Chapter 0

Quantum Basics

0.1 Wave mechanics

Historically, quantum mechanics has been developed in two formulations: the wave mechanics of E. Schrödinger (and others) and the matrix mechanics of W. Heisenberg (and others).

You should be familiar with wave mechanics, and we give a brief reminder here. We start with a quantum particle in one dimension, with x being the position coordinate. The particle's state is characterized by a wavefunction $\psi(x,t) \equiv \langle x|\Psi(t)\rangle$ that solves the Schrödinger equation:

$$\mathrm{i}\hbar\partial_t\psi(x,t) = H\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x,t), \tag{1}$$

where H is the Hamilton operator. The last expression is true for a particle in a (one-dimensional) potential $V(x)$. You get this equation from the classical Hamiltonian function by replacing the momentum by a differential operator,

$$p \mapsto \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x} \tag{2}$$

The generalization to two and three dimensions is immediate. The generalization to a system of two or more particles is immediate as well: one gets a wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2, t)$. 'Quantum statistics' enters here if the particles are indistinguishible: $\psi(\mathbf{r}_2, \mathbf{r}_1, t) = \pm\psi(\mathbf{r}_1, \mathbf{r}_2, t)$, depending on whether the particles are bosons or fermions.

The interpretation of the wavefunction is such that $|\psi(x,t)|^2\mathrm{d}x$ gives the probability to find the particle around position x when a measurement is done. We can thus introduce a probability density $n(x,t)$. Particles do not disappear without reason, this is why normally the probability is conserved (equation of continuity)

$$\partial_t n + \partial_x j = 0 \tag{3}$$

$$j(x,t) = \frac{\hbar}{2\mathrm{i}m}\left[\psi^*(x,t)\frac{\partial}{\partial x}\psi(x,t) - \text{c.c.}\right] = \mathrm{Im}\left[\psi^*(x,t)\frac{p}{m}\psi(x,t)\right] \tag{4}$$

where j is the probability current (density). In three dimensions, this is a vector field and $\partial_x j \mapsto \mathrm{div}\,\mathbf{j}$ in Eq.(3).

A stationary situation is characterized by a time-independent particle density, $\partial_t n = 0$. In that case, $\operatorname{div} \mathbf{j} = 0$, either because the wave function is real (bound state) or because an 'incident current' is balanced by an 'outgoing current'. This can be checked easily in one-dimensional examples.

The following wave function leads to a stationary density, it is therefore called a stationary state and solves the stationary Schrödinger equation:

$$\psi(x,t) = \psi(x)\,\mathrm{e}^{-\mathrm{i}Et/\hbar} \tag{5}$$

$$E\psi(x) = H\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x). \tag{6}$$

This is an eigenvalue equation for the Hamiltonian operator H. Only for specific values of E do solutions to the stationary Schrödinger equation exist.[1] The allowed numbers E are called the 'energy eigenvalues'. Taken together, they form the 'spectrum of the Hamiltonian H'.

Examples.
Harmonic oscillator, $E_n = \hbar\omega(n + \frac{1}{2})$ with $n = 0, 1, \ldots$.
Free particle, $E_p = p^2/2m$ with $p = -\infty \ldots + \infty$.
Hydrogen atom, $E_n = -1/(2n^2)$ in atomic units with $n = 1, 2, \ldots$ (bound states) and $E = \hbar^2 k^2/2m > 0$ ('continuous spectrum').

0.2 Operator mechanics

In the second 'picture' of quantum mechanics, operators play a much more important role. Let us briefly discuss this concept to begin with. In this lecture, we shall not put circumflex accents ('hats') on the letters for operators. You already know the momentum operator p: it is the differential operator given in Eq.(2). It 'acts' on the wavefunction $\psi(x,t)$ by differentiation. On the (Hilbert) space of differentiable functions, the chain rule of differentiation therefore gives the following 'commutator'

$$[x,\, p] \equiv xp - px = \mathrm{i}\hbar. \tag{7}$$

This is the basic difference with respect to classical mechanics, where x and p are numbers. At the most, they act as functions on the phase space (formulation of classical mechanics with Poisson brackets). The nonzero commutator (7) implies the 'Heisenberg indeterminacy relation'

$$\Delta x\, \Delta p \geq \frac{\hbar}{2} \tag{8}$$

where Δx and Δp is the statistical spread (e.g., the standard deviation) of the results of measurement for x and p. The factor $\frac{1}{2}$ is actually a matter of taste and of definition for the statistical spread.

Remark. The Heisenberg relation (8) is actually a consequence of Fourier transformations: the probability of finding a result $p = \hbar k$ when measuring the particle

[1] This is different from the time-dependent equation (1) that can always be solved. For potentials that vanish at infinity, stationary solutions can, as a general rule, also be found for all $E > 0$.

momentum is proportional to $|\tilde{\psi}(k,t)|^2$ where $\tilde{\psi}(k,t)$ is the (spatial) Fourier transformation of $\psi(x,t)$:

$$\tilde{\psi}(k,t) = \int \mathrm{d}x\, \psi(x,t)\, \mathrm{e}^{-\mathrm{i}kx}. \tag{9}$$

A well-known property of Fourier transforms is: if Δx is the 'typical width' of $|\psi(x)|^2$, then the typical width Δk of its Fourier transform $|\tilde{\psi}(k)|^2$ is $\Delta k \approx 1/\Delta x$.

The second formulation of quantum mechanics is called the 'Heisenberg picture'. Here, the time-dependence is carried by the operators, not the wavefunction. The equation of motion of an operator $A(t)$ is given by the commutator with the Hamilton operator:

$$\frac{\mathrm{d}}{\mathrm{d}t} A(t) = \frac{\mathrm{i}}{\hbar} [H,\, A(t)] \tag{10}$$

A convenient initial condition is $A(0) = A$, the operator in the Schrödinger picture.

In the exercises, you show that the Schrödinger and Heisenberg 'pictures' give the same physical predictions. This means that the expectation values

$$\langle A(t) \rangle = \langle \Psi | A(t) | \Psi \rangle \tag{11}$$

are the same as in the Schrödinger picture where one computes $\langle \Psi(t) | A | \Psi(t) \rangle$. In the Heisenberg picture, (average) results of measurements are thus predicted by computing the expectation values (11).

Conserved observables. As a simple consequence of Eq.(10), $H(t) = H$ for all times: energy is conserved. By this we mean that the expectation value $\langle H(t) \rangle$ is time-independent. Indeed, $\langle H(t) \rangle = \langle \Psi | H | \Psi \rangle$ and the state $|\Psi\rangle$ of the system does not depend on time in the Heisenberg picture.

This property holds for all operators K that commute with H: indeed, the differential equation (10) shows that $[K,\, H] = 0$ is equivalent to K being constant. Hence, an observable is conserved if and only if it commutes with H.

'Canonical quantization'. The quantization of a classical system can be performed in the 'canonical way' by starting from its classical Hamiltonian. This is a function $H(x_i, p_j)$ of coordinates and ('canonically conjugate') momenta. One replaces these functions by non-commuting operators such that

$$[x_i,\, p_j] = \mathrm{i}\hbar\, \delta_{ij}, \tag{12}$$

where the Kronecker δ_{ij} appears. The choice (2) is just a convenient way to 'represent' this commutator on a suitable space of functions.

As a reminder from classical mechanics: if you start from a Lagrangian $L = L(x, v)$ that depends on coordinates x and velocities $v = \mathrm{d}x/\mathrm{d}t$, then the canonical momentum is given by

$$p = \frac{\partial L}{\partial v}, \tag{13}$$

and one obtains the Hamiltonian function by the 'Legendre transform'

$$H(x, p) = vp - L(x, v) \tag{14}$$

where on the right hand side, the velocity v must be expressed in terms of the momentum p.

Examples for operators.

- Creation and annihilation operators for the one-dimensional harmonic oscillator

$$a = \frac{1}{a_0\sqrt{2}}\left(x + \mathrm{i}\frac{p}{m\omega}\right), \qquad a^\dagger = \frac{1}{a_0\sqrt{2}}\left(x - \mathrm{i}\frac{p}{m\omega}\right) \tag{15}$$

$$\left[a,\, a^\dagger\right] = 1. \tag{16}$$

  where $a_0 = \sqrt{\hbar/m\omega}$ is the typical size of the ground state wave function of the oscillator.

- Particle density and particle current operators. They are functions of a c-number valued coordinate q:

$$n(q,t) = \delta(q - x(t)), \tag{17}$$

$$j(q,t) = \frac{1}{2m}\left\{p(t),\, \delta(q - x(t))\right\}$$

$$\equiv \frac{1}{2m}\left(p(t)\,\delta(q - x(t)) + \delta(q - x(t))\,p(t)\right) \tag{18}$$

  The curly brackets $\{A,\, B\}$ denote the 'anti-commutator'.

- Orbital angular momentum operator in three dimensions

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = \frac{\hbar}{\mathrm{i}}\mathbf{r} \times \nabla \tag{19}$$

  (the order of the operators is irrelevant here – why?) with the commutation relations

$$[L_x,\, L_y] = \mathrm{i}\hbar\, L_z \tag{20}$$

  and cyclic permutations. Of course, $[L_k,\, L_k] = 0$. You have seen in the quantum mechanics I lecture that in a spherically symmetric potential $V(r)$ (a 'central potential'), the wave functions can be expanded in eigenfunctions of the angular momentum operator. All three components commute with the Hamiltonian for a central potential. In addition, all components commute with the squared angular momentum $\mathbf{L}^2$. One conventionally chooses L_z, $\mathbf{L}^2$ and H as three mutually commuting operators.

