Lectures #15 - 16

Scattering. Differential cross section.

Born approximation. Validity of the Born approximation.

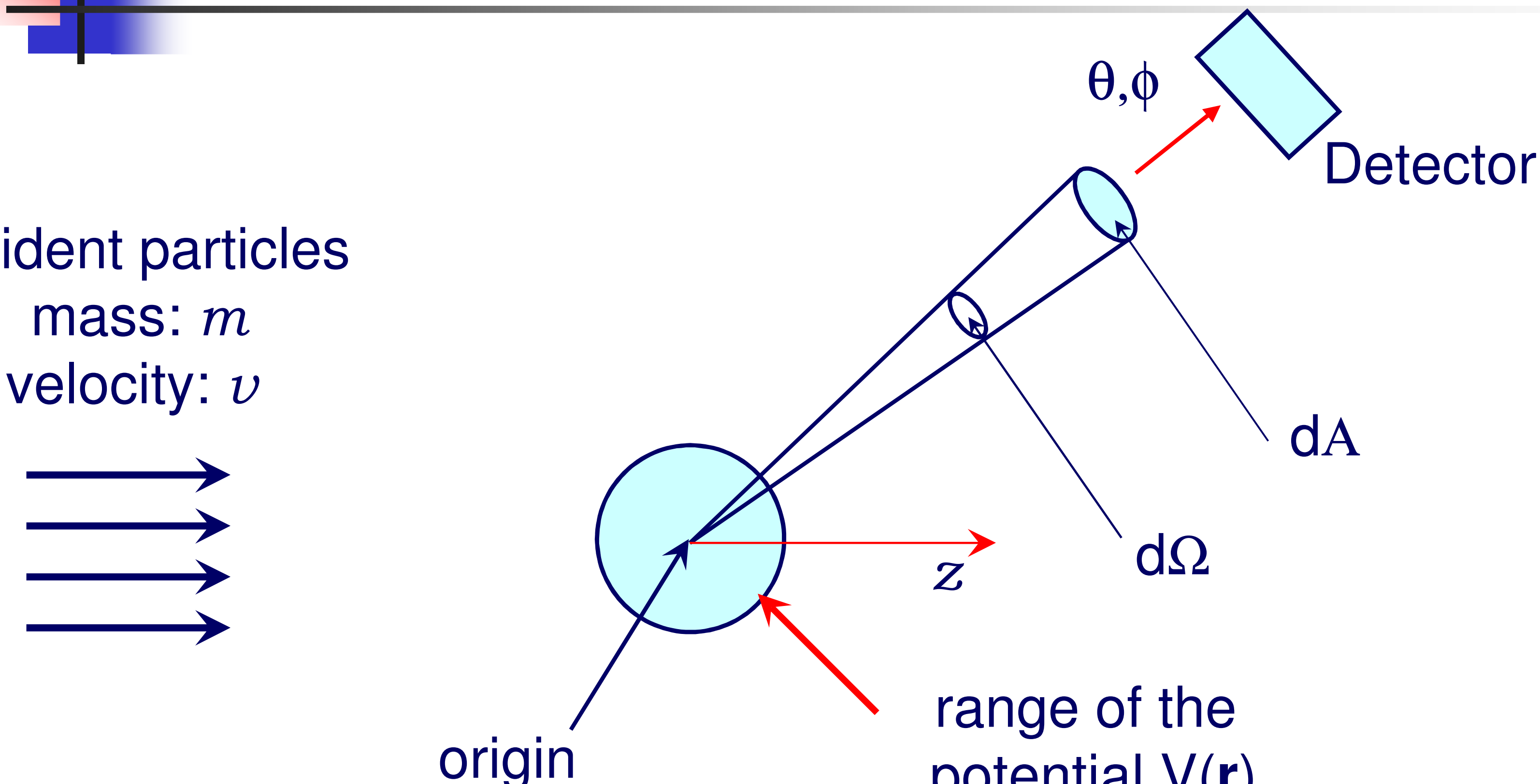
Solving scattering problems: examples.

