QM-18 Lecture Notes

Scattering Theory in Quantum Mechanics

Integral equation and Born approximation

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Introduction

In this unit description of scattering and scheme of computation of cross section in quantum mechanics is introduced. This is achieved by imposing a suitable boundary condition on the solution of the time independent Schrödinger equation and converting Schrödinger equation into an integral equation using the Green function for the free particle Schrödinger equation. A perturbative solution of the integral equation leads to the Born approximation for the scattering amplitude.

§1 Continuous Energy Solutions

§1.1 Asymptotic behaviour of scattering wave function

In this unit description of scattering and scheme of computation of cross section in quantum mechanics is introduced. This is achieved by imposing a suitable boundary condition on the solution of the time independent Schrödinger equation and converting Schrödinger equation into an integral equation using the Green function for the free particle Schrödinger equation. A perturbative solution of the integral equation leads to the Born approximation for the scattering amplitude.

Let us consider a scattering experiment in which a beam of particles is scattered from a target at rest. The frame of reference in which the target is at rest will be called the laboratory frame. After the scattering the particles, at large distances, will be moving, away from the target, like free particles. We assume the potential between an incident particle, position $\vec{r}_1$, and the target, at position $\vec{r}_2$, to be central potential $V(r)$ which depends only on the relative position,$\vec{r} = \vec{r}_1\vec{r}_2$, of the particle and the target. We recall that the two particle problem can then be reduced to the problem of one particle of reduced mass moving in a potential $V(r)$. The cross section calculated for a particle moving in potential $V(r)$ equals the scattering cross sections in the centre of mass frame and must be transformed to the lab frame to establish contact with experiments.

Knowledge of the classical trajectory of a particle, $\vec{r}(t)$ is sufficient to compute the cross section in classical mechanics. The classical physics being deterministic, the particles going into solid angle corresponding to a cone, covering small range $\theta, \theta + d\theta$ of the scattering angle, are precisely those which come from a corresponding range of impact parameter b. Hence we only need to know the relation between the impact parameter and the scattering angle to compute the differential cross section $\sigma(\theta)$. The result is known to be

$$\sigma(\theta) = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| \tag{1}$$

In quantum mechanical framework the particles do not have a well defined trajectory and it is not meaningful to associate a well defined range of impact parameters with a given range of scattering angle. All information about a system has to be obtained from the wave function and must be extracted from the available statistical interpretation of the wave function.

The scattering process, like any other motion, is a problem of time evolution. In a scattering experiment, the incident particle is far off from the target and approaches towards the target reaching a point of closest approach. After that it moves away from the target and goes to infinity. A wave packet description the motion of a particle, in accordance with the time dependent Schrödinger equation, is the framework for a rigorous and a complete description of the scattering problem. It turns out that the scattering process can also the viewed as a stationary state problem and solution of the time independent Schrödinger equation turns out to be adequate as a first introduction for our present purpose.

Let us consider a thought experiment in which a beam of particles is incident and getting scattered for all times from $-\infty$ to ∞. If take a snap shot of the beam in the experiment, it would look the same at all times. It should therefore not come as a surprise that one treat the scattering in terms of using stationary states. This is not something completely new, we are already used to treating motion of electrons in an atom as a stationary process in quantum mechanics. We will, therefore, formulate the scattering problem in terms of stationary state solutions, i.e., the solutions of the time independent Schrodinger equation. Boundary conditions for the wave function Assuming a spherically symmetric potential $V(r)$ which goes to zero for large distances, $E < 0$ corresponds to possible bound states and the continuous energy solution for $E > 0$ is needed for a discussion of to the scattering. The Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi + V(r)\psi = E\psi \tag{2}$$

has an infinite number of solutions $E > 0$. To understand this we look at the free particle solutions. For a given energy the free particle solutions can be written as