  In the exercises, you show that the kinetic energy operator can be written in the form

$$-\frac{\hbar^2}{2m}\triangle = \frac{\hbar^2}{2m\,r}\frac{\partial^2}{\partial r^2}r + \frac{1}{2mr^2}\mathbf{L}^2 \tag{21}$$

  We can write the wave function as a product of an eigenstate of $\mathbf{L}^2$ and of L_z (these functions are called spherical harmonics) and of a 'radial wave function':

$$\psi(\mathbf{r}) = Y_{lm}(\theta,\varphi)R_l(r) \tag{22}$$

  where $l = 0, 1, 2, \ldots$ and $m = -l, \ldots, l-1, l$. The eigenvalue of $\mathbf{L}^2$ is $\hbar^2 l(l+1)$. The radial wavefunction $R_l(r)$ then solves the 'radial Schrödinger equation'

$$ER_l = -\frac{\hbar^2}{2m\,r}\frac{\partial^2}{\partial r^2}rR_l + \frac{\hbar^2 l(l+1)}{2m\,r^2}R_l + V(r)R_l \tag{23}$$

  where the last two potential terms can be combined into an 'effective potential'. As in classical mechanics, one has a 'centrifugal potential' proportional to $l(l+1)/r^2$.

Chapter 1

Scattering Theory

In scattering theory, we are dealing with the 'continuous spectrum' of a Hamiltonian operator and the corresponding wavefunctions. We focus in this chapter on the nonrelativistic theory and shall stay in three dimensions for most of the time.

1.1 Problem formulation

We focus on the scattering of a particle off a potential $V(\mathbf{r})$ that vanishes at infinity. The potential is significantly nonzero around the origin. We shall argue that this scattering process can be described by a stationary Schrödinger equation with a positive energy eigenvalue E. Far from the potential, the wave function of the particle is similar to a plane wave $\mathrm{e}^{\mathrm{i}kz}$ if we choose the z-direction along the incident wavevector (what we shall do), and the energy is given by $E = \hbar^2 k^2/2m$.

In classical potential scattering, the particle follows a trajectory along the (negative) z-axis, changes direction upon scattering and emerges in some direction specified by the angles θ, φ. The relevant quantity is the so-called *differential cross section*. It is defined by the ratio

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{1}{\text{(incident current density)}} \frac{\text{(no. of detected particles)}}{\mathrm{d}t\,\mathrm{d}\Omega} \tag{1.1}$$

In classical mechanics, it can be expressed in terms of the scattering angle $\theta(b)$ that depends on the 'impact parameter' b (a simple exercise, see § 18 in Landau's Mechanics text)

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{b}{\sin\theta} \left| \frac{\mathrm{d}b}{\mathrm{d}\theta} \right| \tag{1.2}$$

In quantum mechanics, we are looking for a specific solution to the stationary Schrödinger equation, a so-called *stationary scattering state*

$$H\psi = -\frac{\hbar^2}{2m}\triangle\psi + V(\mathbf{r})\psi = \frac{\hbar^2 k^2}{2m}\psi. \tag{1.3}$$

This stationary picture corresponds to a steady flow of particles onto the scattering potential. The scattering state is determined by an asymptotic requirement: far from the origin (where the scattering potential is zero), the wave

function should correspond to a sum of an incident wave and a scattered wave:

$$r \to \infty : \quad \psi(\mathbf{r}) \to \mathrm{e}^{\mathrm{i}kz} + f(\mathbf{\Omega})\frac{\mathrm{e}^{\mathrm{i}kr}}{r} \tag{1.4}$$

where $r = |\mathbf{r}|$. The first term describes the incident plane wave with k-vector along the z-axis; the second term an 'outgoing spherical wave'. This form is chosen such that the stationary probability current points radially outward at large r. You have verified this in the exercises. The angular dependence of $f(\mathbf{\Omega})$ ($\mathbf{\Omega}$ combines both θ and φ) specifies the angular distribution of the scattered particles.

Note. A mathematically more precise formulation for the outgoing spherical wave is the so-called Sommerfeld radiation condition:

$$\lim_{r\to\infty} r\left(\mathrm{i}k\psi_{\mathrm{sc}}(\mathbf{r}) - \frac{\partial\psi_{\mathrm{sc}}}{\partial r}\right) = 0. \tag{1.5}$$

This applies only to the scattered part of the wave function, $\psi_{\mathrm{sc}}(\mathbf{r}) = \psi(\mathbf{r}) - \mathrm{e}^{\mathrm{i}kz}$, not the incident one, of course.

The number of particles scattered per unit time into an element of solid angle $\mathrm{d}\Omega$ around the direction $\mathbf{\Omega}$ is given by

$$\frac{\mathrm{d}N_{\mathrm{sc}}}{\mathrm{d}t} = \lim_{r\to\infty} j_r(r\mathbf{\Omega})r^2\mathrm{d}\Omega = \frac{\hbar k}{m}|f(\mathbf{\Omega})|^2\mathrm{d}\Omega, \tag{1.6}$$

where we took into account only the outgoing spherical wave. We use the notation $\mathbf{\Omega}$ for the unit vector specified by the angles θ, φ. A similar calculation for the incident probability current gives $\mathbf{j}_{\mathrm{inc}} = \mathbf{e}_z\hbar k/m$, taking into account only the incident plane wave. A more careful approach would also take into account the interference between the incident and scattered wave. Actually this effect is only important for 'forward scattering' ($\theta = 0$). It leads to the so-called 'optical theorem' that you shall discuss in the exercises.

According to the definition (1.2), the scattering cross section is thus given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\mathbf{\Omega})|^2 \tag{1.7}$$

To summarize, the scattering problem is solved if we know the 'scattering amplitude' $f(\mathbf{\Omega}) = f(\mathbf{\Omega}; k)$ as a function of the scattering angle and the incident wave vector.

1.2 Integral equation

A convenient tool to solve the Schrödinger equation (1.3) is the transformation to an integral equation, called Lippmann–Schwinger equation in quantum mechanics. The advantage of this equation is that it includes the asymptotic boundary conditions (1.4) and that one can formulate easily an approximate scheme to solve it, the so-called Born-von Neumann series.

We start from (1.3) and write it in the form

$$\triangle\psi + k^2\psi = \frac{2m}{\hbar^2}V(\mathbf{r})\psi(\mathbf{r}) \tag{1.8}$$

Formally, we can consider the right hand side as an inhomogeneity or 'source term'. Then, the equation can be solved with the help of a Green function $G(\mathbf{r}, \mathbf{r}'; k)$, as you know from electrodynamics. The Green function is the solution to a point source

$$\left(\triangle + k^2\right) G(\mathbf{r}, \mathbf{r}'; k) = \delta(\mathbf{r} - \mathbf{r}') \tag{1.9}$$

and if we know it, we can write

$$\psi(\mathbf{r}) = \mathrm{e}^{\mathrm{i}kz} + \frac{2m}{\hbar^2} \int \mathrm{d}^3 r'\, G(\mathbf{r}, \mathbf{r}'; k) V(\mathbf{r}') \psi(\mathbf{r}'). \tag{1.10}$$

This is the Lippmann–Schwinger equation. Note that this equation applies for all positions $\mathbf{r}$, not only far away from the scattering potential. The first term is a solution to the 'homogeneous equation'. It is chosen to reproduce the incident wave. The second term gives asymptotically the outgoing spherical wave if we choose the correct (the 'retarded') Green function that behaves like $\mathrm{e}^{\mathrm{i}kr}/r$ for large r. A calculation that we summarize below leads to

$$G(\mathbf{r}, \mathbf{r}'; k) = G(\mathbf{r} - \mathbf{r}'; k) = -\frac{1}{4\pi} \frac{\mathrm{e}^{\mathrm{i}k|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}. \tag{1.11}$$

At large distance from the origin, we can assume that $|\mathbf{r} - \mathbf{r}'| \approx r - \mathbf{r}' \cdot \mathbf{r}/r$ because the integration points $\mathbf{r}'$ remain in a bounded region around the origin (this is due to the potential $V(\mathbf{r}')$ under the integral). The leading order behaviour is thus given by (we write $\mathbf{\Omega} = \mathbf{r}/r$)

$$\frac{2m}{\hbar^2} \int \mathrm{d}^3 r'\, G(\mathbf{r} - \mathbf{r}'; k) V(\mathbf{r}') \psi(\mathbf{r}') \tag{1.12}$$

$$\approx -\frac{2m}{\hbar^2} \frac{\mathrm{e}^{\mathrm{i}kr}}{4\pi r} \int \mathrm{d}^3 r'\, \mathrm{e}^{-\mathrm{i}k\mathbf{\Omega}\cdot\mathbf{r}'} V(\mathbf{r}') \psi(\mathbf{r}') \tag{1.13}$$

$$f(\mathbf{\Omega}) = \frac{m}{2\pi\hbar^2} \int \mathrm{d}^3 r'\, \mathrm{e}^{-\mathrm{i}k\mathbf{\Omega}\cdot\mathbf{r}'} V(\mathbf{r}') \psi(\mathbf{r}') \tag{1.14}$$

This again is not a really useful result: we have only expressed the scattering amplitude in terms of the (unknown) wave function $\psi(\mathbf{r}')$ 'inside the potential'.

