Lippmann-Schwinger eq. in 3D:

- up to now we approached the scattering problem by solving the differential Schrödinger equation: $\left[-\frac{\hbar^2}{2m}\Delta + V(\vec{r})\right]\psi^{(+)}_{\vec{k}}(\vec{r}) = E_k\,\psi^{(+)}_{\vec{k}}(\vec{r})$, $E_k = \frac{k^2}{2m}$

$$+\ \text{b.c.}\ \psi^{(+)}_{\vec{k}}(\vec{r}) \xrightarrow{r\to\infty} e^{i\vec{k}\cdot\vec{r}} + f^{(+)}(\theta,\varphi)\cdot\frac{e^{ik\cdot r}}{r}$$

- the Schr. eq. can be rewritten with the potential term considered as an inhomogeneous term: $\left[\Delta_r + k^2\right]\psi_{\vec{k}}(\vec{r}) = U(\vec{r})\cdot\psi_{\vec{k}}(\vec{r})$, $U(\vec{r}) = -\frac{2m}{\hbar^2}\cdot V(\vec{r})$

- for now we can have $V(\vec{r})$ that is not spherically symmetric but still decaying faster than $\frac{1}{r^2}$ at $r\to\infty$.
- the solution $\psi_{\vec{k}}(\vec{r})$ can be written using the Green's function:

$$\psi_{\vec{k}}(\vec{r}) = \phi_{\vec{k}}(\vec{r}) + \int d^3r'\, G_{0,k}(\vec{r},\vec{r}\,')\,U(\vec{r}\,')\,\psi_{\vec{k}}(\vec{r}\,'),\ \text{where}$$

$$\left[\Delta_r + k^2\right]G_{0,k}(\vec{r},\vec{r}\,') = \delta(\vec{r}-\vec{r}\,'),$$ $G_{0,k}$: Green's function of the free Schrödinger equation.

and $\phi_{\vec{k}}(\vec{r})$ is a solution of the homogeneous eq.:

$$\left[\Delta_r + k^2\right]\phi_{\vec{k}}(\vec{r}) = 0$$

- to simplify the notation I'll further omit the k-dependence in ψ, ϕ, G_0
- for scattering problems we choose: $\phi_{\vec{k}_i}(\vec{r}) = (2\pi)^{-3/2}\cdot\exp[i\vec{k}_i\cdot\vec{r}]$, where the normalization factor $(2\pi)^{-3/2}$ ensures:

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

- without it we would get: $(2\pi)^3\delta(\vec{k}-\vec{k}\,')$
- with $\phi_{\vec{k}_i}$ fixed we get:

$$\psi_{\vec{k}_i}(\vec{r}) = (2\pi)^{-3/2}\exp[i\vec{k}_i\cdot\vec{r}] + \int d^3r'\,G_0(\vec{r},\vec{r}\,')\,U(\vec{r}\,')\,\psi_{\vec{k}_i}(\vec{r}\,')$$

I.E. I've not written the (+) superscript in $\psi_{\vec{k}_i}(\vec{r})$.

Q: what specifies the outgoing b.c.?

A: it is the choice of $G_0(\vec{r}\,',\vec{r})$.

Green's function $G_0(\vec{r}\,',\vec{r})$: we find it by working in the momentum space

$$\left[\Delta_r + k^2\right]G_0(\vec{r}\,',\vec{r}) = \delta(\vec{r}-\vec{r}\,')$$

- using the integral representation of $\delta(\vec{r}-\vec{r}\,')$:

$$\delta(\vec{r}-\vec{r}\,') = (2\pi)^{-3}\int d^3k'\,\exp[i\vec{k}'\cdot(\vec{r}-\vec{r}\,')]$$

- we write G_0 using the Fourier transform:

$$G_0(\vec{r},\vec{r}\,') = (2\pi)^{-3}\int d^3k'\,g_0(\vec{k}',\vec{r}\,')\cdot\exp[i\vec{k}'\cdot\vec{r}]$$

- substitute G_0 into the diff. eq.:

- substitute into the diff eq.:

$$\left[\Delta_r + k^2\right](2\pi)^{-3}\int d^3k'\, g_0(\vec{k}',\vec{r}')\cdot \exp[i\vec{k}'\cdot\vec{r}] = (2\pi)^{-3}\int d^3k' \exp[i\vec{k}'\cdot(\vec{r}-\vec{r}')]$$

$$\left(\Delta_r \exp[i\vec{k}'\vec{r}] = \nabla\cdot i\vec{k}' \exp[i\vec{k}'\vec{r}] = -(k')^2\cdot \exp[i\vec{k}'\vec{r}]\right)$$

$$\int d^3k'\, g_0(\vec{k}',\vec{r}')\cdot\left[k^2-(k')^2\right]\cdot \exp[i\vec{k}'\vec{r}] = \int d^3k' \exp[-i\vec{k}'\cdot\vec{r}']\cdot\exp[i\vec{k}'\vec{r}]$$

$$\Rightarrow g_0(\vec{k}',\vec{r}')\cdot\left[k^2-(k')^2\right] = \exp[-i\vec{k}'\vec{r}']$$

$$g_0(\vec{k}',\vec{r}') = \frac{\exp[-i\vec{k}'\vec{r}']}{k^2-(k')^2}$$

$$\Rightarrow \boxed{G_0(\vec{r},\vec{r}') = -(2\pi)^{-3}\int d^3k' \frac{\exp[i\vec{k}'\cdot(\vec{r}-\vec{r}')]}{(k')^2-k^2}}$$ (I took outside the $\ominus$ from)