Chapter 10, pages 378-393, Jasprit Singh, Quantum Mechanics

Chapter 13, pages 587-595, 608-620, Bransden & Joachain, Quantum Mechanics

Scattering: short-range potential

incident particles
mass: m
velocity: v



Problem: calculate the probability that the particle is scattered into a small solid angle dΩ in the direction θ,φ.

Differential cross section

Problem: calculate the probability that the particle is scattered into a small solid angle dΩ in the direction θ,φ.
How? By solving Schrödinger equation ... again.

This probability is expressed in terms of differential cross section

$$\frac{d\sigma}{d\Omega} = number\ of\ particles\ scattered\ per\ unit\ time\ into\ d\Omega\ in\ the\ direction\ \theta,\phi\ /\ F\ (flux\ of\ the\ incident\ particles)\ d\Omega$$

The total cross section

$$\sigma_{tot} = total\ number\ of\ particles\ scattered\ per\ second\ /\ F$$

is obtained as $\sigma_{tot} = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \frac{d\sigma}{d\Omega}$.

Note: the flux is a number of particles the unit time per unit area so the dimensions of both $\frac{d\sigma}{d\Omega}$ and σ_{tot} are those of the area.

Schrödinger equation … again

Case 1. Free particles: well outside the scattering potential range. Hamiltonian: H_0

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$E = \frac{1}{2}m\upsilon^2 = \frac{\hbar^2 k^2}{2m}$$

$$\left(\nabla^2 + k^2\right)\psi(\mathbf{r}) = 0$$

Case 2. In the presence of the scattering potential. Hamiltonian: $H=H_0+V$

$$\left(\nabla^2 + k^2\right)\psi(\mathbf{r}) = \underbrace{\left(\frac{2m}{\hbar^2}V(\mathbf{r})\right)}_{U(\mathbf{r})}\psi(\mathbf{r})$$

$$\left(\nabla^2 + k^2\right)\psi(\mathbf{r}) = U(\mathbf{r})\psi(\mathbf{r})$$

Wave function at large r & differential cross section

$$\psi(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\,\mathbf{k}\cdot\mathbf{r}} + \frac{f(\theta,\phi)}{r}e^{ikr}$$

Outgoing spherical wave

Incident beam of particles
(plane wave)

Note: potential must decrease faster than $1/r$ with $r\to\infty$.

f: scattering amplitude

Differential cross section is given by $\dfrac{d\sigma}{d\Omega} = \left| f(\theta,\phi) \right|^2$

$$k_{in} = k_{out} : \ \textit{elastic scattering}$$

How to calculate differential cross section?

1. Write the expression for the wave function $\psi(\mathbf{r})$.

2. Determine the asymptotic behavior of this wave function for $r \longrightarrow \infty$.

3. Compare it with $\psi(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\,\mathbf{k}\cdot\mathbf{r}} + \dfrac{f(\theta,\phi)}{r} e^{ikr}$.

4. Determine $f(\theta,\phi)$ from this comparison.

5. Calculate differential cross section using $\dfrac{d\sigma}{d\Omega} = \left| f(\theta,\phi) \right|^2$.

Note: this general procedure is used to derive formula for the differential cross section both using Born approximation and method of partial waves.

Green's function

The equation $\left(\nabla^2 + k^2\right)\psi(\mathbf{r}) = U(\mathbf{r})\psi(\mathbf{r})$ can be solved using Green's function method:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \int G(\mathbf{r},\mathbf{r}')\,U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\,\mathrm{d}\mathbf{r}',$$

where $\phi(\mathbf{r})$ is the solution of the free particle equation $\left(\nabla^2 + k^2\right)\phi(\mathbf{r}) = 0$

and $G(\mathbf{r},\mathbf{r}')$ is a Green's function corresponding to

$$\left(\nabla^2 + k^2\right)G(\mathbf{r},\mathbf{r}') = \delta\left(\mathbf{r}-\mathbf{r}'\right).$$

