Scattering States

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Scattering in a central potential

The problem of collision of two bodies interacting via a central potential $U(r)$ can be reduced to the motion of their reduced mass (m) in a force field centred on the centre-of-mass of the two bodies.
We will work in the C-o-M frame and take the incident particles along the $\hat{z}$ axis.

Incident free particle

A free particle with a definite momentum $\hbar k$ along $\hat{z}$ is described by an incident plane wave

$$\psi_{in} = \exp(ikz)$$

and the corresponding probability current density is

$$\begin{aligned} j_{in} &= \frac{i\hbar}{2m}\left[\psi_{in}\nabla\psi_{in}^{*} - \psi_{in}^{*}\nabla\psi_{in}\right] \\ &= \frac{2\hbar k}{2m} \quad (= v) \end{aligned}$$

Incident wave in terms of radial waves

The incident plane wave can be expanded in terms of the radial waves

$$\psi_{in} = \exp(ikz) = \frac{1}{2ikr} \sum_0^\infty (2\ell + 1) P_l(\cos\theta) \left[(-)^{\ell+1} \exp(-ikr) + \exp(ikr) \right]$$

This form will be useful later when we consider the scattering probability

Scattered Waves

Scattered Waves

At large distance from the scattering centre the amplitude of the scattered wave must fall off as $1/r$ to conserve the flux of particles. Thus the scattered wave must be of the form of a spherical wave with an angular dependence

$$\psi_{sc}(r \to \infty) = f(\theta)\frac{\exp(ikr)}{r}$$

The probability per unit time that the scattered wave will cross a surface $d\vec{S}$ is given by $\vec{j}_{sc} \cdot d\vec{S}$, and since we are looking at radial waves, this reduces to $|j_{sc}|r^2 d\Omega$
j_{sc} is readily found from

$$\begin{aligned} j_{sc} &= \frac{i\hbar}{2m}\left[\psi_{sc}\hat{r}\frac{d}{dr}\psi^*_{sc} - \psi^*_{sc}\hat{r}\frac{d}{dr}\psi_{sc}\right] \\ &= \frac{\hbar k}{mr^2}|f(\theta)|^2 \\ &= \frac{v}{r^2}|f(\theta)|^2 \end{aligned}$$

Scattered Waves

Thus, the probability per unit time that the scattered wave crosses an area dS is

$$\frac{v}{r^2}|f(\theta)|^2 \cdot r^2 d\Omega.$$

The ratio of this probability to the incident current density is $|f(\theta)|^2 d\Omega$

This has dimensions of area. This quantity is the quantum-mechanical analogue of the classical cross-section σ.
Thus $|f(\theta)|^2$ gives the probability per unit time per unit incident flux that the scattered wave wave emerges in a unit solid angle, and hence

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

$f(\theta)$ is called the scattering amplitude

Schrödinger Equation for a central potential

The quantum mechanical scattering problem therefore reduces to the problem of obtaining $f(\theta)$ i.e. obtaining $f(\theta)$ by solving the Schrödinger equation for positive energies.

Schrödinger Equation for a central potential

The Schrödinger equation for positive energies is

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(r)\right]\psi = \frac{\hbar^2 k^2}{2m}\psi$$

where $E = \hbar^2 k^2/2m$, and k is the wavenumber of the incident particles
The general solution is taken in the variable separable form

$$\psi = \sum_{\ell=0}^{\infty} A_\ell R_{k\ell} P_\ell(\cos(\theta))$$

There is no ϕ-dependence in the solution, since the problem has a complete azimuthal symmetry around the $\hat{z}$ axis

Schrödinger Equation for a central potential

The potential is purely radial, so we need to focus on the radial part of the Schrödinger equation:

$$\left[\frac{1}{r^2}\left(\frac{d}{dr}r^2\frac{d}{dr}\right)\right]R - \frac{\ell(\ell+1)}{r^2}R + \frac{2m}{\hbar^2}[E - U(r)]R = 0$$