- this expression is not well-defined since the integral diverges due to the poles in the integrand at $k'=\pm k$!
- we need to remove the singularity: we will do it by moving the poles to the complex plane. We will see that different choices of the poles leads to different boundary conditions! (i.e. $G^{(+)}, G^{(-)}$)

Integration:
- set $\vec{R} = \vec{r}-\vec{r}'$ and choose the coordinates so that $\vec{R} \parallel \hat{z}$ ($\vec{r}$ and $\vec{r}'$ are fixed and I integrate over $\vec{k}'$)
- use spherical polar coordinates and integrate over the angles first:

$$G_0(R) = -(2\pi)^{-3}\int_0^\infty dk'(k')^2\int_0^\pi d\theta'\sin(\theta')\int_0^{2\pi}d\phi' \frac{\exp[ik'R\cos(\theta')]}{(k')^2-k^2} = \left| \begin{array}{l} t = ik'R\cos(\theta') \\ dt = -ik'R\sin(\theta')d\theta' \end{array}\right|$$

$$= -(2\pi)^{-3}\cdot(2\pi)\int_0^\infty dk'(k')^2\int_{ik'R}^{-ik'R} dt\, \frac{-1}{ik'R}\cdot\frac{\exp[t]}{(k')^2-k^2} = \frac{+(2\pi)^{-2}}{iR}\int_0^\infty dk' \frac{k'}{(k')^2-k^2}\cdot\underbrace{\left[\exp[-ik'R]-\exp[ik'R]\right]}_{=-2i\sin(k'R)} =$$

odd function of k'

the integrand is even function of k' so we can write $\int_0^\infty \to \frac{1}{2}\int_{-\infty}^{\infty}$

$$= \left(-\frac{(8\pi^2)^{-1}}{R}\int_0^\infty dk'\, \frac{k'\sin(k'R)}{(k')^2-k^2} = -\frac{(4\pi^2)^{-1}}{R}\int_{-\infty}^{\infty} dk'\, \frac{k'\sin(k'R)}{(k')^2-k^2}\right)$$

the integrand is even function of k' $(k'\sin(k'R))$ so we can write $\int_0^\infty dk' \to \frac{1}{2}\int_{-\infty}^{\infty} dk'$

$$= -\frac{1}{2\cdot 4\pi^2\cdot i\cdot R}\left\{\int_{-\infty}^{\infty} dk'\cdot\exp[ik'R]\cdot\left(\frac{k'}{(k')^2-k^2}\right) - \int_{-\infty}^{\infty} dk'\cdot\exp[-ik'R]\cdot\left(\frac{k'}{(k')^2-k^2}\right)\right\} =$$

I took $\ominus$ from $-\exp[ik'R]$

$$= \frac{A}{k'-k}+\frac{B}{k'+k} = \frac{\frac{1}{2}}{k'-k}+\frac{\frac{1}{2}}{k'+k}$$

$$= -\frac{1}{16\pi^2\cdot i\cdot R}\cdot\left\{\underbrace{\int_{-\infty}^{\infty} dk'\exp[ik'R]\cdot\left[\frac{1}{k'-k}+\frac{1}{k'+k}\right]}_{=I_1} - \underbrace{\int_{-\infty}^{\infty} dk'\exp[-ik'R]\cdot\left[\frac{1}{k'-k}+\frac{1}{k'+k}\right]}_{=I_2}\right\}$$

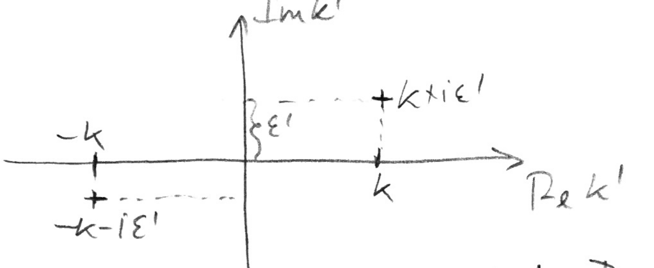
- we're going to integrate over k' in the complex plane:

$$k' = \mathrm{Re}\,k' + i\,\mathrm{Im}\,k'$$

- this ensures that $\exp[ik'R] = \exp[iR\cdot\mathrm{Re}(k')]\cdot\exp[-R\cdot\mathrm{Im}(k')]$ so we can use Jordan's lemma to zero the integral over the semi-circle

- Both I_1 and I_2 have poles at: $k' = \pm k$
- We remove the singularity by <u>displacing the poles slightly</u>:

$$k' = \pm(k + i\varepsilon'), \quad \varepsilon' \to 0_+$$



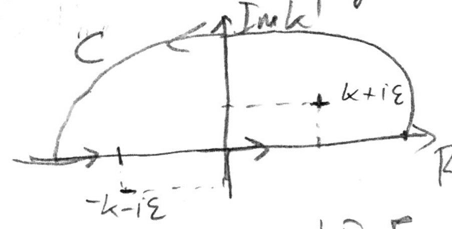
$$(k')^2 = k^2 + i2k\varepsilon' - (\varepsilon')^2 = k^2 + i\varepsilon + O(\varepsilon^2)$$

- I can always set $\varepsilon \equiv 2k\varepsilon'$ since <u>k</u> is fixed in integration over <u>k'</u>.

- <u>substituting $k \to k + i\varepsilon$</u> into I_1 and I_2 we get:

$$I_1 = \oint_C e^{ik' \cdot R}\left[\frac{1}{k'-k-i\varepsilon} + \frac{1}{k'+k+i\varepsilon}\right]dk', \quad \underline{\text{with } \operatorname{Im} k' > 0}$$

- we close the integral over the k' axis by completing the semi-circle in the UHP:

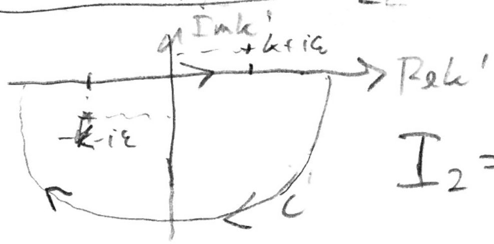


The pole at $k' = -k - i\varepsilon$ does not contribute to the contour integral.