Since we want to obtain the solution which has an asymptotic form

$$\psi(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\,\mathbf{k}\cdot\mathbf{r}} + \frac{f(\theta,\phi)}{r}e^{ikr} \quad \Rightarrow \quad \phi(\mathbf{r}) = e^{i\,\mathbf{k}\cdot\mathbf{r}}.$$

Green's function

$$\psi_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \int G(\mathbf{r},\mathbf{r}')\, U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\, \mathrm{d}\mathbf{r}'$$

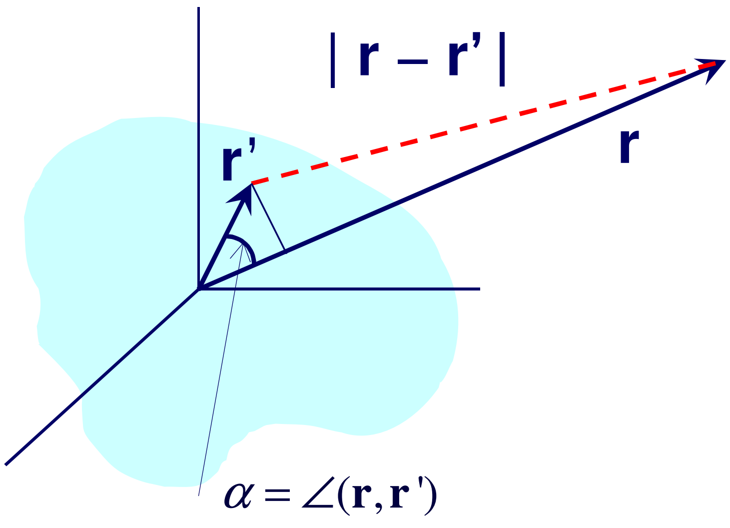
$$G(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$$

⇨ Note: see pages 609-613 of Bransden & Joachain QM book for derivation

$$\psi_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) - \frac{1}{4\pi}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\, \mathrm{d}\mathbf{r}'$$

Asymptotic behavior of ψ(r) $r \to \infty$

$r >> r'$



$$|\mathbf{r}-\mathbf{r}'| = \sqrt{r^2 + 2\mathbf{r}\cdot\mathbf{r}' + r'^2} \approx r - \hat{\mathbf{r}}\cdot\mathbf{r}'$$

$$|\mathbf{r}-\mathbf{r}'| \approx r - r'\cos(\mathbf{r},\mathbf{r}') = r - r'\cos\alpha$$

$$e^{ik|\mathbf{r}-\mathbf{r}'|} \approx e^{ik(r - r'\cos\alpha)} = e^{ikr}e^{-ikr'\cos\alpha}$$

$$= e^{ikr}e^{-i\mathbf{k}'\mathbf{r}'}$$

where $\mathbf{k}' = k\cos\alpha = k\hat{\mathbf{r}}$ points in the direction of the scattering particle

$$\psi_{\mathbf{k}}(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{1}{4\pi}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\,d\mathbf{r}'$$

$e^{ik|\mathbf{r}-\mathbf{r}'|} \to e^{ikr}e^{-i\mathbf{k}'\mathbf{r}'}$

$|\mathbf{r}-\mathbf{r}'| \to$ r

Differential cross-section

Matching

$$\psi_{\mathbf{k}}(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\,\mathbf{k}\cdot\mathbf{r}} - \frac{1}{4\pi}\int \frac{e^{ikr}e^{-i\,\mathbf{k}'\mathbf{r}'}}{r} U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

$$= e^{i\,\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r}\left\{-\frac{1}{4\pi}\int e^{-i\,\mathbf{k}'\mathbf{r}'} U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\,\mathrm{d}\mathbf{r}'\right\}$$

with

$$\psi(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\,\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} f(\theta,\phi)$$

we obtain

$$f(\theta,\phi) = -\frac{1}{4\pi}\int e^{-i\,\mathbf{k}'\mathbf{r}'} U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

Born approximation

$$f(\theta,\phi) = -\frac{1}{4\pi}\int e^{-i\,\mathbf{k}'\mathbf{r}'}U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\,\mathrm{d}\mathbf{r}' = -\frac{1}{4\pi}\left\langle \phi_{\mathbf{k}'}\middle|U\middle|\psi_{\mathbf{k}}\right\rangle$$

Main idea: use perturbation theory to approximate $\psi_{\mathbf{k}}(\mathbf{r})$.
The scattering wave function is expanded in powers of the interaction potential.