Scalar Green function of the Helmholtz equation

The Helmholtz equation is the physicists' name for the differential operator in Eq.(1.9). The spatial Fourier transform of this equation gives

$$G(\mathbf{q}) = \frac{1}{k^2 - \mathbf{q}^2} + C\delta(k^2 - \mathbf{q}^2) \tag{1.15}$$

where the second term corresponds to the 'homogeneous solution', with an amplitude to be fixed by the Sommerfeld condition. A choice that turns out to work is

$$G^{\pm}(\mathbf{q}) = \frac{1}{k^2 - \mathbf{q}^2} \mp \mathrm{i}\pi\delta(k^2 - \mathbf{q}^2) = \lim_{\epsilon \longrightarrow 0} \frac{1}{k^2 - \mathbf{q}^2 \pm \mathrm{i}\epsilon} \tag{1.16}$$

The limit $\epsilon \to 0$ from positive values will not be written explicitly in the following. Indeed, the transformation back to real space gives, as shown in the exercises:

$$\begin{aligned} G^{\pm}(\mathbf{r}) &= \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \frac{\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}}}{k^2 - \mathbf{q}^2 \pm \mathrm{i}\epsilon} \\ &= \frac{1}{4\mathrm{i}\pi^2 r} \int_{-\infty}^{+\infty} \mathrm{d}q \, \frac{\mathrm{e}^{\mathrm{i}qr}}{k^2 - q^2 \pm \mathrm{i}\epsilon} \qquad (1.17) \\ &= -\frac{\mathrm{e}^{\pm \mathrm{i}kr}}{4\pi r} \qquad (1.18) \end{aligned}$$

Within this 'ϵ-trick' that is widely used in quantum field theory, one takes an integration path along the real q-axis in Eq.(1.17). The $+\mathrm{i}\epsilon$ in the denominator shifts the pole $q = +k$ slightly into the upper half-plane. Only poles in this half-plane contribute to the result, and one gets the outgoing spherical wave. More details: see exercises.

An alternative argument that does not use the 'ϵ-trick' is based on a deformation of the integration contour in Eq.(1.17) (written now for $\epsilon = 0$) in the complex q-plane. First observation: for any choice of contour, one has a solution to Eq.(1.9). Second observation: the way one circles around the poles of the denominator, located at $q = \pm k$, one gets different contributions of outgoing and ingoing spherical waves. In fact, the residues of these poles correspond to ingoing and outgoing spherical waves. The contour that encircles the pole at $q = +k$ from below and passes above the pole at $q = -k$ gives the outoing wave only that we focus on here.

Last variation for mathematicians: never ever evaluate Green functions for real values of k, but take a small, positive imaginary part to ensure the Sommerfeld condition (1.5). Indeed, $(k + \mathrm{i}\epsilon)^2 - \mathbf{q}^2 = k^2 - \mathbf{q}^2 + 2\mathrm{i}k\epsilon$ has a form similar to the denominator in the 'ϵ-trick' (although with a different meaning and dimension for ϵ).

1.3 Born–von Neumann series

The Born–von Neumann series is based on an iterative solution of the Lippmann–Schwinger Eq.(1.10). This iteration converges rapidly if the scattering potential is 'weak' since higher-order terms involve higher powers of $V(\mathbf{r}')$. In fact, we are dealing here with a variation of perturbation theory in the context of scattering. (A crash course on perturbation theory follows in an extra section.)

The iteration of the integral equation yields

$$\psi(\mathbf{r}) = \psi^{(0)}(\mathbf{r}) + \psi^{(1)}(\mathbf{r}) + \psi^{(2)}(\mathbf{r}) + \ldots \qquad (1.19)$$

Zero'th term: no scattering at all

$$\psi^{(0)}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}kz} \qquad (1.20)$$

First term: replace $\psi(\mathbf{r})$ by the plane wave $\psi^{(0)}(\mathbf{r})$ under the integral

$$\psi^{(1)}(\mathbf{r}) = -\frac{m}{2\pi\hbar^2} \int \mathrm{d}^3 r' \, \frac{\mathrm{e}^{\mathrm{i}k|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}') \mathrm{e}^{\mathrm{i}kz'} \qquad (1.21)$$

Second term: a double integral

$$\psi^{(2)}(\mathbf{r}) = \frac{m^2}{(2\pi)^2\hbar^4}\int \mathrm{d}^3r'\mathrm{d}^3r''\,\frac{\mathrm{e}^{\mathrm{i}k|\mathbf{r}-\mathbf{r}'|+\mathrm{i}k|\mathbf{r}'-\mathbf{r}''|}}{|\mathbf{r}-\mathbf{r}'||\mathbf{r}'-\mathbf{r}''|}V(\mathbf{r}')V(\mathbf{r}'')\mathrm{e}^{\mathrm{i}kz''} \tag{1.22}$$

and so on.

The expression (1.21) is the '(first order) Born approximation'. It provides us (finally!) with an explicit result for the scattering amplitude:

$$f_{\mathrm{Born}}(\boldsymbol{\Omega}) = -\frac{m}{2\pi\hbar^2}\tilde{V}(\mathbf{q}), \qquad \mathbf{q} = k\boldsymbol{\Omega} - k\mathbf{e}_z = \mathbf{k}' - \mathbf{k} \tag{1.23}$$

where $\tilde{V}(\mathbf{q})$ is the spatial Fourier transform of the scattering potential, evaluated at the 'wave vector transfer' $\mathbf{q}$:

$$\tilde{V}(\mathbf{q}) = \int \mathrm{d}^3r'\,\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}'}V(\mathbf{r}') \tag{1.24}$$

The vector $\mathbf{q}$ is the difference between the outgoing k-vector $\mathbf{k}' = k\boldsymbol{\Omega}$, specified by the observation direction $\boldsymbol{\Omega}$, and the k-vector of the incident plane wave, $\mathbf{k} = k\mathbf{e}_z$.

For a spherically symmetric potential, the scattering amplitude can be written in the form

$$f_{\mathrm{Born}}(\theta) = -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^\infty r\,\mathrm{d}r\,V(r)\sin qr \tag{1.25}$$

as you show in the exercises. Here, $q = 2k\sin(\theta/2)$. We defer a comparison to a square well to a later section when the exact solution in terms of spherical harmonics (partial waves) is available.

Coulomb scattering. For now, let us focus on the example of electron-proton scattering in the nonrelativistic limit. The potential is given by $V(r) = -e^2/(4\pi\varepsilon_0 r)$ where $-e$ is the electron charge. This means that we treat the proton as an immobile and pointlike target and put $\alpha = me^2/(2\pi\hbar^2\varepsilon_0)$. From Eq.(1.25), we get a scattering amplitude

$$f_{\mathrm{Born}}(\boldsymbol{\Omega}) = \frac{\alpha}{q^2} \tag{1.26}$$

Note that the sign of the potential (attractive or repulsive) only enters into the sign of the scattering amplitude, but not into the scattering cross section

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{|\alpha|^2}{q^4} = \frac{m^2e^4}{(2\pi\hbar^2\varepsilon_0)^2[2k\sin(\theta/2)]^4} \tag{1.27}$$

Note the strong angular dependence with a pronounced peak in the forward direction. Any deviation from this result is a signature of the finite size of the target particle. One introduces the technical term of a 'form factor' to quantify this. In particle physics, form factors provide measurements of the size of the proton and the charge distribution of the quarks inside it, for example.

We note that Eq.(1.27) is actually the same result as in classical mechanics, an interesting coincidence. In terms of the incident energy $E = \hbar^2 k^2/2m$, impact parameter b and scattering angle θ are related by (Landau I, § 19):

$$b = \frac{e^2}{8\pi\varepsilon_0 E}\cot(\theta/2) \tag{1.28}$$

and one can easily check that the classical cross section (1.2) gives the same result as the Born approximation (1.26).

Attention. This is a pure coincidence. In fact, the Coulomb potential with its $1/r$ tail decays too slowly to justify the far-field expansion we have done here. The exact wave function can be found (see, e.g., the book by A. Messiah, vol.I, appendix B) and its 'spherically outgoing part' contains terms like

$$f(\theta)\frac{\mathrm{e}^{\mathrm{i}(kr-\gamma\log(2kr))}}{r} \tag{1.29}$$

for large r. Note the logarithmic phase correction that goes with the parameter $\gamma = \alpha/2k$.

Convergence of the Born series

The first Born approximation is sufficient in the majority of physical applications. A large part of crystallography and X-ray scattering is built on it, for example, not to mention high-energy physics. Nevertheless, it is instructive to analyze the range of validity of this approximation. The general rule is that the scattering potential 'be sufficiently weak'. But we shall find that this means different things at low and high energies.

The first, heuristic, idea is to require that the first order term $\psi^{(1)}(\mathbf{r})$ [Eq.(1.21)] be a small correction compared to the zero'th order term $\psi^{(0)}(\mathbf{r})$. Let us check this inequality at $\mathbf{r} = \mathbf{0}$, right in the center of the scattering potential.