Cauchy: $f(z_0) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{z - z_0}dz$

$$I_1 = \oint_C e^{ik' \cdot R}\left[\frac{1}{k'-k-i\varepsilon} + \cancel{\frac{1}{k'+k+i\varepsilon}}\right]dk' = 2\pi i\, e^{i(k+i\varepsilon)\cdot R}$$

<u>Similarly for I_2</u> $(k \to k + i\varepsilon)$ but we need to integrate over LHP:



- here the pole at $k' = k + i\varepsilon$ does not contribute

$$I_2 = \oint_C e^{-ik' \cdot R}\left[\cancel{\frac{1}{k'-k+i\varepsilon}} + \frac{1}{k'+k+i\varepsilon}\right]dk' = -2\pi i\, e^{i(k+i\varepsilon)\cdot R}$$

since the contour C runs in direction $2\pi \to \pi$ (i.e. in the negative sense)

<u>Finally we get:</u>

$$G_0(\vec{r}, \vec{r}\,') = -(2\pi)^{-3} \cdot \lim_{\varepsilon \to 0+} \int \frac{\exp[i\vec{k}' \cdot (\vec{r} - \vec{r}\,')]}{(k')^2 - k^2 - i\varepsilon} d^3k' = -\frac{1}{16\pi^2 iR} \cdot \left[I_1(+\varepsilon) - I_2(+\varepsilon)\right] =$$

$(k')^2 = k^2 + i\varepsilon \Rightarrow (k')^2 - k^2 - i\varepsilon = 0$

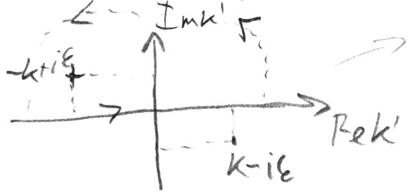
↳ that's the equation for the displaced poles

$$= -\frac{4\pi i}{16\pi^2 iR} \cdot e^{i(k+i\varepsilon)\cdot R} = -\frac{1}{4\pi}\frac{e^{i(k+i\varepsilon)\cdot R}}{R} \xrightarrow{\varepsilon \to 0+} -\frac{1}{4\pi}\frac{e^{ikR}}{R}$$

$$\boxed{G_0^{(+)}(\vec{r}, \vec{r}\,') = -\frac{1}{4\pi} \cdot \frac{e^{ik|\vec{r} - \vec{r}\,'|}}{|\vec{r} - \vec{r}\,'|}}$$

- Choosing the displacement in the <u>opposite direction $k \to k - i\varepsilon$</u>

gives $G^{(-)}(\vec{r},\vec{r}')$:



$$I_1 = \oint_C e^{ik'R}\left[\frac{1}{k'-k+i\varepsilon} + \frac{1}{k'+k-i\varepsilon}\right] = 2\pi i\, e^{i(-k+i\varepsilon)\cdot R}$$

doesn't contribute to the contour integral

$$I_2 = \oint_C e^{-ik'R}\left[\frac{1}{k'-k+i\varepsilon} + \frac{1}{k'+k-i\varepsilon}\right] = -2\pi i\, e^{-i(k-i\varepsilon)\cdot R}$$

$C \to$ in the LHP

due to clockwise direction in LHP

$$\Rightarrow G_0^{(-)}(\vec{r},\vec{r}') = -\frac{1}{16\pi^2 iR}\cdot\left[I_1(-\varepsilon) - I_2(-\varepsilon)\right] = -\frac{1}{4\pi}\frac{e^{-ikR}}{R}$$

$$G_0^{(-)}(\vec{r},\vec{r}') = -(2\pi)^{-3}\lim_{\varepsilon\to 0+}\int d^3k'\,\frac{\exp[i\vec{k}'\cdot(\vec{r}-\vec{r}')]}{(k')^2 - k^2 + i\varepsilon} = -\frac{1}{4\pi}\frac{e^{-ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}$$

$$k' = \pm(k - i\varepsilon) \to (k')^2 = k^2 - i\varepsilon \Rightarrow (k')^2 - k^2 + i\varepsilon = 0$$

$$\Rightarrow \boxed{G_0^{(+)} = \left[G_0^{(-)}\right]^\dagger}$$

- substituting $G_0^{(+)}(\vec{r},\vec{r}')$ into the integral eq. we get:

$$\boxed{\psi_{\vec{k}_i}^{(+)}(\vec{r}) = (2\pi)^{-3/2}\exp[i\vec{k}_i\cdot\vec{r}] + \int d^3r'\, G_0^{(+)}(\vec{r},\vec{r}')\, U(\vec{r}')\, \psi_{\vec{k}_i}^{(+)}(\vec{r}')}$$

Lippmann-Schwinger equation

- it is an implicit <u>integral equation</u> for $\psi_{\vec{k}_i}^{(+)}(\vec{r})$.

- Let's verify that solutions of L-S equation satisfy the scattering b.c.