Born series:

$$\psi_{\mathbf{k}}^{(0)}(\mathbf{r}) = \phi_{\mathbf{k}}(r) = e^{i\,\mathbf{k}\cdot\mathbf{r}}$$

$$\psi_{\mathbf{k}}^{(1)}(\mathbf{r}) = \phi_{\mathbf{k}}(r) + \int G(\mathbf{r},\mathbf{r}')\,U(\mathbf{r}')\psi_{\mathbf{k}}^{(0)}(\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

$$\vdots$$

$$\psi_{\mathbf{k}}^{(1)}(\mathbf{r}) = \phi_{\mathbf{k}}(r) + \int G(\mathbf{r},\mathbf{r}')\,U(\mathbf{r}')\psi_{\mathbf{k}}^{(n-1)}(\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

Born approximation

$$\psi_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(r) + \int G(\mathbf{r},\mathbf{r}')\,U(\mathbf{r}')\phi_{\mathbf{k}}(\mathbf{r}')\,d\mathbf{r}'$$
$$+ \int G(\mathbf{r},\mathbf{r}')\,U(\mathbf{r}')G(\mathbf{r}',\mathbf{r}'')U(\mathbf{r}'')\phi_{\mathbf{k}}(\mathbf{r}'')\,d\mathbf{r}'d\mathbf{r}'' + \ldots$$

We substitute this expansion into the formula for the scattering amplitude

$$f(\theta,\phi) = -\frac{1}{4\pi}\langle \phi_{\mathbf{k}'} | U | \psi_{\mathbf{k}} \rangle$$

$$f(\theta,\phi) = -\frac{1}{4\pi}\langle \phi_{\mathbf{k}'} | U + UGU + UGUGU + \ldots | \phi_{\mathbf{k}} \rangle$$

First term of this series is (first) Born approximation to the scattering amplitude:

$$f^{B}(\theta,\phi) = -\frac{1}{4\pi}\langle \phi_{\mathbf{k}'} | U | \phi_{\mathbf{k}} \rangle$$

Born approximation: just some transformations

$$f^{B}(\theta,\phi) = -\frac{1}{4\pi}\langle \phi_{\mathbf{k}'} | U | \phi_{\mathbf{k}} \rangle = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int e^{-i\,\mathbf{k}'\mathbf{r}'}\,V(\mathbf{r}')\,e^{i\,\mathbf{k}\cdot\mathbf{r}'}\mathrm{d}\mathbf{r}'$$

$$= -\frac{m}{2\pi\hbar^2}\int e^{i\,(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'}\,V(\mathbf{r}')\,\mathrm{d}\mathbf{r}' = -\frac{m}{2\pi\hbar^2}\int e^{i\,\mathbf{q}\cdot\mathbf{r}'}\,V(\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

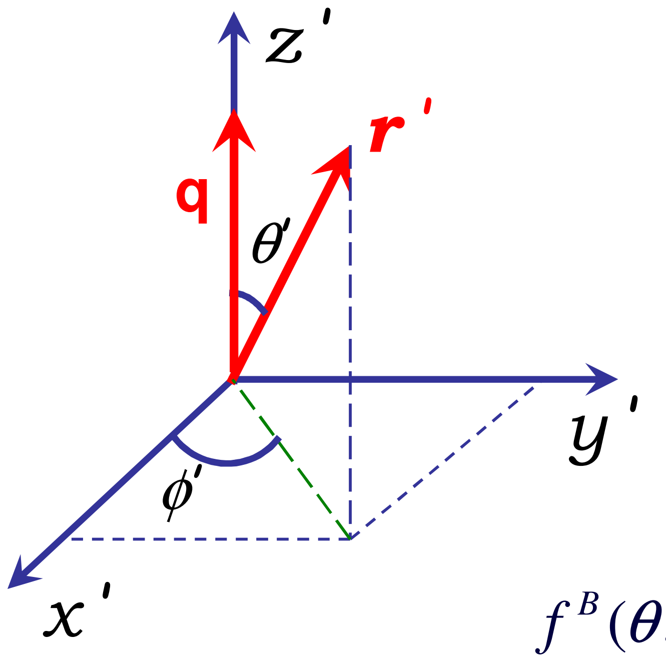
$$\mathbf{q} = \mathbf{k} - \mathbf{k}'$$