$$\psi(\vec{r}) = N\exp(ik\hat{n}\cdot\vec{r}) \tag{3}$$

where $k = \sqrt{2E/2\hbar^2}$ and $\hat{n}$ is a unit vector giving the direction of propagation. For a fixed energy E there are infinitely many plane wave solutions corresponding to the direction of propagation specified by the unit vector $\hat{n}$. Alternately, the solutions can also be written in terms of spherical waves of definite angular momentum ℓ and definite L_z value m

$$\psi(\vec{r}) = C\, j_\ell(kr)Y_{\ell m}(\theta,\phi) \tag{4}$$

The most general solution will be a superposition of the above special solutions. The free particle behaviour will hold for the scattering solutions for a potential which goes to zero for large distances, giving infinite number of solutions. Thus specifying the energy alone is not sufficient to pick a unique solution, it is necessary to specify a boundary condition suited to the scattering problem. In the stationary description, the solution to Schrodinger equation should describe the incident beam and an outgoing scattered wave. For short range potentials this will be a spherical wave with varying amplitude in different directions. We demand that the wave function for a definite energy must satisfy the following boundary condition in the limit $r \to \infty$:

$$\lim \psi(\vec{r}) \to e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \tag{5}$$

The above choice of the boundary condition requires an explanation. The first term has been written for the choice of z axis along the incident beam of definite energy E.

In general, for incident beam having momentum k_i, one must replace the first term by $\exp(-i\vec{k}_i \cdot \vec{r})$. The second term represents an outgoing spherical wave, note that the time dependence of the wave function will $e^{-iEt/\hbar}$. The factor $f(\theta)/r$ represents the amplitude of the wave at large distances in the direction θ. Since the intensity of the scattered beam decreases as $1/r^2$ for large distance, the amplitude must decrease as $1/r$ for large r. As of now, it is not clear that such a solution does exist, in a later subsection we will show that a solution satisfying the boundary condition Eq.(5) does exist.

§1.2 Cross section in quantum Theory

Now we come to computation of cross section for scattering from a potential spherical symmetric, finite range potential $V(r)$. We wish to relate the differential cross section to the scattering amplitude $f(\theta)$. Let us consider a scattering experiment involving a total of N incident particles sent in time T . The number of particles detected per second by a detector in a direction θ will be proportional to the flux of the incident beam and the solid angle subtended by the detector and the constant of proportionality is just the differential cross section. For a detector placed at a distance r from the target and having an opening area ΔS, the solid angle will be $\Delta\Omega = \Delta S/r^2$ Thus we would get

$$\text{No of particle detected per sec} = \sigma(\theta) \times \Delta\Omega \times \text{ Flux of the incident beam.}$$

knowing the wave function, the number of particles detected per second can be computed using the probability current density $\vec{j}$. The opening of the detector is kept perpendicular to the radius vector and usually covers only a small solid angle, the probability of a particle entering the detector per sec is given by the surface integral

$$\iint\limits_S j_r dS \approx j_r \Delta S \tag{6}$$

over the surface of the detector, where j_r is the radial component of the probability current. The total number of particles detected per sec will be N times the expression. Thus Eq.(§1.2) becomes

$$N \times j_r \Delta S = \sigma(\theta) \times \Delta\Omega \times \text{Flux of the incident beam} = \sigma(\theta)\Delta\Omega \times N j_z. \tag{7}$$

where j_z is the z component of the probability current. Using

$$\vec{j} = -\frac{\hbar}{2i\mu}(\psi^* \nabla\psi - \psi\nabla\psi^*) \tag{8}$$

the z component of the probability current for the incident beam e^{ikz} is easily found to be $k/$. Also the radial component of the of the probability current for the scattered wave is obtained by substituting $f(\theta)e^{ikr}/r$ for $\psi(r)$ in Eq.(8) and taking the radial component. Using the most important term in the radial component of the current for the scattered wave becomes