- the term $\exp[i\vec{k}_i\cdot\vec{r}]$ already has the correct form so let's focus on $\psi_{sc}^{(+)}$

$$\psi_{sc}^{(+)}(\vec{r}) = \int d^3r'\, G_0^{(+)}(\vec{r},\vec{r}')\, U(\vec{r}')\, \psi_{\vec{k}_i}^{(+)}(\vec{r}') = -\frac{1}{4\pi}\int d^3r'\,\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}\cdot U(\vec{r}')\,\psi_{\vec{k}_i}^{(+)}(\vec{r}')$$

- we want the form of $\psi_{sc}^{(+)}$ for $r \to \infty$ $\Rightarrow$ we need to expand $|\vec{r}-\vec{r}'|$ (IF $U(\vec{r})$ HAS A FINITE RANGE)

$\vec{r} = r\cdot\hat{r}$

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

small parameter

Taylor expansion around $x = 0$ of $r\cdot\left[1 - 2\vec{x}\cdot\hat{r} + x^2\right]^{1/2}$

$\vec{x} = \frac{\vec{r}'}{r}$

$$\doteq r\cdot\Big[\underbrace{1}_{f(0)} + \underbrace{\frac{1}{2}\left(-2\vec{x}\cdot\hat{r} + \vec{x}\cdot\vec{x}\right)^{-1/2}\Big|_{x=0}\cdot(-2\hat{r})}_{\left.\frac{df}{dx}\right|_{x=0}}\cdot\vec{x} + O(x^2)\Big] \doteq r\left[1 - \hat{r}\cdot\frac{\vec{r}'}{r} + O\left(\left(\frac{r'}{r}\right)^2\right)\right] \sim \boxed{r - \hat{r}\cdot\vec{r}'}$$

- substituting back into $\psi_{sc}^{(+)}(\vec{r})$ we get:

set $\vec{k}_f = k\cdot\hat{r}$ and take the $\exp[ikr]/r$ term outside of the integral

$$\psi_{sc}^{(+)}(\vec{r}) \xrightarrow{r\to\infty} -\frac{1}{4\pi}\int d^3r'\,\frac{e^{ikr}\cdot e^{-ik\hat{r}\cdot\vec{r}'}}{r}\, U(\vec{r}')\,\psi_{\vec{k}_i}^{(+)}(\vec{r}') =$$

$$= -\frac{1}{4\pi}\frac{e^{ikr}}{r}\cdot\int d^3r'\, e^{-i\vec{k}_f\cdot\vec{r}'}\cdot U(\vec{r}')\cdot\psi_{\vec{k}_i}^{(+)}(\vec{r}')$$

- for potentials of "finite" range (i.e. excluding Coulomb) we can assume $U(r') \sim 0$ for $r' > a$, where $\underline{a}$ is the range of the potential (L5)

$$\psi^{(+)}_{\vec{k}_i}(\vec{r}) \xrightarrow[r\to\infty]{} (2\pi)^{-3/2}\cdot \exp[i\vec{k}_i\cdot\vec{r}] + \frac{\exp[ikr]}{r}\cdot\left[-\frac{1}{4\pi}\int d^3r' e^{-i\vec{k}_f\cdot\vec{r}'}U(\vec{r}')\,\psi^{(+)}_{\vec{k}_i}(\vec{r}')\right] =$$

$$= 2\pi^{-3/2}\left[\exp[i\vec{k}_i\cdot\vec{r}] + f(\theta,\varphi)\cdot\frac{e^{ikr}}{r}\right], \text{ where}$$

$$\boxed{f(\theta,\varphi) = -\frac{(2\pi)^{3/2}}{4\pi}\cdot\int d^3r' \exp[-i\vec{k}_f\cdot\vec{r}']\cdot U(\vec{r}')\cdot\psi^{(+)}_{\vec{k}_i}(\vec{r}') = -2\pi^2\langle\phi_{\vec{k}_f}|U|\psi^{(+)}_{\vec{k}_i}\rangle,\quad \phi_{\vec{k}_f} = (2\pi)^{-3/2}\cdot\exp[i\vec{k}_f\cdot\vec{r}]}$$

suitable for making approximations

USE U NOT V

- this is the integral representation of the scattering amplitude
- in terms of the potential $V(\vec{r}) = \frac{\hbar^2}{2m}U(\vec{r})$: $f(\theta,\varphi) = -\frac{(2\pi)^2\cdot m}{\hbar^2}\cdot\langle\phi_{\vec{k}_f}|V|\psi^{(+)}_{\vec{k}_i}\rangle$
- We can now define the T-operator by the requirement : $\boxed{V|\psi^{(+)}_{\vec{k}_i}\rangle = T|\phi_{\vec{k}_i}\rangle}$
- So that: $f(\theta,\varphi) = -\cancel{\frac{(2\pi)^2 m}{\hbar^2}\cdot T_{fi}}\ -2\pi^2 T_{fi}$ and $\frac{d\sigma}{d\Omega} = \cancel{\frac{(2\pi)^4 m^2}{\hbar^4}}\ 4\pi^4\,|T_{fi}|^2$, where

$T_{fi} = \langle\phi_{\vec{k}_f}|T|\phi_{\vec{k}_i}\rangle$; i.e. T operator has a physical interpretation of the transition from the inital momentum to the final momentum state

= expand into partial waves and get it in terms of pw T-matrix elements

~~(one could apply this to T and G-ops too)~~

Born series: demonstrate the use of approximations on L-S form of its implicit form:
- The L-S equation doesn't seem very practical due to its implicit form:

$$\psi^{(+)}_{\vec{k}_i}(\vec{r}) = (2\pi)^{-3/2}\cdot\exp[i\vec{k}_i\cdot\vec{r}] + \int d^3r'\, G_0^{(+)}(\vec{r},\vec{r}')U(\vec{r}')\,\psi^{(+)}_{\vec{k}_i}(\vec{r}')$$

- Note that in the absence of the potential:

$$\psi^{(+)}_{\vec{k}_i}(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) \cancel{+ O(U)}$$

