13 Further Concepts in Quantum Scattering Theory

13.1 Born Series, Green Functions - A Hint of Quantisation of the Field

Solving the Schroedinger equation using Green Functions automatically gives a solution in a form appropriate for scattering. By making the substitution $E = \hbar^2 k^2/2\mu$ and $U(r) = (2\mu/\hbar^2)V(r)$ we can write the TISE as:

$$[\nabla^2 + k^2]\Phi = U(r)\Phi$$

For $U(r) = 0$ this gives $\phi_0(r) = Ae^{\mathbf{ik.r}}$, a travelling wave. We now introduce a 'Green's Function' for the operator $[\nabla^2 + k^2]$, which is the solution to the equation:

$$[\nabla^2 + k^2]G(r) = \delta(r)G(r) \qquad\qquad G(r) = -\exp(ikr)/4\pi r$$

$\delta(r)$ is the Dirac delta-function as is $\delta(r)G(r)$, since G(r) diverges at the origin. G(r) has the property that any function Φ which satisfies

$$\Phi(r) = \phi_0(r) + \int G(r - r')U(r')\Phi(r')d^3r'$$

where $\phi_0(r)$ is the free particle solution, will be a solution to the TISE. Since $\phi_0(r)$ is the unscattered incoming wave, the second term must represent the scattered wave.

Thus the general solution to the TISE is given by:

$$\Phi(r) = Ae^{ik.r} + \int G(r - r')U(r')\Phi(r')d^3r'$$

In this expression, Φ appears on both sides. We can substitute for Φ using the same equation:

$$\Phi(r) = Ae^{ik.r} + \int G(r - r')U(r')Ae^{ik.r'}d^3r' + \int\int G(r - r')U(r')G(r' - r'')U(r'')\Phi(r'')d^3r'd^3r''$$

Repeated substitutions gives the *Born series*, terminated by a term involving $\Phi(r)$ itself. If the potential is weak, the higher order terms can be ignored. The first order term is just the matrix element between the incoming plane wave and the Green function: the Born approximation again! If we think of the potential U as an operator, the first term represents the incoming wavefunction

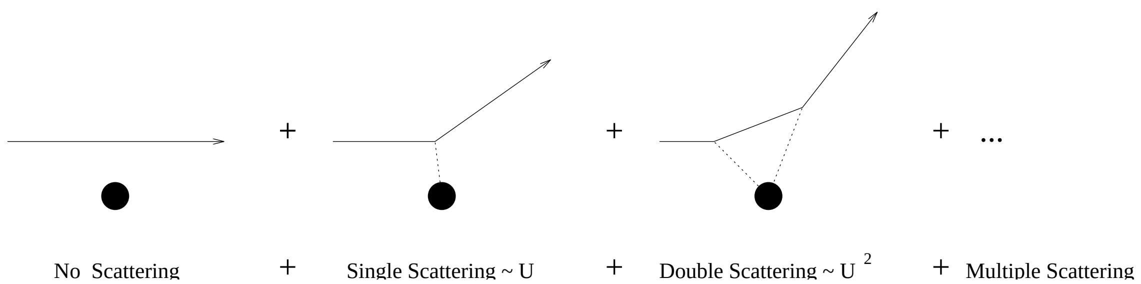

Figure 12: Born Series - scattering as series of terms

being operated on once. The second term represents the incoming wavefunction being operated on twice. And so forth. This suggests a way of *quantising* the effect of the field: The first order term corresponds to a single scattering event, the second order term to double scattering etc.

13.2 Scattering of distinguishable particles and identical particles

Consider two beams of distinguishable particles with the same mass colliding, and scattering through some angle θ. Let the intensity of the scattered particles have angular dependence $|f(\theta)|^2$. Conservation of energy and momentum ensure that the scattering angles are the same for both particles in the COM frame. As usual, the radial part of the wavefunction far from the region of interaction is simply a plane wave so the wavefunction can be written as a function of θ.

The intensity for the process in which both particles are scattered through an angle $(\pi - \theta)$ is $|f(\pi - \theta)|^2$. Note that this process results in particles arriving in the same places as with $f(\theta)$ - it is just the other particles (see diagram).