If $U(r) = 0$, we have the case of a free particle of momentum $\hbar k$, and the equation for $R(r)$ is considerably simplified

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[k^2 - \frac{\ell(\ell+1)}{r^2}\right]R = 0$$

Free Particle States ($U = 0$)

Case 1: $\ell = 0$

The radial equation becomes

$$\frac{d^2(rR)}{dr^2} + k^2(rR) = 0$$

There are four solutions:

$$R(r) = \frac{\sin(kr)}{r}, \frac{\cos(kr)}{r}, \frac{\exp(\pm ikr)}{r}$$

and of these the last two represent ingoing and outgoing waves, while only the first solution is finite at $r = 0$.

Free Particle States ($U = 0$)

Case 2: $\ell \neq 0$

If, instead of solving for $R(r)$, we solve for the function $u(r) = r^l R(r)$, the equation is simplified

$$\frac{d^2 u_{k\ell}}{dr^2} + \frac{2(\ell+1)}{r}\frac{du_{k\ell}}{dr} + k^2 u_{k\ell} = 0$$

To solve this, we differentiate once again w.r.t. r:

$$\frac{d^3 u_{k\ell}}{dr^3} + \frac{2(\ell+1)}{r}\frac{d^2 u_{k\ell}}{dr^2} + \left[k^2 - 2(\ell+1)\right]\frac{du_{k\ell}}{dr} = 0$$

Free Particle States ($U = 0$)

Case 2: $\ell \neq 0$ (contd.)

If we set

$$\frac{du_{k,\ell}}{dr} = r u_{k,\ell+1}(r)$$

the third order differential equation becomes

$$\frac{d^2 u_{k,\ell+1}}{dr^2} + \frac{2(\ell+2)}{r}\frac{du_{k,\ell+1}}{dr} + k^2 u_{k,\ell+1} = 0$$

That is, the same equation is satisfied by $u_{k,\ell+1}$. This implies we have the recursion relation

$$u_{k,\ell+1}(r) = \frac{1}{r}\frac{du_{k,\ell}}{dr}$$

and hence

$$u_{k\ell}(r) = \left[\frac{1}{r}\frac{d}{dr}\right]^{\ell} u_{k0}$$

Type-I Solutions

Recall that u_{k0} is already known, so we have the radial solutions for all ℓ (the sin and exp functions are physically acceptable)

Type-I Solutions

If we choose $u_{k0} = \sin(kr)$ then we get

$$R_{kl}(r) = (-)^l \frac{2r^l}{k^l} \left[\frac{1}{r}\frac{d}{dr}\right]^l \left(\frac{\sin(kr)}{kr}\right)$$

The behaviour of R_{kl} at large r can be found by observing the term in the previous equation that decreases the slowest.

Each differentiation of the RHS creates two new terms, one with an increases power of $1/r$ and the other that that adds $\pi/2$ to the argument of the sin function. (i.e. the sin function toggles between sin and cos).

The sin term has a factor $1/r$ so as $r \to \infty$ this is the only term that is significant

Hence, as $r \to \infty$,

$$R_{kl}(r) \approx \frac{2\sin(kr - l\pi/2)}{r}$$

Type-II Solutions

The same considerations apply if we take $u_{k0} = \exp(\pm ikr)$
The recursion relation yields

$$R^{\pm}_{k\ell}(r) = (-)^{\ell} A^{\ell} \frac{r^{\ell}}{k^{\ell}} \left[\frac{1}{r}\frac{d}{dr}\right]^{\ell} \left[\frac{\exp(\pm ikr)}{kr}\right]$$

and the asymptotic form is

$$R_{k\ell}(r) \approx A \left[\frac{\exp(\pm ikr - \ell\pi/2)}{kr}\right]$$

Solution in the presence of a potential

In the foregoing part we looked at the special case of a free particle.

This was done so as to meet the physical reality, that irrespective of the form of the potential, it tends to zero asymptotically, and this limiting case is represented by our foregoing discussion.