$$(\mathbf{k} - \mathbf{k}')^2 = k^2 + (k')^2 - 2kk'\cos(\mathbf{k},\mathbf{k}') \qquad \theta = \angle(\mathbf{k},\mathbf{k}')$$

$$= 2k^2(1-\cos\theta)$$

$$q = 2k\sin\frac{\theta}{2}$$

Born approximation: central potentials V(r)



$$f^B(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int e^{i\,\mathbf{q}\cdot\mathbf{r}'}\,V(r')\,\mathrm{d}\mathbf{r}'$$

In the case of central potential V(r) we can integrate over θ′ and φ′.
We choose axis *z*′ to be in the direction of **q.**

$$\mathbf{q} = \mathbf{k} - \mathbf{k}'$$

$$q = 2k\sin\frac{\theta}{2}$$

$$\theta = \angle(\mathbf{k},\mathbf{k}')$$

$$f^B(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int_0^\infty dr'(r')^2\int_0^{2\pi} d\phi'\int_0^\pi \sin\theta'\,e^{i\,q\cdot r'\cos\theta'}\,V(r')$$

$$= -\frac{m}{\hbar^2}\int_0^\infty dr'(r')^2\int_{-1}^{1}\mathrm{du}\,e^{i\,q\cdot r' u} = -\frac{m}{\hbar^2}\int_0^\infty dr'(r')^2 V(r')\frac{2\sin(qr')}{qr'}$$

$$= -\frac{2m}{q\hbar^2}\int_0^\infty dr\,r\,V(r)\sin(qr)$$

$$u = \cos\theta'$$

Born approximation: central potential V(r)
How to solve problems: Example 1

Problem: elastic nucleon scattering from heavy nucleus can be represented by a potential

$$V(r) = \begin{cases} -V_0 & r < R \\ 0 & r > R \end{cases} \qquad V_0 > 0$$

Calculate the differential cross section in the lowest order in V.

Solution:

$$f^B(\theta,\phi) = -\frac{2m}{q\hbar^2}\int_0^\infty dr\, r\, V(r)\sin(qr)$$

$$\frac{d\sigma}{d\Omega} = \left|f^B(\theta,\phi)\right|^2$$

$$f^B(\theta,\phi) = V_0\frac{2\mu}{q\hbar^2}\int_0^R dr\, r\ \sin(qr) = V_0\frac{2\mu}{q\hbar^2}\left\{\frac{1}{q^2}\left[\sin(qR) - qR\cos(qR)\right]\right\}$$

$$\frac{d\sigma}{d\Omega} = \frac{4\mu^2 V_0^2}{q^6\hbar^4}\left[\sin(qR) - qR\cos(qR)\right]^2 \qquad q = 2k\sin\frac{\theta}{2}$$

μ : reduced mass

Born approximation: central potential V(r) How to solve problems: Example 2

Problem: a particle of mass m is scattered by a potential

$$V(r) = V_0 e^{-r/a} \qquad a > 0$$

1. Calculate the differential cross section in the lowest order in V.
2. Calculate the total cross section.
3. Define the criteria for the validity of Born approximation