$$j_r = \frac{|f(\theta)|^2}{r^2} + O(1/r^2). \tag{9}$$

Using Eq.(8)-Eq.(9) in Eq.(7) gives

$$(N(|f()|^2/r^2)\Delta S = \sigma(\theta)\Delta\Omega N \tag{10}$$

With $\Delta S = r^2\Delta\Omega$, we get the desired relation

$$\sigma(\theta) = |f(\theta)|^2. \tag{11}$$

We have ignored the terms in the current coming from the interference of the incident and scattered waves. These are of the order of $1/r^2$, and are proportional to $exp(ikr(1cos))$. Due to the presence of large r in the exponential, this term oscillates rapidly with and contributes vanishingly small value to the cross section when summed over a small range of θ values.

§2 Integral Equation

§2.1 A simple example

Setting up integral equation

Very often the problem of solving a linear differential equation can be replaced with solution of an integral equation. An important feature of the integral equation approach is that the initial conditions to be satisfied by the solution is built into the integral equation. The integral equation can be solved many a times by an iterative procedure which we shall illustrate by an example of a simple differential equation.

Suppose we are interested in solving the differential equation

$$\frac{dy}{dx} = \lambda y \tag{12}$$

subject to the boundary condition

$$y(x)|_{x=x_0} = N \tag{13}$$

where N is a constant. To convert Eq.(12) into an integral equation we integrate Eq.(12) to get

$$y(x) = \lambda \int y(x)dx + constant \tag{14}$$

or to be more precise, let us write Eq.(14) as

$$y(x) = \lambda \int_0^x y(t)dt + constant \tag{15}$$

The constant in the above equation is fixed by making use of the initial condition Eq.(13), and we get const= N and

$$y(x) = N + \lambda \int_0^x y(t)dt \tag{16}$$

It is to noted that the unknown function y appears inside the integral sign, hence an equation of this type is called integral equation. This equation can be solved iteratively giving a solution as a series in powers of λ. This method gives the exact answer in the case of this simple example under consideration.

Perturbative Solution

As a first step, we set y equal to y_0 where

$$y_0 = N \tag{17}$$

is the solution in the zeroth order in λ and is simply taken to be equal to the first term Eq.(16). Next the zeroth order 'solution' ,y_0, is substituted in the right hand side of Eq.(16) to get the solution in the first order in λ. Thus we have

$$y_1(x) = N + \lambda \int_0^x y_0 dx \tag{18}$$

$$= N + \lambda \int_0^x N dx \tag{19}$$

$$\therefore \qquad y_1(x) = N(1 + \lambda)x \tag{20}$$

To improve the approximation, we substitute $y_1(x)$ for $y(x)$ in right hand side of Eq.(13) to get the next approximation $y_2(x)$ for our solution.

$$y_2(x) = N + \lambda \int_0^x y_1(x)dx \tag{21}$$

$$= N + \lambda \int_0^x N(1 + \lambda x)dx \tag{22}$$

$$= N\left(1 + \lambda x + \lambda^2 \frac{x^2}{2}\right) \tag{23}$$

continuing in this fashion we get

$$y_3(x) = N + \lambda \int_0^x y_2(x)dx \tag{24}$$

$$= N + N\lambda \int_0^x \left(1 + \lambda x + \lambda \frac{x^2}{2}\right) dx \tag{25}$$

$$= N\left(1 + \lambda x + \frac{\lambda^2 x^2}{2} + \frac{\lambda^3 x^3}{3!}\right) \tag{26}$$

$$y_4(x) = N\left(1 + \lambda x + \frac{\lambda^2 x^2}{2} + \frac{\lambda^3 x^3}{3!} + \frac{\lambda^4 x^4}{4!}\right) \tag{27}$$

Thus we get an infinite series in powers of λ

$$y(x) = N\left(1 + \lambda x + \frac{\lambda^2 x^2}{2} + \frac{\lambda^3 x^3}{3!} + \dots\right) \tag{28}$$

summing the series we get

$$y(x) = Ne^{\lambda x} \tag{29}$$

Note that this is the correct solution for ordinary differential equation and satisfies the given boundary condition $y(0) = N$.