Solution in the presence of a potential

Thus, in the asymptotic limit, the solutions are of the forms discussed earlier, with the generalisation that there can be an additional phase factor

$$R_{k\ell}(r) \approx A \left(\frac{\exp(\pm ikr - \ell\pi/2 + \delta_\ell)}{kr} \right)$$

$$R_{k\ell}(r) \approx \frac{2\sin(kr - \ell\pi/2 + \delta_\ell)}{r}$$

The phase factor allows the asymptotic solution to approach the correct limit in the region with the full form of $U(r)$ in the Schrödinger equation as $r \to 0$

The phase factor can only be determined by solving the exact equation in the limit of small r; there is no general formula for δ_l.

Solution in the presence of a potential

The full solution ψ_{kl} is then

$$\psi_{k\ell}(r \to \infty) = \sum_0^\infty A_\ell \frac{2\sin(kr - \ell\pi/2 + \delta_\ell)}{r} P_\ell(\cos\theta)$$

If we choose

$$A_\ell = \frac{1}{2k}(2\ell+1)i^\ell \exp(i\delta_\ell)$$

and write ψ in the $\exp(\pm ikr + \delta_\ell)$ form, then the asymptotic form of ψ becomes

$$\psi_{kl}(r \to \infty) = \frac{1}{2ikr}\sum_0^\infty (2\ell+1)i^l e^{i\delta_\ell}\left[(-i)^\ell e^{i(kr+\delta_\ell)} - (i)^\ell e^{-i(kr+\delta_\ell)}\right] P_\ell(\cos\theta)$$

Comparison with the Scattering Solution

The case of scattering is a special case of the solution with a non-zero potential in which the incident and outgoing conditions are separately specified

Comparison with the Scattering Solution

As seen at the beginning

$$\psi_{in} = \exp(ikz)$$

The wavefunction in the outgoing state is given by a sum of the incident and the scattered waves $\psi_{out} = \psi_{in} + \psi_{sc}$

$$\psi_{out} = \exp(ikz) + f(\theta)\frac{\exp(ikr)}{r}$$

Comparison with the Scattering Solution

Recall, that the incident wave can be expanded in terms of the radial waves

$$\exp(ikz) = \frac{1}{2ikr}\sum_{0}^{\infty}(2\ell+1)P_l(\cos\theta)\left[(-)^{\ell+1}\exp(-ikr)+\exp(ikr)\right]$$

Comparison with the Scattering Solution

The difference between the general asymptotic wavefunction and the incident wavefunction

$$(\text{as } r \to \infty) \quad \psi_{k\ell} - \exp(ikz)$$

has no terms containing $\exp(-ikr)$.

In other words the difference function has only outgoing radial waves

Comparison with the Scattering Solution

Given that

$$\psi_{out} = \exp(ikz) + f(\theta)\frac{\exp(ikr)}{r}$$

This means that the $f(\theta)$ is equal to the coefficient of $\exp(ikr)/r$ in the difference
This yields

$$f(\theta) = \frac{1}{2ik}\sum_{0}^{\infty} i^{\ell}(2\ell+1)P_{\ell}(\cos\theta)\left[e^{2i\delta_{\ell}} - 1\right]$$

Thus, if the phase shifts are known, the scattering amplitudes and hence the differential cross-section are determined.

Comparison with the Scattering Solution

Integrating the previous expression, we get the required cross-section

$$\sigma = 2\pi \int_0^\pi |f(\theta)|^2 \sin\theta \, d\theta$$

Since the Legendre polynomials are orthonormal, and

$$|P_\ell(\cos\theta)|^2 \sin\theta \, d\theta = 2/(2\ell+1)$$

we get for the total cross-section

$$\sigma = \frac{4\pi}{k^2} 2 \sum_0^\infty (2\ell+1) \sin^2(\delta_\ell).$$

Approximate Solutions

Approximate Solutions

The solution to the free particle Schrödinger equation

$$\nabla^2\psi + k^2\psi = 0; \quad E = \hbar^2 k^2/2m$$

is $\psi^{(0)} = \exp(i\vec{k}\cdot\vec{r})$

Without loss of generality, we may take $\psi^0 = \exp(ikz)$, if needed

Let $\psi = \psi^{(0)} + \psi^{(1)}$ be the solution to the Schrödinger equation with the potential:

$$\nabla^2\psi + k^2\psi - \frac{2mU(r)}{\hbar^2}\psi = 0$$

Substituting, $\psi = \psi^{(0)} + \psi^{(1)}$ in the above, we get

$$\nabla^2\psi^{(1)} + k^2\psi^{(1)} = \frac{2mU(r)}{\hbar^2}\left[\psi^{(0)} + \psi^{(1)}\right]$$

Approximate Solutions (Perturbative Solutions)

The solution to the previous equation is

$$\psi^{(1)}(\vec{r}) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\int [\psi^{(0)}(\vec{r'}) + \psi^{(1)}(\vec{r'})]\, U(r')\, \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r'})}}{|\vec{r}-\vec{r'}|} d\tau'$$

As the simplest approximation we can ignore $\psi^{(1)}(\vec{r'})$ on the RHS, and write the solution as

$$\psi(\vec{r}) = \psi^{(0)} - \frac{2m}{\hbar^2}\frac{1}{4\pi}\int \psi^{(0)}(\vec{r'})\, U(r')\, \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r'})}}{|\vec{r}-\vec{r'}|} d\tau'$$

To determine the conditions under which the perturbative solution is valid, we seek the conditions under which magnitude of the correction to the wavefunction is small, for this we need to estimate the magnitude of the integral above.

Validity of the Perturbative Solutions – Case I

If the energy of the particle is small, i.e. if a is a "range" scale of the potential, $k < 1/a$, then in the integrand we can set

$$\exp(ikr) \approx 1$$

The order of magnitude of the integral is thus $|\psi^{(0)}| \cdot |U| 4\pi r^2/r$

$$\begin{aligned}\psi^{(1)} &\approx \frac{2m}{\hbar^2}\frac{1}{4\pi}|\psi^{(0)}| \cdot |U| \cdot 4\pi a^2 \\ &\approx \frac{2ma^2}{\hbar^2}|\psi^{(0)}| \cdot |U|\end{aligned}$$

Requiring $|\psi^{(1)}| < |\psi^{(0)}|$, we get the condition of validity as

$$|U| \ll \frac{\hbar^2}{2ma^2} \quad \text{or}$$

$$|U| \ll \frac{\hbar^2 k^2}{2m}$$

Validity of the Perturbative Solutions – Case II

The second condition for the validity of the perturbative approach is when the energy of the particle is large: $ka \gg 1$. In this case the exponential part of the integral cannot be ignored.

Let us set $\psi^{(1)} = g \cdot \exp(ikz)$, where $g \ll 1$ and work out the equation for $\psi^{(1)}$, keeping only those terms that have $\exp(ikz)$

$$\frac{\partial^2}{\partial z^2} g e^{ikz} + k^2 g e^{ikz} = \frac{2m}{\hbar^2} U e^{ikz}$$

Noting, that

$$\frac{\partial^2}{\partial z^2} e^{ikz} = -k^2$$
$$\frac{\partial}{\partial z} e^{ikz} = ik$$
$$|g|^2 \ll |g| \ll 1$$

Validity of the Perturbative Solutions – Case II

we get

$$
\begin{aligned}
2ik\frac{\partial g}{\partial z} &= \frac{2mU}{\hbar^2} \\
g &= \frac{-im}{\hbar^2 k}\int U\, dz \\
|g| &= \frac{mUa}{\hbar^2 k}
\end{aligned}
$$

