

For this reason, the solutions $u_{pl}(r)$ are called the normalised solutions. Any other (physically acceptable) solution $\tilde{u}_{pl}(r)$ differs from $u_{pl}(r)$ only in the normalisation. As far as the phase shifts are concerned, the normalisation is not important: since any solution is asymptotically of the form $\tilde{u}_{pl}(r) \simeq A_{pl}e^{ipr} + B_{pl}e^{-ipr}$, the phase shifts are obtained as $e^{2i\delta_l} = \frac{A_{pl}}{B_{pl}}(-1)^{l+1}$, regardless of the normalisation.

6.5 Properties of the phase shifts. The Jost function

The study of the properties of the phase shifts is simpler if we consider a different normalisation for the solution. The convenient choice is to ask for the solution to be proportional to $\hat{\jmath}_l(pr)$ at small r. Denoting the corresponding solution as $\chi_{pl}(r)$, we impose

$$\lim_{r\to 0} \frac{\chi_{pl}(r)}{\hat{\jmath}_l(pr)} = 1 \,. \tag{6.45}$$

The solution $\chi_{pl}(r)$ is called the regular solution. A consequence of our choice is that χ_{pl} is real, since it obeys a real equation and a real boundary condition. In general, the asymptotic behaviour for large r is different from that of u_{pl}, and can be written as

$$\chi_{pl}(r) \simeq \frac{1}{2i}\left[\varphi_l^*(p)e^{i(pr-\frac{\pi}{2}l)} - \varphi_l(p)e^{-i(pr-\frac{\pi}{2}l)}\right] . \tag{6.46}$$

Comparing with Eq. (6.43), we see that

$$\frac{\chi_{pl}(r)}{u_{pl}(r)} = \varphi_l(p)\,, \qquad e^{2i\delta_l(E)} = \frac{\varphi_l^*(p)}{\varphi_l(p)}\,. \tag{6.47}$$

The function φ_l is called the Jost function, and is central in the study of the analyticity properties of the solution and of the S-matrix.

The reason why it is simpler to work with the regular solution rather than the normalised solution becomes apparent when we convert the radial Schrödinger equation and the desired boundary condition into an integral equation. This approach is standard in the study of partial differential equations, but we will not describe it in detail here. Instead, we will just pick the answer out of our hat: in the case at hand, the relevant integral equation for the regular solution is

$$\chi_{pl}(r) = \hat{\jmath}_l(pr) + \lambda\int_0^r dr'\, g_{pl}(r,r')U(r')\chi_{pl}(r')\,, \tag{6.48}$$

where

$$g_{pl}(r,r') = \frac{1}{p}\left[\hat{\jmath}_l(pr)\hat{n}_l(pr') - \hat{n}_l(pr)\hat{\jmath}_l(pr')\right] , \tag{6.49}$$

and we have replaced $U \to \lambda U$ for future convenience. Notice that the integral in Eq. (6.48) extends only up to r: this reflects the fact that our boundary condition is given at a single point, namely $r = 0$. A similar equation can be written also for u_{pl}, but in that case the integral extends up to infinity, reflecting the fact that the normalisation condition involves the function at all points.

To prove that the solution of Eq. (6.48) automatically satisfies both the radial Schrödinger equation and the desired boundary condition one proceeds as follows. Applying the differential operator $\mathcal{O}_r = \frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2} - \lambda U(r) + p^2$ to the right-hand side of Eq. (6.48) we find

$$\begin{aligned}
\mathcal{O}_r\chi_{pl}(r) &= \mathcal{O}_r\left\{\hat{\jmath}_l(pr) + \lambda\int_0^r dr'\, g_{pl}(r,r')U(r')\chi_{pl}(r')\right\} \\
&= -\lambda U(r)\left[\hat{\jmath}_l(pr) + \lambda\int_0^r dr'\, g_{pl}(r,r')U(r')\chi_{pl}(r')\right] + \lambda\left[\frac{\partial}{\partial r}g_{pl}(r,r')\right]_{r=r'} U(r)\chi_{pl}(r) \\
&\quad + \lambda\frac{\partial}{\partial r}\left[g_{pl}(r,r')\big|_{r=r'}\right] U(r)\chi_{pl}(r)\,,
\end{aligned} \tag{6.50}$$

where we have made use of the fact that $\hat{\jmath}_l(pr)$ and $\hat{n}_l(pr)$ satisfy the free equation ($U = 0$). To proceed, notice that $g_{pl}(r,r) = 0$ identically, and that

$$\frac{\partial}{\partial r}g_{pl}(r,r')\big|_{r=r'} = -\frac{1}{p}W(\hat{\jmath}_l(pr),\hat{n}_l(pr))\,, \tag{6.51}$$

where we have introduced the Wronskian of two functions,

$$W(f,g) = fg' - f'g\,. \tag{6.52}$$

Since

$$\frac{\partial}{\partial r}W(f,g) = f\frac{\partial^2 g}{\partial r^2} - \frac{\partial^2 f}{\partial r^2}g\,, \tag{6.53}$$

it is clear that the Wronskian of $\hat{\jmath}_l(pr)$ and $\hat{n}_l(pr)$ is constant, and can be calculated where we find it most convenient. Using the small-p behaviour Eq. (6.14), we obtain $W(\hat{\jmath}_l(pr), \hat{n}_l(pr)) = -p$, and so

$$\mathcal{O}_r\chi_{pl}(r) = -\lambda U(r)\chi_{pl}(r) + \lambda U(r)\chi_{pl}(r) = 0\,, \tag{6.54}$$

as asserted. To prove that the desired boundary condition is satisfied one has to show that the integral vanishes faster than $\jmath_l(pr) \simeq r^{l+1}$ as $r \to 0$, so one has to discuss first the properties of the solution of Eq. (6.48).

To solve Eq. (6.48), one writes $\chi_{pl} = \sum_n \lambda^n \chi_{pl}^{(n)}$ and matches the coefficients of λ^n on both sides of the equation. This leads to the iterative solution

$$\chi_{pl}^{(n+1)}(r) = \int_0^r dr'\, g_{pl}(r,r')U(r')\chi_{pl}^{(n)}(r')\,, \qquad \chi_{pl}^{(0)}(r) = \hat{\jmath}_l(pr)\,. \tag{6.55}$$

One can prove, using appropriate bounds for the Riccati-Bessel and Riccati-Neumann functions, that the power series in λ converges for any *complex* value of λ (so in particular for $\lambda = 1$), so that Eq. (6.55) really provides the solution of Eq. (6.48). As a function of λ, χ_{pl} is thus an entire function. One can also show that the convergence is uniform, so that χ_{pl} is a continuous function of p for all real p. The relevant bounds are

$$|\hat{\jmath}_l(z)| \le \text{const.}\left(\frac{z}{1+z}\right)^{l+1}\,, \quad |\hat{n}_l(z)| \le \text{const.}\left(\frac{z}{1+z}\right)^{-l}\,, \quad z \in \mathbb{R}\,. \tag{6.56}$$

From this it also follows that

$$|\chi_{pl}(r)| \le \text{const.}\left(\frac{pr}{1+pr}\right)^{l+1}\,. \tag{6.57}$$

For $U(r) \sim r'^{\alpha}$ with $\alpha > -2$ for small r, one can thus show that as $r \to 0$

$$\begin{aligned}
&\int_0^r dr'\, g_{pl}(r,r')U(r')\chi_{pl}(r') \\
&\simeq \text{const.}\int_0^r dr'\,\frac{1}{p}\left[(pr)^{l+1}\left(pr'\right)^{-l} - \left(pr'\right)^{l+1}(pr)^{-l}\right] r'^{\alpha}\left(pr'\right)^{l+1} \\
&\simeq \text{const.}'\,(pr)^{l+1}r^{\alpha+2}\,,
\end{aligned} \tag{6.58}$$

which vanishes faster than $\hat{\jmath}_l(pr)$, thus completing our proof.

From Eq. (6.48) one can derive an analogous equation for the Jost function. To this end, consider the Riccati-Hankel functions $\hat{h}_l^{\pm}(z) = \hat{n}_l(z) \pm i\hat{\jmath}_l(z)$. Expressing the Riccati-Bessel and Riccati-Neumann functions in terms of these, one finds

$$\begin{aligned}
\chi_{pl}(r) &= \frac{1}{2i}\left\{\hat{h}_l^+(pr) - \hat{h}_l^-(pr) + \frac{\lambda}{p}\int_0^\infty dr'\,\left[\hat{h}_l^+(pr)\hat{h}_l^-(pr') - \hat{h}_l^-(pr)\hat{h}_l^+(pr')\right]U(r')\chi_{pl}(r')\right\} \\
&= -\frac{1}{2i}\left\{\hat{h}_l^-(pr) + \frac{\lambda}{p}\int_0^\infty dr'\,\hat{h}_l^-(pr)\hat{h}_l^+(pr')U(r')\chi_{pl}(r')\right\} + \text{c.c.}\,.
\end{aligned} \tag{6.59}$$

Using the asymptotic behaviour of $\hat{h}_l^{\pm}(z)$ given in Eq. (6.15), together with Eq. (6.46), we find

$$\varphi_l(p) = 1 + \frac{\lambda}{p}\int_0^\infty dr'\, \hat{h}_l^+(pr')U(r')\chi_{pl}(r')\,. \tag{6.60}$$

We now discuss a few consequences of this result.

