Green Function for Helmholtz Equation

$$(\Delta_{\vec{x}} + k^2)\, G(\vec{x}-\vec{x}') = \delta(\vec{x}-\vec{x}')$$

Fourier transformation: algebraic equation

$$G(\vec{q}) = \frac{-1}{q^2-k^2} \qquad k^2 = \frac{2\mu}{\hbar}\,\varepsilon > 0$$

$$G(\vec{x}-\vec{x}') = \int \frac{d^3q}{(2\pi)^3}\, G(\vec{q})\, e^{i\vec{q}\cdot(\vec{x}-\vec{x}')}$$

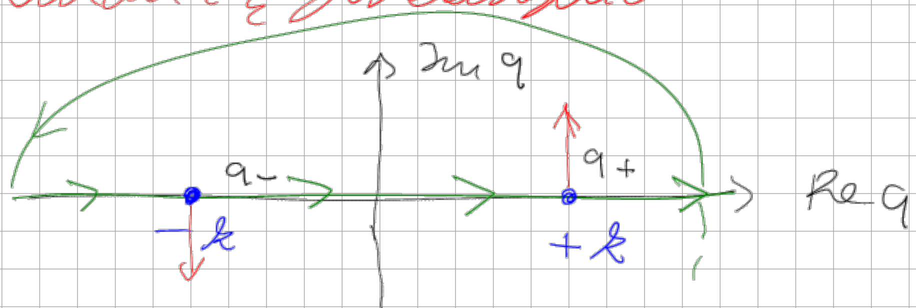
↓ angular degrees

$$= \frac{i}{4\pi^2|\vec{x}-\vec{x}'|} \lim_{\varepsilon \downarrow 0} \int_{-\infty}^{+\infty} dq \, \frac{q}{q^2-k^2-i\varepsilon}\, e^{iq|\vec{x}-\vec{x}'|}$$

causality : Feynman $i\varepsilon$ prescription

zero of denominator:

$$q^2 = \underbrace{k^2 + i\varepsilon}_{\text{cartesian coordinates}} = \underbrace{\sqrt{k^4+\varepsilon^2}\; e^{i\arctan\frac{\varepsilon}{k^2}}}_{\text{polar coordinates}}$$



$$q_\pm = \pm\underbrace{\sqrt[4]{k^4+\varepsilon^2}}_{\approx k\left(1+\frac{1}{4}\frac{\varepsilon^2}{k^4}\right)} \cdot \underbrace{e^{\frac{i}{2}\arctan\frac{\varepsilon}{k^2}}}_{1+\frac{i}{2}\frac{\varepsilon}{k^2}+\dots} \qquad \arctan\frac{\varepsilon}{k^2} \approx \frac{\varepsilon}{k^2}$$

$\varepsilon \downarrow 0$

$$\varepsilon\downarrow 0: \quad = \pm k \pm \frac{i}{2}\frac{\varepsilon}{k} + \dots$$

closing the integration path

$$\Big|\, e^{i\underset{=\mathrm{Re}\,q + i\,\mathrm{Im}\,q}{q}|\vec{x}-\vec{x}'|}\Big| = e^{-\underbrace{(\mathrm{Im}\,q)}_{\overset{!}{>}\,0}\underbrace{|\vec{x}-\vec{x}'|}_{>0}}$$

: closing of path in upper half plane

$$G(\vec{x}-\vec{x}') \overset{\text{residue theorem}}{=} \frac{i}{4\pi^2|\vec{x}-\vec{x}'|}\, 2\pi i \underbrace{\lim_{\varepsilon \downarrow 0} \operatorname*{Res}_{q=q_+} \frac{q}{q^2-k^2-i\varepsilon}\, e^{iq|\vec{x}-\vec{x}'|}}$$

$$= \operatorname*{Res}_{q=+k} \frac{q}{q^2-k^2}\, e^{iq|\vec{x}-\vec{x}'|} = \lim_{q\to +k} \cancel{(q-k)} \frac{q}{\cancel{(q-k)}(q+k)}\, e^{iq|\vec{x}-\vec{x}'|}$$

