11 Fundamentals of Quantum Scattering Theory

11.1 Centre of Mass Frame and the Two-body Problem

The problem of a particle in a given potential can be solved classically from Newton's equations. The Schroedinger equation can be used to describe the behaviour of one particle in a field.

The problem of two particles interacting via conservative fields can be reformulated into two parts: the behaviour of the centre of mass and the behaviour of the relative velocities of the particles. If we work in the centre of mass frame (COM), then the behaviour of the centre of mass is trivial, and we need worry only about the relative motions. This can be described by a *single* effective particle with effective mass $\mu = \frac{m_1 m_2}{m_1+m_2}$. This effective particle can then be treated with one particle equations.

The problem of three interacting particles cannot be reduced in this way. Hence the 'three-body-problem' is in general insoluble.

The COM transformation allows us to treat the scattering problem as a one body problem. For scattering problems we work in the COM frame, describing two real particles as an effective particle moving in a potential. Do not forget that for any experiment we will have to apply the above transformation to relate theory to the experimental results, though if the target particle is much heavier than the other the transformation may be slight. Note also that this transformation is invalid if there is an external field.

11.2 Some terminology for general scattering

The incident flux (I) of particles with momentum $\mathbf{p}= \hbar\mathbf{k}$ is the number of incident particles crossing unit area perpendicular to the beam direction per unit time.

The scattered flux (S) of particles with momentum $\mathbf{p}' = \hbar\mathbf{k}'$, is the number of scattered particles scattered into the element of solid angle $d\Omega$ about the direction θ, ϕ per unit time per unit solid angle.

The differential cross section is the ratio of the scattered flux in direction θ, ϕ to the incident flux.

$$\frac{d\sigma}{d\Omega} = S/I$$

The total cross section is the ratio of the scattered flux in any direction to the incident flux.

$$\sigma_T = \int\int \frac{d\sigma}{d\Omega} \sin\theta d\theta d\phi$$

11.3 Scattering in one dimension- Step function

Firstly, we review the problem of scattering by a step function in one dimension. Consider a particle moving from a region ($x < 0$) where the potential is $V = 0$ to a region ($x > 0$) where the potential is $V = V_0$.

Assuming the particle energy $E > V_0$, this is simply the free particle problem, the spatial solution to which is:

$$\Phi = A\exp(ikx) + B\exp(-ikx) \qquad (x < 0); \qquad \Phi = C\exp(ik'x) + D\exp(-ik'x) \qquad (x > 0)$$

where $k = \sqrt{2mE}/\hbar$ and $k' = \sqrt{2m(E - V_0)}/\hbar$

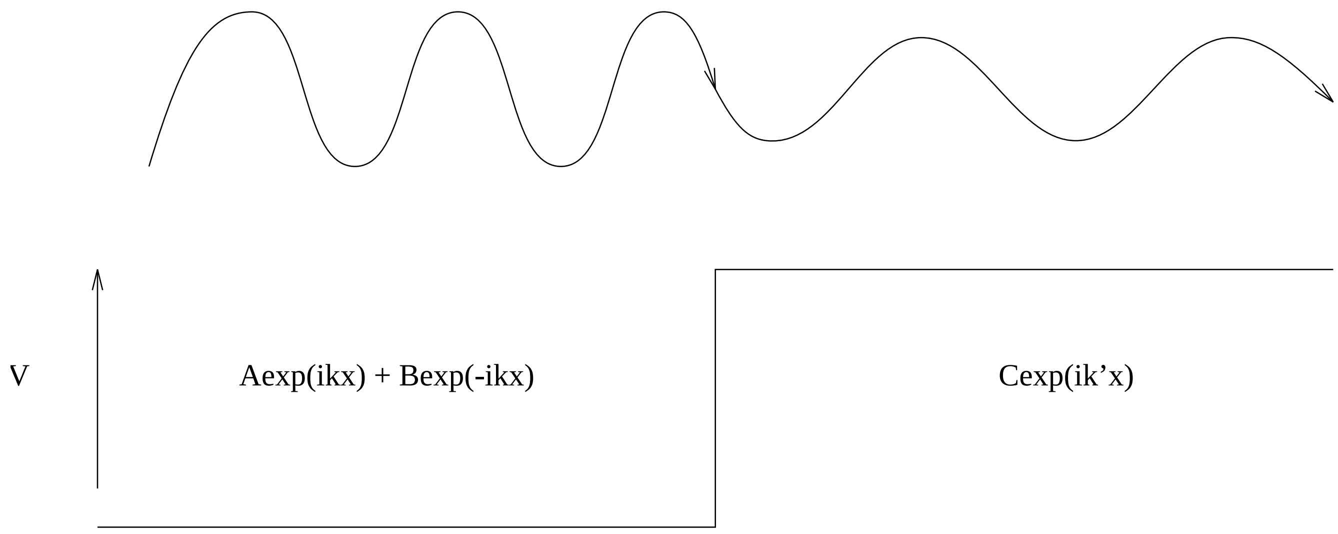

Figure 7: Scattering at a step function.