Small λ and large p limits By properly bounding the integrand [see Eq. (6.56)], one gets from this result that $\varphi_l(p) \to 1$ as either $\lambda \to 0$ or $p \to \infty$, and it does so uniformly in the other variable. This implies in turn that in the same limits $s_l \to 1$, and so $\delta \to n\pi$ for some $n \in \mathbb{Z}$. We see now how one can resolve the modulo-π ambiguity: it is enough to ask for the phase shifts δ_l to be continuous and to tend to 0 (not just any $n\pi$) as $p \to \infty$.

Analyticity in λ and Born series Using the same bounds that allow to prove the convergence of the power series in λ for χ_{pl}, one can show that the series $\varphi_l = \sum_n \lambda^n \varphi_l^{(n)}$ is convergent for any $\lambda \in \mathbb{C}$, i.e., φ_l is an entire function of λ. As long as $\varphi_l(p,\lambda) \neq 0$, one thus finds that also u_{pl} is analytic in λ. If we make explicit the dependence on λ, and we define for general complex λ

$$s_l(p,\lambda) = e^{i2\delta_l(p,\lambda)} = \frac{\varphi_l(p,\lambda^*)^*}{\varphi_l(p,\lambda)}\,, \tag{6.61}$$

we see that also s_l is analytic in λ, provided $\varphi_l(p,\lambda) \neq 0$. Notice that we are considering now s_l and δ_l as functions of p rather than E. In both cases, the radius of convergence of the power-series expansion in λ (i.e., the Born series) of the normalised solution and of the S-matrix is determined by the position $\lambda_0(p)$ of the zero of the Jost function closest to the origin (certainly $\lambda_0(p) \neq 0$ since $\varphi(p,0) = 1$). Furthermore, for $|\lambda| \leq 1$ and large p, one has that since the Jost function converges to 1 uniformly in λ as $p \to \infty$, it is possible to find p_0 such that for $p > p_0$ one has, say, $|\varphi(p,\lambda)| > \frac{1}{2}$ inside the whole unit circle. Setting $\lambda = 1$, this implies that the Born series converges for any potential (satisfying our "reasonableness" assumptions, pag. 20) if the energy is sufficiently large.

Amplitude from the Jost function Recall that $f_l = \frac{s_l - 1}{2ip}$. Using Eq. (6.61) we find

$$f_l(p) = \frac{\varphi_l(p,\lambda^*)^* - \varphi_l(p,\lambda)}{2ip\varphi_l(p,\lambda)}\,, \tag{6.62}$$

where we keep λ complex for generality, and we are considering $f_l(p)$ as a function of p. Using the fact that $h_l^{\pm}(z)^* = h_l^{\mp}(z)$ and the expression Eq. (6.60), we find that

$$\begin{aligned}\varphi_l(p,\lambda^*)^* - \varphi_l(p,\lambda) &= \frac{\lambda}{p}\int_0^\infty dr\,[\hat{h}_l^-(pr) - \hat{h}_l^+(pr)]U(r)\chi_{pl}(r) \\ &= -2i\frac{\lambda}{p}\int_0^\infty dr\,\hat{\jmath}_l(pr)U(r)\chi_{pl}(r)\,,\end{aligned} \tag{6.63}$$

and so

$$f_l(p) = -\frac{\lambda}{p^2\varphi_l(p,\lambda)}\int_0^\infty dr\,\hat{\jmath}_l(pr)U(r)\chi_{pl}(r)\,. \tag{6.64}$$

Small p behaviour of the amplitude We now focus on the physical case, setting $\lambda = 1$ and dropping it from the notation. What we want to derive is the small-p behaviour of the amplitude. Using Eqs. (6.56), (6.57), and (6.64), we have that

$$|f_l(p)| \leq \frac{1}{p^2|\varphi_l(p)|} \int_0^\infty dr\, |U(r)| \left(\frac{pr}{1+pr}\right)^{2(l+1)} . \tag{6.65}$$

Let us now assume that $\varphi_l(0) \neq 0$. If $U(r)$ vanishes faster than any inverse power of r at large r, we can drop the denominator in the integrand of Eq. (6.65) and obtain $|f_l(p)| \leq \text{const.} \times p^{2l}$. Since the contribution from small r is precisely of this order, we have $f_l(p) = \mathcal{O}(p^{2l})$ as $p \to 0$. If $U(r)$ vanishes like $r^{-\nu}$, this result still holds for $2l + 2 - \nu < -1$. For $l > (\nu - 3)/2$ we split the integral as $\int_0^\infty = \int_0^1 + \int_1^\infty$: for the first term the bound above still applies. For the second contribution we have instead

$$\begin{aligned} &\int_1^\infty dr\, U(r) \left(\frac{pr}{1+pr}\right)^{2(l+1)} \leq \text{const.} \int_1^\infty \frac{dr}{r^\nu} \left(\frac{pr}{1+pr}\right)^{2(l+1)} \\ &= p^{\nu-1}\text{const.} \int_p^\infty \frac{dr}{r^\nu} \left(\frac{r}{1+r}\right)^{2(l+1)} \leq p^{\nu-1}\text{const.} \int_0^\infty \frac{dr}{r^\nu} \left(\frac{r}{1+r}\right)^{2(l+1)} , \end{aligned} \tag{6.66}$$

where the last integral is convergent since $2l + 2 - \nu > -1$. Since $2l > \nu - 3$, the second term is dominant at small p, and $|f_l(p)| \leq \text{const.} \times p^{\nu-3}$. Again, since the large-r contribution is precisely of this order, we have for $l > (\nu - 3)/2$ that $f_l(p) = \mathcal{O}(p^{\nu-3})$ as $p \to 0$. When $l = (\nu - 3)/2$, the last integral in Eq. (6.66) is logarithmically divergent as $p \to 0$, and so $f_l(p) = \mathcal{O}(p^{\nu-3} \ln(p_0/p))$ with p_0 some fixed momentum scale.

We have thus shown that f_l vanishes as $p \to 0$ like

$$f_l(p) \simeq -a_l p^{2l} \quad \text{or} \quad -a_l p^{\nu-3} . \tag{6.67}$$

The constants a_l are known as scattering lengths; for $l = 0$, a_0 has indeed dimensions of length. It is clear from the above that at very low energy the scattering amplitude is dominated by the s-wave ($l = 0$), so that it is isotropic, and that it is energy-independent. For the S-matrix the results above imply

$$s_l(p) = 1 + \mathcal{O}(p^{2l+1}) \Longrightarrow \delta_l(p) = n'\pi + \mathcal{O}(p^{2l+1}) , \tag{6.68}$$

for rapidly vanishing potentials, and for potentials vanishing like $r^{-\nu}$ when $l \leq (\nu - 3)/2$, or

$$s_l(p) = 1 + \mathcal{O}(p^{\nu-2}) \Longrightarrow \delta_l(p) = n'\pi + \mathcal{O}(p^{\nu-2}) , \tag{6.69}$$

for potentials vanishing like $r^{-\nu}$ and $l \geq (\nu - 3)/2$. We thus have that $\delta_l(p)$ becomes an integer multiple of π both at large and small energies, although possibly with different proportionality constants. In particular, if we resolve the modulo-π ambiguity as discussed above by setting $\delta_l(\infty) = 0$, then $\delta_l(0)$ will be in general a nonzero multiple of π. Is there some physics hidden in this constants? As we will see below, the answer is yes.

The results above hold if $\varphi_l(0) \neq 0$: this case can be handled as well, and if φ_l vanishes at zero like p^α, then the powers of the power-law terms in the expressions above have to be reduced by α.

Large-l behaviour of the phase shifts There is one more property of the phase shifts worth discussing. Returning to the radial Schrödinger equation Eq. (6.10), it is clear that as $l \to \infty$ the repulsive centrifugal barrier dominates over the potential (unless this has a "long tail"). The larger l, the smaller becomes the chance that the incident particle penetrate the barrier and reach into the region where the potential is non-negligible. This means that it will be essentially unaffected by the potential, so that it will behave as a free particle, and thus the phase shift will be zero (modulo π). If a is the range of the potential, one can estimate the height of the centrifugal barrier at the edge of the interaction region as $h = l^2/(2ma^2)$. In order to penetrate the barrier one needs that $E = \frac{p^2}{2m} > h$, so for $E \ll h$ one will not have any appreciable effect. This means that for $l \gg pa$ all the phase shifts will be small. Classically, one has that $l = pb$ where b is the impact parameter: if $b \gg a$ one does not have scattering at all, and this corresponds to $l \gg pa$.