Solution: 1. $f^B(\theta,\phi) = -\frac{2m}{q\hbar^2}\int_0^\infty dr\, r\, \{V_0 e^{-r/a}\}\sin(qr)$

```
> assume(a>0);
> Q:=simplify(int(r*exp(-r/a)*sin(q*r),r=0...infinity));
```

$$Q := \frac{2\, q\, a\sim^3}{(1+q^2 a\sim^2)^2}$$

```
> DQ:=((2*m*V/(q*h^2))*Q)^2;
```

$$DQ := \frac{16\, m^2\, V^2\, a\sim^6}{h^4\,(1+q^2 a\sim^2)^4}$$

$$\frac{d\sigma}{d\Omega} = [DQ] = \frac{16\, m^2 V_0^2 a^6}{\hbar^2 \left(1+q^2a^2\right)^4}$$

Born approximation: central potentials V(r)
How to solve problems: Example 2

Solution: 2. The total cross-section is given by the integral

$$\sigma_{tot} = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \frac{d\sigma}{d\Omega} = \frac{16\, m^2 V_0^2 a^6}{\hbar^2} 2\pi \int_0^{\pi} d\theta \sin\theta \left(1 + 4k^2 a^2 \sin(\theta/2)\right)^{-4}$$

$$q = 2k \sin\frac{\theta}{2}$$

```
> q:=2*k*sin(theta/2);
> DQ;
> R:=2*Pi*int(DQ*sin(theta),theta=0...Pi);
> factor(R);
```

$$\sigma_{tot} = \frac{64\,\pi\, m^2 V^2 a\sim^6 (3 + 12\,k^2 a\sim^2 + 16\,k^4 a\sim^4)}{3\,h^4 (1 + 4\,k^2 a\sim^2)^3}$$

Validity of the Born approximation

This method is based on treating the scattering potential as a perturbation.

Therefore, for this approach to be valid, the correction to the wave function which is introduced by a potential (our first order correction $\Delta\psi_{\mathbf{k}}^{(1)}(\mathbf{r})$) must be small in comparison to the wave function in the absence of the potential (in our case $\psi_{\mathbf{k}}^{(0)}(\mathbf{r})$).

Using this statement as a guide we use the following criteria for the validity of the Born approximation:

$$\left|\frac{\Delta\psi_{\mathbf{k}}^{(1)}(0)}{\psi_{\mathbf{k}}^{(0)}(0)}\right| << 1$$

Validity of the Born approximation

We need to evaluate this expression: $\left|\dfrac{\Delta\psi_{\mathbf{k}}^{(1)}(0)}{\psi_{\mathbf{k}}^{(0)}(0)}\right| << 1$

$$\psi_{\mathbf{k}}^{(0)}(\mathbf{r}) = e^{i\,\mathbf{k}\cdot\mathbf{r}} \quad \rightarrow \psi_{\mathbf{k}}^{(0)}(0) = 1$$

$$\Delta\psi_{\mathbf{k}}^{(1)}(\mathbf{r}) = -\frac{1}{4\pi}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

$$\Delta\psi_{\mathbf{k}}^{(1)}(0) = -\frac{1}{4\pi}\int \frac{e^{ikr'}}{r'} U(\mathbf{r}')\,e^{i\mathbf{k}\cdot\mathbf{r}'}\,\mathrm{d}\mathbf{r}'$$

$$\left|\frac{\Delta\psi_{\mathbf{k}}^{(1)}(0)}{\psi_{\mathbf{k}}^{(0)}(0)}\right| = \left|\frac{m}{2\pi\hbar^2}\int \frac{e^{ikr'}}{r'} V(\mathbf{r}')\,e^{i\mathbf{k}\cdot\mathbf{r}'}\,\mathrm{d}\mathbf{r}'\right| << 1$$

Validity of the Born approximation: central potential

$$\left|\frac{\Delta\psi_{\mathbf{k}}^{(1)}(0)}{\psi_{\mathbf{k}}^{(0)}(0)}\right| = \left|\frac{m}{2\pi\hbar^2}\int \frac{e^{ikr'}}{r'}V(\mathbf{r}')\, e^{i\mathbf{k}\cdot\mathbf{r}'}\, \mathrm{d}\mathbf{r}'\right| << 1$$

