CHAPTER 4

Scattering of quantum particles

Deadline for exercises: This weeks *-exercises should be uploaded via SDU Assignment before Tuesday 8/3 at 2pm.

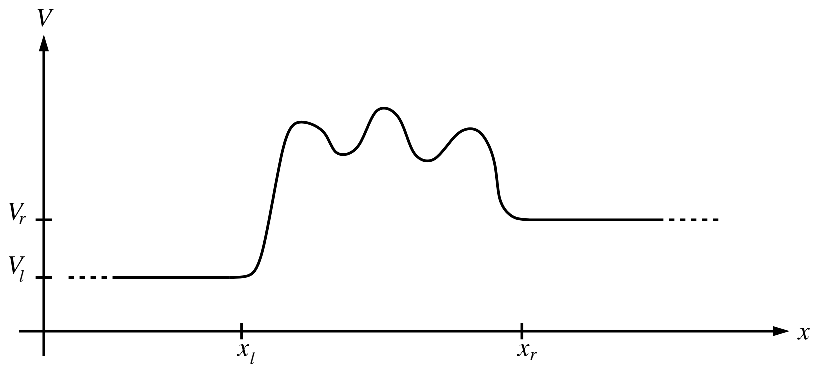
4.1 Transfer matrices

Subject keywords: transfer matrices, potential steps and barriers with constant potential.

Literature: "Notes on transfer matrices" below. The other sections on scattering will be used in the next class and thus serve for this class only as motivation for calculating transfer matrices.

Exercises: below the notes.

Notes on scattering:



Imagine a particle with definite energy $E = \hbar\omega$ and therefore a wave function that separates as $\Psi(x,t) = \psi(x)e^{-i\omega t}$. Initially the particle is moving toward the right on the left side of the potential barrier shown above (i.e., at $x < x_l$) with definite momentum $p = \hbar k_l = \sqrt{2m(E - V_l)}$. Thus the incident particle is represented by the spatial wave function

$$\psi_{\text{in}} = Ae^{ik_l(x-x_l)}, \quad x < x_l, \tag{4.1}$$

where A is a constant and the shift by x_l has been introduced for later convenience. If you are uneasy about representing a particle by a non-normalizable wave function such as this one, then you can imagine that the wave function instead represents a constant current of particles. The particle (or particle current) might be reflected backwards when it hits the barrier. To take this into account we include a left-moving component to the wave function, such that the full wave function to the left of the barrier is given by the form

$$\psi = Ae^{ik_l(x-x_l)} + Be^{-ik_l(x-x_l)}, \quad x < x_l, \tag{4.2}$$

with B another at the moment unknown constant. Also, the particle might pass across the barrier, so to the right of the barrier we have

$$\psi = Ce^{ik_r(x-x_r)}, \quad x > x_r. \tag{4.3}$$

with C yet another unknown constant and $k_r = \sqrt{2m(E - V_r)/\hbar^2}$.

Let us first recall the probability flows corresponding to these wave functions. Remember that the probability density $\rho = |\psi|^2$ obeys the continuity equation

$$\frac{\partial \rho}{\partial t} = -\frac{\partial j}{\partial x} \tag{4.4}$$

where the current of probability is given by

$$j = \frac{i\hbar}{2m}\left(\Psi\frac{\partial \Psi^*}{\partial x} - \Psi^*\frac{\partial \Psi}{\partial x}\right) = \frac{i\hbar}{2m}\left(\psi\frac{\partial \psi^*}{\partial x} - \psi^*\frac{\partial \psi}{\partial x}\right) \tag{4.5}$$

In week 3 you calculated the current corresponding to the given parts of the above wave function and found (or at least was supposed to find)

$$j = \begin{cases} \hbar k_l|A|^2/m - \hbar k_l|B|^2/m & , \quad x < x_l \\ \hbar k_r|C|^2/m & , \quad x > x_r \end{cases}. \tag{4.6}$$

In particular you should have noticed that there is no cross term between the flow of probability from the incident and reflected parts. Thus on the left side we can interpret $\hbar k_l|A|^2/m$ as the probability flow of the incoming wave and $\hbar k_l|B|^2/m$ as the probability flow of the reflected outgoing wave. The ratio of these two probability flows

$$r = \frac{|B|^2}{|A|^2} \tag{4.7}$$

will correspond to the fraction of particles that are reflected by the barrier and we will call it the reflection coefficient. Similarly, the ratio

$$t = \frac{k_r|C|^2}{k_l|A|^2} \tag{4.8}$$

gives the fraction that penetrates to the right hand side, and we will call this the transmission coefficient. Notice here the factor k_r/k_l, which will be unity only if $V_l = V_r$. Also notice that the parts of the current given in Eq. (4.6) are constant in space and time. In fact, given that we study a stationary situation with ρ independent of time t, then we see immediately from Eq. (4.4) that j must equal the same constant everywhere in space. Therefore the two expressions for the current in Eq. (4.6) must be equal, and we have

$$k_l|A|^2 - k_l|B|^2 = k_r|C|^2. \tag{4.9}$$

From this we obtain that we will always have $r + t = 1$. The particles thus have a probability of one to be either reflected or transmitted, which of course must be the case. To be able to calculate the specific values of r and t for a given potential it is convenient to introduce the method of using transfer matrices.