7 Analyticity properties of the S-matrix

The study of the analyticity properties of the S-matrix allows to uncover many useful results, both in the non-relativistic and in the relativistic case. In the simple case of non-relativistic, single-channel, elastic two-body scattering there are several rigorous results, which we now discuss.

7.1 Analytic properties of the regular solution

We begin our analysis by studying the analyticity properties of the regular solution. As we have already said, this is that solution of the radial Schrödinger equation,

$$\left(\frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2} - U(r) + p^2\right)\chi_{pl}(r) = 0\,, \tag{7.1}$$

that behaves like $\chi_{pl}(r) \sim \hat{\jmath}_l(pr)$ for $r \to 0$. Although in the physical case p is a real quantity, there is in principle nothing preventing us to consider the equation for complex p. As for the boundary condition, $\hat{\jmath}_l(pr)$ is an entire function of p (i.e., analytic for all p). As in the case of real p, the Schrödinger equation plus the boundary condition are equivalent to the integral equation

$$\chi_{pl}(r) = \hat{\jmath}_l(pr) + \int_0^r dr'\, g_{pl}(r,r')U(r')\chi_{pl}(r')\,, \tag{7.2}$$

where

$$g_{pl}(r,r') = \frac{1}{p}\left[\hat{\jmath}_l(pr)\hat{n}_l(pr') - \hat{n}_l(pr)\hat{\jmath}_l(pr')\right]\,, \tag{7.3}$$

which is again an entire function of p. The integral equation Eq. (7.2) can be solved by iteration, as we did in the real-p case, setting $\chi_{pl}(r) = \sum_n \chi_{pl}^{(n)}(r)$ with

$$\chi_{pl}^{(n+1)}(r) = \int_0^r dr'\, g_{pl}(r,r')U(r')\chi_{pl}^{(n)}(r')\,, \qquad \chi_{pl}^{(0)}(r) = \hat{\jmath}_l(pr)\,. \tag{7.4}$$

One can show that the series converges for all complex p, and does so uniformly in p; moreover, each term is analytic in p, and therefore so is the sum of the series, i.e., the regular solution.

One thus concludes that $\chi_{pl}(r)$ is an entire function of p. It is easy to generalise the proof to the case $U \to \lambda U$ with complex λ, in which case the solution is entire both in p and in λ.

In order to prove the statements above, one needs the generalisation of the bounds Eq. (6.56) to the case of complex arguments:

$$|\hat{\jmath}_l(z)| \leq \text{const.} \left(\frac{|z|}{1+|z|}\right)^{l+1} e^{|\mathrm{Im}\, z|}\,, \quad |\hat{n}_l(z)| \leq \text{const.} \left(\frac{|z|}{1+|z|}\right)^{-l} e^{|\mathrm{Im}\, z|}\,. \tag{7.5}$$

Moreover, since

$$g_{pl}(r,r') = \frac{1}{2ip}\left[\hat{h}_l^+(pr)\hat{h}_l^-(pr') - \hat{h}_l^-(pr)\hat{h}_l^+(pr')\right], \tag{7.6}$$

and

$$\hat{h}_l^\pm(z) \underset{|z|\to\infty}{\to} e^{\pm i(z-\frac{\pi}{2}l)}\,, \tag{7.7}$$

one has for $r \geq r'$

$$|g_{pl}(r,r')| \leq \frac{\text{const.}}{|p|} e^{|\mathrm{Im}\, p|(r-r')} \left(\frac{|p|r}{1+|p|r}\right)^{l+1} \left(\frac{|p|r'}{1+|p|r'}\right)^{-l}. \tag{7.8}$$

The n-th term of the iteration reads

$$\begin{aligned}\chi_{pl}^{(n)}(r) = &\int_0^r dr_n\, g_{pl}(r,r_n)U(r_n) \int_0^{r_n} dr_{n-1}\, g_{pl}(r_n,r_{n-1})U(r_{n-1})\ldots \\ &\times \int_0^{r_3} dr_2\, g_{pl}(r_3,r_2)U(r_2) \int_0^{r_2} dr_1\, g_{pl}(r_2,r_1)U(r_1)\hat{\jmath}_l(pr_1)\,.\end{aligned} \tag{7.9}$$

Taking the modulus and using the bounds above we find

$$\begin{aligned}|\chi_{pl}^{(n)}(r)| &\leq \text{const.}^n \times \frac{1}{|p|^n} e^{|\mathrm{Im}\, p|r} \left(\frac{|p|r}{1+|p|r}\right)^{l+1} \int_0^r dr_n \ldots \int_0^{r_2} dr_1 \prod_{i=1}^n \frac{|p|r_i}{1+|p|r_i}|U(r_i)| \\ &= \text{const.}^n \times e^{|\mathrm{Im}\, p|r} \left(\frac{|p|r}{1+|p|r}\right)^{l+1} \int_0^r dr_n \ldots \int_0^{r_2} dr_1 \prod_{i=1}^n \frac{r_i}{1+|p|r_i}|U(r_i)| \\ &= \text{const.}^n \times e^{|\mathrm{Im}\, p|r} \left(\frac{|p|r}{1+|p|r}\right)^{l+1} \frac{1}{n!}\left[\int_0^r dr' \frac{r'}{1+|p|r'}|U(r')|\right]^n \\ &\leq \text{const.}^n \times e^{|\mathrm{Im}\, p|r} \left(\frac{|p|r}{1+|p|r}\right)^{l+1} \frac{1}{n!}\left[\int_0^r dr'\, r'\, |U(r')|\right]^n.\end{aligned} \tag{7.10}$$

This bound has three important consequences.

1. It shows that $|\chi_{pl}^{(n)}(r)| \to 0$ as $n \to \infty$. It also shows that $|\chi_{pl}^{(n)}(r)| \to 0$ faster than r^{l+1} as $r \to 0$, which implies that $\chi_{pl}(r)$ as given by Eq. (7.2) really satisfies its boundary condition at $r = 0$.

2. The series is bounded by a convergent one, so it is convergent:

$$|\chi_{pl}(r)| = \Big|\sum_n \chi_{pl}^{(n)}(r)\Big| \leq e^{\text{const.}\times\alpha(r)} e^{|\mathrm{Im}\, p|r} \left(\frac{|p|r}{1+|p|r}\right)^{l+1}, \quad \alpha(r) = \int_0^r dr'\, r'\, |U(r')|\,. \tag{7.11}$$

This provides also a bound on the regular solution. Finally, this also shows that $|\chi_{pl}(r)| \to 0$ like $|p|^l$ as $|p| \to 0$, a result that we used in the previous section, in the case of real p, to determine the small-p behaviour of the scattering amplitude.

3. For p in any bounded complex domain, the series converges uniformly in p.

Moreover, each term of the recursion is analytic: assuming that the nth term is analytic in p, the $(n+1)$-th one is analytic in p as well, being obtained via Eq. (7.4) as the integral in r' of a function which is both analytic in p and continuous in r' (see, e.g., [Titchmarsh], §2.83). Since the zeroth term is analytic in p and continuous in r, each term is. Combined with uniform convergence of the series, this implies that the regular solution is analytic for all p.

Notice the following symmetry property of $\chi_{pl}(r)$. Since the radial Schrödinger equation depends only on p^2, and its solution is unique up to normalisation, it follows that $\chi_{pl}(r)$ and $\chi_{-pl}(r)$ must be proportional, $\chi_{-pl}(r) = C\chi_{pl}(r)$. Since $\hat{\jmath}_l(-z) = (-1)^{l+1}\hat{\jmath}_l(z)$, we have

$$C = \frac{\chi_{-pl}(r)}{\chi_{pl}(r)} = \lim_{r\to 0} \frac{\chi_{-pl}(r)}{\chi_{pl}(r)} = \lim_{r\to 0} \frac{\hat{\jmath}_l(-pr)}{\hat{\jmath}_l(pr)} = (-1)^{l+1}\,, \tag{7.12}$$

i.e., $\chi_{-pl}(r) = (-1)^{l+1}\chi_{pl}(r)$, exactly like the free solution.

7.2 Analytic properties of the Jost function

From the analyticity properties of the regular solution we can obtain those of the Jost function. For real p, we know that the Jost function is related to the regular solution via Eq. (6.60),

$$\varphi_l(p) = 1 + \frac{1}{p}\int_0^\infty dr'\, \hat{h}_l^+(pr')U(r')\chi_{pl}(r')\,. \tag{7.13}$$

If the upper bound of integration were finite, this expression would define an analytic function of p. If we can show that the integral converges uniformly at least for p in some complex domain connected to the real positive axis, then we would have found the unique analytic extension of the Jost function.