We get, of course, $\psi^{(0)}(\mathbf{0}) = 1$ and

$$\psi^{(1)}(\mathbf{0}) = -\frac{2m}{\hbar^2 k}\int_0^\infty \mathrm{d}r\,\mathrm{e}^{\mathrm{i}kr}V(r)\sin(kr) \tag{1.30}$$

where $V(r)$ is assumed with spherical symmetry, for simplicity. To proceed, we shall assume that the radial integral is actually limited to a range $r \le R$. The length R is called the 'range' of the scattering potential.

In the regime of high energies, one has $kR \gg 1$, and the integral (1.30) can be handled by partial integration:

$$kR \gg 1: \qquad \psi^{(1)}(\mathbf{0}) = -\frac{\mathrm{i}m}{\hbar^2 k}\int_0^R \mathrm{d}r\,\left(1-\mathrm{e}^{2\mathrm{i}kr}\right)V(r) \tag{1.31}$$

$$\approx -\frac{\mathrm{i}m}{\hbar^2 k}\left(\int_0^R \mathrm{d}r\,V(r) - \frac{1}{2\mathrm{i}k}\left[\mathrm{e}^{2\mathrm{i}kr}V(r)\right]_0^R + \frac{1}{2\mathrm{i}k}\int_0^R \mathrm{d}r\,\mathrm{e}^{2\mathrm{i}kr}\partial_r V(r)\right) \tag{1.32}$$

When the potential is sufficiently smooth (certainly not the case for the Coulomb potential), the second line in Eq.(1.32) is smaller compared to the first by a factor $1/(kR)$ and can be neglected. Hence to leading order, the inequality $|\psi^{(1)}(\mathbf{0})| \ll 1$ leads to the criterion

$$\frac{m}{\hbar^2}\int_0^R \mathrm{d}r\ |V(r)| \ll k, \tag{1.33}$$

the scattering potential times its range must be 'small' compared to the incident momentum. This can always be satisfied at 'sufficiently high' energy, but remember that our treatment is not valid in the relativistic regime.

In the opposite case, low incident energy, we have $kR \ll 1$, and the integral (1.30) becomes

$$\frac{2m}{\hbar^2}\int_0^R \mathrm{d}r\, r\ |V(r)| \ll 1, \tag{1.34}$$

the scattering potential times its range squared must be 'small' in absolute value. (A note on units: $(2m/\hbar^2)V$ has the units of wavevector squared, hence multiplied by R^2, one gets a dimensionless number.)

Finally, a note for mathematical physicists: the Born series can be seen as a geometrical series to invert an integral operator, and this series converges if the operator in the series has a norm smaller than 'unity'. Let us write $U(\mathbf{r}) = (m/2\pi\hbar^2)V(\mathbf{r})$ and re-scale the wave function as $\phi(\mathbf{r}) = |U(\mathbf{r})|^{1/2}\psi(\mathbf{r})$. The Lippmann-Schwinger equation then becomes

$$\begin{aligned}\phi(\mathbf{r}) &= \phi_{\mathrm{inc}}(\mathbf{r}) - \int \mathrm{d}^3r'\, \frac{\mathrm{e}^{\mathrm{i}k|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}|U(\mathbf{r})|^{1/2}\frac{U(\mathbf{r}')|}{|U(\mathbf{r}')|^{1/2}}\phi(\mathbf{r}') &(1.35)\\ &= \phi_{\mathrm{inc}}(\mathbf{r}) + \int \mathrm{d}^3r'\, K(\mathbf{r},\mathbf{r}')\phi(\mathbf{r}') &(1.36)\end{aligned}$$

where $K(\mathbf{r},\mathbf{r}')$ is the 'kernel' of an integral operator that can be formally written as $\hat{K}$. The Born series thus takes the form

$$\phi = \left(\hat{1}-\hat{K}\right)^{-1}\phi_{\mathrm{inc}} = \phi_{\mathrm{inc}} + \hat{K}\phi_{\mathrm{inc}} + \hat{K}^2\phi_{\mathrm{inc}} + \ldots \tag{1.37}$$

The functional analysis of this kind of series gives the convergence criterion

$$1 > \|\hat{K}\|^2 \equiv \int \mathrm{d}^3r\,\mathrm{d}^3r'\ \left|K(\mathbf{r},\mathbf{r}')\right|^2 = \int \mathrm{d}^3r\,\mathrm{d}^3r'\,\frac{|U(\mathbf{r})U(\mathbf{r}')|}{|\mathbf{r}-\mathbf{r}'|^2}. \tag{1.38}$$

More details can be found in the mathematical physics literature on scattering theory or in the mathematics literature on so-called 'Fredholm integral equations'.

Extra: quantum perturbation theory

The Born–von Neumann series is an example of perturbation expansions that occur very often in quantum mechanics. We recall here the general flavor of such an expansion.

In the Born series, the wave function is expanded in a series in the scattering potential, with the energy held fixed. In many other cases, also the energy

is changed by some interaction Hamiltonian. We consider here this more general setting. We keep to the stationary Schrödinger equation, however. Time-dependent perturbation theory is needed later.

Suppose you have a quantum mechanical system described by the Hamiltonian

$$H = H_0 + \epsilon V \tag{1.39}$$

where H_0 is the part you know already and ϵV is a "small potential" that one wants to take into account.

The "part you know already" provides you with energies E_n and the corresponding eigenstates ψ_n. We suppose that these are normalized and restrict to the subspace spanned by these states (i.e., they form a complete basis):

$$\langle\psi_n|\psi_m\rangle = \delta_{nm}, \qquad \mathbb{1} = \sum_n |\psi_n\rangle\langle\psi_n| \tag{1.40}$$

where $\mathbb{1}$ is the unit operator (on the chosen subspace).

The stationary Schrödinger equation one wants to solve is, of course,

$$0 = (H_0 + \epsilon V)\,\psi - E\psi, \tag{1.41}$$

where V is the 'difficult' part. We now seek the solution to (1.41) in the form of a power series in ϵ:

$$E = E^{(0)} + E^{(1)} + E^{(2)} + \ldots, \tag{1.42}$$
$$\psi = \psi^{(0)} + \psi^{(1)} + \psi^{(2)} + \ldots, \tag{1.43}$$

where the terms with superscript $^{(n)}$ are of order n in ϵ. We insert this expansion into the Schrödinger Eq.(1.41), and require that this equation holds "order by order" in ϵ. (This is an equality in a space of polynomials whose coefficients are states/elements of the Hilbert space.) Taking terms up to the second order, we have

$$\begin{aligned} 0 &= H_0\psi^{(0)} - E^{(0)}\psi^{(0)} && (1.44)\\ &+ H_0\psi^{(1)} + \epsilon V\psi^{(0)} - E^{(1)}\psi^{(0)} - E^{(0)}\psi^{(1)} && (1.45)\\ &+ H_0\psi^{(2)} + \epsilon V\psi^{(1)} - E^{(2)}\psi^{(0)} - E^{(1)}\psi^{(1)} - E^{(0)}\psi^{(2)} && (1.46)\\ &+ \ldots \end{aligned}$$

Each line must be zero separately.

To zeroth order, we recognize the eigenvalue problem for H_0. Hence, we can take

$$\psi^{(0)} = \psi_n, \qquad E^{(0)} = E_n \tag{1.47}$$

for some eigenfunction ψ_n. This one will be 'perturbed' by the potential ϵV.

To first order, we have, using the results of the zeroth order:

$$0 = H_0\psi^{(1)} + \epsilon V\psi_n - E^{(1)}\psi_n - E_n\psi^{(1)} \tag{1.48}$$

To proceed, we project this equation onto ψ_n and observe that $\langle\psi_n|H_0|\psi^{(1)}\rangle = E_n\langle\psi_n|\psi^{(1)}\rangle$ because H_0 can be made to "act to left" onto its eigenvector. Hence the only terms that remain from (1.48) give

$$\boxed{E^{(1)} = \epsilon\langle\psi_n|V|\psi_n\rangle} \tag{1.49}$$

This the most useful result of perturbation theory: *if you want to know the change in energy of a quantum state ψ_n, evaluate the 'diagonal matrix element' of the perturbation ϵV with respect to your state.*

The information about the perturbed wave function can be found if we project Eq.(1.48) onto the 'other states' ψ_m with $m \neq n$. Now, the third term cancels because of orthogonality, Eq.(1.40). The first and last terms combine to give $(E_m - E_n)\langle\psi_m|\psi^{(1)}\rangle$, so that we finally get (here, the completeness of the basis state is used)

$$\psi^{(1)} = -\sum_{m\neq n} \frac{\epsilon\langle\psi_m|V|\psi_n\rangle}{E_m - E_n}\psi_m \tag{1.50}$$

— well, if the denominator $E_m - E_n$ is not zero. This case is treated in a note below.