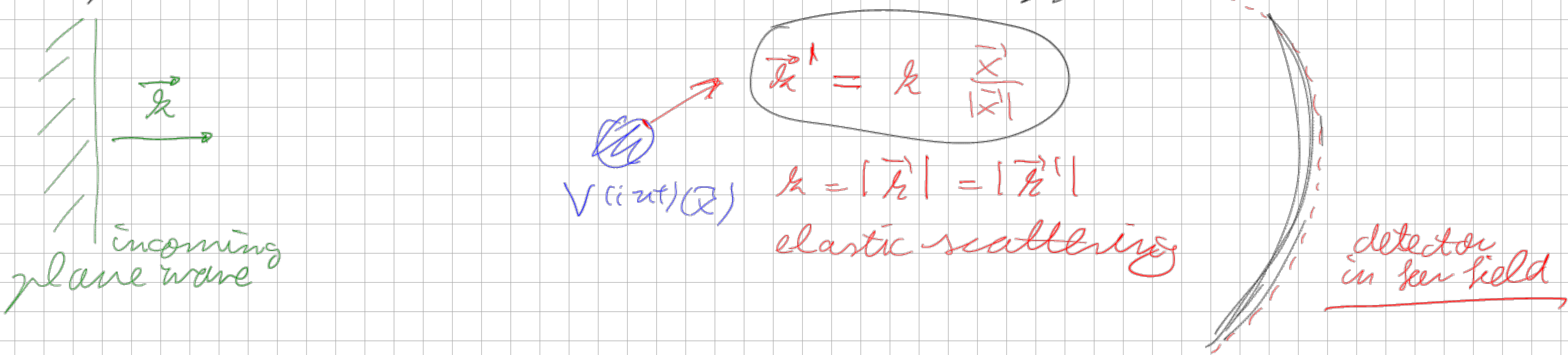
$$= \frac{k}{2k}\, e^{ik|\vec{x}-\vec{x}'|} = \frac{e^{ik|\vec{x}-\vec{x}'|}}{2}$$

$$\Rightarrow G(\vec{x}-\vec{x}') = -\underbrace{\frac{e^{ik|\vec{x}-\vec{x}'|}}{4\pi|\vec{x}-\vec{x}'|}}_{\text{spherical wave}}$$

Implication for solution of Lippmann-Schwinger equation:

$$\psi(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} - \frac{m}{2\pi\hbar^2}\int d^3x'\, \frac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}\, V^{(int)}(\vec{x}')\,\psi(\vec{x}')$$

What implications does this have for the scattering problem?



$$|\vec x - \vec x'| = \sqrt{(\vec x - \vec x')^2} = \sqrt{\vec x^2 - 2\vec x\cdot\vec x' + \vec x'^2}$$

$$= |\vec x|\sqrt{1 - 2\frac{\vec x\cdot\vec x'}{\vec x^2} + \frac{\vec x'^2}{\vec x^2}} \approx |\vec x|\left\{1 - \cancel{\tfrac{1}{2}}\,\cancel{2}\,\frac{\vec x\cdot\vec x'}{\vec x^2} + \dots\right\}$$

far field $|\vec x'| \gg |\vec x|$

$$\psi(\vec x) = e^{i\vec k\cdot\vec x} - \frac{m}{2\pi\hbar^2}\int d^3x' \, \frac{e^{i|\vec x|\left(1 - \frac{\vec x\cdot\vec x'}{\vec x^2} + \dots\right)k}}{|\vec x| + \dots} V^{(int)}(\vec x')\,\psi(\vec x')$$

$$= \underbrace{e^{i\vec k\cdot\vec x}}_{\text{incoming plane wave}} - \frac{m}{2\pi\hbar^2}\underbrace{\frac{e^{ikr}}{r}}_{\text{outgoing spherical wave}}\int d^3x' \, e^{-i\underbrace{\boxed{k\frac{\vec x}{|\vec x|}}}_{\vec k'}\cdot\vec x'} V^{(int)}(\vec x')\,\psi(\vec x')$$

$$\vec k' = k\begin{pmatrix}\sin\vartheta\cos\varphi\\ \sin\vartheta\sin\varphi\\ \cos\vartheta\end{pmatrix}$$

$$\psi(\vec x) = e^{i\vec k\cdot\vec x} + \frac{e^{ikr}}{r}\underbrace{f(\vartheta,\varphi)}_{\text{scattering amplitude}} \; ; \quad f(\vartheta,\varphi) = -\frac{m}{2\pi\hbar^2}\int d^3x' \, e^{-i\vec k'\cdot\vec x'}V^{(int)}(\vec x')\,\psi(\vec x')$$