Requiring $|g| \ll 1$, we have the condition

$$
\begin{aligned}
U &\ll \hbar^2 k/ma \\
&\ll \hbar v/a
\end{aligned}
$$

Validity of the Perturbative Solutions – Case III

For the special case of the Coulomb potential (very important in atomic physics !), the condition for validity of the perturbative formulation appear would fail, because there is no definable "range" of the potential, (a). However, we note, that $U(r) = \alpha/r$ for this potential, so we can write the condition as

$$\frac{\alpha}{r} \ll \hbar v/r$$

$$\text{i.e.} \quad \frac{\alpha}{\hbar v} \ll 1$$

Approximate Solutions : Scattering Amplitude

Approximate Solutions : Scattering Amplitude

Let us re-visit the perturbative solution, with a goal to obtain the scattering amplitude

$$\psi^{(1)}(\vec{r}) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\int [\psi^{(0)}(\vec{r'}) + \psi^{(1)}(\vec{r'})]\, U(r')\, \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r'})}}{|\vec{r}-\vec{r'}|} d\tau'$$

Earlier, in order to obtain the validity condition, we had ignored the $\psi^{(1)}(\vec{r'})$ *on the RHS.*

In the full form, i.e. not caring about the number of terms in the perturbative expansion, this equation is

$$\psi(\vec{r}) = \psi^{(0)} - \frac{2m}{\hbar^2}\frac{1}{4\pi}\int \psi(\vec{r'})\, U(r')\, \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r'})}}{|\vec{r}-\vec{r'}|} d\tau'$$

This is called the Lippmann–Schwinger Equation

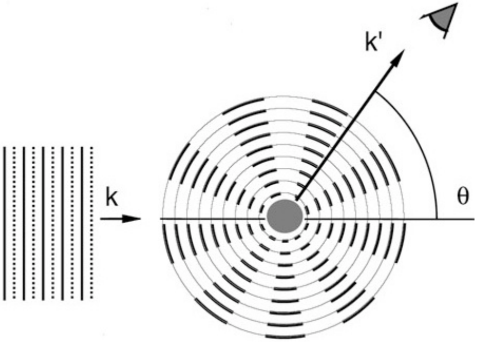
Approximate Solutions : Scattering Amplitude

At large distances from the scatterer in the (elastic) scattering problem, we can make the approximation

$$|\vec{r} - \vec{r'}| = r\,[1 - \hat{k}' \cdot r' + \frac{1}{2}(\hat{k} \cdot r')^2 + \ldots]$$

so that

$$\frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r'})}}{|\vec{r} - \vec{r'}|} \approx \frac{e^{ikr}}{r} e^{-i\vec{k}'\cdot\vec{r'}}$$



Approximate Solutions : Scattering Amplitude

Hence, in the equation

$$\psi = \psi^{(0)} - \frac{2m}{\hbar^2}\frac{1}{4\pi}\int [\psi^{(0)}(\vec{r'}) + \psi^{(1)}(\vec{r'})]\, U(r')\, \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r'})}}{|\vec{r}-\vec{r'}|} d\tau'$$

we get

$$\psi = \psi^{(0)} - \frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}\int [\psi^{(0)}(\vec{r'}) + \psi^{(1)}(\vec{r'})]\, U(r')\, e^{-i\vec{k}'\cdot\vec{r'}} d\tau'$$

Comparing this with

$$\psi_{out} = \exp(ikz) + f(\theta)\frac{\exp(ikr)}{r}$$

we immediately recognise

$$f(\theta) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\int [\psi^{(0)}(\vec{r'}) + \psi^{(1)}(\vec{r'})]\, U(r') e^{-i\vec{k}'\cdot\vec{r'}} d\tau'$$

Approximate Solutions : Scattering Amplitude

We can rewrite

$$f(\theta) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\int [\psi^{(0)}(\vec{r'}) + \psi^{(1)}(\vec{r'})]\, U(r') e^{-i\vec{k'}\cdot\vec{r'}} d\tau'$$

as

$$f(\theta) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\int \psi(\vec{r'})\, U(r')\psi_{k'}^{(0)*}(\vec{r'}) d\tau'$$

From this last equation, we see that to calculate $f(\theta)$ we need to know $\psi(\vec{r'})$.

But to obtain $\psi(\vec{r'})$ we need to know $f(\theta)$.