For complex p, in general $\chi_{pl}(r) \sim e^{|\mathrm{Im}\, p|r}$ at large r, while $\hat{h}_l^+(pr') \sim e^{-\mathrm{Im}\, pr}$. For $\mathrm{Im}\, p > 0$ we have that the exponentials cancel out, and the integral can be convergent. More precisely, using the bounds Eqs. (7.5) and

$$|\hat{h}_l^+(z)| \le \text{const.} \times e^{-\mathrm{Im}\, z}\left(\frac{|z|}{1+|z|}\right)^{-l}\,, \tag{7.14}$$

we find

$$|\varphi_l(p) - 1| \le \frac{\text{const.}}{|p|}\int_0^\infty dr'\, |U(r')| e^{(|\mathrm{Im}\, p| - \mathrm{Im}\, p)r'}\frac{|p|r'}{1+|p|r'}\,. \tag{7.15}$$

When $\mathrm{Im}\, p > 0$, the exponentials cancel out as anticipated, and the integral converges uniformly in p: since the integrand is analytic in p and continuous in r, this implies that $\varphi_l(p)$, as defined by Eq. (7.13), is analytic in the upper half of the complex plane. Moreover, the integral converges uniformly in p for $\mathrm{Im}\, p \ge 0$, where the integrand is continuous both in p and in r, so $\varphi_l(p)$ is continuous in $\mathrm{Im}\, p \ge 0$. This means that the physically relevant Jost function (real positive p) is continuously connected to an analytic function in the whole upper half-plane.

It is rather straightforward to generalise the results above to the case in which one makes explicit the dependence of the potential on an overall scale λ, i.e., for Hamiltonians of the form $H = H_0 + \lambda V$. Since χ_{pl} is in this case an entire function of λ, and the only change in Eq. (7.13) is the replacement $U \to \lambda U$, it follows that $\varphi_l(p, \lambda)$ is entire in λ.

An important property of the Jost function is that it is real on the imaginary axis. To prove this result, recall that $\chi_{pl}(r)$ is a real function of p for real p, so by Schwartz's reflection principle $\chi_{p^*l}(r) = \chi_{pl}(r)^*$. As we saw above, the regular solution satisfies $\chi_{-pl}(r) = (-1)^{l+1}\chi_{pl}(r)$. Recall furthermore the following symmetry property of the Riccati functions, $\hat{\jmath}_l(-z) = (-1)^{l+1}\hat{\jmath}_l(z)$ and $\hat{n}_l(-z) = (-1)^l \hat{n}_l(z)$, from which it follows $\hat{h}_l^{\pm}(-z) = (-1)^l \hat{h}_l^{\mp}(z) = (-1)^l \hat{h}_l^{\pm}(z^*)^*$. Inserting this into Eq. (7.13) we find

$$\begin{aligned} \varphi_l(-p) &= 1 + \frac{1}{-p}\int_0^\infty dr'\, \hat{h}_l^+(-pr')U(r')\chi_{-pl}(r') \\ &= 1 + \frac{1}{-p}\int_0^\infty dr'\, \hat{h}_l^+(p^*r')^*(-1)^l U(r')\chi_{p^*l}(r')^*(-1)^{l+1} = \varphi_l(p^*)^* \,. \end{aligned} \tag{7.16}$$

This relation can be written equivalently as

$$\varphi_l(p) = \varphi_l(-p^*)^* \,, \tag{7.17}$$

and for purely imaginary $p = -p^*$ one sees that the Jost function is real.

So far we have shown that the Jost function is analytic in the upper half-plane, but in order for analytic properties to be useful in the physical region, we need that the domain of analyticity extends into the lower half-plane. For this to be possible we need more restrictive requirements on the potential, which should vanish sufficiently fast to kill the exponential growth of the Riccati-Hankel function and of the regular solution. An obvious possibility is that the potential is exponentially bounded at large r, $U(r) \lesssim e^{-\mu r}$. In this case for $\mu - |\mathrm{Im}\, p| + \mathrm{Im}\, p \geq 0$ one still has uniform convergence of the integral in Eq. (7.13), so the region of analyticity is extended to include the strip $0 \geq \mathrm{Im}\, p > -\frac{\mu}{2}$.

An interesting class of potentials is that of analytic potentials, which contains potentials which are analytic functions of r, and that moreover satisfy our "reasonableness" conditions along any ray $r = \rho e^{i\theta}$ in the right half of the complex plane, i.e., for $\mathrm{Re}\, r > 0$ (for the "reasonableness" conditions see section 4.1, pag. 20). One such potential is the Yukawa potential. For such potentials, one has that the regular solution is also analytic for complex r in $\mathrm{Re}\, r > 0$ (this is shown making use of the iterative solution). By deforming the contour of integration one can thus identically write

$$\varphi_l(p) = 1 + \frac{1}{p}\int_0^\infty dr'\, \hat{h}_l^+(pr')U(r')\chi_{pl}(r') = 1 + \frac{e^{i\theta}}{p}\int_0^\infty dr'\, \hat{h}_l^+(pe^{i\theta}r')U(e^{i\theta}r')\chi_{pl}(e^{i\theta}r') \,. \tag{7.18}$$

The same argument given above allows to extend the second integral into that part of the complex plane for which $\mathrm{Im}\,(pe^{i\theta}) > 0$. This part of the complex plane overlaps with the upper half-plane and extends into the lower half-plane: due to the uniqueness of the analytic extension, the second expression in Eq. (7.18) provides the analytic extension of $\varphi_l(p)$ into part of the lower half-plane. Repeating the argument for all θ, one can continue $\varphi_l(p)$ in the whole lower half-plane, with the negative imaginary axis excluded. For a Yukawa potential one can combine the results obtained from analyticity and from the exponential boundedness, so adding to the general analyticity domain also the interval $(-\frac{\mu}{2}, 0]$ on the negative imaginary axis, where the Jost function is real.

7.3 Analytic properties of the S-matrix

The reason why we were interested in extending the domain of analyticity of the Jost function into the lower half-plane becomes clear if we recall the expression for the S-matrix elements in terms of $\varphi_l(p)$, Eq. (6.47), which we rewrite here:

$$s_l(p) = e^{2i\delta_l(p)} = \frac{\varphi_l^*(p)}{\varphi_l(p)}\,. \tag{7.19}$$

This expression is valid for physical p. In order to extend it to complex momenta, we notice that for real p one clearly has $\varphi_l^*(p) = \varphi_l^*(p^*)$. The second expression is however analytic in p. Moreover, exploiting Eq. (7.17) we have $\varphi_l(p^*)^* = \varphi_l(-p)$, so we can write

$$s_l(p) = e^{2i\delta_l(p)} = \frac{\varphi_l(-p)}{\varphi_l(p)}\,. \tag{7.20}$$

For this expression to have any meaning for nonreal p, we need that both the numerator and the denominator be analytic in the same complex domain, and this is possible only if the domain of analyticity of $\varphi_l(p)$ extends into the lower half-plane. If this is the case, we have immediately the following result: the S-matrix has a pole whenever the Jost function vanishes. Nice, but what is the physical content of this?

We prove now a crucial result, relating the zeros of the Jost function and the discrete spectrum of the Hamiltonian: $\varphi_l(p)$ vanishes at $\bar{p}$ in the upper half-plane if and only if $\bar{p}$ is purely imaginary and the Hamiltonian has a bound state of energy $E = \frac{\bar{p}^2}{2m} < 0$. To do so, let us introduce first the Jost solutions $J_{lp}^{\pm}(r)$ of the radial Schrödinger equation, identified by the boundary condition $J_{lp}^{\pm}(r) \to \hat{h}_l^{\pm}(pr)$ as $r \to \infty$.[39] As usual, the equation plus boundary condition are equivalent to an integral equation, which now takes the form

$$J_{pl}^{\pm}(r) = \hat{h}_l^{\pm}(pr) - \int_r^{\infty} dr'\, g_{pl}(r,r')U(r')J_{pl}^{\pm}(r')\,. \tag{7.21}$$

Using the by now familiar technique of iterative solution, one can show that under our usual assumptions on the potential the Jost solutions exist and are continuous in $\mathrm{Im}\, p \geq 0$, and moreover they are analytic in $\mathrm{Im}\, p > 0$.

From the asymptotic behaviours Eqs. (6.46) and (6.15) we find that for real p

$$\chi_{pl}(r) = \frac{1}{2i}\left[\varphi_l^*(p)J_{pl}^{+}(r) - \varphi_l(p)J_{pl}^{-}(r)\right] = \frac{1}{2i}\left[\varphi_l(-p)J_{pl}^{+}(r) - \varphi_l(p)J_{pl}^{-}(r)\right]\,. \tag{7.22}$$

Recalling the definition given in Eq. (6.52) of the Wronskian $W(f,g)$ of two functions f, g, we see that

$$W(J_{pl}^{+}, \chi_{pl}) = -\frac{1}{2i}\varphi_l(p)W(J_{pl}^{+}, J_{pl}^{-})\,. \tag{7.23}$$

Since $J_{lp}^{\pm}$ are both solutions of the same Schrödinger equation, we have that their Wronskian is constant:

$$\frac{d}{dr}W(J_{pl}^{+}, J_{pl}^{-}) = J_{pl}^{+}\frac{d^2J_{pl}^{-}}{dr^2} - \frac{d^2J_{pl}^{+}}{dr^2}J_{pl}^{-} = 0\,, \tag{7.24}$$

[39] Notice that the Jost solutions need not vanish at $r = 0$.

and so it can be evaluated where desired. Since we know the asymptotic behaviour $J^{\pm}_{pl} \sim e^{\pm i(pr - l\frac{\pi}{2})}$, one can compute the Wronskian at $r \to \infty$, and obtain $W(J^+_{pl}, J^-_{pl}) = -2ip$, so that

$$\varphi_l(p) = \frac{1}{p} W(J^+_{pl}, \chi_{pl})\,. \tag{7.25}$$

This relation can be analytically continued in the upper half plane, since both J^+_{pl} and χ_{pl} are analytic there.

