

QM-18 Lecture Notes

Scattering Theory in Quantum Mechanics*

18.3 Perturbative Solution of Integral Equation and Born Approximation

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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

$$\psi(\vec{r}) = \exp(i\vec{k}_i \cdot \vec{r}) - \frac{1}{4\pi} \int \frac{\exp\{ik|\vec{r} - \vec{r}'|\}}{|\vec{r} - \vec{r}'|} U(\vec{r}') \psi(\vec{r}') d^3r' \quad (1)$$

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 between \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)

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

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

$$\psi_0(\vec{r}) = \exp(i\vec{k}_i \cdot \vec{r}) \quad (2)$$

Using this approximation for $\psi(\vec{r})$ from Eq.(20) in the right hand side of Eq.(20), we get the next order solution, denoted as $\psi_1(\vec{r})$, given by

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

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The next approximation to the solution, $\psi_2(\vec{r})$, is obtained by replacing $\psi(\vec{r})$ in Eq.(20) with $\psi_1(\vec{r})$. Thus

$$\psi_2(\vec{r}) = e^{i\vec{k}_i \cdot \vec{r}} - \frac{1}{4\pi} \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} U(\vec{r}') \psi_1(\vec{r}') d^3 r' \quad (4)$$

$$\begin{aligned} &= e^{i\vec{k}_i \cdot \vec{r}} - \frac{1}{4\pi} \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} U(\vec{r}') e^{i\vec{k}_i \cdot \vec{r}'} d^3 r' \quad (5) \\ &+ \frac{1}{(4\pi)^2} \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} U(\vec{r}') \int \frac{e^{ik|\vec{r}'-\vec{r}''|}}{|\vec{r}'-\vec{r}''|} U(\vec{r}'') e^{i\vec{k}_i \cdot (\vec{r}'+\vec{r}'')} d^3 r'' d^3 r' \end{aligned}$$

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

$$f(\theta, \phi) = -\frac{1}{4\pi} \int \exp(-i\vec{k}_f \cdot \vec{r}') U(r') \psi(r') d^3 r' \quad (7)$$

$$= -\left(\frac{\mu}{2\pi\hbar^2}\right) \int \exp(-i\vec{k}_f \cdot \vec{r}') V(r') \psi(r') d^3 r' \quad (8)$$

for the scattering amplitude, giving

$$f(\theta, \phi) \approx -\frac{\mu}{2\pi\hbar^2} \int e^{i(\vec{k}_i - \vec{k}_f) \cdot \vec{r}} V(r) d^3 r, \quad (9)$$

or

$$f(\theta, \phi) \approx -\frac{\mu}{2\pi\hbar^2} \int e^{-i\vec{q} \cdot \vec{r}} V(r) d^3 r, \quad (10)$$

where $\vec{q} = \vec{k}_i - \vec{k}_f$ is the momentum transfer. The result Eq.(25) is the well known, first order, Born approximation result for the scattering amplitude.

2 Validity of Born approximation

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

$$\psi(\vec{r}) = e^{i\vec{k}_i \cdot \vec{r}} - \left(\frac{\mu}{2\pi\hbar^2}\right) \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi(\vec{r}') d^3 r' \quad (11)$$

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

$$\psi(\vec{r}) \approx \exp(i\vec{k}_i \cdot \vec{r}) \quad (12)$$

and substitute in the right hand side of Eq.(20). The second term on the right hand side of Eq.(20) gives a correction to plane wave form. If Eq.(20) 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

$$\left| \left(\frac{\mu}{2\pi\hbar^2}\right) \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi(\vec{r}') d^3 r' \right| < \left| e^{i\vec{k}_i \cdot \vec{r}} \right| \quad (13)$$

or

$$\left| \left(\frac{\mu}{2\pi\hbar^2}\right) \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \exp(i\vec{k}_i \cdot \vec{r}') d^3 r' \right| < 1 \quad (14)$$

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 $r \rightarrow \infty$, assuming that the potential is of short range and that most significant effect comes for $r \approx 0$, we apply the condition Eq.(22) for $r = 0$ and get

$$\left| \left(\frac{\mu}{2\pi\hbar^2}\right) \int \frac{e^{ikr'}}{r'} V(\vec{r}') \exp(i\vec{k}_i \cdot \vec{r}') d^3 r' \right| < 1 \quad (15)$$

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

$$\left(\frac{\mu}{2\pi\hbar^2} \right) \left| \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \int_0^\infty \frac{e^{ikr}}{r} V(r) e^{ikr \cos\theta} r^2 dr \right| < 1 \quad (16)$$

The ϕ integration gives 2π and the θ integral is

$$\int_0^\pi \sin\theta d\theta e^{ikr \cos\theta} = \int_{-1}^1 \exp(ikrt) dt \quad (17)$$

$$= \frac{1}{ikr} (e^{ikr} - e^{-ikr}) \quad (18)$$

Substituting Eq.(26) in Eq.(24) we get

$$\frac{\mu}{\hbar^2 k} \left| \int_0^\infty (e^{2ikr} - 1) V(r) dr \right| < 1 \quad (19)$$

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

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.(19) takes the form

$$\frac{\mu V_0}{\hbar^2 k} \left| \int_0^{R_0} (e^{2ikr} - 1) dr \right| = \frac{\mu V_0}{\hbar^2 k} \left| \frac{e^{2ikR_0} - 1}{2ik} - R_0 \right| \quad (20)$$

$$= \frac{\mu V_0}{2\hbar^2 k^2} \left| e^{2ikR_0} - 2ikR_0 - 1 \right| \quad (21)$$

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

$$\frac{\mu V_0}{2\hbar^2 k^2} (\rho^2 - 2\rho \sin \rho - 2 \cos \rho + 2)^{\frac{1}{2}} \ll 1 \quad (22)$$

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.* $2kR_0 \ll 1$. We then have

$$\begin{aligned} \rho^2 & - 2\rho \sin \rho + 2 \cos \rho \\ & \approx \rho^2 - 2\rho \left(\rho - \frac{\rho^3}{6} + \dots \right) - 2 \left(1 - \frac{\rho^2}{2} + \frac{\rho^4}{24} + \dots \right) + 2 \\ & = \frac{\rho^4}{4} \end{aligned} \quad (23)$$

Hence at low energies the Born approximation is applicable if

$$\frac{\mu V_0}{2\hbar^2 k^2} \frac{\rho^2}{2} = \frac{\mu V_0 R_0^2}{\hbar^2} \ll 1 \quad (24)$$

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 $\rho \gg 1$ and we get

$$(\rho^2 - 2\rho \sin \rho - 2 \cos \rho + 2)^{\frac{1}{2}} \approx \rho \quad (25)$$

and hence the Born approximation is valid if

$$\frac{\mu V_0}{2\hbar^2 k^2} \rho \ll 1 \quad (26)$$

or

$$\frac{\mu V_0 a}{\hbar v} \ll 1 \quad (27)$$

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