We thus see that the perturbed state is proportional, on the one hand, to the "matrix elements" $\langle\psi_m|V|\psi_n\rangle$ of the perturbation. This is a typical feature of quantum mechanics: *if you want to generate some probability amplitude in a different ('target') state, you need an interaction Hamiltonian that has a nonzero matrix element between your initial and target states.* In addition: *the probability amplitude you get is large, if initial and target states are near in energy.* It is difficult to generate states with a very different energy.[1]

Finally, the second order: following the same procedure, one finds for the energy shift:

$$\boxed{E^{(2)} = -\sum_{m\neq n} \frac{\epsilon^2\,|\langle\psi_m|V|\psi_n\rangle|^2}{E_m - E_n}} \tag{1.51}$$

Here again, the denominator $E_m - E_n$ must not be zero. In words: second-order energy shifts are proportional to squared matrix elements, and inversely proportional to the difference in energy. The largest contributions come again from nearly degenerate states ψ_m.

Two general comments can be made here. Let us specialize to the ground state $\psi_n = \psi_g$ where all energy differences $E_m - E_g > 0$ for $m \neq g$. We then find: $E^{(2)} < 0$ because it is a sum of negative terms. Hence: any perturbation (that vanishes in first order) when applied to the ground state lowers the energy of this state.

Let us focus on two states ψ_g and ψ_e and assume that the state ψ_e is the only one that is "coupled to ψ_g by the perturbation" (i.e., the matrix elements of ϵV are nonzero only between these two states). Then the sum for the second order shift (1.51) becomes a single term. This is the shift for the state ψ_g, $E_g^{(2)}$.

We can also compute, within the same approximations, the energy shift for the other state, $E_e^{(2)}$. Since the same matrix elements are involved, we find that

$$E_e^{(2)} + E_g^{(2)} = 0 \tag{1.52}$$

$$E_e^{(2)} - E_g^{(2)} = 2\frac{\epsilon^2\,|\langle\psi_e|V|\psi_g\rangle|^2}{E_e - E_g} > 0 \tag{1.53}$$

[1] That sounds like energy conservation. However, the "admixture" (1.50) to the original state has, strictly speaking, a different energy. Sometimes, one is talking about a "virtual transition", in distinction to "real transitions" where energy must be conserved. In particular, the energy shift in Eq.(1.51) is often said to be due to virtual transitions $\psi_n \to \psi_m$.

hence, the "mean energy" is not changed by the perturbation, and the difference in energy is increased. One says that the "levels are pushed apart" by the perturbation. This is also a general feature.

What to do with 'degenerate states' with $E_m = E_n$? The idea is to change the basis in this subspace such that the perturbation ϵV contains only diagonal elements. In the first-order equation

$$E^{(1)}\delta_{mn} = (E_m - E_n)\,\langle\psi_m|\psi^{(1)}\rangle + \epsilon\langle\psi_m|V|\psi_n\rangle \tag{1.54}$$

we then have only two cases: either $m = n$, and one gets the first-order energy shift (1.49). Or $m \neq n$, but then we simply have $0 = 0$ since $E_m = E_n$ by assumption and the off-diagonal matrix element $\langle\psi_m|V|\psi_n\rangle = 0$ by construction because the $\psi_{m,n}$ are chosen as eigenvectors of V.

The sums in Eqs.(1.50, 1.51) then run only over those states which have a different energy so that the denominators $E_m - E_n$ are never zero.

1.4 Partial wave expansion

We now turn to a second method to solve the scattering problem. It is particularly useful in the case of a spherically symmetric potential. The result for the scattering amplitude will be of the form

$$f(\mathbf{\Omega}) = \sum_{l=0}^{\infty} \frac{2l+1}{2ik}\left(\mathrm{e}^{2i\delta_l(k)} - 1\right) P_l(\cos\theta) \tag{1.55}$$

where $\delta_l(k)$ is a phase shift that can be computed from a radial Schrödinger equation and where $P_l(\cos\theta)$ are Legendre polynomials.

Let us explain how this comes about. We shall start from the stationary Schrödinger equation (1.3):

$$-\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\mathbf{L}^2}{\hbar^2 r^2}\right)\psi + V(r)\psi = k^2\psi, \tag{1.56}$$

where we have taken units with $2m/\hbar^2 = 1$. We expand the wave function in spherical harmonics [Eq.(22)]

$$\psi(\mathbf{r}) = \sum_{lm} c_{lm} Y_{lm}(\theta,\varphi) R_l(r) \tag{1.57}$$

where the coefficients c_{lm} must be found and the 'radial wave functions' $R_l(r)$ are unknown as well. Since the spherical harmonics form a complete basis for the dependence on the angles θ, φ, we get for each lm the radial Schrödinger equation

$$-\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}rR_l + \frac{l(l+1)}{r^2}R_l + V(r)R_l = k^2 R_l \tag{1.58}$$

The solution to this equation can be found subject to the requirement that the wavefunction be regular at the origin. We shall study the behaviour there in a second. The coefficients c_{lm} are fixed by (i) the expansion of the 'incident' wave in spherical harmonics and by (ii) the asymptotic behaviour of $R_l(r)$.

Incident wave

The expansion of the incient wave in spherical harmonics is done with the following identity:

$$\mathrm{e}^{\mathrm{i}kr\cos\theta} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \mathrm{i}^l \sqrt{4\pi(2l+1)}\delta_{m,0} Y_{lm}(\theta,\varphi) j_l(kr) \tag{1.59}$$

Explanations, please. The spherical harmonics occur only for $m = 0$. This could have been expected since the incident wave propagates along the z-axis, and it has no dependence on φ. But all possible values of l occur in the sum. The dependence on θ comes from the spherical harmonics that simplify here to the following form

$$Y_{l0}(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta) \tag{1.60}$$

where $P_l(\cos\theta)$ are Legendre polynomials.

The Legendre polynomials are polynomials of order l in $\cos\theta$ that are orthogonal on the interval $\theta = 0 \ldots \pi$ with respect to the integration measure $\sin\theta$. They are normalized such that $P_l(1) = 1$. The first few Legendre polynomials look like

$$\begin{aligned} P_0(\cos\theta) &= 1 \\ P_1(\cos\theta) &= \cos\theta \\ P_2(\cos\theta) &= \tfrac{1}{2}\left(3\cos^2\theta - 1\right) \end{aligned} \tag{1.61}$$

The normalization integral is $\int_{-1}^{+1} \mathrm{d}\cos\theta \; [P_l(\cos\theta)]^2 = 2/(2l+1)$.

Finally, the radial dependence is carried by the function $j_l(kr)$, the so-called 'spherical Bessel function'. This function is the regular solution to the radial Schrödinger equation for a free particle:

$$-\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}(rR_l) + \frac{l(l+1)}{r^2} R_l = k^2 R_l \tag{1.62}$$

Indeed, the incident plane wave $\mathrm{e}^{\mathrm{i}kr\cos\theta}$ describes a free particle as well. With the change of variable $x = kr$, one immediately gets from (1.62)

$$\frac{1}{x}\frac{\mathrm{d}^2}{\mathrm{d}x^2}(xR_l) + R_l - \frac{l(l+1)}{x^2} R_l = 0 \tag{1.63}$$

This second-order differential equation has two solutions, the spherical Bessel functions $j_l(x)$ and $y_l(x)$. You can find their properties in Abramowitz & Stegun, chap. 10; Gradshteyn & Ryzhik, § 8.46. They are polynomials of finite degree in $1/x$ with coefficients $\sin x$, $\cos x$:

$$y_l(x) + \mathrm{i} j_l(x) = \frac{\mathrm{i}^{-l}\,\mathrm{e}^{\mathrm{i}x}}{x} \sum_{k=0}^{l} \frac{(l+k)!}{k!\,(l-k)!} \left(\frac{\mathrm{i}}{2x}\right)^k \tag{1.64}$$

The short distance asymptotics is not easy to work out from this formula because one has to expand the exponential $\mathrm{e}^{\mathrm{i}x}$. The results are

$$x \to 0: \qquad j_l(x) \to \frac{x^l}{(2l+1)!!}, \qquad y_l(x) \to \frac{(2l-1)!!}{x^{l+1}}, \tag{1.65}$$

where $(2l+1)!! = 1 \cdot 3 \cdots (2l+1)$ is the 'odd factorial'. Note that $y_l(x)$ diverges at the origin for all values of $l \geq 0$. It is hence excluded as a physical solution of the radial Schrödinger equation. The large distance asymptotics can be found from the lowest order term ($k = 0$) in the expansion (1.64):

$$x \to \infty : \qquad j_l(x) \to \frac{\mathrm{Im}(\mathrm{i}^{-l}\,\mathrm{e}^{\mathrm{i}x})}{x} = \frac{\sin(x - l\pi/2)}{x}, \qquad y_l(x) \to \frac{\cos(x - l\pi/2)}{x} \tag{1.66}$$

The regular solution to the general radial equation, including the scattering potential, is of a similar asymptotic form. This motivates the definition of a so-called 'partial wave phase shift'.

Phase shifts

Let us go back to the radial Schrödinger Eq.(1.58):

$$-\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2} r R_l + \frac{l(l+1)}{r^2} R_l + V(r) R_l = k^2 R_l \tag{1.67}$$

At large distance where the potential vanishes, its solution must look like the solution for a free particle, hence it must be a combination of spherical Bessel functions. Since these behave like $\sin(kr)/r$ and $\cos(kr)/r$, we can introduce a phase shift $\delta_l(k)$ by the following asymptotics

$$r \to \infty : \qquad R_l(r) \to A j_l(kr) + B y_l(kr) \to \frac{c}{kr} \sin[kr - l\pi/2 + \delta_l(k)] \tag{1.68}$$

where c is a normalization constant that depends on l. This scattering phase is defined such that $\delta_l(k) = 0$ if there is no scattering potential. We then recover the asymptotics of the regular $j_l(kr)$ solution, Eq.(1.66).