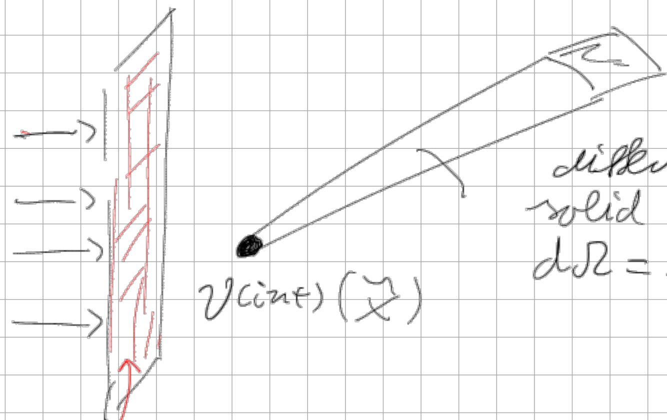
not yet normalised

with $[f] = 1\,m$

Scattering Cross-Section:

differential cross-section

$$\frac{d\sigma}{d\vartheta} = \frac{\text{count scattered particles per solid angle } d\Omega \text{ per time}}{\text{number of incoming particles per time and area}} = \frac{dN(\Omega)}{dt\,d\Omega\,j_{in}}$$



differential solid angle $d\Omega = \sin\vartheta\, d\vartheta\, d\varphi$

Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = \left\{-\frac{\hbar^2}{2m}\Delta + V^{(int)}(\vec x)\right\}\psi \quad \Big|\cdot\psi^*$$

$$-i\hbar\frac{\partial\psi^*}{\partial t} = \left\{-\frac{\hbar^2}{2m}\Delta + V^{(int)}(\vec x)\right\}\psi^* \quad \Big|\cdot\psi$$

subtract: $\underbrace{i\hbar\left[\psi^*\frac{\partial\psi}{\partial t}+\psi\frac{\partial\psi^*}{\partial t}\right]}_{\frac{\partial}{\partial t}\psi^*\psi} = -\frac{\hbar^2}{2\mu}\big(\underbrace{\psi^*\Delta\psi-\psi\Delta\psi^*}_{=\vec\nabla(\psi^*\nabla\psi-\psi\vec\nabla\psi^*)}\big)$

continuity equation: $\frac{\partial}{\partial t}\underbrace{(\psi^*\psi)}_{=\rho \text{ probability density}}+\vec\nabla\underbrace{\left[\frac{\hbar}{2\mu i}(\psi^*\nabla\psi-\psi\nabla\psi^*)\right]}_{\vec j = \text{probability current density}}=0$

$\frac{\partial\rho}{\partial t}+\operatorname{div}\vec j=0$ local conservation law

$\frac{\partial}{\partial t}\underbrace{\int d^3\rho}_{\text{probability}} = -\int d^3x\,\operatorname{div}\vec j \underset{\text{Gauss}}{=} -\oint_{\Gamma}\vec j\cdot d\vec S = 0$

Γ boundary at infinity

$\psi_{in}(\vec x)=e^{i\vec k\cdot\vec x}$ $\quad \vec\nabla\psi = i\vec k\, e^{i\vec k\vec x}$

$\vec j_{in}(\vec x)=\frac{\hbar}{2\mu i}\left\{e^{-i\vec k\vec x}\, i\vec k\, e^{i\vec k\vec x}-e^{i\vec k x}(-i\vec k)e^{-i\vec k\vec x}\right\}=\boxed{\frac{\hbar\vec k}{\mu}}$

$\psi_{out}(\vec x)=\frac{e^{ikr}}{r}\,f(\vartheta,\varphi)$

$\vec j_{out}(\vec x)=\vec e_r\, j_{out},\quad j_{out}=\frac{\hbar}{2\mu i}\left\{\psi^*\frac{\partial}{\partial r}\psi-\psi\frac{\partial}{\partial r}\psi^*\right\}=\frac{\hbar k}{\mu r^2}|f|^2$

