Helmholtz Green's Function

For QM scattering, we have:

$$\psi = A\left[\underset{\substack{\uparrow\\ \text{incident}\\ \text{"beam"}}}{e^{ikz}} + \underset{\substack{\uparrow\\ \text{scattered}\\ \text{"free particle"}}}{f(\theta)\frac{e^{ikr}}{r}}\right]$$

& conservation of probability gives:

$$d\sigma = \underbrace{|f(\theta)|^2}_{=D(\theta)\ \text{diff cross-section}} d\Omega$$

We want to find $f(\theta)$ using Schrödinger's eqn.:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi = E\psi$$

which we rewrote as:

$$\nabla^2\psi + k^2\psi = s \quad \text{for } k^2 = \frac{2mE}{\hbar^2} \text{ \& "source"}$$

function $s = \frac{2m}{\hbar^2}U\psi$ ...

If you had the Green's function $G(\vec{r},\vec{r}\,')$ solving

$$\nabla^2 G(\vec{r},\vec{r}\,') + k^2 G(\vec{r},\vec{r}\,') = \delta^3(\vec{r}-\vec{r}\,'), \quad \text{then}$$

$$\psi(\vec{r}) = \int_{\substack{\text{all}\\ \text{space}}} G(\vec{r},\vec{r}\,')\, s(\vec{r}\,')\, d\tau'$$

solves: $$\nabla^2\psi + k^2\psi = \int_{\substack{\text{all}\\ \text{space}}} \underbrace{(\nabla^2+k^2)G(\vec{r},\vec{r}\,')}_{=\delta^3(\vec{r}-\vec{r}\,')} s(\vec{r}\,')\,d\tau' = s(\vec{r})\ \checkmark$$

1. set $\vec{r}\,'=0$, & assume spherical symmetry: $G(\vec{r},0) = G(r)$

2. solve: $(\nabla^2+k^2)G(r) = \delta^3(\vec{r})$ at points away from $\vec{r}=0$:

$$\frac{1}{r}(rG)'' + k^2 G = 0 \Rightarrow (rG)'' = -k^2(rG), \text{ so}$$

$$rG = Ae^{\pm ikr} \Rightarrow G = \frac{Ae^{\pm ikr}}{r}$$

3. "Normalize" to the δ source - int. $(\nabla^2+k^2)G = \delta^3(\vec{r})$ over a ball of radius ϵ (centered at the origin):

$$\int_{B(\epsilon)} \nabla^2 G\, d\tau + k^2 \int_{B(\epsilon)} G\, d\tau = \int_{B(\epsilon)} \delta^3(\vec{r})\, d\tau$$

"div. thm"

$$\oint_{\partial B} (\nabla G)\cdot d\vec{a} + k^2 \int_{B(\epsilon)} G\, d\tau = 1$$

you can solve the above, for $\epsilon \to 0$, for A - turns out that k drops out of that process, so set $k=0$

$$\oint\left(-\frac{A}{\epsilon^2}\right)da = 1 \Rightarrow -A\cdot 4\pi = 1 \Rightarrow A = -\frac{1}{4\pi}$$

pick the "outgoing" one

$$\text{so} \quad G(r) = -\frac{1}{4\pi}\frac{e^{ikr}}{r}$$

4. Move the source back to $\vec{r}\,'$: $r \to |\vec{r}-\vec{r}\,'|$

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

Perturbation Expansion

We have $G(\vec{r},\vec{r}')$, & can construct the integral solution:

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \frac{2m}{\hbar^2}\int_{\text{all space}} G(\vec{r},\vec{r}')\,U(\vec{r}')\,\psi(\vec{r}')\,d\tau' \quad (*)$$

w/

$$(\nabla^2 + k^2)\,\psi_0(\vec{r}) = 0$$

The issue is the apperance of the unknown on the right.

Suppose the potential energy function is "small"

$$U = \epsilon \bar{U}$$

& take: $\psi = \psi_0 + \epsilon\psi_1 + \epsilon^2\psi_2 + \cdots$

That gives us an interpretation for ψ_0 – it's the original, incoming "beam" – the full solution for $\epsilon = 0$.

Now $(*)$ looks like:

$$\psi_0 + \epsilon\psi_1 + \epsilon^2\psi_2 + \cdots = \psi_0 + \frac{2m}{\hbar^2}\int_{\text{all space}} G(\vec{r},\vec{r}')\,\epsilon\bar{U}(\vec{r}') \times [\psi_0(\vec{r}') + \epsilon\psi_1(\vec{r}') + \cdots]\,d\tau'$$

then, collecting in powers of ϵ:

ϵ^0: $\psi_0 = \psi_0$ ✓

$$\epsilon^1: \psi_1(\vec{r}) = \frac{2m}{\hbar^2}\int_{\text{all space}} G(\vec{r},\vec{r}')\,\bar{U}(\vec{r}')\,\psi_0(\vec{r}')\,d\tau' \quad (+)$$

$$\epsilon^2: \psi_2(\vec{r}) = \frac{2m}{\hbar^2}\int_{\text{all space}} G(\vec{r},\vec{r}')\,\bar{U}(\vec{r}')\,\psi_1(\vec{r}')\,d\tau'$$

in general, we have:

$$\psi_{j+1}(\vec{r}) = \frac{2m}{\hbar^2}\int_{\text{all space}} G(\vec{r},\vec{r}')\,\bar{U}(\vec{r}')\,\psi_j(\vec{r}')\,d\tau'$$

written this way, the situation is relatively clear.