Alternate approach – Using series expansion

The above method of solution is equivalent to the following alternate sequence of steps. We want to solve

$$y(x) = N + \lambda \int_0^x y(t)dt \tag{30}$$

we assume that the solution can be written as a series in λ

$$y(x) = \alpha_0 + \lambda\alpha + \lambda^2\alpha^2 + \cdots + \alpha^n\lambda^n + \cdots \tag{31}$$

we substitute Eq.(31) in Eq.(30) and compare powers on both the sides. Therefore we get

$$\alpha_0(x) + \lambda\alpha_1(x) + \lambda^2\alpha_2(x) + \dots \lambda^n\alpha_n(x) + \dots \tag{32}$$

$$= N + \lambda \int_0^x \left\{\alpha_0(t) + \lambda\alpha_1(t) + \lambda^2(t)\alpha_2(t) + \cdots\right\} dt \tag{33}$$

on comparing coefficients of different powers of λ we successively get

$$\begin{aligned}
\alpha_0(x) &= N \\
\alpha_1(x) &= \int_0^x \alpha_0(t)dt = Nx \\
\alpha_2(x) &= \int_0^x \alpha_1(t)dt = N\frac{x^2}{2} \\
\alpha_1(x) &= \int_0^x \alpha_2(t)dt = N\frac{x^3}{3!} \\
\alpha_k(x) &= \int_0^x \alpha_{k-1}(t)dt = N\frac{x^k}{k!}
\end{aligned} \tag{34}$$

Therefore we get

$$y(x) = N\left(1 + \lambda x + \frac{\lambda^2}{2!}x^2 + \cdots + \frac{\lambda^n}{n!}x^n + \cdots\right) \tag{35}$$

§2.2 Green function for Poisson equation

In electromagnetic theory the electric potential satisfies the Poisson equation

$$\nabla^2 \Phi = -\frac{\rho}{\varepsilon_0}, \tag{36}$$

where $\rho(\vec{r})$ is the volume charge density. The Green function for the Poisson equation is defined by

$$\nabla^2 G(\vec{r}) = -\delta^3(\vec{r}) \tag{37}$$

If $\phi_0(\vec{r})$ is a solution of the Laplace equation

$$\nabla^2 \phi_0(\vec{r}) = 0, \tag{38}$$

then

$$\Phi(\vec{r}) = \phi_0(\vec{r}) + \int G(\vec{r} - \vec{r}') \frac{\rho(\vec{r}')}{\varepsilon_0} d^3 r' \tag{39}$$

is a solution of the Poisson equation which can be easily verified by applying ∇^2 on both sides of Eq.(39).

$$\nabla^2 \Phi(\vec{r}) = \nabla^2 \phi_0(\vec{r}) + \nabla^2 \int G(\vec{r} - \vec{r}') \frac{\rho(\vec{r}')}{\varepsilon_0} d^3 r' \tag{40}$$

$$= \int \nabla^2 G(\vec{r} - \vec{r}') \frac{\rho(\vec{r}')}{\varepsilon_0} d^3 r' \tag{41}$$

$$= -\frac{1}{\varepsilon_0} \int \delta^3(\vec{r} - \vec{r}') \rho(\vec{r}') d^3 \vec{r}' \tag{42}$$

$$= -\frac{\rho(\vec{r})}{\varepsilon_0} \tag{43}$$

It can be shown that one solution of Eq.(37) is

$$G(\vec{r}) = \frac{1}{4\pi r}. \tag{44}$$

This Green function gives the potential due to a charge distribution subject to the condition that the potential vanishes at infinity. The exact form of the Green function and the solution ϕ_0 of the Laplace equation is determined by the boundary conditions of the problem.