$\boxed{dN = j_{out}\,dt\,\underbrace{r^2\,d\Omega}_{dS} = \frac{\hbar k}{\mu \cancel{r^2}}|f|^2\,dt\,\cancel{r^2}\,d\Omega = \frac{\hbar k}{\mu}|f|^2\,dt\,d\Omega}$

$$\frac{d\sigma}{d\Omega} = \frac{dN}{dt\,d\Omega\, j_{in}} = \cancel{\frac{\hbar k}{\mu}} |f|^2 \cancel{dt\,d\Omega} \frac{1}{\cancel{dt\,d\Omega}\,\cancel{\frac{\hbar k}{\mu}}} = |f(\vartheta,\varphi)|^2$$

$$\left[\frac{d\sigma}{d\Omega}\right] = 1\,m^2$$, generic unit: 1 barn ("Scheune") $= 10^{-24}\,cm^2$

total cross-section:

$$\sigma = \int d\Omega \left(\frac{d\sigma}{d\Omega}\right)$$

Result: General structure of scattering theory is now available

Problem remains: how to determine $\psi(\vec{x})$?

- Exact solution for $\psi(\vec{x})$ is only available for a few problems as, e.g. the Fermi pseudopotential $\Rightarrow$ afterwards calculate $f(\vartheta,\varphi;\underbrace{k}_{=\sqrt{\frac{2\mu E}{\hbar^2}}})$
  $\Rightarrow \left(\frac{d\sigma}{d\Omega}\right) = |f(\vartheta,\varphi;k)|^2$
- Born approximation: perturbation theory of first order

Born approximation:

$$\psi^{(n+1)}(\vec{x}) = e^{i\vec{k}\vec{x}} - \frac{\mu}{2\pi\hbar^2}\int d^3x'\, e^{-i\vec{k}'\cdot\vec{x}'}\, V^{(int)}(\vec{x}')\, \psi^{(n)}(\vec{x}')\, \frac{e^{ikr}}{r}$$

Lippmann-Schwinger equation in far field

in general: self-consistent result needed

$$\psi^{(1)}(\vec{x}) = e^{i\vec{k}\vec{x}} - \frac{\mu}{2\pi\hbar^2}\int d^3x'\, \underline{e^{-i\vec{k}'\vec{x}'}}\, V^{(int)}(\vec{x}')\, \underbrace{\psi^{(0)}(\vec{x}')}_{=e^{i\vec{k}\vec{x}'}}\, \frac{e^{ikr}}{r}$$

$$= e^{i\vec{k}\vec{x}} + \frac{e^{ikr}}{r}\, \underbrace{f^{(1)}(\vartheta,\varphi)}_{= -\frac{\mu}{2\pi\hbar^2}\underbrace{\int d^3x'\, e^{i(\vec{k}-\vec{k}')\vec{x}'}\, V^{(int)}(\vec{x}')}_{= V^{(int)}(\vec{k}-\vec{k}')}}$$

Result: In Born approximation the scattering amplitude is given by the Fourier transformed of interaction potential

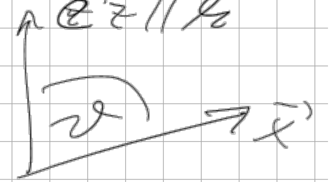
$$V^{(int)}(\vec{x}) = \frac{Q_1 Q_2}{4\pi\varepsilon_0 |\vec{x}|} \;\rightarrow\; V^{(int)}(\vec{k}) = ?$$

$$V^{(int)}(\vec{x}) = \int \frac{d^3k}{(2\pi)^3}\, V^{(int)}(\vec{k})\, e^{i\vec{k}\vec{x}}, \qquad V^{(int)}(\vec{k}) = \int d^3x\, e^{-i\vec{k}\vec{x}}\, V^{(int)}(\vec{x})$$

general statement: symmetry in $V^{(int)}(\vec{x})$ gets inherited by $V^{(int)}(\vec{k})$