Notes on transfer matrices: The time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi \tag{4.10}$$

is an ordinary second order differential equation with a general solution that has two arbitrary integration constants. Thus, if we specify the values $\psi(x_0)$ and its spatial derivative $\psi'(x_0) = \partial\psi/\partial x|_{x=x_0}$ at some point x_0, i.e., specify the vector

$$\mathbf{X}(x_0) = \begin{pmatrix} \psi(x_0) \\ \psi'(x_0) \end{pmatrix} \tag{4.11}$$

then we can find these integration constants. And knowing the integration constants we can find the value of the vector $\mathbf{X}(x_1)$ at any other point x_1 in space. Since the Schrödinger equation is linear then the mapping from $\mathbf{X}(x_0)$ to $\mathbf{X}(x_1)$ will also be linear. Thus we can write the mapping as a product with a matrix

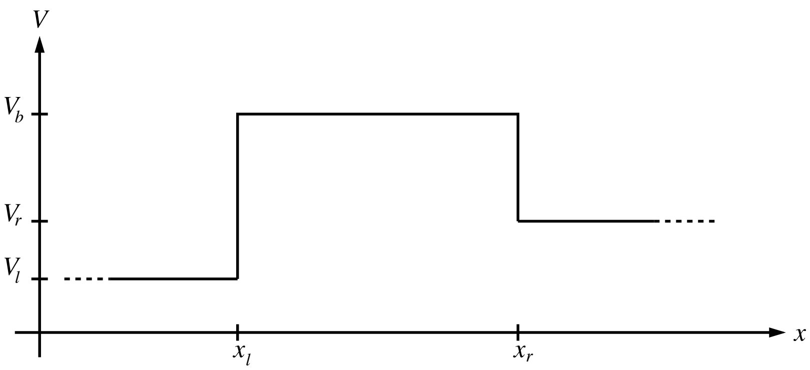
$$\mathbf{X}(x_1) = \mathbf{T}(x_1, x_0)\mathbf{X}(x_0) \tag{4.12}$$

where the 2×2 matrix $\mathbf{T}(x_1, x_0)$, called a transfer matrix, depends on the energy E and the potential V in between x_0 and x_1. Similarly, if we want to map $\mathbf{X}(x_1)$ to the value of the vector $\mathbf{X}(x_2)$ at x_2, then we need to multiply by the transfer matrix $\mathbf{T}(x_2, x_1)$ between these two points. But this means that the transfer matrix between x_0 and x_2 is given by

$$\mathbf{T}(x_2, x_0) = \mathbf{T}(x_2, x_1)\mathbf{T}(x_1, x_0) \tag{4.13}$$

Thus if we can divide a potential into intervals for which we know the transfer matrices, then we can quickly find the overall transfer matrix by multiplying the transfer matrices for each interval.

Application to scattering: As an example of the use of transfer matrices consider the situation in the notes on scattering with the following simple potential:



For this potential we can calculate the transfer matrix immediately as

$$\mathbf{T}(x_r^+, x_l^-) = \mathbf{T}(x_r^+, x_r^-)\mathbf{T}(x_r^-, x_l^+)\mathbf{T}(x_l^+, x_l^-) \tag{4.14}$$

if we have figured out the transfer matrices for finite potential jumps and finite stretches of constant potential. Notice that we, due to the singular behavior of the potential, are careful about whether we are just to the left of a singular point, e.g. x_l^-, or just to the right, e.g. x_l^+. Knowing the transfer matrix $\mathbf{T}(x_r^+, x_l^-)$ we can then write out the equation $\mathbf{X}(x_r^+) = \mathbf{T}(x_r^+, x_l^-)\mathbf{X}(x_l^-)$ more explicitly as

$$\mathbf{T}(x_r^+, x_l^-)\begin{pmatrix} A+B \\ ik_l(A-B) \end{pmatrix} = \begin{pmatrix} C \\ ik_rC \end{pmatrix} \tag{4.15}$$

which becomes 2 equations with the 3 unknowns A, B and C when the matrix multiplication has been carried out. This is not enough equations to solve explicitly for the three unknowns. However, we can obtain explicit expressions for the ratios B/A and C/A, which is enough to calculate the reflection coefficient r and transmission coefficient t explicitly for these kinds of scattering problems.

4.1.1 Exercise: Calculations of transfer matrices

Find the transfer matrices for the following situations

(*a) For a finite potential step as in the figure above, from just to the left of the step at x_l^- to just to the right at x_l^+.

(*b) For a finite stretch of length a where the potential has the constant value V_b, which is smaller than the energy E. *Hint*: the final result is

$$\mathbf{T}(x_r^-, x_l^+) = \begin{pmatrix} \cos(k_b a) & \frac{1}{k_b}\sin(k_b a) \\ -k_b\sin(k_b a) & \cos(k_b a) \end{pmatrix} \tag{4.16}$$

where $a = x_r - x_l$ and $k_b = \sqrt{2m(E-V_b)/\hbar^2}$.

(*c) Same question, but now with $V_b > E$.

(*d) From x_l^- to x_r^+ for the potential in the figure just above.

(e) The transfer matrix that you found in the previous question should become the identity matrix for some values of the energy E. For these situations, find out how the wavelength of the wave function inside the barrier is related to the width $a = x_r - x_l$ of the barrier.