Born approximation in time-independent description

In this approach, the central problem is to solve

$$\left(\nabla^2 + k^2\right)\psi_{\vec{k}} = \frac{2\mu}{\hbar^2} V \psi_{\vec{k}}$$

for the full Hamiltonian with boundary conditions such that $\psi_{\vec{k}}$ takes the form

$$\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \psi_{sc}(\vec{r}), \quad \psi_{sc}(\vec{r}) \xrightarrow[r\to\infty]{} f(\vartheta,\varphi)\frac{e^{ikr}}{r}$$

(ϑ, φ measured relative to $\vec{k} \parallel \vec{e}_z$.)

We solve this as we solve the Helmholtz equation in electrodynamics: First solve the equation for a point source to get the Green function $G^0(\vec{r},\vec{r}\,')$

$$\left(\nabla^2 + k^2\right) G^0(\vec{r},\vec{r}\,') = \delta(\vec{r}-\vec{r}\,')$$

then get the full soln. by superposition of point sources:

$$\psi_{\vec{k}}(\vec{r}) = \psi^0(\vec{r}) + \frac{2\mu}{\hbar^2}\int d^3r'\, G^0(\vec{r},\vec{r}\,')\, V(\vec{r}\,')\, \psi_k(\vec{r}\,')$$

where $\psi^0(\vec{r})$ is a solution of the homogeneous eq.

$$\left(\nabla^2 + k^2\right)\psi^0 = 0$$

chosen such that ψ_k has the correct boundary conditions.

Of course, this solution is not explicit, but in the form of an integral equation. We solve it again iteratively, generating a perturbative series.

If we turn off the potential (zeroth order in V), $\psi_{sc} \equiv 0$, i.e. $\psi_k(\vec{r}) = \psi^0(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}$

This fixes ψ^0, and we have to solve for $V \neq 0$

$$\boxed{\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \frac{2\mu}{\hbar^2}\int d^3r'\, G^0(\vec{r},\vec{r}\,')\, V(\vec{r}\,')\, \psi_k(\vec{r}\,')}$$

At first order in V, we get

$$\psi^{(1)}_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}\,'} + \frac{2\mu}{\hbar^2}\int d^3r'\, G^0(\vec{r},\vec{r}\,')\, V(\vec{r}\,')\, e^{i\vec{k}\cdot\vec{r}\,'}$$

Reinserting this we get symbolically

$$\psi^{(2)}_k = \psi^0 + \frac{2\mu}{\hbar^2} G^0 V \psi^0 + \left(\frac{2\mu}{\hbar^2}\right)^2 G^0 V G^0 V \psi^0$$

etc. etc.

From electrodynamics we know the Green function for the Helmholtz equation:

$$G^0(\vec{r},\vec{r}\,') = G^0(\vec{r}-\vec{r}\,') = \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{4\pi\,|\vec{r}-\vec{r}\,'|}$$

$$\Rightarrow \boxed{\begin{aligned}\psi_{\vec{k}}(\vec{r}) &= e^{i\vec{k}\cdot\vec{r}} - \frac{2\mu}{4\pi\hbar^2}\int d^3\vec{r}\,'\ \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}V(\vec{r}\,')\,\psi_{\vec{k}}(\vec{r}\,') \\ &= e^{i\vec{k}\cdot\vec{r}} + \psi_{sc}(\vec{r})\end{aligned}}$$

Does this have the correct asymptotic form as $r \to \infty$?

$$\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} \xrightarrow[r\to\infty]{} \frac{e^{ikr}}{r}\left(1 + O\left(\frac{r'}{r}\right)\right)$$

Since the r' integral receives contribution only from the region $r' \lesssim r_0$ where $V(r')$ is significant, we are inclined to drop the $O(r'/r)$ terms. But then all dependence on ϑ, φ (the direction of $\vec{k}_f$) vanishes. So this must be wrong. Let's see whether we can find out what went wrong by keeping the next terms. We need for the denominator

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

$$\approx r\left(1 - \frac{\vec{r}\cdot\vec{r}\,'}{r^2} + O\left(\left(\frac{r'}{r}\right)^2\right)\right)$$

$$\Rightarrow \frac{1}{|\vec{r}-\vec{r}\,'|} \approx \frac{1}{r}\left(1 + \frac{\vec{r}\cdot\vec{r}\,'}{r^2}\right) \xrightarrow[r\to\infty]{} \frac{1}{r}$$

For the numerator we get similarly

$$k|\vec{r}-\vec{r}'| \approx kr\left(1-\frac{\vec{r}\cdot\vec{r}'}{r^2}\right) = kr - k\vec{e}_r\cdot\vec{r}'$$
$$= kr - \vec{k}_f\cdot\vec{r}'$$

But since this is in the exponent, the second term does not become small in magnitude compared to the first one – it add just a (more slowly varying) phase.

