Computation of G_k

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- Definition: $\left(\nabla^2 + k^2\right) G_k(\vec{r}, \vec{r}\,') = \delta^3(\vec{r} - \vec{r}\,')$
- Fourier transform: $G_k(\vec{r}, \vec{r}\,') \equiv G_k(\vec{r} - \vec{r}\,') = \int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}\, \tilde{G}_k(\vec{q})$
- Representation of the δ-Funktion: $\delta^3(\vec{r} - \vec{r}\,') = \int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}$

$\Rightarrow$ $\left(\nabla^2 + k^2\right) G_k(\vec{r}, \vec{r}\,') = \int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}\, (\vec{k}^{\,2} - \vec{q}^{\,2})\, \tilde{G}_k(\vec{q}) \overset{!}{=} \int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}$

$\Rightarrow$ $\tilde{G}_k(\vec{q}) = \frac{1}{\vec{k}^{\,2} - \vec{q}^{\,2}}$ (Here we wrote $\vec{k}^{\,2}$ for k^2 because eventually $\vec{k}$ will be identified with the wave vector of the incoming wave.)

$\tilde{G}_k(\vec{q})$ diverges at $\vec{q}^{\,2} = \vec{k}^{\,2}$

$\longrightarrow$ introduce an infinitesimal imaginary term to circumvent the pole:

$$\tilde{G}_k^{(\pm)}(\vec{q}) = \frac{1}{\vec{k}^{\,2} - \vec{q}^{\,2} \pm i\varepsilon}$$

- explicit evaluation of the Fourier integral (→ exercises):

$$\boxed{G_k^{(\pm)}(\vec{r},\vec{r}\,') = -\frac{1}{4\pi}\,\frac{e^{\pm ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}}$$

- asymptotic behavior (→ exercises):

$$G_k^{(\pm)}(\vec{r},\vec{r}\,') \overset{r\gg r'}{\longrightarrow} -\frac{1}{4\pi}\,\frac{e^{\pm ikr}}{r}\,e^{\mp i\vec{k}\,'\cdot\vec{r}\,'}, \qquad \vec{k}\,' \equiv k\frac{\vec{r}}{r}$$

  - $G_k^{(+)}$: outgoing spherical wave → correct asymptotics
  - $G_k^{(-)}$: incoming spherical wave → wrong asymptotics

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

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- $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \frac{2\mu}{\hbar^2} \int d^3r' \, G_k^{(+)}(\vec{r}, \vec{r}\,') \, V(\vec{r}\,') \, \psi_{\vec{k}}(\vec{r}\,')$

$$\xrightarrow{r \gg r'} e^{i\vec{k}\cdot\vec{r}} - \frac{\mu}{2\pi\hbar^2} \frac{e^{ikr}}{r} \int d^3r' \, e^{-i\vec{k}\,'\cdot\vec{r}\,'} \, V(\vec{r}\,') \, \psi_{\vec{k}}(\vec{r}\,')$$

$$\Rightarrow \boxed{f(\vec{k}\,', \vec{k}) = -\frac{\mu}{2\pi\hbar^2} \int d^3r' \, e^{-i\vec{k}\,'\cdot\vec{r}\,'} \, V(\vec{r}\,') \, \psi_{\vec{k}}(\vec{r}\,')}$$

2.4 The Born series

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- So far:

  Schrödinger equation not yet solved,
  we just transformed an differential equation into an integral equation:

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

- Advantages:
  - boundary conditions already incorporated
  - starting point for numerical or approximative solutions:

    For weak potentials the integral is only a small correction to the incoming wave.

    $\rightarrow$ iterative solution

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

$$\Rightarrow \quad \psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \int d^3r' \, G_k^{(+)}(\vec{r},\vec{r}\,') \, U(\vec{r}\,') \, \psi_{\vec{k}}(\vec{r}\,')$$

$$= e^{i\vec{k}\cdot\vec{r}} + \int d^3r' \, G_k^{(+)}(\vec{r},\vec{r}\,') \, U(\vec{r}\,') \Big[e^{i\vec{k}\cdot\vec{r}\,'} + \int d^3r'' \, G_k^{(+)}(\vec{r}\,',\vec{r}\,'') \, U(\vec{r}\,'') \, \psi_{\vec{k}}(\vec{r}\,'') \Big]$$

$$= e^{i\vec{k}\cdot\vec{r}} + \int d^3r' \, G_k^{(+)}(\vec{r},\vec{r}\,') \, U(\vec{r}\,') \, e^{i\vec{k}\cdot\vec{r}\,'} + \int d^3r' \int d^3r'' \, G_k^{(+)}(\vec{r},\vec{r}\,') \, U(\vec{r}\,') \, G_k^{(+)}(\vec{r}\,',\vec{r}\,'') \, U(\vec{r}\,'') \, e^{i\vec{k}\cdot\vec{r}\,''} + \ldots$$

→ Born series:

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \sum_{j=1}^{\infty} \int d^3r'\, K_k^{(j)}(\vec{r},\vec{r}\,')\, e^{i\vec{k}\cdot\vec{r}\,'}$$

with

$$K_k^{(1)}(\vec{r},\vec{r}\,') = G_k^{(+)}(\vec{r},\vec{r}\,')\, U(\vec{r}\,')$$

$$K_k^{(j+1)}(\vec{r},\vec{r}\,') = \int d^3r''\, G_k^{(+)}(\vec{r},\vec{r}\,'')\, U(\vec{r}\,'')\, K_k^{(j)}(\vec{r}\,'',\vec{r}\,')$$

→ Born series:

$$\boxed{\begin{aligned}&\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \sum_{j=1}^{\infty} \int d^3r'\, K_k^{(j)}(\vec{r},\vec{r}\,')\, e^{i\vec{k}\cdot\vec{r}\,'}\\ &\text{with}\\ &K_k^{(1)}(\vec{r},\vec{r}\,') = G_k^{(+)}(\vec{r},\vec{r}\,')\, U(\vec{r}\,')\\ &K_k^{(j+1)}(\vec{r},\vec{r}\,') = \int d^3r''\, G_k^{(+)}(\vec{r},\vec{r}\,'')\, U(\vec{r}\,'')\, K_k^{(j)}(\vec{r}\,'',\vec{r}\,')\end{aligned}}$$

- Scattering amplitude: $f(\vec{k}\,',\vec{k}) = -\frac{1}{4\pi} \int d^3r'\, e^{-i\vec{k}\,'\cdot\vec{r}\,'}\, U(\vec{r}\,')\, \psi_{\vec{k}}(\vec{r}\,')$

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→ Born series:

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \sum_{j=1}^{\infty} \int d^3r'\, K_k^{(j)}(\vec{r},\vec{r}\,')\, e^{i\vec{k}\cdot\vec{r}\,'}$$

with

$$K_k^{(1)}(\vec{r},\vec{r}\,') = G_k^{(+)}(\vec{r},\vec{r}\,')\, U(\vec{r}\,')$$

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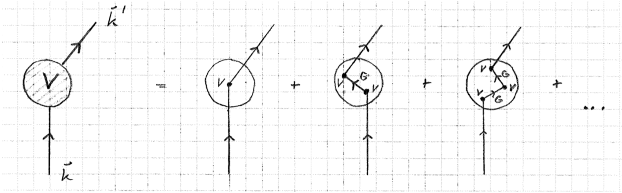
$$\Rightarrow \quad f(\vec{k}\,',\vec{k}) = -\frac{1}{4\pi} \Big\{ \int d^3r'\, e^{-i\vec{k}\,'\cdot\vec{r}\,'}\, U(\vec{r}\,')\, e^{i\vec{k}\cdot\vec{r}\,'} + \int d^3r' \int d^3r''\, e^{-i\vec{k}\,'\cdot\vec{r}\,'}\, U(\vec{r}\,')\, G_k^{(+)}(\vec{r}\,',\vec{r}\,'')\, U(\vec{r}\,'') e^{i\vec{k}\cdot\vec{r}\,''} + \dots \Big\}$$

- Born series for the scattering amplitude:

$$f(\vec{k}\,', \vec{k}) = -\frac{1}{4\pi}\Big\{ \int d^3r'\, e^{-i\vec{k}\,'\cdot\vec{r}\,'}\, U(\vec{r}\,')\, e^{i\vec{k}\cdot\vec{r}\,'} + \int d^3r' \int d^3r''\, e^{-i\vec{k}\,'\cdot\vec{r}\,'}\, U(\vec{r}\,')\, G_k^{(+)}(\vec{r}\,', \vec{r}\,'')\, U(\vec{r}\,'') e^{i\vec{k}\cdot\vec{r}\,''} + \ldots \Big\} = \sum_{j=1}^{\infty} f^{(j)}(\vec{k}\,', \vec{k})$$

- Interpretation:



single scattering + double scat. + triple scat. + ...

(First-order) Born approximation

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- Only consider the first term:

$$f(\vec{k}\,', \vec{k}) \approx f^{(1)}(\vec{k}\,', \vec{k}) = -\frac{1}{4\pi} \int d^3r'\, e^{-i\vec{k}\,'\cdot\vec{r}\,'}\, U(\vec{r}\,')\, e^{i\vec{k}\cdot\vec{r}\,'}$$

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

(First-order) Born approximation

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$$f(\vec{k}\,', \vec{k}) \approx f^{(1)}(\vec{k}\,', \vec{k}) = -\frac{1}{4\pi} \int d^3r'\, e^{-i\vec{k}\,'\cdot\vec{r}\,'}\, U(\vec{r}\,')\, e^{i\vec{k}\cdot\vec{r}\,'}$$

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

$\Rightarrow$

$$f^{(1)}(\vec{k}\,', \vec{k}) = -\frac{\mu}{2\pi\hbar^2} \tilde{V}(\vec{q})$$

$$\tilde{V}(\vec{q}) = \int d^3r'\, e^{-i\vec{q}\cdot\vec{r}\,'}\, V(\vec{r}\,')$$ Fourier transform of the Potential

$$\vec{q} = \vec{k}\,' - \vec{k}$$ „momentum transfer"