Now we consider this condition for the case of the central potential

$$\frac{m}{2\pi\hbar^2}\int \frac{e^{ikr'}}{r'}V(r')\, e^{i\mathbf{k}\cdot\mathbf{r}'}\, \mathrm{d}\mathbf{r}' = \frac{m}{2\pi\hbar^2}\int_0^\infty dr'(r')^2\int_0^{2\pi} d\phi'\int_0^\pi d\theta' \sin\theta' \frac{e^{ikr'}}{r'}V(r')\, e^{ikr'\cos\theta'}$$

$$= \frac{m}{\hbar^2}\int_0^\infty dr'(r')^2\frac{e^{ikr'}}{r'}V(r')\frac{2\sin(kr')}{kr'} = \frac{2m}{k\hbar^2}\int_0^\infty dr'\, e^{ikr'}V(r')\sin(kr')$$

Validity of the Born approximation condition for the central potential

$$\left|\frac{2m}{k\hbar^2}\int_0^\infty dr\, e^{ikr}V(r)\sin(kr)\right| << 1$$

Validity of the Born approximation
How to solve problems: back to Example 2

Problem: a particle of mass m is scattered by a potential

$$V(r) = V_0 e^{-r/a} \qquad a > 0$$

3. Define the criteria for the validity of the Born approximation

Solution: 3.

$$\left| \frac{2mV_0}{k\hbar^2} \int_0^\infty dr\, e^{ikr} e^{-r/a} \sin(kr) \right| << 1$$

```
> assume(k>0);
> assume(a>0);
> (2*m*V/(k*h^2))*abs(int(exp(I*k*r)*exp(-r/a)*sin(k*r),r=0...infinity));
```

$$\frac{2\, m\, V\, a\sim^2}{h^2 \sqrt{1 + 4\, k\sim^2\, a\sim^2}}$$

$$\frac{2m|V_0|a^2}{\hbar^2\sqrt{1+4k^2a^2}} << 1$$

Validity of the Born approximation
How to solve problems: back to Example 2

$$\frac{2m|V_0|a^2}{\hbar^2\sqrt{1+4k^2a^2}} << 1$$

1. Low k limit (slow particles) $ka << 1 \rightarrow \quad |V_0| << \dfrac{\hbar^2}{2ma^2}$

2. High k limit (fast particles) $ka >> 1 \rightarrow \quad |V_0| << \dfrac{\hbar^2 k}{ma}$

Note that the validity of the Born approximation is considerably extended in this case as $|V_0| << \dfrac{\hbar^2 (ka)}{ma^2}$ and $ka >> 1$

$(\textit{compare with the other condition})$

Validity of the Born approximation

General condition: $|\Delta\psi^{(1)}| << |\psi^{(0)}|$

The results derived above may also be obtained for an arbitrary potential if we take the $|V_0|$ to be the average value of the potential and a to be the range over which the potential is significant.

Case 1. Potential is sufficiently weak or sufficiently localized (or the particle speed is slow enough). $e^{ik|\mathbf{r}-\mathbf{r}'|} \approx 1$

$$|\Delta\psi^{(1)}| \le \frac{m}{2\pi\hbar^2}\int \frac{|V(\mathbf{r}')|}{|\mathbf{r}-\mathbf{r}'|} |\psi^{(0)}(\mathbf{r}')| \mathrm{d}\mathbf{r}' \approx \frac{m}{2\pi\hbar^2}|V_0||\psi^{(0)}| 4\pi\frac{a^2}{2} = \frac{m}{\hbar^2}|V_0||\psi^{(0)}| a^2$$

$$\left|\frac{\Delta\psi^{(1)}}{\psi^{(0)}}\right| \approx \frac{m}{\hbar^2}|V_0| a^2 << 1 \rightarrow \qquad |V_0| << \frac{\hbar^2}{ma^2}$$

Case 2. Fast particles $ka >> 1$ $\qquad |V_0| << \frac{\hbar^2 k}{ma} = \frac{\hbar \upsilon}{m}$.