Assume now that $\varphi_l(\bar{p}) = 0$ for some $\bar{p}$, $\mathrm{Im}\,\bar{p} > 0$. From Eq. (7.25), we see that $\chi_{\bar{p}l} \propto J^+_{\bar{p}l}$; moreover, $J^+_{\bar{p}l}$ is a normalisable eigenfunction of the Hamiltonian with eigenvalue $\frac{\bar{p}^2}{2m}$, since $|J^+_{\bar{p}l}| \sim e^{-\mathrm{Im}\,\bar{p}r}$ at large r. Since the Hamiltonian is self-adjoint, it has only real eigenvalues and so $\bar{p}$ must be purely imaginary. Conversely, if the Hamiltonian has a bound state of energy $E < 0$, then we can set $E = \frac{\bar{p}^2}{2m}$ with $\bar{p}$ purely imaginary, and the corresponding eigenfunction $\chi_{\bar{p}l}$ must be exponentially decaying at large r, and thus proportional to the Jost solution at $\bar{p}$, see Eq. (7.22). It then follows that $\varphi_l(\bar{p}) = 0$. This proves our statement about the one-to-one correspondence between bound states and zeros of the Jost function in the upper half plane.

It is worth noticing that this result is actually independent of the possibility of continuing the Jost function into the lower half-plane. When this is possible, however, we can relate the presence of a bound state in the spectrum with the appearance of a pole in the S-matrix. This is the way the result is usually presented, for several reasons: for the physically interesting cases the relevant analytic continuation into the lower half-plane can be made; for the full amplitude (as opposed to the partial-wave amplitude) the complications related to the analytic continuation do not appear and poles of the amplitude are in one-to-one correspondence with the bound states; finally, in the relativistic case it is not clear whether a Jost function can be defined, while the existence of the S-matrix is established.

There are a few more results to be discussed concerning the zeros of the Jost function. First of all, we show that there are no zeros on the real axis, except perhaps at $p = 0$. Indeed, if $\varphi_l(\bar{p}) = 0$ for real $\bar{p}$, then from the first equality in Eq. (7.22) we see that χ_{pl} would vanish identically, but since $\chi_{pl} \propto (pr)^{l+1}$ as $r \to 0$ this is impossible, as long as $p \neq 0$. Secondly, from the bound Eq. (7.15) one sees that for $\mathrm{Im}\,p \geq 0$ the Jost function tends to 1 uniformly in p as $|p| \to \infty$, decaying at least like some power of p. This implies that it has no zeros for $|p| > R$ for some R. Since an analytic function can have at most a finite number of zeros in a bounded region (see [Titchmarsh], §2.6), it follows that there is only a finite number of bound states for any angular momentum l.[40]

Finally, one can show that the zeros of φ_l at a bound state are always simple (unless $p = 0$: see below). To see this one proceeds as follows. From Eq. (7.25) we have

$$\frac{d}{dp}\varphi_l(p) = -\frac{1}{p}\varphi_l(p) + \frac{1}{p} W\left(\frac{d}{dp} J^+_{pl}, \chi_{pl}\right) + \frac{1}{p} W\left(J^+_{pl}, \frac{d}{dp}\chi_{pl}\right)\,. \tag{7.26}$$

Moreover, from

$$\frac{d}{dr} W(J^+_{pl}, \chi_{p'l}) = (p^2 - p'^2) J^+_{pl} \chi_{p'l}\,, \tag{7.27}$$

[40] The zeros of an analytic function cannot have an accumulation point (and therefore there must be a finite number of them) in a bounded region if the function is nonzero on the boundary. If we assume $\varphi_l(0) \neq 0$, then there is no place on the boundary $\mathrm{Im}\,p = 0$ of the analyticity domain $\mathrm{Im}\,p > 0$ of φ_l where zeros could accumulate. If $\varphi_l(0) = 0$, then it must vanish linearly or quadratically, as we will see below, so that the origin is an isolated zero.

from

$$W(J^+_{\bar{p}l}, \chi_{pl})|_{r=0} = 0\,, \tag{7.28}$$

which follows from $J^+_{\bar{p}l}$ vanishing at 0 since it is proportional to the regular solution, and from

$$W(J^+_{pl}, \chi_{\bar{p}l})|_{r\to\infty} = 0\,, \tag{7.29}$$

since $\chi_{\bar{p}l}$ and J^+_{pl} (for $\mathrm{Im}\, p > 0$) vanish at infinity, we find

$$\begin{aligned} W(J^+_{\bar{p}l}, \chi_{pl}) &= \int_0^r dr'\, (\bar{p}^2 - p^2) J^+_{\bar{p}l}(r') \chi_{pl}(r')\,, \\ W(J^+_{pl}, \chi_{\bar{p}l}) &= -\int_r^\infty dr'\, (p^2 - \bar{p}^2) J^+_{pl}(r') \chi_{\bar{p}l}(r')\,. \end{aligned} \tag{7.30}$$

Taking derivatives with respect to p, setting $p = \bar{p}$, and adding the two terms we obtain

$$\frac{d}{dp}\varphi_l(\bar{p}) = -2\int_0^\infty dr'\, J^+_{\bar{p}l}(r')\chi_{\bar{p}l}(r') = -2\kappa \int_0^\infty dr'\, \chi^2_{\bar{p}l}(r')\,, \tag{7.31}$$

where κ is the nonzero proportionality constant between the regular and the Jost solutions, and $\chi_{\bar{p}l}$ is a real quantity, so that the right-hand side in the equation above is nonzero.

Bound states at threshold What happens when $p = 0$? In this case the radial Schrödinger equation reads

$$\left(\frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2} - U(r)\right)\tilde{\chi}_l(r) = 0\,, \tag{7.32}$$

and one sees that the general solution behaves both at small and large r like a linear combination of r^{l+1} and r^{-l}. Imposing regularity at the origin, one is left in general with a divergent $\tilde{\chi}_l(r)$ as $r \to \infty$. For specific choices of the potential it is possible that the r^{l+1} term vanishes: if $l > 0$ one has therefore a normalisable solution, while for $l = 0$ the solution is asymptotically constant and so not normalisable. In other words, bound states at $p = 0$ might exist only for $l > 0$.

The use of a different notation for the solution at $p = 0$ is due to the fact that $\tilde{\chi}_l$ is not the limit of χ_{pl} as $p \to 0$, for the latter function vanishes identically. Instead, given that χ_{pl} satisfies the integral equation Eq. (6.48) and that $\hat{\jmath}_l(pr) \propto (pr)^{l+1}$ as $p \to 0$, one easily sees that $\tilde{\chi}_l = \lim_{p\to 0} p^{-(l+1)}\chi_{pl}$ indeed satisfies Eq. (7.32). Since $\lim_{p\to 0} p^{-(l+1)}\hat{\jmath}_l(pr) = \frac{r^{l+1}}{(2l+1)!!}$, the boundary condition is $\tilde{\chi}_l(r) \to \frac{r^{l+1}}{(2l+1)!!}$ as $r \to 0$. One similarly finds that $\lim_{p\to 0} p^l \hat{n}_l(pr) = \lim_{p\to 0} p^l \hat{h}^\pm_l(pr) = \frac{(2l-1)!!}{r^l}$. A reasoning similar to that used for the regular solution shows that the appropriate limit for the Jost solutions is $\tilde{J}^\pm_l = \lim_{p\to 0} p^l J^\pm_{pl}$, with boundary condition $\tilde{J}^\pm_l(r) \to \frac{(2l-1)!!}{r^l}$ as $r \to \infty$.

Rewriting now the Jost function as

$$\varphi_l(p) = \frac{1}{p} W(J^+_l, \chi_{pl}) = W(p^l J^+_l, p^{-(l+1)}\chi_{pl})\,, \tag{7.33}$$

we see that in the limit $p \to 0$

$$\varphi_l(0) = W(\tilde{J}^+_l, \tilde{\chi}_l)\,, \tag{7.34}$$

and therefore $\varphi_l(0) = 0$ if and only if $\tilde{\chi}_l$ ($\propto r^{l+1}$ as $r \to 0$) is proportional to $\tilde{J}_l^+$ ($\propto r^{-l}$ as $r \to \infty$), and so, for $l > 0$, a bound state at $p = 0$ exists if and only if the Jost function vanishes there. If for the s-wave $\varphi_0(0) = 0$, one talks instead of a virtual state.