(First-order) Born approximation

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- Only consider the first term:

$$f(\vec{k}\,', \vec{k}) \approx f^{(1)}(\vec{k}\,', \vec{k}) = -\frac{1}{4\pi} \int d^3r' \, e^{-i\vec{k}\,'\cdot\vec{r}\,'} \, U(\vec{r}\,') \, e^{i\vec{k}\cdot\vec{r}\,'}$$

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$\Rightarrow$

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- central potential: $V(\vec{r}) = V(r) \quad \Rightarrow \quad \tilde{V}(\vec{q}) = \tilde{V}(q)$

(First-order) Born approximation

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- Only consider the first term:

$$f(\vec{k}\,', \vec{k}) \approx f^{(1)}(\vec{k}\,', \vec{k}) = -\frac{1}{4\pi} \int d^3r'\, e^{-i\vec{k}\,'\cdot\vec{r}\,'}\, U(\vec{r}\,')\, e^{i\vec{k}\cdot\vec{r}\,'}$$

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

$\Rightarrow$

$$\boxed{\begin{aligned} f^{(1)}(\vec{k}\,', \vec{k}) &= -\frac{\mu}{2\pi\hbar^2}\, \tilde{V}(\vec{q}) \\ \tilde{V}(\vec{q}) &= \int d^3r'\, e^{-i\vec{q}\cdot\vec{r}\,'}\, V(\vec{r}\,') \qquad \text{Fourier transform of the Potential} \\ \vec{q} &= \vec{k}\,' - \vec{k} \qquad \text{„momentum transfer”} \end{aligned}}$$

- central potential: $V(\vec{r}) = V(r) \quad \Rightarrow \quad \tilde{V}(\vec{q}) = \tilde{V}(q)$

$$\vec{q}\,^2 = (\vec{k}\,' - \vec{k})^2 = \vec{k}\,'^2 + \vec{k}\,^2 - 2\vec{k}\,'\cdot\vec{k} \overset{k'=k}{=} 2k^2(1-\cos\theta) = 4k^2\sin^2\frac{\theta}{2}$$

$q = 2k\,\sin\frac{\theta}{2} \;\rightarrow\; f^{(1)}(\vec{k}\,', \vec{k}) \equiv f_k^{(1)}(\theta)$ depends only on k and θ
(holds for higher orders as well)

Second-order Born approximation

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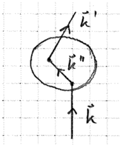
- $f(\vec{k}\,', \vec{k}) \approx f^{(1)}(\vec{k}\,', \vec{k}) + f^{(2)}(\vec{k}\,', \vec{k})$
- $f^{(2)}(\vec{k}\,', \vec{k}) = -\frac{1}{4\pi} \left(\frac{2\mu}{\hbar^2}\right)^2 \int d^3r' \int d^3r'' \, e^{-i\vec{k}\,'\cdot\vec{r}\,'} \, V(\vec{r}\,') \, G_k^{(+)}(\vec{r}\,', \vec{r}\,'') \, V(\vec{r}\,'') \, e^{i\vec{k}\cdot\vec{r}\,''}$
- $G_k^{(+)}(\vec{r}\,', \vec{r}\,'') = \int \frac{d^3k''}{(2\pi)^3} \, e^{i\vec{k}\,''\cdot(\vec{r}\,' - \vec{r}\,'')} \, \frac{1}{\vec{k}^{\,2} - \vec{k}\,''^2 + i\varepsilon}$

$$\Rightarrow \quad f^{(2)}(\vec{k}\,', \vec{k}) = -\frac{1}{4\pi} \left(\frac{2\mu}{\hbar^2}\right)^2 \int \frac{d^3k''}{(2\pi)^3} \left(\int d^3r' \, e^{-i\vec{k}\,'\cdot\vec{r}\,'} \, V(\vec{r}\,') \, e^{i\vec{k}\,''\cdot\vec{r}\,'} \right) \frac{1}{\vec{k}^{\,2} - \vec{k}\,''^2 + i\varepsilon}$$

$$\times \left(\int d^3r'' \, e^{-i\vec{k}\,''\cdot\vec{r}\,''} \, V(\vec{r}\,'') \, e^{i\vec{k}\cdot\vec{r}\,''} \right)$$

$$= -\frac{1}{4\pi} \left(\frac{2\mu}{\hbar^2}\right)^2 \int \frac{d^3k''}{(2\pi)^3} \, \tilde{V}(\vec{k}\,' - \vec{k}\,'') \, \frac{1}{\vec{k}^{\,2} - \vec{k}\,''^2 + i\varepsilon} \, \tilde{V}(\vec{k}\,'' - \vec{k})$$



$$= -\frac{\mu}{2\pi\hbar^2} \int \frac{d^3k''}{(2\pi)^3} \, \tilde{V}(\vec{k}\,' - \vec{k}\,'') \, \frac{1}{E - E'' + i\varepsilon} \, \tilde{V}(\vec{k}\,'' - \vec{k})$$

with $E = \frac{\hbar^2 k^2}{2\mu}$ und $E'' = \frac{\hbar^2 k''^2}{2\mu}$