If the two particle beams are distinguishable they cannot interfere and differential cross section for either particle to be detected at θ is:

$$I_{dis} = |f(\theta)|^2 + |f(\pi - \theta)|^2$$

If, however, the particles are indistinguishable bosons(fermions), they can interfere and the combined wavefunction must (anti)symmetric under exchange of labels:

$$\Phi^{bos}_{fer} = f(\theta) \pm f(\pi - \theta) \qquad\qquad I^{bos}_{fer} = |f(\theta) \pm f(\pi - \theta)|^2$$

Taking the specific extreme example of scattering through $\pi/2$, the differential cross section is $2|f(\pi/2)|^2$ for distinguishable particles, $4|f(\pi/2)|^2$ for identical bosons, and 0 for identical fermions.

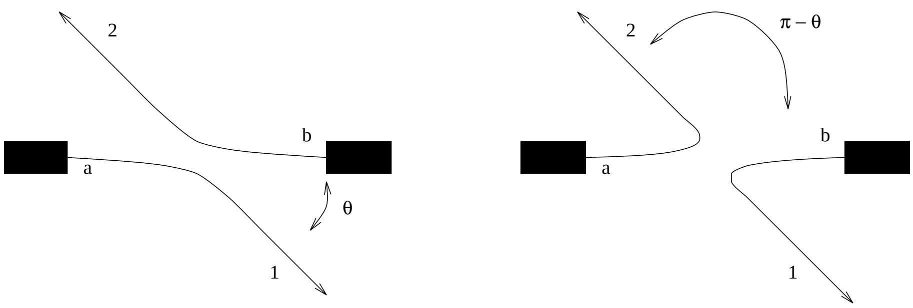

Figure 13: Two indistinguishable scattering processes.

13.3 Scattering of indistinguishable particles into the same state

Consider scattering of two indistinguishable bosons by an external potential. The wavefunction describing the bosons must be *symmetric* with respect to exchange.Thus the cross section for scattering of both through the same angle is: $|2f(\theta)|^2$: two bosons are twice as likely to be scattered into the same state as two distinguishable particles. For many bosons the effect is even more pronounced, and the probability of scattering *out* of the state is similarly reduced.

The tendency for bosons to clump into one state leads to superfluid behaviour in He^4 and superconductivity: α particles and Cooper pairs behave as bosons. All the particles are in the same state and cannot be scattered out.

For fermions, the cross section for being scattered into the same state is $|f(\theta) - f(\theta)|^2 = 0$, as we would expect from the exclusion principle.

13.4 Collision between two unpolarised electron beams

In this case, half the collisions will be between like-polarised electrons, so will involve interference, and half will be between unlike electrons: so there would be no interference. In both cases $|f(\theta)|^2$ represents Rutherford scattering. The differential cross section of finding an electron scattered through an angle θ is thus:

$$I = \frac{1}{2}(I_{dis} + I_{ind}) = \frac{1}{2}(|f(\theta)|^2 + |f(\pi-\theta)|^2) + \frac{1}{2}|f(\theta) - f(\pi-\theta)|^2$$

Consider $\theta = \pi/2$. The like polarised beams give zero probability, so unpolarised beams give only half what we would expect from Coulomb scattering of distinguishable particles. Furthermore, the spins of pairs of electrons scattered through $\theta = \pi/2$ are always observed to be opposite.

An alternate philosophy is that we should treat the spins as a symmetric triplet and an antisymmetric singlet, with probabilities $\frac{3}{4}$ and $\frac{1}{4}$. Then the spatial scattering process must be antisymmetric in the first case and symmetric in the second. This gives the same answer!

13.5 Scattering of identical free particles with a periodic potential

For a free particle moving in a 1D region of space there are two degenerate wavefunctions ($\Phi = e^{\pm ikx}$). If there is a weak periodic potential, $V \cos ax$, to evaluate the energy shift to first order in degenerate perturbation theory the relevant matrix elements are:

$$\int e^{\pm ikx} V \cos ax e^{\mp ikx} dx = \int V \cos ax dx = 0\,; \qquad \int e^{\pm ikx} V \cos ax e^{\pm ikx} dx = \int V \cos ax \cos 2kx dx$$

The second term is also zero, except in the case $2k = a$. This gives rise to the remarkable result: *To first order, free particles are unaffected by a periodic potential unless it has half the wavelength.* This is the basis of Bragg's Law, x-ray and neutron diffraction.

13.6 Scattering of free electrons in metals

If we describe an electron bound in a solid or liquid as a free electron, we see that scattering occurs only for those electrons with wavenumbers close to periodic repeats. For simple metals (Li, Na etc) the highest occupied free-electron level has wavelength greater than any crystal spacing, so it only sees the average of the ionic potential.