- This suggests that one way of solving L-S equation is by iteration:

$$\psi_0(\vec{r}) = \phi_{\vec{k}_i}(\vec{r})$$
$$\psi_1(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \int G_0^{(+)}(\vec{r},\vec{r}')\,U(\vec{r}')\,\phi_{\vec{k}_i}(\vec{r}')\,d^3r'$$
$$\psi_2(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \int G_0^{(+)}(\vec{r},\vec{r}')\,U(\vec{r}')\,\psi_1(\vec{r}')\,d^3r'$$
$$\vdots$$
$$\psi_n(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \int G_0^{(+)}(\vec{r},\vec{r}')\,U(\vec{r}')\,\psi_{n-1}(\vec{r}')\,d^3r'$$

- The Born series is therefore a perturbation series in powers of the potential. Interpretation in terms of multiple-scattering with U providing the interaction

L5

<u>Lippmann-Schwinger eq</u>: <u>explicit solution</u>

$$\psi^{(+)}_{\vec{k}_i} = \phi_{k_i}(\vec{r}) + \int d^3r' \, G_0(\vec{r},\vec{r}') \, U(\vec{r}') \, \psi^{(+)}_{\vec{k}_i}(\vec{r}')$$ ... in braket notation: $\boxed{|\psi^{(+)}_{k_i}\rangle = |\phi_{k_i}\rangle + G_0 U |\psi^{(+)}_{k_i}\rangle}$

– this has the form

$$(1) \quad \psi^{(+)}_{\vec{k}_i} = \phi_{\vec{k}_i}(\vec{r}) + \underbrace{\psi^{(+)}_{sc}(\vec{r})}$$ → we don't know that

– we know that $\psi^{(+)}_{k_i}$ satisfies Schrödinger equation:

$$[\Delta + k^2]\, \psi^{(+)}_{\vec{k}_i} = U(\vec{r})\, \psi^{(+)}_{\vec{k}_i} \quad (2)$$

– substitute (1) into (2) and obtain equation for $\psi^{(+)}_{sc}(\vec{r})$: $\left([\Delta + k^2]\, \phi_{\vec{k}_i} = 0\right)$

$$[\Delta + k^2]\, \psi^{(+)}_{sc} = U(\vec{r})\, \phi_{k_i}(\vec{r}) + U(\vec{r})\, \psi^{(+)}_{sc}$$ / put $U(\vec{r})\psi^{(+)}_{sc}$ on LHS

$$\Rightarrow [\Delta + k^2 - U(\vec{r})]\, \psi^{(+)}_{sc} = U(\vec{r})\, \phi_{k_i}(\vec{r})$$

the full Green's function of Schr. equation satisfies: $[\Delta + k^2 - U]\, G^{(+)}(\vec{r},\vec{r}') = \delta(\vec{r}-\vec{r}')$ ... we need $G^{(+)}(r,r')$ to give the scattering b.c.

– we can write explicitly

$$\psi^{(+)}_{sc}(\vec{r}) = \int d^3r' \, G^{(+)}(\vec{r},\vec{r}')\, U(\vec{r}')\, \phi_{\vec{k}_i}(\vec{r}')$$

– and the full solution (1) is <u>explicitly</u> (i.e. not an implicit equation)

$$\psi^{(+)}_{\vec{k}_i} = \phi_{\vec{k}_i}(\vec{r}) + \int d^3r' \, G^{(+)}(\vec{r},\vec{r}')\, U(\vec{r}')\, \phi_{\vec{k}_i}(\vec{r}')$$

in bra-ket notation this is:

$$|\psi^{(+)}_{\vec{k}_i}\rangle = |\phi_{\vec{k}_i}\rangle + \hat{G}^{(+)}\hat{U}\,|\phi_{\vec{k}_i}\rangle = (1 + \hat{G}^{(+)}\hat{U})\,|\phi_{\vec{k}_i}\rangle$$

Therefore the <u>T-matrix element</u> is ~~defined~~: (i.e. the <u>scattering amplitude</u>)

$$T_{fi} = \langle \phi_{\vec{k}_f} | U | \psi^{(+)}_{\vec{k}_i}\rangle = \langle \phi_{\vec{k}_f} | \underbrace{U + UG^{(+)}U}_{\text{operator}} | \phi_{\vec{k}_i}\rangle =$$ explicit form: $\boxed{T = U + UG^{(+)}U}$

$$= \langle \phi_{\vec{k}_f} | T | \phi_{\vec{k}_i}\rangle$$ i.e. definition from yesterday ... to <u>know the T-operator</u> means to know <u>the full solution of the Schrödinger equation</u>

~~you can express the scattering ampl. also using $\psi^{(-)}$: $|\psi^{(-)}\rangle = |\phi_{k_i}\rangle + G^{(-)}_0 U |\psi^{(-)}\rangle$~~

5 cont.