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

We need this phase to obtain the (ϑ,φ)-dependence of the scattering amplitude.

Plugging this in we find

$$\psi_{\vec{k}}(\vec{r}) \xrightarrow[r\to\infty]{} e^{i\vec{k}\cdot\vec{r}} - \frac{e^{ikr}}{r} \underbrace{\frac{2\mu}{4\pi\hbar^2}\int d^3r'\, e^{-i\vec{k}_f\cdot\vec{r}'} V(\vec{r}')\psi_{\vec{k}}(\vec{r}')}_{-f(\vartheta,\varphi)}$$

This is still an integral equation.

Solving it iteratively we find

$$\psi^{(0)}_{\vec{k}}(\vec{r}) \xrightarrow[r\to\infty]{} e^{i\vec{k}_i\cdot\vec{r}} \qquad \text{(we wrote } \vec{k}\to\vec{k}_i \text{ for clarity)}$$

$$\psi^{(1)}_{\vec{k}}(\vec{r}) \xrightarrow[r\to\infty]{} e^{i\vec{k}_i\cdot\vec{r}} + \frac{e^{ikr}}{r}\underbrace{\left(-\frac{2\mu}{4\hbar^2\pi}\int d^3r'\, e^{-i\vec{k}_f\cdot\vec{r}'} V(\vec{r}') e^{i\vec{k}_i\cdot\vec{r}'}\right)}_{f^{(1)}(\vartheta,\varphi)}$$

$$\Rightarrow \boxed{f^{(1)}(\vartheta,\varphi) = -\frac{\mu}{2\pi\hbar^2}\int d^3r'\, e^{-i\vec{q}\cdot\vec{r}'} V(\vec{r}')} \qquad (\vec{q}=\vec{k}_f-\vec{k}_i)$$

as before ✓

Here the phase factor -1 is a result of the calculation and need not be assumed.

Validity of the Born approximation

We obtained the Born approximation by replacing under the integral

$$\psi_{\vec{k}} = e^{i\vec{k}\cdot\vec{r}'} + \psi_{sc}(\vec{r}') \longmapsto e^{i\vec{k}\cdot\vec{r}'}$$

$\Rightarrow$ Need $|\psi_{sc}| \ll e^{i\vec{k}\cdot\vec{r}'}$ where it matters,

i.e. in the region $|\vec{r}'| \lesssim r_0$. Let us analyze this near $|\vec{r}'| = 0$, assuming that the potential is largest there:

$$\frac{|\psi_{sc}(0)|}{|e^{i\vec{k}\cdot\vec{0}}|} = |\psi_{sc}(0)| = \left| \frac{2\mu}{4\pi\hbar^2} \int d^3r' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') e^{-i\vec{k}_i\cdot\vec{r}'} \right|_{\vec{r}=0}$$

assume $V(\vec{r}) = V(r)$

$$= \left| \frac{2\mu}{\hbar^2 k} \int e^{ikr'} \sin(kr') V(r')\, dr' \right| \overset{!}{\ll} 1$$

- At low energies $kr' \to 0$, $e^{ikr'} \to 1$, $\sin(kr') \to kr'$ this requires

$$\frac{2\mu}{\hbar^2} \left| \int_0^\infty r' V(r')\, dr' \right| \ll 1$$

If $V(r)$ has range r_0 and effective depth V_0

$$\Rightarrow \frac{\mu V_0 r_0^2}{\hbar^2} \ll 1 \Rightarrow \boxed{V_0 \ll \frac{\hbar^2}{\mu r_0^2}}$$

If $V(r)$ had a bound state, its size would be $\lesssim r_0$, its momentum $p \gtrsim \frac{\hbar}{r_0}$, and its kinetic energy $\gtrsim \frac{\hbar^2}{\mu r_0^2}$. The condition $V_0 \ll \frac{\hbar^2}{\mu r_0^2}$ says that no such bound state can exist (its kinetic energy would always overwhelm the potential energy).