We can also discuss how $\varphi_l(p)$ vanishes as $p \to 0$ (in case it does so). First of all notice that, since $\hat{\jmath}_l(pr) = (pr)^{l+1} F_l^{(j)}\left((pr)^2\right)$ and $\hat{n}_l(pr) = (pr)^{-l} F_l^{(n)}\left((pr)^2\right)$, one has that $\chi_{pl}(r) = (pr)^{l+1} F_l^{(\chi)}\left((pr)^2\right)$. To see this, observe that $\chi_{pl}(r)$ can be constructed through the iterative solution Eq. (7.4), and that at each step one is convoluting $g_{pl}(r, r') = \tilde{g}_l(r, r', p^2)$ with p^{l+1} times a function of p^2. From the relation Eq. (6.60) between the Jost function and the regular solution (for $\lambda = 1$) we find for small p

$$\begin{aligned} \varphi_l(p) &= 1 + \frac{1}{p}\int_0^\infty dr'\, \hat{n}_l(pr') U(r') \chi_{pl}(r') + \frac{i}{p}\int_0^\infty dr'\, \hat{\jmath}_l(pr') U(r') \chi_{pl}(r') \\ &= 1 + (\alpha_l^{(0)} + \alpha_l^{(1)} p^2 + \ldots) + i p^{2l+1} (\beta_l^{(1)} + \beta_l^{(2)} p^2 + \ldots)\,, \end{aligned} \tag{7.35}$$

with real coefficients $\alpha_l^{(n)}$ and $\beta_l^{(n)}$. The Jost function vanishes at the origin if $1 + \alpha_l^{(0)} = 0$, and in that case it behaves like p^2 if $l > 0$, i.e., a double zero, or like ip if $l = 0$, i.e., a simple zero. This can be seen also from Eq. (7.31): for $l > 0$, one has that

$$\begin{aligned} \frac{d}{dp}\varphi_l(\bar{p}) &= -2\int_0^\infty dr'\, J_{\bar{p}l}^+(r') \chi_{\bar{p}l}(r') = -2\bar{p}\int_0^\infty dr'\, \bar{p}^l J_{\bar{p}l}^+(r') \bar{p}^{-(l+1)} \chi_{\bar{p}l}(r') \\ &\underset{\bar{p}\to 0}{\to} -2\bar{p}\int_0^\infty dr'\, \tilde{J}_l^+(r') \tilde{\chi}_l(r') = -2\gamma\bar{p}\int_0^\infty dr'\, [\tilde{\chi}_l(r')]^2\,, \end{aligned} \tag{7.36}$$

and so $\varphi_l(p)$ vanishes quadratically as the integral in Eq. (7.36) is nonzero. For $l = 0$ this argument does not work since in that case this integral diverges. Instead, by noticing that $J_{\bar{p}0}^+ \sim 1$ at large r and $\chi_{\bar{p}0} \propto p$ as $p \to 0$, so that $J_{\bar{p}0}^+ = \bar{p}\gamma\chi_{\bar{p}0}$ as $\bar{p} \to 0$,[41] we can write (recall $\operatorname{Re}\bar{p} = 0$ if $\operatorname{Im}\bar{p} > 0$)

$$\begin{aligned} \frac{d}{dp}\varphi_0(\bar{p}) &= -2\gamma\bar{p}\int_0^\infty dr'\, [J_{\bar{p}0}^+(r')]^2 = -2i\gamma\int_0^\infty dr'\, \left[J_{\bar{p}0}^+\left(\tfrac{r'}{\operatorname{Im}\bar{p}}\right)\right]^2 \\ &\underset{\bar{p}\to 0}{\to} -2i\gamma\int_0^\infty dr'\, e^{-2r'} = -i\gamma\,, \end{aligned} \tag{7.37}$$

so that $\varphi_0(p)$ vanishes linearly at the origin (if at all).

These results lead to the following remark. From the relation Eq. (7.19) we find, for general l, when $\varphi_0(0) = 0$, that at low energies (p real positive)

$$s_l(p) = \frac{\varphi_l^*(p)}{\varphi_l(p)} \simeq \frac{\alpha_l^{(1)} p^2 - i p^{2l+1} \beta_l^{(1)}}{\alpha_l^{(1)} p^2 + i p^{2l+1} \beta_l^{(1)}} \underset{p\to 0}{\to} \begin{cases} +1 - 2i\frac{\beta_l^{(1)}}{\alpha_l^{(1)}} p^{2l-1}\,, & \text{if } l > 0\,, \\ -1 - 2i\frac{\alpha_l^{(1)}}{\beta_l^{(1)}} p\,, & \text{if } l = 0\,. \end{cases} \tag{7.38}$$

Plugging this into Eq. (6.33) we find that

$$f_l(p) = \frac{s_l(p) - 1}{2ip} \underset{p\to 0}{\to} \begin{cases} -\frac{\beta_l^{(1)}}{\alpha_l^{(1)}} p^{2(l-1)}\,, & \text{if } l > 0\,, \\ \frac{i}{p} - \frac{\alpha_l^{(1)}}{\beta_l^{(1)}}\,, & \text{if } l = 0\,. \end{cases} \tag{7.39}$$

[41] Imagine that we are controlling the position of $\bar{p}$ by changing the overall strength of the potential.

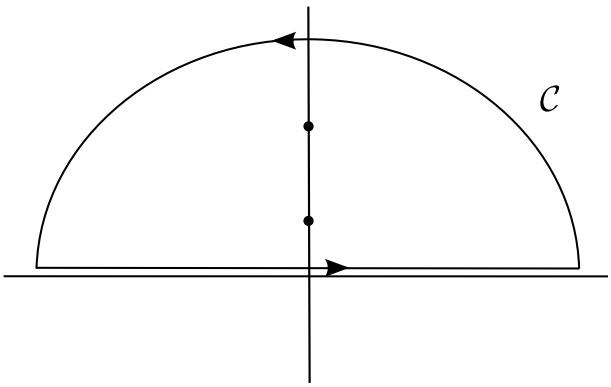

Figure 7: Path of integration in the complex plane used in the proof of Levinson's theorem.

We thus see that in the presence of a virtual state [i.e., $\varphi_0(0)$] one has a diverging s-wave scattering amplitude $f_0(p)$ as $p \to 0$. For higher angular momenta the vanishing behaviour at $p = 0$ is instead reduced by a power of 2; in particular, for the p-wave one finds a finite amplitude at $p = 0$.

7.4 Levinson's theorem

We are now ready to prove an important result concerning the phase shifts, known as Levinson's theorem:

> For any "reasonable" spherical potential, the phase shifts $\delta_l(p)$ and the number n_l of bound states of angular momentum l satisfy the relation
>
> $$\delta_l(0) - \delta_l(\infty) = n_l \pi \,, \tag{7.40}$$
>
> as long as the Jost function $\varphi_l(p)$ does not vanish at $p = 0$. If $\varphi_l(0) = 0$ then
>
> $$\delta_l(0) - \delta_l(\infty) = \begin{cases} n_l \pi & \text{if } l > 0 \,, \\ \left(n_l + \frac{1}{2}\right) \pi & \text{if } l = 0 \,. \end{cases} \tag{7.41}$$

In the case $\varphi_l(0) \neq 0$ the proof is rather straightforward. Consider the complex integral

$$I = \oint_{\mathcal{C}} dz \frac{\frac{d}{dz}\varphi_l(z)}{\varphi_l(z)} \,, \tag{7.42}$$

on the semicircular contour $\mathcal{C}$ closed in the upper half-plane, see Fig. 7. The integrand is analytic everywhere in the upper half-plane, except at the zeros of the Jost function, where it has a pole with residue 1 (here one has to make use of the fact that the zeros are simple). Therefore, by a simple application of Cauchy's residue theorem we find

$$I = 2\pi i n_l \,, \tag{7.43}$$

where n_l is the number of zeros of φ_l, which lie on the positive imaginary axis. Of course n_l matches the number of bound states of angular momentum l. On the other hand, for real p we

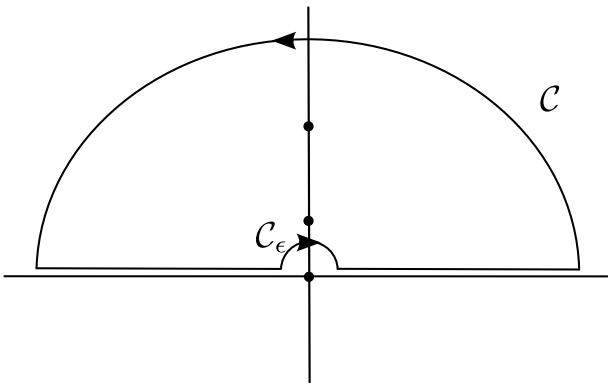

Figure 8: Modified path of integration in the complex plane used in the proof of Levinson's theorem when $\varphi_l(0) = 0$.

can write the Jost function as $\varphi_l(p) = |\varphi_l(p)|e^{-i\delta_l(p)}$ [see Eq. (6.47)]. Moreover, since $\varphi_l(p)$ tends to 1 at large $|p|$, one sees that the semicircle gives no contribution to the integral, and thus

$$I = \int_{-\infty}^{\infty} dp\, \frac{d}{dp} \log \varphi_l(p) = \int_{-\infty}^{\infty} dp\, \frac{d}{dp} \left\{ \ln |\varphi_l(p)| - i\delta_l(p) \right\} . \tag{7.44}$$

Since, for real p, $\varphi_l(-p) = \varphi_l(p)^*$, we have that $|\varphi_l(-p)|e^{-i\delta_l(-p)} = |\varphi_l(p)|e^{i\delta_l(p)}$, i.e., the modulus is an even function of p while the phase is an odd function of p. The contribution of the modulus thus cancels in Eq. (7.44), and we are left with

$$I = -2i[\delta_l(\infty) - \delta_l(0)] . \tag{7.45}$$

Comparing Eqs. (7.43) and (7.44), the desired result Eq. (7.40) follows.