§2.3 Integral Equation for Scattering

In order to convert the Schrodinger equation

$$\left\{ \frac{-\hbar^2}{2\mu} \nabla^2 + v(r) \right\} \psi = E\psi \tag{45}$$

into an integral equation we first rewrite it as

$$\left(\nabla^2 + k^2\right)\psi = u(\vec{r})\psi(\vec{r}) \tag{46}$$

where $k^2 = \dfrac{2\mu E}{\hbar^2}$, $U(r) = \dfrac{2\mu}{\hbar^2}V(r)$ and we have defined Green function $G(\vec{r})$ as a solution of

$$\left(\nabla^2 + k^2\right)G(\vec{r}) = -\delta(\vec{r}) \tag{47}$$

and it was found that several solutions of Eq.(47) exist.Thus $G(\overrightarrow{r})$ can

$$G_{\pm}(\vec{r}) = \frac{1}{4\pi r}\exp \pm kr \tag{48}$$

$$G_0(\vec{r}) = \frac{1}{4\pi r}\cos(kr) \tag{49}$$

using the Green function we shall now write down a "formal" solution of Eq.(46) as a solution of integral equation. Next we shall determine the behaviour of the solution as $r \to \infty$ and show that the choice

$$G(\vec{r}) = \frac{1}{4\pi r}\exp ikr \tag{50}$$

leads to the correct boundary condition on the wave function. Using a Green function which is a solution of Eq.(47) a formal solution for Eq.(46) can be written as

$$\psi(\vec{r}) = \phi(\vec{r}) - \int G(|\vec{r} - \vec{r}\,'|)U(|\vec{r}\,'|)\psi(\vec{r}\,')d^3r' \tag{51}$$

where $\phi(\vec{r})$ is a solution of the equation

$$\left(\nabla^2 + k^2\right)\phi(\vec{r}) = 0 \tag{52}$$

For the scattering problem we must select

$$\phi(\vec{r}) = \exp(i\vec{k_i}.\vec{r}) \tag{53}$$

where $\vec{k_i}$ is the momentum of the incident particles.Substituting Eq.(50) Eq.(53) in Eq.(51) we get the integral equation for the scattering to be

$$\psi(\vec{r}) = \exp(i\vec{k_i}.\vec{r}) - \frac{1}{4\pi}\int \frac{\exp^{ik|\vec{r}-\vec{r'}|}}{|\vec{r} - \vec{r'}|}U(\vec{r'})\psi(\vec{r'})d^3r\prime \tag{54}$$

To verify that $\psi(\vec{r})$ given by Eq.(54) does indeed have correct asymptotic property we expand $|\vec{r} - \vec{r'}|$ in powers of $\dfrac{\vec{r}}{\vec{r'}}$ we shall assume that the potential is short range potential so that the contribution to integral over $\vec{r'}$ comes from small value of r'. Expand $|\vec{r} - \vec{r'}|$ in powers of r'

$$|\vec{r} - \vec{r'}| = \sqrt{r^2 + r'^2 - 2\vec{r}\cdot\vec{r'}} \tag{55}$$

$$= r\left(1 - 2\frac{\vec{r}\cdot\vec{r'}}{r^2} + \frac{r'^2}{r^2}\right)^{1/2} \tag{56}$$

Using binomial expansion we get

$$|\vec{r} - \vec{r'}| = r\left(1 - \frac{\vec{r}\cdot\vec{r'}}{r^2} + O\left(\frac{r'^2}{r^2}\right)^2\right) \tag{57}$$

We substitute Eq.(57) in the exponential and in the factor $\dfrac{1}{|\vec{r}-\vec{r'}|}$ in Eq.(54) and write $\dfrac{1}{|\vec{r}-\vec{r'}|} \approx \dfrac{1}{r}$ to get

$$\begin{aligned}
\psi(\vec{r}) \quad &\longrightarrow \quad \exp(i\vec{k}_i\cdot\vec{r}) - \frac{1}{4\pi r}\int \exp\left(ikr - ik\frac{\vec{r}\cdot\vec{r'}}{r^2}\right)U(\vec{r'})\psi(\vec{r'})d^3r' && (58)\\
&= \quad \exp(i\vec{k}_i\cdot\vec{r}) - \frac{e^{ikr}}{4\pi r}\int \exp(-ik\hat{n}\cdot\vec{r'})U(r')\psi(r')d^3r' && (59)
\end{aligned}$$

