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

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

- $\int \frac{d^3k''}{(2\pi)^3}$ ➞ in general: $E'' \neq E$: virtual intermediate state
- energy denominator: $\frac{1}{E - E'' + i\varepsilon}$ (cf. perturbation theory)

  ➞ Intermediate states with $E'' \approx E$ contribute most.
- In fact: Performing the integral with the residue theorem:

  Ultimately only states with $k'' = k \;\Leftrightarrow\; E'' = E$ contribute.

- *n*th order:

$$\boxed{\begin{aligned} f^{(n)}(\vec{k}\,', \vec{k}) \;=\; -\tfrac{\mu}{2\pi\hbar^2} \int \tfrac{d^3k_1}{(2\pi)^3} \,\dots\, \tfrac{d^3k_{n-1}}{(2\pi)^3}\; \tilde{V}(\vec{k}\,' - \vec{k}_{n-1})\, \tfrac{1}{E-E_{n-1}+i\varepsilon} \\ \times \quad \tilde{V}(\vec{k}_{n-1} - \vec{k}_{n-2})\, \tfrac{1}{E-E_{n-2}+i\varepsilon} \,\dots\, \tfrac{1}{E-E_1+i\varepsilon}\; \tilde{V}(\vec{k}_1 - \vec{k}) \end{aligned}}$$

2.5 Representation independent approach to scattering theory

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- Hamiltonian: $\hat{H} = \hat{H}_0 + \hat{V}$
  - free part: $\hat{H}_0 = \hat{H}_0(\hat{\vec{p}}) = \frac{\hat{\vec{p}}^{\,2}}{2\mu}, \quad \hat{\vec{p}} = \hbar\hat{\vec{k}}$
  - potential: $\hat{V} = \hat{V}(\hat{\vec{r}})$ (by our assumption)
- Eigenstates with energy E:
  - $\hat{H}\,|\psi\rangle = E\,|\psi\rangle$
  - $\hat{H}_0\,|\phi\rangle = E\,|\phi\rangle$
- Momentum eigenstates: $\hat{\vec{k}}\,|\vec{k}\rangle = \vec{k}\,|\vec{k}\rangle \quad \Rightarrow \quad \hat{\vec{p}}\,|\vec{k}\rangle = \hbar\vec{k}\,|\vec{k}\rangle$

$\Rightarrow \quad \hat{H}_0\,|\vec{k}\rangle = \frac{\hat{\vec{p}}^{\,2}}{2\mu}\,|\vec{k}\rangle = \frac{\hbar^2\vec{k}^{\,2}}{2\mu}\,|\vec{k}\rangle = E\,|\vec{k}\rangle$ with $E = \frac{\hbar^2\vec{k}^{\,2}}{2\mu} \quad \Rightarrow \quad |\vec{k}\rangle \in \{|\phi\rangle\}$

- Schrödinger equation: $\hat{H}\,|\psi\rangle = E\,|\psi\rangle$

  $\Rightarrow \quad \left(E - \hat{H}\right)|\psi\rangle = \left(E - \hat{H}_0 - \hat{V}\right)|\psi\rangle = 0$

  $\Rightarrow \quad \left(E - \hat{H}_0\right)|\psi\rangle = \hat{V}\,|\psi\rangle$

- formal solution:

  $$|\psi\rangle = |\phi\rangle + \left(E - \hat{H}_0\right)^{-1}\hat{V}\,|\psi\rangle \equiv |\phi\rangle + \hat{G}_0(E)\,\hat{V}\,|\psi\rangle$$

  with $\hat{G}_0(z) = \left(z - \hat{H}_0\right)^{-1}$, $z \in \mathbb{C}$, „Green's operator", „resolvent"

- $\hat{G}_0^{-1}(E)\,|\phi\rangle = \left(E - \hat{H}_0\right)|\phi\rangle = 0$

  $\Rightarrow \quad |\phi\rangle = \hat{G}_0(E)\,\hat{G}_0^{-1}(E)\,|\phi\rangle = \hat{G}_0(E)\,0 \quad \Rightarrow$ $\hat{G}_0(z)$ is singular at $z = E$

  ➞ evade the singularity in the complex energy plane

- Boundary condition:

  plane wave + outgoing scattering wave (as before)