If the potential is regular at the origin, we can make the *Ansatz* around the origin

$$R_l(r) \to c r^s \tag{1.69}$$

where c and s remain to be fixed. We put this *Ansatz* into the radial Schrödinger equation and single out the 'most singular terms' (those that scale like R_l/r^2). If the potential is less singular than $1/r^2$ at the origin, we get for the exponent

$$s(s+1) = l(l+1) \tag{1.70}$$

with the solutions $s = l$ or $s = -(l+1)$. (Exactly these exponents also occur for the spherical Bessel functions (1.65).) The solution $s = -(l+1)$ leads to a function that is locally not integrable at the origin for $l \geq 1$. But also for $l = 0$, this solution can be discarded.

> The case $l = 0$ is more subtle because if $R_l \to c/r$, this is still square integrable due to the integration measure $r^2 \mathrm{d}r\mathrm{d}\Omega$. However, the (full) Laplace operator acting on a function with the behavior c/r gives $4\pi c\delta(\mathbf{r})$, and this singularity cannot be balanced by the (regular!) potential in the Schrödinger equation.

The regular solution thus starts like r^l at the origin. The constant c is arbitrary for the moment, and we can choose it equal to unity. By integrating the differential equation outward, one gets, in the asymptotic region, a real wave function from which we can read off the scattering phase shift $\delta_l(k)$, by comparing to Eq.(1.68).

It is curious to note that these 'partial waves' $R_l(r)$, as they are called, are all real and contain at large distances both 'ingoing' and 'outgoing' spherical waves ($\mathrm{e}^{\pm \mathrm{i}kr}/r$). None of these solutions is thus suited to the asymptotic conditions for the stationary scattering state. But as we show now, this can be done from the knowledge of the phase shifts $\delta_l(k)$.

If we write the radial wavefunction in terms of $u = rR_{kl}(r)$, then from the radial Schrödinger Eq.(1.58), we get

$$u'' + \left(\frac{l(l+1)}{r^2} + V(r) \right) u = k^2 u \tag{1.71}$$

which looks like a one-dimensional problem. The only difference is that the point $r = 0$ is special: the physical solution goes like $u \sim r^{l+1}$ at $r \to 0$, in particular it vanishes as $r \to 0$.

Scattering amplitude

At large distance, we thus get the following expansion for the wave function:

$$\psi(\mathbf{r}) \to \sum_{lm} c_{lm} Y_{lm}(\theta, \varphi) \frac{\sin(kr - l\pi/2 + \delta_l(k))}{kr} \tag{1.72}$$

where we now have to determine the coefficients c_{lm}. We require that this expansion matches the usual one,

$$\psi(\mathbf{r}) \to \mathrm{e}^{\mathrm{i}kr\cos\theta} + f(\theta, \varphi) \frac{\mathrm{e}^{\mathrm{i}kr}}{r} \tag{1.73}$$

We proceed by re-arranging

$$\psi(\mathbf{r}) - \mathrm{e}^{\mathrm{i}kr\cos\theta} \to f(\theta, \varphi) \frac{\mathrm{e}^{\mathrm{i}kr}}{r} \tag{1.74}$$

i.e., the difference between the full wave function and the incident wave is a purely outgoing spherical wave. With the help of the expansion (1.59), we have

$$\begin{aligned} \mathrm{e}^{\mathrm{i}kr\cos\theta} &= \sum_{l=0}^{\infty} (2l+1) \mathrm{i}^l P_l(\cos\theta) j_l(kr) && (1.75) \\ &\to \sum_{l=0}^{\infty} \frac{(2l+1)\mathrm{i}^l}{kr} P_l(\cos\theta) \sin(kr - l\pi/2) && (1.76) \end{aligned}$$

The difference (1.74) thus becomes

$$\begin{aligned} \psi(\mathbf{r}) - \mathrm{e}^{\mathrm{i}kr\cos\theta} \to\ & \frac{\mathrm{e}^{\mathrm{i}kr}}{2\mathrm{i}kr} \sum_{lm} \Big(c_{lm} Y_{lm}(\theta, \varphi) \mathrm{e}^{-\mathrm{i}l\pi/2 + \mathrm{i}\delta_l} \\ & \qquad - \delta_{m0} (2l+1) \mathrm{i}^l P_l(\cos\theta) \mathrm{e}^{-\mathrm{i}l\pi/2} \Big) \\ & + \frac{\mathrm{e}^{-\mathrm{i}kr}}{2\mathrm{i}kr} \sum_{lm} \Big(c_{lm} Y_{lm}(\theta, \varphi) \mathrm{e}^{\mathrm{i}l\pi/2 - \mathrm{i}\delta_l} \\ & \qquad - \delta_{m0} (2l+1) \mathrm{i}^l P_l(\cos\theta) \mathrm{e}^{\mathrm{i}l\pi/2} \Big) \end{aligned} \tag{1.77}$$

The third and fourth line contain the spherically ingoing wave with the 'wrong asymptotics'. Hence the coefficients of this sum must be zero for each lm. (Here, the completeness of the spherical harmonics is used.) We obviously get $c_{lm} = \delta_{m0} c_l$ and furthermore, using the formula (1.60)

$$c_l \sqrt{\frac{2l+1}{4\pi}} \mathrm{e}^{-\mathrm{i}\delta_l} \stackrel{!}{=} (2l+1)\mathrm{i}^l \quad \Longrightarrow \quad c_{lm} = \delta_{m0} \mathrm{i}^l \mathrm{e}^{\mathrm{i}\delta_l} \sqrt{4\pi(2l+1)} \tag{1.78}$$

The wave function is now completely specified. From the outgoing spherical wave, we read off the scattering amplitude

$$f(\mathbf{\Omega}) = \sum_{l=0}^{\infty} \frac{2l+1}{2\mathrm{i}k} \left(\mathrm{e}^{2\mathrm{i}\delta_l(k)} - 1 \right) P_l(\cos\theta) \tag{1.79}$$

This is the 'partial wave expansion' for the scattering amplitude. Note that in general, different angular momentum waves interfere in the cross section $\mathrm{d}\sigma/\mathrm{d}\Omega = |f(\mathbf{\Omega})|^2$.

Discussion

The scattering cross section, from Eq.(1.79) does not depend on φ, it is rotationally symmetric around the axis of the incoming beam direction. This is intuitively clear because we deal with a spherically symmetric potential. ("Left-right" asymmetries are often signatures of 'hidden' vectors, spins etc. that break that symmetry.)

If there is no scattering potential, the phase shifts of the partial waves are $\delta_l(k) = 0$, and $f(\mathbf{\Omega}) = 0$. For small phase shifts, we have a linear dependence:

$$f(\mathbf{\Omega}) \approx \sum_{l=0}^{\infty} (2l+1) \frac{\delta_l(k)}{k} P_l(\cos\theta) \tag{1.80}$$

This is the starting for a perturbation scheme. It is not necessarily equivalent to the Born approximation: that depends on the way the phase shifts are computed.

Optical theorem and unitarity limit. The maximum value for the scattering amplitude, for a given partial wave, is reached when $\mathrm{e}^{2\mathrm{i}\delta_l(k)} = -1$, hence for $\delta_l(k) = (\pi/2) \bmod \pi$. This case is called the "unitarity limit". This limit is also relevant for the total scattering cross section. The easiest way to get it is to apply the optical theorem (see the exercises):

$$\sigma = \frac{4\pi}{k} \mathrm{Im}\, f(\mathbf{e}_z) \tag{1.81}$$

$$= \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) P_l(1) \sin^2 \delta_l(k) \tag{1.82}$$

The Legendre polynomials $P_l(1) = 1$ occur because $\cos\theta = 1$ in forward scattering. (See around Eq.(1.61).) Hence,

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l(k) \tag{1.83}$$

This is a sum of positive terms, σ_l, say, and we have the upper limit

$$\sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l(k) \leq \frac{4\pi}{k^2}(2l+1). \tag{1.84}$$

Of course, this limit is not sufficient to make the sum over l converge in (1.83). But it is sometimes the case that only small values of l contribute with a significant amount. The inequality (1.84) thus provides an upper limit to these partial cross sections. It is interesting that one indeed finds an upper limit: it means that whatever the strength of the potential, there is an upper limit on the amount of scattering.

Low-energy scattering

Why only low partial waves are relevant. (i) Classical path: does not hit the potential if $b > r_0$, b: impact parameter and r_0: potential range. Translated into angular momentum $L = |\mathbf{r} \times \mathbf{p}| = b\hbar k$, hence partial waves with $kb = l > kr_0$ are not scattered.

(ii) Semiclassical approximation: wave function oscillates in classically allowed region $r > r_l$, with $V_{\text{eff}}(r_l) = k^2$. If $r_l > r_0$, then scattering potential irrelevant in this region. If l is large, $r_l \approx l/k$. Corresponds again to $l/k > r_0$.