example: $V^{(int)}(\vec{x}) = v(|\vec{x}|)$ rotational symmetry

$\vec{e}_z \parallel \vec{k}$



$$V^{(int)}(\vec{k}) \underset{\uparrow}{=} \int_0^{2\pi} d\varphi \int_0^{\pi} d\vartheta \sin\vartheta \int_0^{\infty} dr\, r^2\, e^{-i\underbrace{kr\cos\vartheta}_{\vec{k}\cdot\vec{x}}}\, v^{(int)}(r)$$

spherical coordinates

$$\vec{k} = k\begin{pmatrix}0\\0\\1\end{pmatrix}, \qquad \vec{x} = \begin{pmatrix}\vdots\\ r\cos\vartheta\end{pmatrix}$$

$$= 2\pi \int_0^{\infty} dr\, v^{(int)}(r)\, \underbrace{\int_0^{\pi} d\vartheta \sin\vartheta\, e^{-ikr\cos\vartheta}}$$

$$\underset{u=\cos\vartheta}{=} \int_{-1}^{+1} du\, e^{-ikru} = \frac{e^{-ikr} - e^{+ikr}}{-ikr} = \frac{-2i\sin kr}{-ikr}$$

$$V^{(int)}(\vec{k}) = \frac{4\pi}{k}\int_0^{\infty} dr\, r\, \sin(kr)\, v^{(int)}(r) \longleftarrow$$

$\rightarrow$ also rotationally invariant

Yukawa potential $\hat{=}$ screened Coulomb potential

$$V_Y^q(\vec{x}) = C \frac{1}{|\vec{x}|} e^{-q|\vec{x}|}$$ q: screening parameter, $\frac{1}{q}$ screening length

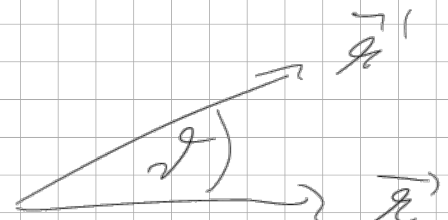
$$V_C(\vec{x}) = \lim_{q \downarrow 0} V_Y^q(\vec{x}) = \frac{C}{|\vec{x}|}, \quad C = \frac{Q_1 Q_2}{4\pi\varepsilon_0}$$

$$V_Y^q(\vec{k}) = \frac{4\pi}{k}\int_0^\infty dr\, \cancel{r} \sin(kr)\, \underbrace{V_Y^q(\vec{x})}_{= C \cancel{\frac{1}{r}} e^{-qr}}$$ convergence factor

$$= \frac{4\pi C}{k} \underbrace{\int_0^\infty dr \sin(kr) e^{-qr}}_{= \mathrm{Im} \int_0^\infty dr\, e^{(-q+ik)r} \,=\, \mathrm{Im} \left.\frac{e^{(-q+ik)r}}{-q+ik}\right|_0^\infty \,=\, \mathrm{Im} \frac{1}{q-ik}}$$

$$\Rightarrow V_Y^q(\vec{k}) = \frac{4\pi C}{\cancel{k}} \frac{\cancel{k}}{q^2+k^2} \xrightarrow{q \downarrow 0} \frac{4\pi C}{k^2}$$

Born approximation for Coulomb potential:



$$f(\vartheta, \varphi) = -\frac{\mu}{2\pi\hbar^2} \frac{Q_1 Q_2}{\varepsilon_0} \frac{1}{(\vec{k} - \vec{k}')^2}$$

$$= -\frac{\mu}{2\pi\hbar^2} \frac{Q_1 Q_2}{\varepsilon_0} \frac{1}{4k^2 \sin^2\vartheta}$$

$$\left(\frac{d\sigma}{d\Omega}\right)(\vartheta) = |f(\vartheta)|^2 \sim \frac{1}{\sin^4\frac{\vartheta}{2}}$$ Rutherford scattering formula

$$(\vec{k} - \vec{k}')^2 = k^2 - 2\vec{k}\cdot\vec{k}' + \vec{k}'^2$$
$$= k^2(2 - 2\cos\vartheta) = k^2 4\sin^2\frac{\vartheta}{2}$$