If $\varphi_l(0) = 0$, then we have to modify the contour $\mathcal{C}$ in Eq. (7.42) by avoiding the origin on a small semicircular contour, see Fig. 8. In this way Eq. (7.43) remains unchanged. On the other hand, Eq. (7.44) contains now the contribution from this small contour, which reads ($dz = i\epsilon e^{i\theta} d\theta = iz d\theta$)

$$\int_{\mathcal{C}_\epsilon} dz \frac{\frac{d}{dz}\varphi_l(z)}{\varphi_l(z)} = \begin{cases} 2\displaystyle\int_{\mathcal{C}_\epsilon} \frac{dz}{z} = -2\pi i , & \text{if } l > 0 , \\ \displaystyle\int_{\mathcal{C}_\epsilon} \frac{dz}{z} = -\pi i , & \text{if } l = 0 . \end{cases} \tag{7.46}$$

We thus find $2\pi n_l = -2\pi + \delta_l(0) - \delta_l(\infty)$ if $l > 0$, and $2\pi n_l = -\pi + \delta_l(0) - \delta_l(\infty)$ if $l = 0$, from which Eq. (7.42) follows.

Combined with the choice $\delta_l(\infty) = 0$, Levinson's theorem shows that the scattering phase at zero momentum is just $n_l\pi$ (except for the s-wave in the presence of a virtual state). As p is increased from 0 to ∞, $\delta_l(p)$ passes several times through multiples of π, and at those energies one finds no contribution to the total cross section from the partial wave of momentum l. In particular, this might happen to $\delta_0(p)$ at energies low enough so that the other partial waves are completely negligible. In this case one observes that the target is transparent to the beam at a particular energy: this is the Ramsauer-Townsend effect.

7.5 Resonances

We conclude this section discussing the phenomenon of resonances, and their relation with the zeros of the Jost function in the lower half plane.

It is a fact of life that in certain scattering processes, the cross section shows one or more pronounced peaks in correspondence with specific values E_R of the energy. These peaks are called resonances. The theoretical interpretation of this phenomenon is that when the scattering system has energy near E_R, it can form a metastable state, that quickly decays again into stable objects. More precisely, in the non-relativistic setting, the resonance is related to the existence of an almost-bound state of the two particles involved in the process: if the energy of the system is near E_R, then the two particles can be temporarily captured into this state, and this causes the sharp variation of the cross section.

To see in more detail how this can happen in the single-channel scattering system discussed in this section, assume that the Jost function can be analytically continued in the lower half plane, and that it has a simple zero at some $p = \bar{p} = p_R - ip_I$ with $p_I > 0$.[42] Since $\varphi_l(p)$ and $\varphi_l(-p)$ cannot both vanish, this implies that the S-matrix has a pole at $\bar{p}$. A zero of the Jost function in the lower half plane does not correspond to a bound state: $\varphi_l(\bar{p}) = 0$ means that the regular solution is proportional to the Jost solution $J^+_{\bar{p}l}$, but since $\operatorname{Im}\bar{p} < 0$ this is not normalisable, and thus not a proper eigenfunction of the Hamiltonian.

In the vicinity of $\bar{p}$, the Jost function can be approximated as

$$\varphi_l(p) \approx \varphi_l'(\bar{p})(p - \bar{p})\,. \tag{7.47}$$

If $\bar{p}$ is close to the real axis, then there is an interval around p_R where this approximation is good. From the relation between the S-matrix and the Jost function we find for real p that

$$s_l(p) = e^{2i\delta_l(p)} = \frac{\varphi_l(p)^*}{\varphi_l(p)} \approx \frac{\varphi_l'(\bar{p})^*(p-\bar{p})^*}{\varphi_l'(\bar{p})(p-\bar{p})} = e^{2i(\delta_{\rm bg}+\delta_{\rm res}(p))}\,, \tag{7.48}$$

where

$$\delta_{\rm res}(p) = -\arg(p-\bar{p})\,, \qquad \delta_{\rm bg} = -\arg\varphi_l'(\bar{p})\,, \tag{7.49}$$

are respectively the resonant part of the phase shift, and the background phase shift. From Eq. (7.49)

$$\tan\delta_{\rm res}(p) = \frac{p_I}{p_R - p}\,, \tag{7.50}$$

and we see that as we increase p past p_R, the resonant part grows from zero to π, taking the value $\delta_{\rm res}(p_R) = \frac{\pi}{2}$ at p_R. This rapid increase of the phase shift from $\delta_{\rm bg}$ to $\delta_{\rm bg} + \pi$ is the signature of a resonance.

From Eq. (6.35) we see that the contribution σ_l of the l-th partial wave to the total cross section reads

$$\sigma_l(p) = \frac{4\pi}{p^2}(2l+1)\sin^2\delta_l(p) = \frac{4\pi}{p^2}(2l+1)\sin^2(\delta_{\rm bg}+\delta_{\rm res}(p))\,. \tag{7.51}$$

In general $\delta_{\rm bg}$ can take any value, but if $\bar{p}$ is close to zero, then, as we will see below, $\delta_{\rm bg}$ will be small. In this case one has that $\sin^2\delta_l(p) \simeq \sin^2\delta_{\rm res}(p)$ takes its maximal value at p_R. Since

[42] While zeros in the upper half plane must be simple, there is no general principle guaranteeing that it is so in the lower half plane.

usually the cross section is expressed as a function of the energy $E = \frac{p^2}{2m}$, we now describe how the analytic structure of the S-matrix in the complex-p plane translates into the analytic structure in the complex-E plane.

As a function of E, the Jost function reads $\varphi_l(p) = \varphi_l(\sqrt{2mE}) = \tilde{\varphi}_l(E)$, where the tilde is used temporarily to distinguish the two functions. The presence of the square root in this expression implies that $\tilde{\varphi}_l(E)$ has a branching point at $E = 0$, and to make it a single-valued function one needs two Riemann sheets, i.e., two copies of the complex plane. The first ("physical") sheet is cut from 0 to ∞ along the real axis, and when one crosses the cut one goes into the second sheet. Crossing the cut on the second sheet one goes back into the physical sheet. The upper complex-p half plane is mapped into the first sheet, with the physical region $p \geq 0$ being mapped to the upper rim of the cut. The lower complex-p half plane is mapped instead into the second sheet. More precisely, pairs $\pm p$ with $\mathrm{Im}\, p > 0$ are mapped to the same value of E, but while p is mapped into the first sheet, $-p$ is mapped into the second sheet. It is now clear what the analytic structure of $\tilde{\varphi}_l(E)$ lools like: a zero at $p_{\rm bound}$ on the positive imaginary axis in the p-plane, corresponding to a bound state, is mapped into $E_{\rm bound} = \frac{p^2_{\rm bound}}{2m}$ on the negative real axis in the first sheet, while a resonance zero at $p_{\rm res}$ is mapped into a point in the second Riemann sheet. If $p_{\rm res}$ is below and close to the positive real axis, then $E_{\rm res} = \frac{p^2_{\rm res}}{2m}$ will be below and close to the positive real axis, but on the second sheet: in other words, $E_{\rm res}$ is on the second sheet slighly below the cut.