$\Rightarrow$ for Born to work at low energies, potential must be too shallow to bind a particle to a region $\lesssim r_0$.

- At high energies, $kr_0 \gg 1$

$$e^{ikr'} \sin kr' = \frac{e^{2ikr'} - 1}{2i}$$

The exponential oscillates rapidly and averages to zero:

$$\Rightarrow \left| \frac{2\mu}{\hbar^2 k} \int_0^\infty \frac{-1}{2i} V(r')\,dr' \right| \ll 1$$

$$\Rightarrow \boxed{\frac{\mu V_0 r_0^2}{\hbar^2} \ll k r_0}$$

So if the Born approx. is valid at low energies, $V_0 \ll \frac{\hbar^2}{\mu r_0^2}$, then it is automatically valid at all energies.

The Helmholtz propagator from Cauchy's theorem:

Fourier transform the eq. $(\nabla^2+k^2)G^0(\vec{r}) = \delta(\vec{r})$:

$$\frac{1}{(2\pi)^{3/2}}\int d^3r\, e^{-i\vec{q}\cdot\vec{r}}(\nabla^2+k^2)\,G^0(\vec{r}) = \frac{1}{(2\pi)^{3/2}}$$

Integrate twice by parts, assuming $G^0(r) \xrightarrow[r\to\infty]{} 0$:

$$(k^2-q^2)\int\frac{d^3r}{(2\pi)^{3/2}}\,e^{-i\vec{q}\cdot\vec{r}}\,G^0(\vec{r}) = (k^2-q^2)\,G^0(\vec{q}) = \frac{1}{(2\pi)^{3/2}}$$

$$\Rightarrow G^0(\vec{q}) = \frac{1}{(2\pi)^{3/2}(k^2-q^2)}$$

This diverges at $k=q$! The reason is that

$$(\nabla^2+k^2)\psi = 0$$

has non-vanishing solutions (plane waves), called "zero modes", so (∇^2+k^2) is not invertible (it has zero eigenvalues):

$$\Rightarrow (\hat{D}^2+k^2)\,\hat{G}^0 = \hat{\mathbb{1}} \text{ has no solution } \hat{G}^0.$$

Let's therefore consider a slightly different operator,

$$\hat{D}^2+k^2+i\varepsilon \qquad (\varepsilon>0,\ \varepsilon\to 0^+)$$

Its zero eigenvalues correspond to complex k, so the corresponding eigenfunctions are not normalizable to δ-functions (the norm diverges exponentially). So within the Hilbert space of normalizable states $\hat{D}^2+k^2+i\varepsilon$ is invertible:

$$G^0_\varepsilon(\vec{q}) = \frac{1}{(2\pi)^{3/2}} \frac{1}{k^2 - q^2 + i\varepsilon}$$

Its Fourier transform is the Green function $G^0_\varepsilon(\vec{r})$.

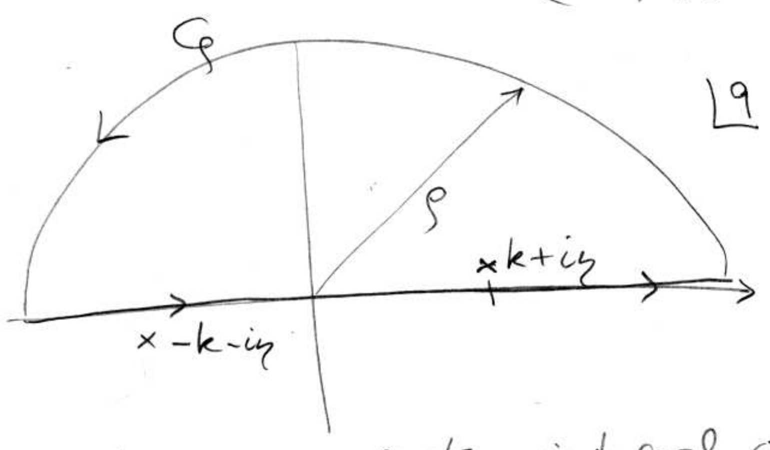
$$G^0_\varepsilon(\vec{r}) = \frac{1}{(2\pi)^3} \int d^3q \, \frac{e^{i\vec{q}\cdot\vec{r}}}{k^2 + i\varepsilon - q^2}$$

$$= \frac{1}{4\pi^2} \int_0^\infty q^2 dq \int_{-1}^{1} d\cos\vartheta \, \frac{e^{iqr\cos\vartheta}}{k^2 + i\varepsilon - q^2}$$