  $\rightarrow$ $\boxed{|\psi_{\vec{k}}\rangle = |\vec{k}\rangle + \hat{G}_0(E + i\varepsilon)\,\hat{V}\,|\psi_{\vec{k}}\rangle}$

  Lippmann-Schwinger equation for the state $|\psi\rangle$

Position-space and momentum-space representation

- Eigenstates of position and momentum operator:

$$\hat{\vec{r}}\,|\vec{r}\rangle = \vec{r}|\vec{r}\rangle\,, \qquad \hat{\vec{k}}\,|\vec{k}\rangle = \vec{k}|\vec{k}\rangle$$

- Orthogonality, normalization and completeness:

$$\langle\vec{r}\,'|\vec{r}\rangle = \delta^3(\vec{r}\,' - \vec{r})\,, \qquad \int d^3r\,|\vec{r}\rangle\langle\vec{r}| = \mathbb{1}$$

$$\langle\vec{k}\,'|\vec{k}\rangle = (2\pi)^3\,\delta^3(\vec{k}\,' - \vec{k})\,, \qquad \int \frac{d^3k}{(2\pi)^3}\,|\vec{k}\rangle\langle\vec{k}| = \mathbb{1}$$

(Caution: Some authors have different normalization conventions!)

Consistency:

$$|\vec{r}\,'\rangle = \int d^3r\,|\vec{r}\rangle\langle\vec{r}|\vec{r}\,'\rangle = \int d^3r\,|\vec{r}\rangle\,\delta^3(\vec{r}\,' - \vec{r}) \quad \checkmark$$

$$|\vec{k}\,'\rangle = \int \frac{d^3k}{(2\pi)^3}\,|\vec{k}\rangle\langle\vec{k}|\vec{k}\,'\rangle = \int \frac{d^3k}{(2\pi)^3}\,|\vec{k}\rangle(2\pi)^3\,\delta^3(\vec{k}\,' - \vec{k}) \quad \checkmark$$

- Wave functions
  - position-space representation: $\psi(\vec{r}) = \langle \vec{r} | \psi \rangle$
  - momentum-space representation: $\tilde{\psi}(\vec{k}) = \langle \vec{k} | \psi \rangle$

$$\Rightarrow \quad \tilde{\psi}(\vec{k}) = \langle \vec{k} | \psi \rangle = \int d^3r \, \langle \vec{k} | \vec{r} \rangle \langle \vec{r} | \psi \rangle = \int d^3r \, \langle \vec{k} | \vec{r} \rangle \, \psi(\vec{r}) \stackrel{!}{=} \int d^3r \, e^{-i\vec{k}\cdot\vec{r}} \, \psi(\vec{r})$$

$$\Rightarrow \quad \langle \vec{k} | \vec{r} \rangle = e^{-i\vec{k}\cdot\vec{r}}$$

$$\Leftrightarrow \quad \langle \vec{r} | \vec{k} \rangle = \langle \vec{k} | \vec{r} \rangle^* = e^{i\vec{k}\cdot\vec{r}}$$ pos.-space wave fct. of the momentum eigenstate

- Potential

$$V(\vec{r}\,', \vec{r}) \equiv \langle \vec{r}\,' | \hat{V}(\hat{\vec{r}}) | \vec{r} \rangle = V(\vec{r}) \, \langle \vec{r}\,' | \vec{r} \rangle = V(\vec{r}) \, \delta^3(\vec{r}\,' - \vec{r})$$ "local potential"

$$\langle \vec{k}\,' | \hat{V} | \vec{k} \rangle = \int d^3r' \int d^3r \, \langle \vec{k}\,' | \vec{r}\,' \rangle \langle \vec{r}\,' | \hat{V}(\vec{r}) | \vec{r} \rangle \langle \vec{r} | \vec{k} \rangle$$

$$= \int d^3r' \int d^3r \, e^{-i\vec{k}\,'\cdot\vec{r}\,'} \, V(\vec{r}) \delta^3(\vec{r}\,' - \vec{r}) \, e^{i\vec{k}\cdot\vec{r}} = \int d^3r \, e^{-i\vec{q}\cdot\vec{r}} \, V(\vec{r}) = \tilde{V}(\vec{q})$$

($\vec{q} = \vec{k}\,' - \vec{k}$ = momentum transfer)