From the boundary condition that all particles start from $x = -\infty$, we can immediately set D=0.

From the condition of continuity of Φ and $d\Phi/dx$ at $x = 0$ we also require $A + B = C$ and $k(A - B) = k'C$

This gives the reflected amplitude $B/A = (k - k')/(k + k')$ and the transmitted amplitude $C/A = 2k/(k + k')$

The reflected flux is thus

$$\frac{\hbar k}{m} A^2 \left(\frac{k - k'}{k + k'} \right)^2$$

and the transmitted flux is

$$\frac{\hbar k'}{m} A^2 \left(\frac{2k}{k + k'} \right)^2$$

Note that $A^2 \neq B^2 + C^2$. The conserved quantity is the *flux* of particles, not the probability density. In this case the transmitted particles are moving more slowly than the incident ones.

Notice that if V_0 is negative, the transmitted flux gets smaller as $|V_0|$ gets larger: it is difficult to fall off a big cliff! This anomaly is due to the unphysical potential - the discontinuous first derivative at $x = 0$.

We have not considered the case of $E < V_0$. Now the square root is imaginary and $\Phi(x > 0) = Ce^{-\kappa' x}$ where we define a *real* quantity $\kappa' = ik' = \sqrt{2m(V_0 - E)}/\hbar$. The boundary conditions are then $A+B = C$ and $ik(A-B) = \kappa' C$, which gives the reflected amplitude $B/A = (ik-\kappa')/(ik+\kappa')$ and the transmitted amplitude $C\kappa'/Ak = 2ik/(ik + \kappa')$.

Now the reflected flux is equal to the incident flux, and although the wavefunction penetrates the region $x > 0$, it decays exponentially and there is no propagating wave.

11.4 Scattering in one dimension - Square Well

The square well potential has $V(x<0) = V(x>a) = 0; V(0<x<a) = V_0$. As with the step function, we can write the wavefunction as a plane wave in each of the three regions.

$$\Phi(x<0) = A\exp(ikx) + B\exp(-ikx)$$
$$\Phi(0<x<a) = F\exp(ik'x) + G\exp(-ik'x)$$
$$\Phi(x>a) = C\exp(ikx) + D\exp(-ikx)$$

Once again there is no wave coming back from $x=\infty$ $(D=0)$.

There are now four boundary conditions from continuity of the wave function and its derivative at x=0 and x=a. The solving of four equations in four unknowns is straightforward but tedious. Eventually one can obtain ratios for reflected and transmitted flux:

$$B/A = \frac{(k^2-k'^2)(1-e^{2ik'a})}{(k+k')^2-(k-k')^2e^{2ik'a}}$$

$$C/A = \frac{4kk'e^{i(k'-k)a}}{(k+k')^2-(k-k')^2e^{2ik'a}}$$

where $k^2 = 2mE/\hbar^2$ and $k'^2 = 2m(E-V_0)/\hbar^2$. Since the wavenumber is the same on both sides of the barrier, the reflection and transmission coefficients are just:

$$|B/A|^2 = \left[1+\frac{4k^2k'^2}{(k^2-k'^2)^2\sin^2 k'a}\right]^{-1} = \left[1+\frac{4E(E-V_0)}{V_0^2\sin^2 k'a}\right]^{-1}$$

$$|C/A|^2 = \left[1+\frac{(k^2-k'^2)^2\sin^2 k'a}{4k^2k'^2}\right]^{-1} = \left[1+\frac{V_0^2\sin^2 k'a}{4E(E-V_0)}\right]^{-1}$$

We get complete transmission when $k'a = n\pi$, i.e. when an exact number of half waves fit in the well.

Assuming that $E > V_0$. Looking at the limits of this, we see that as $E \to V_0$ then $\sin^2(k'a) \to k'a$ and the transmission coefficient

$$|C/A|^2 \to \left[1+\frac{mV_0a^2}{2\hbar^2}\right]^{-1}$$

As the incoming particle energy is increased, the transmission oscillates between $\left[1+\frac{V_0^2}{4E(E-V_0)}\right]^{-1}$ and 1 at $k'a = n\pi$. The lower limit itself increases to 1 as E increases.

For the tunnelling case where $E < V_0$ we can use these solutions for B/A and C/A, except that k' is now imaginary. This gives

$$|C/A|^2 = \left[1+\frac{4E(E-V_0)}{V_0^2\sinh^2|k'|a}\right]^{-1}$$

which decreases monotonically with decreasing E. Thus a small change in V_0 can give a large change in $|C/A|^2$. This is the principle on which the transistor and the tunnelling electron microscope are based.

Note that the transmitted wave $\Phi(x>a) = C\exp(ikx)$, differs from the incident wave only by a phase - it has the same wavevector. Thus the only effect of the potential on the transmitted particles is to change their *phase*, an idea we shall meet again.