In the last step we have introduced a unit vector $\hat{n} = \vec{r}/r$. The Eq.(59) gives the probability amplitude (wave function) at $\vec{r}$. If the particles are to reach at a detector at $\vec{r}$, the vector $\hat{n}$ must be in the direction of the final momentum and parallel to k_f. Note that

$$|\vec{k}_i| = |\vec{k}_f| = k \tag{60}$$

holds as a consequence of energy conservation and hence

$$k(\hat{n}\cdot\vec{r'}) = \vec{k}_f\cdot\vec{r} \tag{61}$$

Thus Eq.(59) takes the form

$$\psi(\vec{r}) \approx \exp(i\vec{k}_i\cdot\vec{r}) - \frac{e^{ikr}}{4\pi r}\int \exp(-i\vec{k}\cdot\vec{r'})U(r')\psi(r')d^3r' \tag{62}$$

This asymptotic behaviour is of the for expected for large r

$$\psi(\vec{r}) \approx \exp(i\vec{k}_i\cdot\vec{r}) - \frac{e^{ikr}}{r}f(\theta,\phi). \tag{63}$$

Comparing Eq.(62) with Eq.(63) we see that the scattering amplitude is given by

$$\begin{aligned}
f(\theta,\phi) \quad &= \quad -\frac{1}{4\pi}\int \exp(-i\vec{k}_f\cdot\vec{r'})U(r')\psi(r')d^3r' && (64)\\
&= \quad -\left(\frac{\mu}{2\pi\hbar^2}\right)\int \exp(-i\vec{k}_f\cdot\vec{r'})V(r')\psi(r')d^3r' && (65)
\end{aligned}$$

It must be noted that the integral equation Eq.(54) and the expression for the scattering amplitude in Eq.(65) are **exact** results. We shall next discuss how to use (54) and (65) to obtain scattering amplitude in the Born approximation.

§3 Born Approximation

§3.1 Perturbation series and first Born approximation

The energy eigenfunctions, with a correct asymptotic behaviour corresponding to the scattering solutions satisfy the following integral equation

$$\psi(\vec{r}) = \exp(i\vec{k}_i.\vec{r}) - \frac{1}{4\pi}\int \frac{\exp\{ik|\vec{r}-\vec{r}\,'|\}}{|\vec{r}-\vec{r}\,'|}U(\vec{r}\,')\psi(\vec{r}\,')d^3r\prime \tag{66}$$

where we have used the notation

$\vec{k}_i$ = momentum of the incident beam

$\vec{k}_f$ = momentum of the scattered beam

θ= scattering angle = angle bewteen $\vec{k}_i$ and $\vec{k}_f$.

$V(\vec{r})$ = potential due the target

μ= mass of the incident particle (reduced mass for two body problem)

$U(\vec{r})$= $\dfrac{2\mu}{\hbar^2}V(\vec{r})$

An iterative solution of the integral equation can be obtained by assuming that in the lowest order approximation $\psi(\vec{r})$ is equal to $\psi_0(\vec{r})$ given by

$$\psi_0(\vec{r}) = \exp(i\vec{k}_i\cdot\vec{r}) \tag{67}$$

Using this approximation for $\psi(\vec{r})$ from Eq.(67) in the right hand side of Eq.(66), we get the next order solution, denoted as $\psi_1(\vec{r})$, given by

$$\psi_1(\vec{r}) = \exp(i\vec{k}_i\cdot\vec{r}) - \frac{1}{4\pi}\int \frac{\exp\{ik|\vec{r}-\vec{r}\,'|\}}{|\vec{r}-\vec{r}\,'|}U(\vec{r}\,')\exp(i\vec{k}_i\cdot\vec{r}\,')d^3r\prime \tag{68}$$