L–S equation for the T-operator and for the Green's function

– we know that $\langle \phi_{\vec{k}_f} | U | \psi^{(+)}_{\vec{k}_i} \rangle = \langle \phi_{\vec{k}_f} | T | \phi_{\vec{k}_i} \rangle$

$$\Rightarrow \quad U |\psi^{(+)}_{\vec{k}_i}\rangle = T |\phi_{\vec{k}_i}\rangle$$

– we derive L–S eq. for T-operator starting from L–S eq. for $\psi^{(+)}_{\vec{k}_i}$

$$|\psi^{(+)}_{\vec{k}_i}\rangle = |\phi_{\vec{k}_i}\rangle + G_0^{(+)} U |\psi^{(+)}_{k_i}\rangle \qquad \Big/ \text{ mult. by } U \text{ from the left}$$

$$\underbrace{U|\psi^{(+)}_{k_i}\rangle}_{T|\phi_{k_i}\rangle} = U|\phi_{\vec{k}_i}\rangle + U G_0^{(+)} \underbrace{U|\psi^{(+)}_{k_i}\rangle}_{T|\phi_{k_i}\rangle}$$

$$T|\phi_{k_i}\rangle = U|\phi_{k_i}\rangle + U G_0^{(+)} T |\phi_{k_i}\rangle \Rightarrow \boxed{T = U + U G_0^{(+)} T}$$ L–S equation for T-operator

L–S equation for the Green's function:

– the full Green's function of the Schr. eq. satisfies

$$[\Delta + k^2 - U]\, G^{(+)}(\vec{r},\vec{r}') = \delta(\vec{r}-\vec{r}')$$

$$[\Delta + k^2]\, G^{(+)}(\vec{r},\vec{r}') = \underbrace{\delta(\vec{r}-\vec{r}')}_{} + U(\vec{r})\, G^{(+)}(\vec{r},\vec{r}')$$

$$\Rightarrow [\Delta + k^2]\, G_0^{(+)}(\vec{r},\vec{r}') = \delta(\vec{r}-\vec{r}')$$ Green's function of the free Schr. equation

$$[\Delta + k^2]\, G^{(+)}(\vec{r},\vec{r}') = [\Delta + k^2]\, G_0^{(+)}(\vec{r},\vec{r}') + U(\vec{r})\, G^{(+)}(\vec{r},\vec{r}')$$

$$[\Delta + k^2]\underbrace{\left(G^{(+)}(\vec{r},\vec{r}') - G_0^{(+)}(\vec{r},\vec{r}')\right)}_{} = U(\vec{r})\, G^{(+)}(\vec{r},\vec{r}')$$

– the solution can be found again using the free Green's function integrated with the source term on RHS

$$G^{(+)}(\vec{r},\vec{r}') - G_0(\vec{r},\vec{r}') = \int dr''\, G_0^{(+)}(\vec{r},\vec{r}'')\, U(\vec{r}'')\, G^{(+)}(\vec{r}'',\vec{r}')$$

$$G^{(+)}(\vec{r},\vec{r}') = G_0(\vec{r},\vec{r}') + \int dr''\, G_0^{(+)}(\vec{r},\vec{r}'')\, U(\vec{r}'')\, G^{(+)}(\vec{r}'',\vec{r}')$$

written indep. of representation:

$$\boxed{G^{(+)} = G_0^{(+)} + G_0^{(+)} U G^{(+)}}$$ L–S equation for Green's operator

Relation to pw T-matrix elements:

$$f(\vec{k}_i,\vec{k}_f) = \overset{(-2\pi^2)}{\cdot}\langle \phi_{\vec{k}_f} | T | \phi_{\vec{k}_i} \rangle = \Big| \phi_{\vec{k}} = (2\pi)^{-3/2} \cdot \exp[i\vec{k}\cdot\vec{r}] = \frac{4\pi}{(2\pi)^{3/2}} \cdot \sum_{lm} i^l j_l(kr) \cdot Y^*_{lm}(\vec{k}) Y_{lm}(\vec{r}) \Big| =$$

$$= \frac{(4\pi)^2 \cdot (-2\pi^2)}{(2\pi)^3} \sum_{lm} \sum_{l'm'} i^{l-l'} Y_{l'm'}(\vec{k}_i^*) Y_{lm}(\vec{k}_f) \underbrace{\langle j_l Y_{lm} | T | j_{l'} Y_{l'm'} \rangle}_{\sim \delta_{l,l'} \cdot \delta_{m,m'} \text{ for sph. sym. } U(\vec{r})} = \underbrace{\frac{(4\pi)^2 (-2\pi^2)}{(2\pi)^3}}_{-4\pi} \sum_{l,m} Y_{lm}(\vec{k}_i^*) Y_{lm}(\vec{k}_f) \cdot T_{l,l} =$$

$$= \Big| P_l(\vec{k}_i \cdot \vec{k}_f) = P_l(\cos\theta) = \frac{4\pi}{2l+1} \sum_{m} Y^*_{lm}(\vec{k}_i) Y_{lm}(\vec{k}_f) \Big| = -4\pi \cdot \sum_l T_{l,l} \cdot \frac{2l+1}{4\pi} \cdot P_l(\cos\theta) = -\sum_l T_l (2l+1) \cdot P_l(\cos\theta)$$

$T_l = T_{l,l}$ defined for <u>spherical Bessel functions</u>

– compare with partial-wave amplitude defined earlier (for $\vec{k}_i \parallel \vec{z}$)

$$f(\theta) = \sum_l \frac{2l+1}{2ik} \underbrace{\left(e^{2i\delta_l} - 1\right)}_{= t_l \dots \text{ for Riccatti-Bessel functions}} P_l(\cos\theta) = \sum_l \frac{t_l}{2ik} (2l+1) \cdot P_l(\cos\theta) \Rightarrow \boxed{T_l = -\frac{t_l}{2ik} = \frac{t_l \cdot i}{2k}}$$

⇒ <u>message is:</u> partial-wave T-matrix elements can be used to reconstruct scattering amplitudes for specific directions

– we see here again ~~the~~ <u>importance of the partial-wave basis</u>!

cont.