- Green's operator:

$$\langle\vec{k}\,''|\hat{G}_0(z)|\vec{k}\,'\rangle = \langle\vec{k}\,''|(z-\hat{H}_0)^{-1}|\vec{k}\,'\rangle = \left(z - \frac{\hbar^2\vec{k}\,'^2}{2\mu}\right)^{-1}\langle\vec{k}\,''|\vec{k}\,'\rangle$$

$$= \left(z - \frac{\hbar^2\vec{k}\,'^2}{2\mu}\right)^{-1}(2\pi)^3\delta^3(\vec{k}\,''-\vec{k}\,')$$

$$\Rightarrow\ \langle\vec{k}\,''|\hat{G}_0(E+i\varepsilon)|\vec{k}\,'\rangle \overset{E=\frac{\hbar^2\vec{k}^2}{2\mu}}{=} \frac{2\mu}{\hbar^2}\frac{1}{\vec{k}^{\,2}-\vec{k}\,'^2+i\varepsilon}(2\pi)^3\delta^3(\vec{k}\,''-\vec{k}\,')$$

$$= \frac{2\mu}{\hbar^2}\,\tilde{G}_k^{(+)}(\vec{k}\,')\,(2\pi)^3\delta^3(\vec{k}\,''-\vec{k}\,')$$

$$\Rightarrow\ \langle\vec{r}|\hat{G}_0(E+i\varepsilon)|\vec{r}\,'\rangle = \int\frac{d^3k''}{(2\pi)^3}\int\frac{d^3k'}{(2\pi)^3}\,\langle\vec{r}|\vec{k}\,''\rangle\langle\vec{k}\,''|\hat{G}_0(E+i\varepsilon)|\vec{k}\,'\rangle\langle\vec{k}\,'|\vec{r}\,'\rangle$$

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

$$= \frac{2\mu}{\hbar^2}\,G_k^{(+)}(\vec{r},\vec{r}\,')$$

- Lippmann-Schwinger equation: $|\psi_{\vec{k}}\rangle = |\vec{k}\rangle + \hat{G}_0(E + i\varepsilon)\,\hat{V}\,|\psi_{\vec{k}}\rangle$
- Position-space representation:

$$\langle\vec{r}|\psi_{\vec{k}}\rangle = \langle\vec{r}|\vec{k}\rangle + \langle\vec{r}|\hat{G}_0(E + i\varepsilon)\,\hat{V}\,|\psi_{\vec{k}}\rangle$$

$$= \langle\vec{r}|\vec{k}\rangle + \int d^3r' \int d^3r'' \langle\vec{r}|\hat{G}_0(E + i\varepsilon)|\vec{r}\,'\rangle\langle\vec{r}\,'|\hat{V}|\vec{r}\,''\rangle\langle\vec{r}\,''|\psi_{\vec{k}}\rangle$$

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

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

T-matrix

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- Def: $\hat{T}\,|\vec{k}\rangle \equiv \hat{V}|\psi_{\vec{k}}\rangle$ T-matrix

$$\Rightarrow \hat{T}\,|\vec{k}\rangle \overset{\text{LSE}}{=} \hat{V}\left(|\vec{k}\rangle + \hat{G}_0\hat{V}|\psi_{\vec{k}}\rangle\right) = \left(\hat{V} + \hat{V}\hat{G}_0\hat{T}\right)|\vec{k}\rangle$$

$\Rightarrow$ $\boxed{\hat{T} = \hat{V} + \hat{V}\hat{G}_0\hat{T}}$ Lippmann-Schwinger equation for the T-matrix

  - valid for $\hat{G}_0(E + i\varepsilon)$
  - generalization: $\hat{G}_0(z) \;\rightarrow\; \hat{T}(z)$

- Matrix elements:

$$\langle\vec{k}\,'|\hat{T}\,|\vec{k}\rangle = \langle\vec{k}\,'|\hat{V}|\psi_{\vec{k}}\rangle = \int d^3r \int d^3r'\,\langle\vec{k}\,'|\vec{r}\,'\rangle\langle\vec{r}\,'|\hat{V}|\vec{r}\rangle\langle\vec{r}|\psi_{\vec{k}}\rangle$$

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

$$\Rightarrow \boxed{f(\vec{k}\,',\vec{k}) = -\frac{\mu}{2\pi\hbar^2}\,\langle\vec{k}\,'|\hat{T}(E + i\varepsilon)\,|\vec{k}\rangle}$$