$$= \frac{1}{4\pi^2} \int_0^\infty q^2 dq \, \frac{1}{k^2 + i\varepsilon - q^2} \, \frac{e^{iqr} - e^{-iqr}}{iqr}$$

$$= \frac{1}{4\pi} \int_{-\infty}^{\infty} \frac{q^2 dq}{k^2 + i\varepsilon - q^2} \, \frac{e^{iqr}}{iqr}$$

$$= \frac{-i}{4\pi^2 r} \int_{-\infty}^{\infty} \frac{e^{iqr} q \, dq}{(k + q + i\eta)(k - q + i\eta)} \qquad \left(\eta = \frac{\varepsilon}{2k} \to 0^+\right)$$



We need only the integral over real q. But we can add to this the integral over the semicircle C_ρ,

$$\lim_{\rho\to\infty} \int_{C_\rho} e^{iqr} \underbrace{\frac{dq}{q}}_{i\,d\varphi} = i\int_0^\pi d\varphi \, e^{iq\rho(\cos\varphi + i\sin\varphi)} \qquad q = \rho e^{i\varphi} \quad dq = \rho e^{i\varphi} i \, d\varphi$$

$$= \lim_{\rho\to\infty} i \int_0^\pi d\varphi \, e^{iq\rho\cos\varphi} \underbrace{e^{-q\rho\sin\vartheta}}_{\text{vanishes exponentially}} = 0$$

So the semicircle, in the limit $\rho \to \infty$, adds nothing to the integral, making the desired integral $\int_{-\infty}^{\infty} dq$ identical to the closed-contour integral shown in the sketch, which we can evaluate with the residue theorem:

$$G^{\circ}_{\eta}(\vec{r}) = -\frac{i}{4\pi^2 r}\left(2\pi i\right)\frac{e^{ir(k+i\eta)}\,(k+i\eta)}{2\,(k+i\eta)}$$

In the limit $\eta \to 0+$ we get

$$\boxed{G^{\circ}(\vec{r}) = -\frac{e^{ikr}}{4\pi r}}\,.$$

This has the correct behavior at large r (outgoing spherical wave). The reason is that we ensured this by judiciously moving the pole of $G_{\eta}(\vec{q})$ at $q = k + i\eta$ into the upper plane and the one at $q = -k - i\eta$ into the lower half plane. Other pole prescriptions are possible, but lead to different asymptotic behavior (i.e. correspond to different boundary conditions).

$\Rightarrow$ The $i\varepsilon$-prescription fixes the boundary conditions.

Partial wave expansion

For $V(\vec{r}) = V(r)$, $f(\vartheta,\varphi)$ depends only on the angle ϑ and the incoming wave number k, i.e. the energy $E = \frac{\hbar^2 k^2}{2\mu}$ of the projectile at $t=-\infty$:

Let us expand

$$\boxed{f(\vartheta, k) = \sum_{l=0}^{\infty} (2l+1)\, a_l(k)\, P_l(\cos\vartheta)}$$

"partial wave expansion"

$a_l(k) = l^{th}$ partial wave amplitude

Use

$$e^{ikz} = e^{ikr\cos\vartheta} = \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(kr)\, P_l(\cos\vartheta)$$

Since the potential is spherically symmetric $\sim Y_{00}$, it carries no angular momentum (it conserves angular momentum, or $\hat{L}^2$ commutes with it), each partial wave scatters independently.

The amplitude l is a measure of scattering in the angular momentum l sector.

If we have a uniform beam and consider particles with impact parameter between ρ and $\rho+d\rho$, they have angular momentum

$$l\hbar \approx p\rho = \hbar k \rho$$

If the potential has range r_0, only particles with $\rho \lesssim r_0$ will be scattered

$$\Rightarrow l \lesssim l_{max} = k r_0$$

So we expect that, for low energies $k \to 0$, we need to consider only a few low-order partial waves.

How do we compute the $a_l(k)$ from the potential?