Validity of the Born approximation:

- From the L-S equation we can express the difference:

$$\left|\psi^{(+)}_{\vec{k}_i}(\vec{r}) - \phi_{\vec{k}_i}(\vec{r})\right| = \frac{1}{4\pi}\left|\int d^3r' \, \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} \cdot \frac{2m}{\hbar^2} V(\vec{r}\,') \, \psi^{(+)}_{\vec{k}_i}(\vec{r}\,')\right|$$

- if Born approximation is valid then the replacement $\psi^{(+)}_{\vec{k}_i}(\vec{r}) \to \phi_{\vec{k}_i}(\vec{r})$ means $|\psi^{(+)}_{\vec{k}_i}(\vec{r}) - \phi_{\vec{k}_i}(\vec{r})| \ll 1$ (i.e. the difference between exact and pw is small)
- in particular this condition must be satisfied for $\vec{r}=0$ where we assume that the potential is the strongest.
- therefore we set $\vec{r}=0$ and $\psi^{(+)}_{\vec{k}_i} = (2\pi)^{-3/2} \exp[i\vec{k}_i \cdot \vec{r}\,']$ and obtain the condition:

$$\boxed{\frac{2\pi^{-3/2}}{4\pi}\left|\int d^3r' \, \frac{e^{i(k\cdot r' + \vec{k}_i \cdot \vec{r}\,')}}{r'} \cdot \frac{2m}{\hbar^2} V(r')\right| \ll 1}$$

- this is satisfied if the potential is weak or k is large.

Example: scattering of charged particles by neutral atoms

- charge of the particle is: c
- the potential energy is: $V(\vec{r}\,') = c \cdot \frac{1}{4\pi\varepsilon_0} \int d^3r'' \, \frac{-Zq_e \, \delta(\vec{r}\,'') + \rho(\vec{r}\,'')}{|\vec{r}\,' - \vec{r}\,''|}$

ATOMIC NUMBER, elem. charge, electronic charge density

- scattering amplitude in the first Born approx:

$$f^{(1)}(\theta,\varphi) = -\frac{m}{2\pi\hbar^2}\int d^3r' \, e^{-i\vec{q}\cdot\vec{r}\,'} \, V(\vec{r}\,') = -\frac{m\cdot c}{8\pi^2\varepsilon_0\hbar^2} \int d^3r' \, e^{-i\vec{q}\cdot\vec{r}\,'} \int d^3r'' \, \frac{-Zq_e\,\delta(\vec{r}\,'') + \rho(\vec{r}\,'')}{|\vec{r}\,' - \vec{r}\,''|}$$

- We would like to perform the integral over $\vec{r}\,'$ first otherwise we would have to deal (due to $\rho(\vec{r}\,'')$) with an integral over $\vec{r}\,'$ with some general function.
- However the $\vec{r}\,'$ integral diverges (consider: $\int d^3r \, e^{-i\vec{q}\cdot\vec{r}} \, \frac{e^{-\alpha r}}{r} = \dots 2\pi \cdot \frac{1}{iq}\left[\frac{e^{(-\alpha+iq)r}}{-\alpha+iq} + \frac{e^{-(\alpha+iq)r}}{\alpha+iq}\right]_0^\infty$

α eliminates the divergence at ∞)

- Therefore we bypass the problem introducing the convergence factor $\alpha > 0$:

$$f^{(1)}(\theta,\varphi) = -\frac{m\cdot c}{8\pi^2\varepsilon_0\hbar^2} \cdot \lim_{\alpha\to 0} \int d^3r' \, e^{-i\vec{q}\cdot\vec{r}\,'} \int d^3r'' \, \frac{e^{-\alpha|\vec{r}\,'-\vec{r}\,''|}}{|\vec{r}\,'-\vec{r}\,''|} \cdot \left(-Zq_e\,\delta(\vec{r}\,'') + \rho(\vec{r}\,'')\right) =$$

change the order of integrations

$$= -\frac{m\cdot c}{8\pi^2\varepsilon_0\hbar^2} \int d^3r'' \left[-Zq_e\,\delta(\vec{r}\,'') + \rho(\vec{r}\,'')\right] \cdot \lim_{\alpha\to 0} \int d^3r' \, e^{-i\vec{q}\cdot\vec{r}\,'} \, \frac{e^{-\alpha|\vec{r}\,'-\vec{r}\,''|}}{|\vec{r}\,'-\vec{r}\,''|} =$$

$$= -\frac{m\cdot c}{8\pi^2\varepsilon_0\hbar^2} \cdot \int d^3r'' \left(-Zq_e\,\delta(\vec{r}\,'') + \rho(\vec{r}\,'')\right) e^{-i\vec{q}\cdot\vec{r}\,''} \lim_{\alpha\to 0} \int d^3s \, \frac{\exp[-\alpha\cdot s - i\vec{q}\cdot\vec{s}]}{s} =$$

shift the integrand: $\vec{r}\,' = \vec{s} + \vec{r}\,''$

$$\lim_{\alpha\to 0} \frac{4\pi}{\alpha^2+q^2} = \frac{4\pi}{q^2} \quad \text{(HOMEWORK)}$$

First Born approximation:

– the exact amplitude is given by:

$$f(\theta,\varphi) = -2\pi^2 \langle \phi_{k_f} | U | \psi^{(+)}_{\vec{k}_i} \rangle = -\frac{(2\pi)^{3/2}}{4\pi} \int d^3r' \exp[-i\vec{k}_f\cdot\vec{r}\,'] U(\vec{r}\,') \cdot \psi^{(+)}_{\vec{k}_i}(\vec{r}\,')$$