To first order, only electrons with the periodicity of the lattice are scattered. To second order in perturbation theory, the potential can mix states:

$$\Delta E = \frac{|V_{ij}|^2}{(E_j - E_i)}; \qquad V_{ij} = \int e^{\pm i(a/2+\delta)x} V \cos ax e^{\pm i(a/2-\delta)x} \neq 0$$

which gives significant energy shifts for states $\pm\delta$ from the lattice periodicity ($E_j - E_i = -\hbar^2 a\delta/m$). Thus free-electron levels with $k \approx a/2$ are split by periodic potentials giving a *bandgap* in the density of allowed states. At first glance, this may seem to be totally different physics from the LCAO band gaps we saw earlier. In fact, its simply another manifestation of using two different *mathematical* basis sets to describe the same *physical* phenomenon.

13.7 Low energy Scattering: Partial Waves

The Born Approximation is a perturbation method based on the Fermi Golden Rule and is therefore valid when the incoming particle energy is large compared to the potential. An alternative approach is needed at low energy. For a central potential, scattering geometry plane wave in, radial wave out, implies a wavefunction:

$$|\Psi\rangle = \text{IncidentWave} \;+\; \text{ScatteredWave} \;=\; = e^{ikz} + f(\theta)e^{ikr}/r$$

The incident flux is $I = ve^{iKz}e^{-iKz} = v = \hbar k/m$. The scattered flux must be a normalisable plane wave (hence e^{-iKr}/r), with a θ dependence arising from the scattering. By symmetry, there is no ϕ dependence. Thus the scattered flux per unit area will be: $vf^*(\theta)f(\theta)/r^2$. The cross section $d\sigma/d\Omega = S(\theta)/I = f^*(\theta)f(\theta)$, and all we need do is solve the Schroedinger equation and calculate $f(\theta)$.

For a spherically symmetric potential, the angular parts of the wavefunction are simply spherical harmonics, so scattering is described by the radial equation:

$$\frac{d^2u_l(r)}{dr^2} - \frac{l(l+1)}{r^2}u_l(r) + \frac{2\mu}{\hbar^2}[E - V(r)]u_l(r) = 0$$

where $u_l(r) = rR_l(r)$, the same substitution as in the atomic hydrogen problem. Assuming a short range potential, $V(r \to \infty) = 0$, $R_l(Kr \to \infty)$ describes a free particle, with some phase $l\pi/2 - \delta_l$.

$$R_l(Kr) = \sin(Kr - l\pi/2 + \delta_l)/Kr$$

Thus the effect of the scattering at long range can be described by a set of *phase shifts* δ_l.

To solve further, we expand a plane wave into angular momentum components using a complete set of spherical harmonics and Bessel Functions:

$$\exp(iKr\cos\theta) = \sum_{l=0}^{\infty} i^l j_l(Kr)(2l+1)P_l(\cos\theta)$$

so that we can write:

$$\Psi(\mathbf{r}) = e^{iKz} + f(\theta)\frac{e^{iKr}}{r} = \sum_{l=0}^{\infty} i^l j_l(Kr)(2l+1)P_l(\cos\theta) + f(\theta)\frac{e^{iKr}}{r} = \sum_{l=0}^{\infty} b_l R_l(Kr)P_l(\cos\theta)$$

where b_l are expansion coefficients for the expression of Ψ in the *partial wave* basis, which can be determined from the boundary $r \to \infty$, giving:

$$f(\theta) = K^{-1}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta)$$

From this we can calculate $d\sigma/d\Omega = |f(\theta)|^2$ and $\sigma = 2\pi\int |f(\theta)|^2 d\theta$. Differential cross sections $d\sigma/d\Omega$ are complicated, involving many cross terms. However, when integrated over all θ these cross terms vanish due to orthogonality of the Legendre polynomials $\langle P_l|P_{l'}\rangle = 0$ $(l \neq l')$, and

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

Hence scattering cross sections are completely determined by $|K|$ and the phase shifts δ_l. This is most useful in the low energy limit (*S-wave scattering*) where any particle with $l > 0$ must be so far from the target (*impact parameter* $b = l/\hbar k$) that it will miss.

Note the term (2l+1). This can be related to the classical 'impact parameter' mentioned above. The angular momentum of a particle of velocity v is $mvb = \sqrt{l(l+1)}\hbar$. Thus a classical (large l) particle with angular momentum $l\hbar$ would pass between a ring of radius $b = l\hbar/mv$ and one of radius $b = (l+1)\hbar/mv$. The area between these rings is $(2l+1)\pi(\hbar/mv)^2$ so for a uniform beam the probability of a particle having angular momentum l is proportional to (2l+1).