The next approximation to the solution, $\psi_2(\vec{r})$, is obtained by replacing $\psi(\vec{r})$ in Eq.(66) with $\psi_1(\vec{r})$. Thus

$$\begin{aligned}
\psi_2(\vec{r}) &= e^{i\vec{k}_i.\vec{r}} - \frac{1}{4\pi}\int \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}U(\vec{r}\,')\psi_1(\vec{r}\,')d^3r\prime && (69)\\
&= e^{i\vec{k}_i\cdot\vec{r}} - \frac{1}{4\pi}\int \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}U(\vec{r}\,')e^{(i\vec{k}_i\cdot\vec{r}\,')}d^3r\prime && (70)\\
&\quad + \frac{1}{(4\pi)^2}\int \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}U(\vec{r}\,')\int \frac{e^{ik|\vec{r}\,'-\vec{r}\,''|}}{|\vec{r}\,'-\vec{r}\,''|}U(\vec{r}\,'')e^{i\vec{k}_i\cdot(\vec{r}\,'+\vec{r}\,'')}d^3r'd^3r'' && (71)
\end{aligned}$$

This process can be continued indefinitely and it becomes very cumbersome to compute the wave function beyond first few orders.

The first order Born approximation consists in using the first, the plane wave term in the above series as approximate wave function in the expression

$$f(\theta,\phi) = -\frac{1}{4\pi}\int \exp(-i\vec{k}_f\cdot\vec{r}')U(r')\psi(r')d^3r' \tag{72}$$

$$= -\left(\frac{\mu}{2\pi\hbar^2}\right)\int \exp(-i\vec{k}_f\cdot\vec{r}')V(r')\psi(r')d^3r' \tag{73}$$

for the scattering amplitude, giving

$$f(\theta,\phi) \approx -\frac{\mu}{2\pi\hbar^2}\int e^{i(\vec{k}_i-\vec{k}_f)\cdot\vec{r}}V(r)d^3r, \tag{74}$$

or

$$f(\theta,\phi) \approx -\frac{\mu}{2\pi\hbar^2}\int e^{-i\vec{q}\cdot\vec{r}}V(r)d^3r, \tag{75}$$

where $\vec{q} = \vec{k}_i - \vec{k}_f$ is the momentum transfer. The result Eq.(75) is the well known, first order, Born approximation result for the scattering amplitude.

§3.2 Validity of Born approximation

The integral equation for the energy eigen functions was derived to be

$$\psi(\vec{r}) = e^{i\vec{k}_i\cdot\vec{r}} - \left(\frac{\mu}{2\pi\hbar^2}\right)\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}V(\vec{r}')\psi(\vec{r}')d^3r' \tag{76}$$

In the derivation of the integral equation it is assumed that it is good approximation to take $\psi(\vec{r})$ to be plane wave

$$\psi(\vec{r}) \approx \exp(i\vec{k}_i\cdot\vec{r}) \tag{77}$$

and substitute in the right hand side of Eq.(76). The second term on the right hand side of Eq.(76)gives a correction to plane wave form. If Eq.(77) is a good approximation to the wave function, the correction must be small compared to the plane wave term. Hence the condition, under which the Born approximation is valid, is given by

$$\left|\left(\frac{\mu}{2\pi\hbar^2}\right)\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}V(\vec{r}')\psi(\vec{r}')d^3r'\right| < \left|e^{i\vec{k}_i\cdot\vec{r}}\right| \tag{78}$$

or

$$\left|\left(\frac{\mu}{2\pi\hbar^2}\right)\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}V(\vec{r}')\exp(i\vec{k}_i\cdot\vec{r}')d^3r'\right| < 1 \tag{79}$$