(iii) Bethe's formula and the Born approximation.

$$k\sin(\delta_1 - \delta_2) = \int_0^\infty \mathrm{d}r\, r^2 R_1(r)R_2(r)\left(V_1(r) - V_2(r)\right) \tag{1.85}$$

for scattering problems $1, 2$ with the same k, l. This holds only with the normalization of the radial wave functions to asymptotics $R_l(r) \to \sin(kr - l\pi/2 + \delta_l(k))/r$. Born approximation: take for 2 a free particle and approximate $R_1(r) \approx kj_l(kr)$ (free radial wave function):

$$\sin\delta_1 \approx k\int_0^\infty \mathrm{d}r\, r^2 \left[j_l(kr)\right]^2 V_1(r) \tag{1.86}$$

and the function $j_l(kr)$ is small for $kr < l$, hence this region of the potential does not contribute. Hence weak scattering or no scattering at all if $r_0 < l/k$.

Angular dependence. Let us assume that the phase shifts behave like $1 \gg \delta_0 \gg \delta_1 \gg \ldots$. In that case, the leading order terms in the scattering amplitude (1.80) are

$$f(\mathbf{\Omega}) \approx \frac{\delta_0(k)}{k} + 3\frac{\delta_1(k)}{k}\cos\theta \tag{1.87}$$

To lowest order, this gives a spherically symmetric cross section $\sigma_0 = |\delta_0(k)/k|^2$. This behaviour is typical for low energies. Indeed, we found in the Born approximation also, Eq.(1.34), $f_{\text{B}} = \int_0^R \mathrm{d}r\, r\, V(r)$, independent of the momentum transfer $q = 2k\sin(\theta/2)$.

If only the p-wave is present[2], one gets a cross-section $\sigma_1 \propto \cos^2\theta$ with peaks in the forward and backward directions.

[2]This may happen if $\mathrm{e}^{2\mathrm{i}\delta_0} = 1$ or for reasons of particle symmetry.

If both s- and p-waves are present, the cross section shows a forward-backward asymmetry because of the *interference* between the two partial waves:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{|\delta_0(k) + 3\delta_1(k)\cos\theta|^2}{k^2} \tag{1.88}$$

From the angular dependence, one can thus measure both $\delta_0(k)$ and $\delta_1(k)$.

Scattering length for the square well. We now discuss the absolute magnitude of the scattering cross section in the low-energy limit. We have seen that the ratio $\delta_0(k)/k$ determines the scattering amplitude. This motivates the following definition for the (s-wave) 'scattering length' a_s

$$k \to 0: \qquad \delta_0(k) \to -ka_\mathrm{s}. \tag{1.89}$$

The differential scattering cross section is then $|a_\mathrm{s}|^2$, which integrates over all angles to $\sigma_\mathrm{tot} = 4\pi|a_\mathrm{s}|^2$. *The s-wave scattering length thus defines an equivalent 'absorbing sphere' with radius $2a_\mathrm{s}$ that gives the same cross section.*

To elaborate on the physical interpretation of this quantity, let us go back to the example of a square well that has been discussed in the exercises. The square well potential $V(r)$ has the value $-V_0$ for $0 < r < a/2$ and vanishes for $r > a/2$. Inside the potential, the solutions to the radial Schrödinger equation are of the form (we write $R(r)$ instead of $R_0(r)$ for simplicity)

$$R(r) = \frac{\sin(\kappa r)}{r} \qquad \text{and} \qquad R(r) = \frac{\cos(\kappa r)}{r} \tag{1.90}$$

where $\kappa^2 = k^2 + V_0$. The first solution has the correct behavior at the origin (it goes to a constant), while the second one diverges. Note that the regular solution can be extended as an odd function to negative values of r. This is how you found it in the exercises, see Fig.**??**.

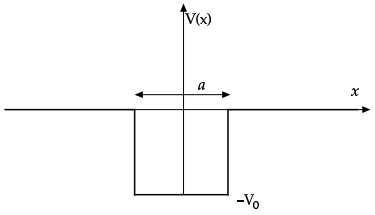

Figure 1.1: Square potential well. In the radial Schrödinger equation, only $x > 0$ is actually meaningful.

At the radius $r = a/2$, we can match our solution to spherical Bessel functions $j_0(kr)$ and $y_0(kr)$, but these are for $l = 0$ of a simple form, and we can make the ansatz

$$r > a/2: \qquad R(r) = C\frac{\sin(kr + \delta)}{r} \tag{1.91}$$

Note that with this ansatz, δ is identical to the scattering phase δ_0 The matching equations are (note that from the form of the radial kinetic energy in the

radial Schrödinger equation, it is the function rR that is continuous and differentiable)

$$\sin(\kappa a/2) = C\sin(ka/2+\delta) \tag{1.92}$$
$$\kappa\cos(\kappa a/2) = Ck\cos(ka/2+\delta) \tag{1.93}$$

We get rid of the constant C by taking the ratio of both equations and get

$$\frac{k}{\kappa}\tan(\kappa a/2) = \tan(ka/2+\delta) \tag{1.94}$$
$$\delta(k) = -\frac{ka}{2} + \arctan\left[\frac{k}{\kappa}\tan(\kappa a/2)\right] \tag{1.95}$$

This result is valid for any k and V_0, but only in s-wave scattering, of course.

Let us now consider the low-energy limit where $ka \ll 1$. We keep κa arbitrary, compute the linear expansion and find a scattering length:

$$k\to 0: \qquad \delta(k)\to -ka_{\rm s}, \qquad a_{\rm s} = \frac{a}{2} - \frac{\tan(\kappa a/2)}{\kappa} \tag{1.96}$$

For $\tan(\kappa a)$ of order unity, the scattering length is of the order of a: *the "size" of the scattering potential determines the scattering length and hence the cross section* $\sim a^2$.

But if $\kappa a/2 = \pi/2, 3\pi/2, \ldots$, the scattering length (1.96) diverges. This condition is similar to the quantization of bound states in the potential well.[3] In fact, the wave function then has a maximum at $r = a/2$: the scattering from the square potential looks like the scattering from a 'loose end' of a string (no phase shift instead of a π shift from a 'fixed end'). This phenomenon is called 'resonant potential scattering'. It occurs when something like a bound state is entering from below the continuum of scattering states.

The scattering amplitude does not diverge, however: we find a phase shift δ_0 close to $\pi/2$ and

$$f_0 = \frac{1}{2{\rm i}k}\left(\mathrm{e}^{-{\rm i}ka}\frac{\kappa + {\rm i}k\tan(\kappa a/2)}{\kappa - {\rm i}k\tan(\kappa a/2)} - 1\right) \to -\frac{\mathrm{e}^{-{\rm i}ka}+1}{2{\rm i}k} \approx \frac{\rm i}{k} \tag{1.97}$$

This corresponds to the unitary limit discussed in Eq.(1.84).

Scattering length, general case. Our third illustration for the scattering length is valid for any potential. We focus again on the low-energy limit $kr_0 \ll 1$ where the range r_0 of the potential is small compared to the incident wavelength. Consider first the range of distances defined by the inequalities $1/k \gg r_0 > r$: the potential $V(r)$ is relevant here. If we express the radius in terms of $\tilde{r} = r/r_0$, the radial Schrödinger equation becomes (for the partial wave $l = 0$)

$$-\frac{1}{\tilde{r}}\frac{\mathrm{d}^2}{\mathrm{d}\tilde{r}^2}(\tilde{r}R_0) + r_0^2 V(r_0\tilde{r})R_0 - (kr_0)^2 R_0 = 0 \tag{1.98}$$

[3] There is a slight shift: the odd bound states in the well $-a/2 < r < a/2$, the quantized states satisfy $\kappa a/2 = \pi, 2\pi$, right "in between" the divergences we encouter here.

In the low-energy limit, we can consider $(kr_0)^2$ to be small compared to $r_0^2 V(r_0\tilde{r})$ and neglect the last term. This gives (going back to the unscaled units)

$$1/k \gg r_0 > r: \qquad -\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}(rR_0) + V(r)R_0 = 0 \tag{1.99}$$

which is nothing else than the Schrödinger equation at zero energy. The regular solution R_0 to this equation starts as a constant at the origin and is for $r > r_0$ a 'free particle at zero energy':

$$1/k \gg r > r_0: \qquad -\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}(rR_0) = 0, \qquad R_0 = c_0\frac{a-r}{r} \tag{1.100}$$

The wave function 'outside the potential' thus behaves (removing the $1/r$ factor) like a linear function that intersects the r-axis at the coordinate a. We now show that this a is nothing but the scattering length.

In fact, at $r > r_0$, the potential is zero, and we know that the solution goes over into the phase-shifted spherical Bessel function $R_0 \to C\sin(kr+\delta)/r$ This function can be expanded in the range $1/k \gg r$ and gives

$$1/k \gg r > r_0: \qquad R(r) \to C\frac{kr+\delta}{r} \tag{1.101}$$

The comparison of the constant and linear terms of these two functions gives $\delta = -ka$, and from the definition (1.89), the s-wave scattering length is indeed $a = a_\mathrm{s}$.