– we approximate: $\psi^{(+)}_{\vec{k}_i}(\vec{r}\,') \sim \phi_{\vec{k}_i}(\vec{r}\,') = (2\pi)^{-3/2} \exp[i\vec{k}_i\cdot\vec{r}\,']$

$$f(\theta,\varphi) \sim -\frac{1}{4\pi}\int d^3r' \exp[-i\vec{k}_f\cdot\vec{r}\,'] U(\vec{r}\,') \exp[i\vec{k}_i\cdot\vec{r}\,'] =$$

$$= -\frac{1}{4\pi}\int d^3r' \exp[-i\vec{q}\cdot\vec{r}\,'] U(\vec{r}\,'),$$ where $\boxed{\vec{q} = \vec{k}_f - \vec{k}_i}$ is the momentum transfer: $q = 2k\cdot\sin(\frac{\theta}{2})$:

– Commonly $f^{(1)}(\theta,\varphi)$ is written in terms of the potential V: $U = \frac{2m}{\hbar^2}V$

$$\boxed{f^{(1)}(\theta,\varphi) = -\frac{m}{2\pi\cdot\hbar^2}\int d^3r' \exp[-i\vec{q}\cdot\vec{r}\,'] V(\vec{r}\,')}$$

the scattering amplitude is a FT of the potential!

– in the first Born approx. the scattering amplitude is a function of the momentum transfer only

– for inverse symmetric potentials $V(\vec{r}) = V(-\vec{r})$ the Born amplitude is real

$$[f^{(1)}(\theta,\varphi)]^* = -\frac{m}{2\pi\hbar^2}\cdot\int d^3r' \exp[-i\vec{q}\cdot(-\vec{r}\,')] V(\vec{r}\,') = \left| \begin{array}{l} \vec{r} = -\vec{r}\,' \text{ and noting} \\ \text{that } V(\vec{r}\,') = V(-\vec{r}\,') \end{array} \right| =$$

$$= -\frac{m}{2\pi\hbar^2}\cdot\int d^3r \exp[-\vec{q}\,\vec{r}] V(\vec{r}) = f^{(1)}(\theta,\varphi)$$

– this is valid in particular for radially symmetric potentials:

$$f^{(1)}(\theta,\varphi) = -\frac{m}{2\pi\hbar^2}\int_0^\infty dr'(r')^2 \int_0^{2\pi} d\varphi' \int_0^{\pi} d\theta' \sin(\theta')\cdot \exp[-iq\,r'\cos\theta'] V(r') =$$

$$= \left| \begin{array}{l} t = -iqr'\cos\theta' \\ dt = +iqr'\sin(\theta')\,d\theta' \end{array} \right| = -\frac{m}{2\pi\hbar^2}\cdot 2\pi\int_0^\infty dr'(r')^2 \frac{V(r')}{iqr'}\cdot \left[\exp[-iqr'\cdot\underbrace{\cos(\pi)}_{=-1}] - \exp[-iqr'\cos(0)] \right] =$$

$$= -\frac{m}{\hbar^2}\int_0^\infty dr'\cdot\frac{(r')^2 V(r')}{iq\cdot r'}\underbrace{\left(\exp[iqr'] - \exp[-iqr']\right)}_{=2i\sin(qr')} = \boxed{-\frac{2m}{\hbar^2}\int_0^\infty dr'(r')^2\,\frac{\sin(qr')}{qr'}\cdot V(r')}$$

($\Rightarrow$ the angular dep. of $f^{(1)}$ is given by: $q = 2p\cdot\sin(\frac{\theta}{2})$)

– The FT property of Born approximation allows to use the inverse FT to determine $V(\vec{r})$:

$$V(\vec{r}) = -\frac{\hbar^2}{4\pi m}\int d^3q\, e^{i\vec{q}\cdot\vec{r}}\cdot f(\vec{q}).$$ ← we need $f(\vec{q})$ for all momenta

– However experimentally we know only the D.C.S.: $\frac{d\sigma}{d\Omega} = |f(\theta,\varphi)|^2$ ⇒

⇒ only if $f(\theta,\varphi)$ is real we can determine $V(\vec{r})$

→ Finally due to properties of FT we see that if $f(\vec{q})$ is poorly determined for large q we cannot determine the details of $V(r)$ (i.e. for small r)

⇒ to probe details of $V(r)$ we need to use large energies

$$= \boxed{-\frac{m\cdot c}{2\pi\varepsilon_0\hbar^2 q^2}\int d^3r''\, e^{-i\vec{q}\cdot\vec{r}''}\left(-Zq_e\cdot\delta(\vec{r}'')+\rho(\vec{r}'')\right)}$$

- simplification for case of radially-symmetric densities (e.g. H atom)

$\rho(\vec{r}'') = \rho(r'')$:

$$\int d^3r''\, e^{-i\vec{q}\cdot\vec{r}''}\left(-Zq_e\cdot\delta(\vec{r}'')+\rho(\vec{r}'')\right) = -Zq_e + F(\theta),\ \text{where}$$

$$\boxed{F(\theta) = \frac{4\pi}{q}\int_0^\infty dr''\, r''\rho(r'')\sin(q r'')} \quad \text{FORM-FACTOR}$$

angular integral over $d\Omega''$

(the FT of $\rho(r'')$ was evaluated like in case of Born ampl. for radial potential)

- putting the Form factor into the expression for the scattering ampl. we get:

$$f^{(1)}(\theta) = -\frac{m\cdot c}{8\pi\varepsilon_0\cdot\hbar^2 k^2\sin^2(\theta/2)}\left[-Zq_e+F(\theta)\right]$$

$$\left[\frac{q}{2}=k\cdot\sin\left(\frac{\theta}{2}\right)\right]^2$$

$\Rightarrow \dfrac{d\sigma}{d\Omega} = |f^{(1)}(\theta)|^2$ ... therefore we can measure the Form-factor

- and using the inverse FT we can therefore determine the electronic charge distribution

- alternatively in nuclear physics we could determine the structure of the nucleus.