The effect of the potential is to distort the wave function and make it different from the plane wave and clearly this distortion is expected to be maximum where the potential is large. The potential is assumed to tend to zero as $r\to\infty$, assuming that the potential is of short range and that most significant effect comes for $r\approx 0$, we apply the condition Eq.(79)for $r=0$ and get

$$\left|\left(\frac{\mu}{2\pi\hbar^2}\right)\int \frac{e^{ikr'}}{r'}V(\vec{r}')\exp(i\vec{k}_i\cdot\vec{r}')d^3r'\right| < 1 \tag{80}$$

Changing the integration variable name from r' to r, assuming the potential to be spherically symmetric we get

$$\left(\frac{\mu}{2\pi\hbar^2}\right)\left|\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \int_0^{\infty} \frac{e^{ikr}}{r} V(r) e^{ikr\cos\theta} r^2 dr\right| < 1 \tag{81}$$

The ϕ integration gives 2π and the θ integral is

$$\int_0^{\pi} \sin\theta d\theta e^{ikr\cos\theta} = \int_{-1}^{1} \exp(ikrt)dt \tag{82}$$

$$= \frac{1}{ikr}\left(e^{ikr} - e^{-ikr}\right) \tag{83}$$

Substituting Eq.(83) in Eq.(81) we get

$$\frac{\mu}{\hbar^2 k}\left|\int_0^{\infty}\left(e^{2ikr} - 1\right) V(r) dr\right| < 1 \tag{84}$$

In the next subsection we shall derive, the condition for validity of the Born approximation for the square well potential.

§3.3 Square Well potential

For a square well potential of strength V_0 and range R_0, the expression in the left hand side Eq.(84) takes the form

$$\frac{\mu V_0}{\hbar^2 k}\left|\int_0^{R_0}\left(e^{2ikr} - 1\right) dr\right| = \frac{\mu V_0}{\hbar^2 k}\left|\frac{e^{2ikR_0} - 1}{2ik} - R_0\right| \tag{85}$$

$$= \frac{\mu V_0}{2\hbar^2 k^2}\left|e^{2ikR_0} - 2ikR_0 - 1\right| \tag{86}$$

Using the notation $\rho = 2kR_0$ the condition, that the Born approximation be valid, takes the form

$$\frac{\mu V_0}{2\hbar^2 k^2}\left(\rho^2 - 2\rho\sin\rho - 2\cos\rho + 2\right)^{\frac{1}{2}} << \tag{87}$$

we shall consider the low energy and high energy cases separately.

Low energy scattering

At low energy the de Broglie wave length is much larger than the range of the potential *i.e.* $2kR_0 << 1$. We then have

$$\begin{aligned} \rho^2 &- 2\rho\sin\rho + 2\cos\rho \\ &\approx \rho^2 - 2\rho\left(\rho - \frac{\rho^3}{6} + \cdots\right) - 2\left(1 - \frac{\rho^2}{2} + \frac{\rho^4}{24} + \cdots\right) + 2 \\ &= \frac{\rho^4}{4} \end{aligned} \tag{88}$$

Hence at low energies the Born approximation is applicable if

$$\frac{\mu V_0}{2\hbar^2 k^2}\frac{\rho^2}{2} = \frac{\mu V_0 R_0^2}{\hbar^2} << 1 \tag{89}$$

The above condition implies that the potential is so weak that the bound state does not exist.

High energy limit

In the high energy limit $\rho >> 1$ and we get

$$\left(\rho^2 - 2\rho\sin\rho - 2\cos\rho + 2\right)^{\frac{1}{2}} \approx \rho \tag{90}$$

and hence the Born approximation is valid if

$$\frac{\mu V_0}{2\hbar^2 k^2}\rho << 1 \tag{91}$$

or

$$\frac{\mu V_0 a}{\hbar v} << 1 \tag{92}$$