After this digression, we can repeat the analysis of the phase shifts given above, this time in terms of E. A resonance zero lies now at $\bar{E} = \frac{\bar{p}^2}{2m} = E_R - i\frac{\Gamma}{2}$ on the second Riemann sheet of $\varphi_l(E)$ (where we have now dropped the tilde), and close to the cut. For real positive energies near E_R

$$\varphi_l(E) \approx \varphi_l'(\bar{E})(E - \bar{E})\,, \tag{7.52}$$

and the phase shift reads

$$\delta_l(E) = \delta_{\rm res}(E) + \delta_{\rm bg}\,, \qquad \delta_{\rm res}(E) = -\arg(E - \bar{E})\,, \qquad \delta_{\rm bg} = -\arg\varphi_l'(\bar{E})\,. \tag{7.53}$$

Furthermore,

$$\tan\delta_{\rm res}(E) = \frac{\frac{\Gamma}{2}}{E_R - E}\,, \tag{7.54}$$

and

$$\sigma_l(E) = \frac{2\pi}{mE}(2l+1)\sin^2\delta_l(E) = \frac{2\pi}{mE}(2l+1)\sin^2(\delta_{\rm bg} + \delta_{\rm res}(E))\,. \tag{7.55}$$

For small $\delta_{\rm bg}$ we can retain only the resonant part, so that

$$\sin^2(\delta_{\rm bg} + \delta_{\rm res}(E)) \simeq \sin^2\delta_{\rm res}(E) = \frac{\tan^2\delta_{\rm res}(E)}{1 + \tan^2\delta_{\rm res}(E)} = \frac{\frac{\Gamma^2}{4}}{(E_R - E)^2 + \frac{\Gamma^2}{4}}\,. \tag{7.56}$$

Up to a factor $1/E$, Eq. (7.56) gives the energy dependence of the cross section near the peak: this is the celebrated Breit-Wigner formula.

Let us now briefly repeat the argument in terms of poles of the S-matrix. If s_l has a pole at $\bar{p} = p_R - ip_I$ ($p_I > 0$), then $s_l(p) = r(p)/(p - \bar{p})$ with $r(\bar{p}) \neq 0$. For real p, unitary implies $|r(p)| = |p - \bar{p}|$, so $r(p) = e^{2i\tilde{\delta}(p)}(p - \bar{p}^*)$, since $r(p)$ cannot vanish at $\bar{p}$. Analyticity then dictates that for general complex p

$$s_l(p) = e^{2i\tilde{\delta}(p)}\frac{p - \bar{p}^*}{p - \bar{p}}\,, \tag{7.57}$$

and for real p near p_R (if p_I is small) one finally finds

$$s_l(p) \simeq e^{2i\tilde{\delta}(\bar{p})} \frac{p - \bar{p}^*}{p - \bar{p}}\,, \tag{7.58}$$

so that $\delta_l(p) \simeq \delta_{\rm bg} + \delta_{\rm res}(p)$, with $\delta_{\rm bg} = \tilde{\delta}(\bar{p})$, and $\delta_{\rm res}(p)$ as above in Eq. (7.49).

The result Eq. (7.58) shows that a resonance does not correspond to large values of the amplitude due to the vicinity of a pole: for real p near $\bar{p}$ the numerator in Eq. (7.49) is as small in absolute value as the denominator, thus keeping $|s_l(p)| = 1$, as it should. Similarly, the contribution of the resonance to $\sigma_l(p)$ can take any value, depending on the value of the background phase. The really distinctive feature of a resonance is instead the rapid change of the phase shift by an amount of π.

Resonances and bound states We have seen that zeros of the Jost function (or poles of the S-matrix) in the upper half p-plane correspond to bound states, and that zeros of the Jost function (or poles of the S-matrix) in the lower half p-plane correspond to resonances. This similarity is the basis for the interpretation of resonances as the consequence of the presence of an almost-bound state. To see this, consider a Hamiltonian of the form $H = H_0 + \lambda V$. The Jost function $\varphi_l(p, \lambda)$ is entire in λ and analytic in p in the upper half plane; we assume that it is analytic also in the lower half plane. Suppose now that for some real λ_0 there is a zero at threshold, $\varphi_l(0, \lambda_0) = 0$: for $l > 0$ this indicates the presence of a bound state and the zero is double, while for $l = 0$ there is a virtual state and the zero is simple. If we now increase λ, making the potential more attractive, then the zero will move up to some $\bar{p}(\lambda)$ on the positive imaginary axis (i.e., there will be a larger binding energy, or the virtual state can become a true bound state). If we make λ smaller, instead, the bound state will cease to exist (or the virtual state will be made "more virtual"), and the zero will move down in the lower half plane.

To see this in more detail, notice first that the zero has to move as λ moves away from λ_0: if it did not for λ in an interval around λ_0, then it would not for any λ due to analyticity; but $\varphi_l(p, 0) = 1$, so this is impossible. Next, expand $\varphi_l(p, \lambda)$ both in p and λ around some λ_0,

$$\begin{aligned}\varphi_l(p, \lambda) &= \varphi_l(p, \lambda_0) + \dot{\varphi}_l(p, \lambda_0)(\lambda - \lambda_0) + \dots \\ &= \varphi_l(0, \lambda_0) + \varphi_l'(0, \lambda_0)p + \frac{1}{2}\varphi_l''(0, \lambda_0)p^2 + \dot{\varphi}_l(0, \lambda_0)(\lambda - \lambda_0) + \dot{\varphi}_l'(0, \lambda_0)(\lambda - \lambda_0)p + \dots\end{aligned} \tag{7.59}$$

where prime and dot indicate the derivative with respect to p and λ, respectively. Imposing now $\varphi_l(p, \lambda_0) = 0$, and recalling from Eq. (7.35) the small p behaviour of $\varphi_l(p, \lambda_0)$, we have to lowest order $[b \equiv \dot{\varphi}_l(0, \lambda_0)]$

$$\varphi_l(p, \lambda) \simeq b(\lambda - \lambda_0) + \begin{cases} ic_0 p & (l = 0)\,, \\ c_l p^2 & (l > 0)\,, \end{cases} \tag{7.60}$$

with real c_l, $l \geq 0$. For $l = 0$, the zero of the Jost function is thus at

$$\bar{p} = \frac{ib}{c_0}(\lambda - \lambda_0)\,; \tag{7.61}$$

if for $\lambda > \lambda_0$ there is a bound state and thus $\mathrm{Im}\,\bar{p} > 0$ (which requires $b/c_0 > 0$), then $\bar{p}$ moves down along the imaginary axis as λ is decreased, until it crosses zero and goes on the negative

imaginary axis as λ becomes smaller than λ_0. For $l > 0$ we have instead two zeros,

$$\bar{p} = \pm i \sqrt{\frac{b}{c_l}(\lambda - \lambda_0)}\,; \tag{7.62}$$

assuming that for $\lambda \geq \lambda_0$ there is a bound state, so that $\bar{p}$ are purely imaginary in that case (which requires $b/c_l > 0$), then we see that the two zeros get closer to the origin as λ is decreased, until they finally join into a double zero at $\lambda = \lambda_0$, and then part ways again as λ becomes smaller than λ_0. They will not move into the upper half plane (they could only move along the imaginary axis, but as the potential is made less attractive it will not support bound states anymore), and there cannot be zeros on the really axis, so they will move in the lower half plane, symmetrically away from the imaginary axis, since $\varphi_l(p) = \varphi_l(-p^*)^*$ implies that if $\varphi_l(\bar{p}) = 0$, then also $\varphi_l(-\bar{p}^*) = 0$. From Eq. (7.35) one sees that the imaginary part of the zero satisfies (to lowest order) $\mathrm{Re}\,\bar{p}\mathrm{Im}\,\bar{p} \propto \mathrm{Re}\,\bar{p}^{2l+1}$, and so $\mathrm{Im}\,\bar{p} \propto (\lambda - \lambda_0)^l$: this means that for resonances of higher angular momentum the resonance zero will stay closer to the real axis, thus leading to a sharper resonance due to a more rapid change of phase.

Background phase for low-energy resonances We now return on the background phase and show that it must be small when the resonance is at low energy. Consider first the case $l > 0$. As a function of energy, $\varphi_l(E, \lambda)$ is real on the negative real axis (reflecting the fact that it is real on the positive imaginary axis in the p-plane), and so must be its derivative; therefore, $\frac{d\varphi_l}{dE}|_{E=\bar{E}}$ is a real function of (real) λ as long as $\lambda > \lambda_0$ and the potential supports a bound state. By continuity, it will be almost real also in an interval with $\lambda < \lambda_0$, since it does not vanish at $\lambda = \lambda_0$ ($\varphi_l \propto E$ in that case). Therefore, δ_{bg} will be small as long as the zero is near threshold. For $l = 0$ it is more convenient to consider $\varphi_l(p, \lambda)$ as a function of p. In this case, $\varphi_l(p, \lambda)$ is real on the positive imaginary axis, and so $\frac{d\varphi_l}{dp}|_{p=\bar{p}}$ is real as long as $\lambda > \lambda_0$. Since it does not vanish when the zero is at threshold, by continuity it will remain real also for $\lambda - \lambda_0 < 0$ as long as this is small.

As a final comment, we remark that the relation between resonances and zeros of the Jost function in the lower half plane is not as mathematically compelling as the one between bound states and zeros in the upper half plane. Indeed, zeros in the lower half plane have physical implications only if they are close enough to the real axis, i.e., not every zero with negative imaginary part gives rise to a resonance. Conversely, it is theoretically possible to have the same physical effects typical of a resonance without there being any zero in the lower half plane. Nevertheless, the picture discussed here allows to satisfactorily describe most of the experimental results.

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