In the case of resonant scattering, the phase shift δ may be large and we match Eq.(1.100) to

$$1/k \gg r > r_0: \qquad R(r) \to C\frac{\sin(\delta) + kr\cos(\delta)}{r} \tag{1.102}$$

and this gives

$$a = -\frac{\tan\delta}{k} \tag{1.103}$$

This formula serves to *define* the scattering length whenever resonances are present in the scattering. It goes over into our previous definition (1.89) when $\delta(k) \to 0$ at low energy. The more general expression (1.103) displays a divergence whenever $\delta = \pi/2, 3\pi/2, \ldots$ ($\tan\delta = \pm\infty$). In that case, the wave function 'outside the potential' becomes a constant that never intersects the r-axis. Around this situation, the "scattering length" *defined* by Eq.(1.103) changes rapidly from $-\infty$ to $+\infty$. These resonances have recently played an important role in the scattering between pairs of ultracold atoms. The maximum value of the (s-wave) scattering cross section does not diverge, however: at fixed (but small) k, it is limited by the "unitarity limit" (1.84) to $\sigma_0 \leq 4\pi/k^2$.

1.5 Formal scattering theory

Lippmann-Schwinger equation

$$|\psi_k^{(+)}\rangle = |\varphi_k\rangle + G_0^{(+)}(k^2)V|\psi_k^{(+)}\rangle \tag{1.104}$$

with scattering state $|\psi_k^{(+)}\rangle$ (superscript $^{(+)}$ denotes spherically outgoing or "retarded" solution), plane wave (free particle) state $|\varphi_k\rangle$ and (retarded) Green operator

$$G_0^{(\pm)}(k^2) = \lim_{\epsilon \to 0} \left(k^2 - H_0 \pm \mathrm{i}\epsilon\right)^{-1} \tag{1.105}$$

with free particle Hamiltonian H_0.

the limit of the resolvent operator

$$G_0(z) = (z - H_0)^{-1} \tag{1.106}$$

as the complex energy $z \to E$ from the upper half-plane on the real axis.

Properties of resolvent operator:

poles at eigenvalues of H_0

"cut" along real axis where H_0 has a continuous spectrum. (Local) density of states

$$\langle \mathbf{x}|\mathrm{Im}\, G_0^{(+)}(E)|\mathbf{x}\rangle = -\pi\rho(\mathbf{x}, E) = -\pi \sum_n \delta(E - E_n) \left|\psi_n(\mathbf{x})\right|^2 \delta(E - E_n) \tag{1.107}$$

last expression strictly speaking applies only for the discrete energy eigenvalues. Sum degenerates into an integral in the continuum. In a quantization box of volume $V = L^3$ with periodic boundary conditions:

$$\begin{aligned} &\sum_n |\psi_n(\mathbf{x})|^2 = \sum_{\mathbf{k}} \delta(E - E_n) \left|\psi_n(\mathbf{x})\right|^2 \\ &= \left(\frac{L}{2\pi}\right)^2 \int \mathrm{d}^3k \delta(E - k^2) \frac{1}{V} = \frac{1}{4\pi^2}\sqrt{E} \end{aligned} \tag{1.108}$$

Note that the *local* density of states goes to a finite limit in the "continuum limit" $V \to \infty$. Compare to imaginary part of Green function:

$$\begin{aligned} &\langle \mathbf{x}|\mathrm{Im}\, G_0^{(+)}(E)|\mathbf{x}\rangle = \lim_{\mathbf{x}' \to \mathbf{x}} \mathrm{Im} G_0^{(+)}(\mathbf{x} - \mathbf{x}'; E) \\ &= -\frac{1}{4\pi} \lim_{\mathbf{x}' \to \mathbf{x}} \frac{\mathrm{e}^{\mathrm{i}k|\mathbf{x} - \mathbf{x}'|}}{|\mathbf{x} - \mathbf{x}'|} = -\frac{\sqrt{E}}{4\pi} \end{aligned} \tag{1.109}$$

where the limit $\mathbf{x}' \to \mathbf{x}$ is required to get a finite imaginary part and $k = \sqrt{E}$.

Dyson equation for Green function including potential V:

$$G = G_0 + G_0 V G \tag{1.110}$$

iterative solution gives multiple scattering series, Feynman graphs etc. $G(z)$s a function of (complex) energy z, physical values only required for real values $z \to E + \mathrm{i}\varepsilon$.

1.5.1 T-matrix and S-matrix

Defined by the requirement that

$$V|\psi_k^{(+)}\rangle = T(E_k)|\varphi_k\rangle. \tag{1.111}$$

Manipulations with Lippmann-Schwinger equation give

$$V|\psi_k^{(+)}\rangle = V|\varphi_k\rangle + G_0^{(+)}(E_k)V|\psi_k^{(+)}\rangle \quad (1.112)$$

$$= V|\varphi_k\rangle + \int \mathrm{d}^3k'\, G_0^{(+)}(E_k)|\varphi_{k'}\rangle\langle\varphi_{k'}|V|\psi_k^{(+)}\rangle \quad (1.113)$$

and hence

$$T(E) = V + G_0^{(+)}(E)VT(E). \quad (1.114)$$

What is the T-matrix good for? Eq.(1.111) is fundamentally important: instead of acting with the potential on the "unknown" scattering state $|\psi_k^{(+)}\rangle$, act with the T-matrix on the free particle state $|\varphi_k\rangle$ and get the same result. In particular for scattering amplitude:

$$f(\mathbf{k},\mathbf{k}') == -\frac{m}{2\pi\hbar^2}\langle\varphi_{k'}|V|\psi^{(+)}k\rangle = -\frac{m}{2\pi\hbar^2}\langle\varphi_{k'}|T(E_k)|\varphi_k\rangle \quad (1.115)$$

Hence the scattering amplitudes are essentially the matrix elements of the T-matrix.

Feynman graphs: "strip off the legs" corresponding to the Green functions. Expansion of the total scattering vertex into a Born series.

"Optical theorem":

$$T^\dagger(E) - T(E) = 2\pi\mathrm{i}T^\dagger(E)\delta(E - H_0)T(E) \quad (1.116)$$

Historical note. (From Sakurai's book.) Optical theorem usually attributes to Bohr, Peierls, and Placzek. But first account given by E. Feenberg (1932). That paper published on 01 April 1932, but "received" date is 08 Sep 1932.

Explicit expression

$$\mathrm{Im}\langle\varphi_k|T(E_k)|\varphi_k\rangle = -\frac{\pi m}{\hbar^2}\int \mathrm{d}\Omega(\mathbf{k}')\,|\langle\varphi_{k'}|T(E_k)|\varphi_k\rangle|^2 \quad (1.117)$$

Definition of S-matrix via its matrix elements:

$$\langle\varphi_{k'}|S|\varphi_k\rangle = \delta(\mathbf{k}' - \mathbf{k}) - 2\pi\mathrm{i}\,\delta(E_{k'} - E_k)\langle\varphi_{k'}|T(E_k)|\varphi_k\rangle \quad (1.118)$$

Is a transformation between free particle states. Formally, a mapping between "incident waves" (described by eigenstates of H_0 with wavevector $\mathbf{k}$ and "outgoing waves" (with wavevector $\mathbf{k}'$).

Physically expected: "no particles lost" (norms = probability of outgoing state is the same as norm of ingoing state) and hence S is unitary. Exercise: prove this.

1.5.2 Subtleties in the continuum

Free particles states are not normalizable in an infinite volume. But consider

$$\psi(\mathbf{x};c) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}c(\mathbf{k} - \bar{\mathbf{k}})\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{x}) \quad (1.119)$$

With a suitable smooth function $c(\mathbf{k}-\bar{\mathbf{k}})$ peaked around $\bar{\mathbf{k}}$, one can have a wave function whose average momentum is $\hbar\bar{\mathbf{k}}$ and whose momentum spread is arbitarily small. The condition of normalization for $\psi(\mathbf{x};c)$ is (Parceval theorem)

$$\int \mathrm{d}^3x\, |\psi(\mathbf{x};c)|^2 = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\, \left|c(\mathbf{k}-\bar{\mathbf{k}})\right|^2 = 1 \tag{1.120}$$

Hence c must be a function in $L^2(\mathbb{R}^3)$.

Physicists often work with non-normalizable states $|\varphi_k\rangle$ that behave like

$$\langle\varphi_{k'}|\varphi_k\rangle = \delta(\mathbf{k}'-\mathbf{k}) \tag{1.121}$$

It is clear that these states have infinite norm. A suitable wavefunction is

$$\langle\mathbf{x}|\varphi_k\rangle = \varphi_k(\mathbf{x}) = (2\pi)^{-3/2}\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{x}). \tag{1.122}$$

Show that $|c(\mathbf{k}-\bar{\mathbf{k}})|^2$ is the probability distribution for momentum measurements: evaluate characteristic function

$$\chi(\xi) \equiv \langle \mathrm{e}^{\mathrm{i}\xi p}\rangle \tag{1.123}$$

as an expectation value taken within the state (1.119). Known from theory of characteristic functions: $\chi(\xi)$ it is the Fourier transform of the probability distribution for the random variable p (here: an operator whose measurement outcomes are statistically distributed).

Other topics in scattering theory

multi-channel scattering (different spin states etc.), resonances, elastic/inelastic scattering.

analytical properties for complex k, E and bound states

center of mass system, relative mass, pair interaction potential

interpretations of scattering amplitude: index of refraction, frequency shift of incident plane wave. Sum over plane wave modes: Lamb shift

propagation in random media, effective medium theory, connection to radiative transfer/quantum kinetic theory