Consider the solution to the Schrödinger eq. for angular momentum l. The incoming free particle wave can be written $\left(j_l(kr) \xrightarrow[r\to\infty]{} \dfrac{\sin(kr - \frac{l\pi}{2})}{kr} \right)$

$$e^{ikz} \xrightarrow[r\to\infty]{} \frac{1}{2ik} \sum_{l=0}^{\infty} i^l (2l+1) \left(\frac{e^{i(kr - \frac{l\pi}{2})}}{r} - \frac{e^{-i(kr - \frac{l\pi}{2})}}{r} \right) P_l(\cos\theta)$$

$(i = e^{i\pi/2})$
$$= \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \left(\frac{e^{ikr}}{r} - \frac{e^{-i(kr - l\pi)}}{r} \right) P_l(\cos\theta)$$

outgoing   incoming wave of same amplitude

$\Rightarrow$ no net probability flux into the origin $r=0$, for each l.

When we turn on the potential, and go to $r\to\infty$, the radial wavefunction must go again to a free wave function, but with a phase shift $\delta_l(k)$ from the potential:

$$R_\ell(r) = \frac{u_\ell(r)}{r} \xrightarrow[r\to\infty]{} A_\ell \frac{\sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell(k)\right)}{r}$$

$$\Rightarrow \psi_{\vec{k}}(\vec{r}) \xrightarrow[r\to\infty]{} \sum_{\ell=0}^{\infty} A_\ell \frac{e^{i(kr - \frac{\ell\pi}{2} + \delta_\ell)} - e^{-i(kr - \frac{\ell\pi}{2} + \delta_\ell)}}{r} P_\ell(\cos\vartheta)$$

Since $V(r)$ produces only an outgoing wave, the incoming part of $\psi_{\vec{k}}(r)$ must come from the e^{ikz} part of $\psi_{\vec{k}}^{\circ}$: $\Rightarrow A_\ell = \frac{2\ell+1}{2ik} e^{i(\frac{\ell\pi}{2} + \delta_\ell)}$

$$\Rightarrow \psi_{\vec{k}}(\vec{r}) \xrightarrow[r\to\infty]{} \frac{1}{2ikr} \sum_{\ell=0}^{\infty} (2\ell+1)\left[e^{ikr} e^{2i\delta_\ell} - e^{-i(kr - \ell\pi)}\right] P_\ell(\cos\vartheta)$$

$$= e^{ikz} + \Bigg[\underbrace{\sum_{\ell=0}^{\infty} (2\ell+1) \frac{e^{2i\delta_\ell} - 1}{2ik} P_\ell(\cos\vartheta)}_{f(\vartheta, k)}\Bigg] \frac{e^{ikr}}{r}$$

$$\Rightarrow \boxed{a_\ell(k) = \frac{e^{2i\delta_\ell} - 1}{2ik}} \equiv \frac{S_\ell(k) - 1}{2ik}$$

To get $a_\ell(k)$, we need to find the asymptotic phase shifts δ_ℓ in the scattered partial wave ℓ.

$S_\ell(k) = e^{2i\delta_\ell(k)}$ = partial wave S matrix element.

Since V conserves ℓ, $\hat{S}$ is diagonal in the partial wave basis

Rewrite $\frac{e^{2i\delta_\ell}-1}{2ik} = \frac{e^{i\delta_\ell}\sin\delta_\ell}{k}$

$$\Rightarrow \boxed{f(\vartheta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\, e^{i\delta_\ell}\sin\delta_\ell\, P_\ell(\cos\vartheta)} \quad (*)$$

Total cross section

$$\sigma = \int d\Omega\, |f(\vartheta,\varphi)|^2$$

$$= \boxed{\frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell} \quad (**) \qquad \left(\int_{-1}^{1} P_\ell P_{\ell'}\, d\cos\vartheta = \frac{2}{2\ell+1}\delta_{\ell\ell'}\right)$$

$$= \sum_{\ell=0}^{\infty}\sigma_\ell$$

$$\boxed{\sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_\ell \quad \text{total cross section in partial wave } \ell}$$

Each σ_ℓ is bounded by its unitarity limit

$$\boxed{\sigma_\ell < \sigma_\ell^{max} = \frac{4\pi}{k^2}(2\ell+1)}$$

To saturate the unitarity bound, the phase shift must be $\boxed{\delta_\ell = \frac{n\pi}{2},\ n \text{ odd}}$

Comparing $(*)$ with $(**)$ and using $P_\ell(1)=1$ at $\vartheta=0$, we find

$$\boxed{\sigma = \frac{4\pi}{k}\operatorname{Im} f(0)}$$

"Optical theorem"
(extinction at $\vartheta=0$ $\leftrightarrow$ scattering into $\vartheta \neq 0$)