If you write the terms out explicitly:

$$\psi_2(\vec{r}) = \frac{2m}{\hbar^2}\int_{\text{all space}} G(\vec{r},\vec{r}')\,\bar{U}(\vec{r}')\left[\int_{\text{all space}} G(\vec{r}',\vec{r}'')\,\bar{U}(\vec{r}'')\,\psi_0(\vec{r}'')\,d\tau''\right]d\tau'$$

$$= \left(\frac{2m}{\hbar^2}\right)^2 \int\!\!\int G(\vec{r},\vec{r}')\,G(\vec{r}',\vec{r}'')\,\bar{U}(\vec{r}')\,\bar{U}(\vec{r}'')\,\psi_0(\vec{r}'')\,d\tau'\,d\tau''$$

you need a diagrammatic system to keep track of the perturbative order.

Born Approximation

For our Green's function, $(*)$ looks like:

$$\psi(\vec{r}) = \underset{\text{beam}}{\psi_0(\vec{r})} - \underbrace{\frac{2m}{\hbar^2}\int_{\text{all space}} \frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|}\,U(\vec{r}')\,\psi(\vec{r}')\,d\tau'}_{\approx \frac{f(\theta)}{r}e^{ikr} \text{ far away}}$$

we'll use the perturbation expansion to approximate $f(\theta)$.

Imagine a completely localized source, like the "soft sphere"

$$U(r) = \begin{cases} 0 & r>R \\ U_0 & r<R \end{cases}$$

the integration over $\vec{r}\,'$ will extend out to R - suppose we are interested in $\psi(\vec{r})$ for $r \gg R$, then

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

can be approximated, in the Green's function:

$$\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{4\pi|\vec{r}-\vec{r}\,'|} \approx \frac{e^{ikr(1-\hat{r}\cdot\vec{r}\,'/r)}}{4\pi r} + \dots \approx \frac{e^{ikr}\,e^{-ik\hat{r}\cdot\vec{r}\,'}}{4\pi r}$$

& we have

isolated spherical wave piece

$$\psi(\vec{r}) \approx \psi_0(\vec{r}) - \underbrace{\frac{\frac{2m}{\hbar^2}e^{ikr}}{4\pi r}\int_{\text{all space}} e^{-ik\hat{r}\cdot\vec{r}\,'}\,U(\vec{r}\,')\psi(\vec{r}\,')\,d\tau'}_{\sim f(\theta)}$$

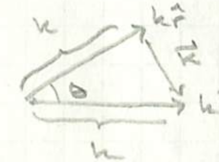
& $f(\theta) = -\dfrac{m}{2\pi\hbar^2}\displaystyle\int_{\text{all space}} e^{-ik\hat{r}\cdot\vec{r}\,'}\,U(\vec{r}\,')\psi(\vec{r}\,')\,d\tau'$ (□)

We'll use $\psi \to \psi_0$ in the integral, (the ϵ^1 level of approximation, (+1)).

$$\psi_0(\vec{r}\,') = e^{ikz'}$$

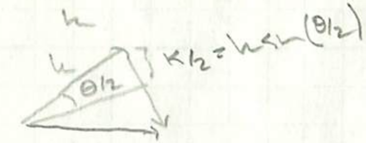
& then $e^{-ik\hat{r}\cdot\vec{r}\,'}\psi_0(\vec{r}\,') = e^{ik(z'-\hat{r}\cdot\vec{r}\,')} = e^{i(k\hat{z}-k\hat{r})\cdot\vec{r}\,'}$

let $\vec{K} = k\hat{z} - k\hat{r}$



w/ $k\hat{r} + \vec{K} = k\hat{z}$

the magnitude of $\vec{K}$ is:



$$K = 2k\sin(\theta/2).$$

the exponential of interest to us is: $e^{i(k\hat{z}-k\hat{r})\cdot\vec{r}\,'} = e^{i\vec{K}\cdot\vec{r}\,'}$

Align the $\hat{z}'$ axis w/ $\vec{r}\,'$ (for the prime integration)

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int_{\text{all space}} e^{i\vec{K}\cdot\vec{r}\,'}\,U(\vec{r}\,')\,d\tau'$$

$$= -\frac{m}{2\pi\hbar^2}\int_0^\infty\int_0^{2\pi}\int_0^\pi e^{iKr'\cos\theta'}\,U(r')\,r'^2\sin\theta'\,d\theta'\,d\phi'\,dr'$$

If $U(\vec{r}\,') = U(r')$ (spherically symmetric pot'l)

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\cdot 2\pi\int_0^\infty\int_0^\pi \frac{d}{d\theta}\left(\frac{-e^{iKr'\cos\theta'}}{iKr'}\right)U(r')\,r'^2\,d\theta'\,dr'$$

$$= \frac{m}{\hbar^2}\int_0^\infty \frac{r'^2}{iKr'}\underbrace{\left(e^{-iKr'} - e^{+iKr'}\right)}_{=-2i\sin(Kr')}U(r')\,dr'$$

$$= -\frac{2m}{\hbar^2 K}\int_0^\infty r'\sin(Kr')\,U(r')\,dr'$$

w/ $K = 2k\sin(\theta/2)$ & $k^2 = \dfrac{2mE}{\hbar^2}$.