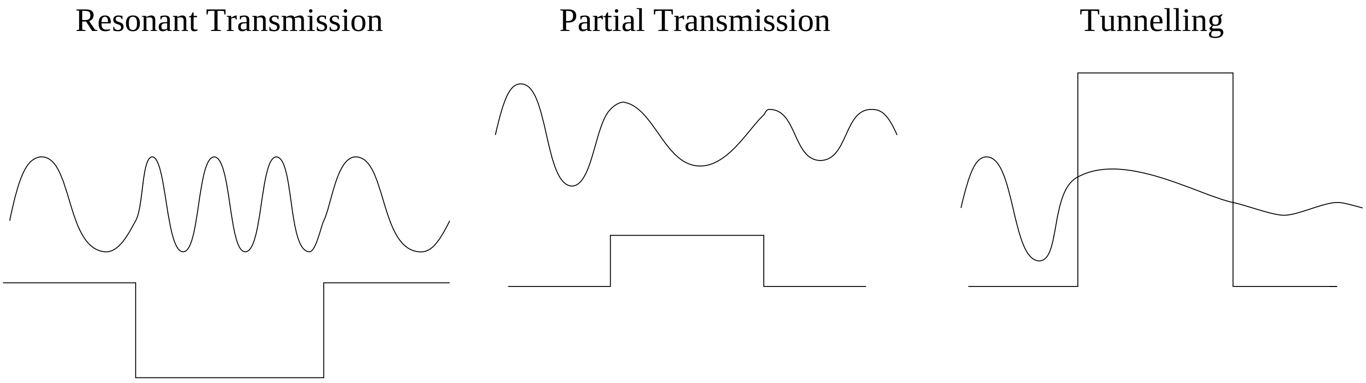

Figure 8: Forward moving wavefunctions passing a square well potential

11.5 The transistor (1956 Nobel) and giant magneto-resistance (2007 Nobel)

Transistors can be modelled as a barrier potential, with the voltage across them represented by different potentials on either side.

The rapid variation in transmission coefficient (current) with change in potential barrier (voltage) is the basis of the transistor The name come from ‘transfer resistor’. The resistance to motion of electrons past the barrier is determined by the voltage V_0 in the barrier region more than the voltage difference across the transistor.

Actual behaviour also depends on the availability of electrons for conduction, which depends in turn on the material in question, since there must be available electron states of appropriate energy on each side of the barrier.

In GMR a series of barriers are created from layers of ferromagnetic material and a spacer chosen to make the layer align antiferromagnetically (e.g. FeCrFe). Conduction electrons with spin opposite to the magnetic moment pass easily through iron (there are many state available to them). So oppositely aligned layers form a series of barriers to either spin. An external magnetic field applied to the GMR causes all the ferromagnetic layers to align, meaning there is no barrier to antialigns conduction electrons. Thus a magnetic field causes a change in resistance: GMR heads are used to “read” the magnetisation states in computer hard disks.

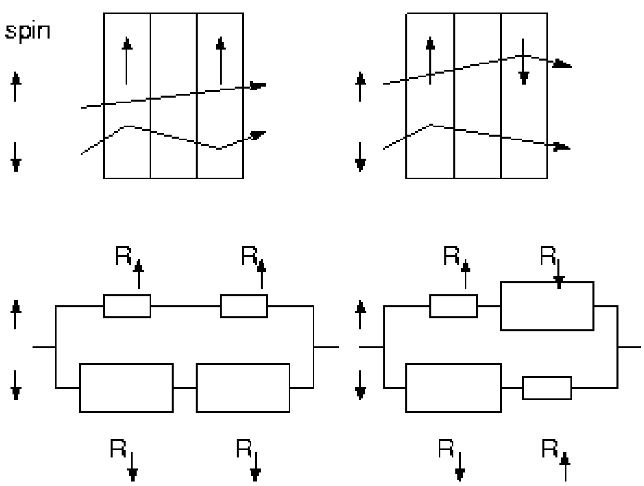

Figure 9: Giantmagnetoresistance

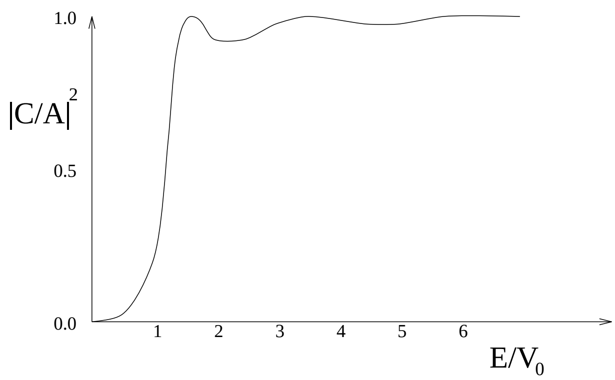

Figure 10: Transmission in a 1D square well