This can be calculated by an iterative correction to $\psi(\vec{r'})$: initially set $\psi(\vec{r'}) = \psi^{(0)}(\vec{r'})$ (zeroth approximation), and then do a serial calculation.

Approximate Solutions : Born Approximation

This series expression is called the Born Series for the scattering amplitude.
The leading term is called the First Born Approximation

$$f_{\text{Born}} = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\langle\psi_{k'}^{(0)}|U|\psi_{k}^{(0)}\rangle$$

The change in the momentum of the incident particle is $\vec{q} = \vec{k'} - \vec{k}$. We can write the integral in terms of q:

$$f_{\text{Born}} = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3r' e^{-iqr'}U(r')$$

The first Born term is the Fourier transform of the potential from ordinary space to the momentum transfer space

Note that $|q| = 2k\sin(\theta/2)$

Born Approximation : Coulomb Case

For the case of the Coulomb potential, we saw earlier that the boundary condition in terms of a, k cannot be applied. In the present context this implies that the intergral for calculating f does not converge.

So, we do a trick: instead of the Coulomb potential, we solve for a screened Coulomb potential

$$U_s(r) = \frac{\alpha \exp(-\beta r)}{r}$$

which falls off faster than $1/r$ so that the integral can be evaluated, and then after obtaining the integral let $\beta \to 0$

Born Approximation : Coulomb Case

This yields

$$f_{\text{Born}} = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\frac{\alpha}{\beta^2 + q^2}$$

which in the limit $\beta \to 0$ becomes

$$f_{\text{Born}}(\theta) = \frac{2m}{\hbar^2}\frac{\alpha}{[2k\sin(\theta/2)]^2}$$

The differential cross-section is

$$\frac{d\sigma}{d\Omega} = |f_{\text{Born}}(\theta)|^2 = \left[\frac{2m}{\hbar^2}\right]^2 \frac{\alpha^2}{16k^2\sin^4(\theta/2)}$$

$$= \frac{(Z_1 Z_2)^2}{(2mv^2)^2\sin^4(\theta/2)}$$

Approximate Solutions (Using Green's Function)

Approximate Solutions (Using Green's Function)

Returning to the wavefunction, we recall that

$$\psi = \psi^{(0)} - \frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}\int [\psi^{(0)}(\vec{r'}) + \psi^{(1)}(\vec{r'})]\, U(r')\, e^{-i\vec{k}\cdot\vec{r'}}\, d\tau'$$

which is usually written as

$$\psi = \psi^{(0)} + \int G(\vec{r},\vec{r'})\frac{2m}{\hbar^2}U(r')\,\psi(\vec{r'})d\tau'$$

where G is the Green's function

$$G = -\frac{1}{4\pi}\frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r'})}}{|\vec{r}-\vec{r'}|}$$

Approximate Solutions (Using Green's Function)

The iterative solution to ψ can be written in a coordinate-free form as

$$|\psi\rangle = |\psi^{(0)}\rangle + \hat{G}\hat{U}|\psi^{(0)}\rangle + \hat{G}\hat{U}\hat{G}\hat{U}|\psi^{(0)}\rangle$$

in which the integral over $d\tau'$ is implied, and $\hat{U}$ includes the factor $2m/\hbar^2$. Since

$$f(\theta) = \frac{2m}{\hbar^2}\frac{1}{4\pi}\int \psi_k(\vec{r'})\, U(r')\psi_{k'}^{(0)*}(\vec{r'})d\tau'$$

we can also write $f(\theta)$ in a simpler (appearing!) form

$$f(\theta) = -\frac{1}{4\pi}\langle\psi_{k'}^{(0)}|U(r')|\psi_k\rangle$$

This second form is very useful in identifying the series solution for $f(\theta)$

$$f(\theta) = -\frac{1}{4\pi}\langle\psi_{k'}^{(0)})|\hat{U} + \hat{U}\hat{G}\hat{U} + \hat{U}\hat{G}\hat{U}\hat{G}\hat{U} + \ldots|\psi_k^{(0)}\rangle$$