Lippmann – Schwinger: integral equation for Schrödinger equation

time-dependent perturbation: application to elastic scattering problem

$$\underbrace{|\psi\rangle}_{\text{final state}} = \underbrace{|\phi\rangle}_{\text{initial state}} + \hat{G}_0 \hat{V} |\psi\rangle$$

interaction potential

self – consistency equation

$$= \lim_{\varepsilon \downarrow 0} \frac{-1}{\hat{H}_0 - E - i\varepsilon}$$

"resolvent

convert Dirac notation into representation $\hat{\vec{x}}\,|\vec{x}\rangle = \vec{x}\,|\vec{x}\rangle$

$$\underbrace{\langle \vec{x} | \psi \rangle}_{= \psi(\vec{x})} = \underbrace{\langle \vec{x} | \phi \rangle}_{= \phi(\vec{x})} + \langle \vec{x} | \hat{G}_0 \hat{V} \underbrace{1}_{= \int d^3x' |\vec{x}'\rangle\langle\vec{x}'|} | \psi \rangle$$

$= \psi(\vec{x})$ scattered wave function

$= \phi(\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}_i\vec{x}}$ plane wave

$$= \int d^3x' \underbrace{\hat{V} |\vec{x}'\rangle}_{= |\vec{x}'\rangle V(\vec{x}')} \underbrace{\langle \vec{x}' | \psi \rangle}_{= \psi(\vec{x}')}$$

$V(\vec{x}')$: scattering potential

$$= \int d^3x' \langle \vec{x} | \hat{G}_0 | \vec{x}' \rangle \, V(\vec{x}') \, \psi(\vec{x}')$$

$$= \lim_{\varepsilon \downarrow 0} \underbrace{\langle \vec{x} | \frac{1}{\hat{H}_0 - E - i\varepsilon} | \vec{x}' \rangle} \quad ; \quad \hat{H}_0 = -\frac{\hbar^2}{2m}\Delta = \frac{\vec{P}^2}{2m}$$

$$= \int d^3q \, \underbrace{\langle \vec{x} | \vec{q} \rangle}_{\frac{1}{(2\pi)^3} e^{+i\vec{x}\vec{q}}} \underbrace{\langle \vec{q} | \frac{1}{\hat{H}_0 - E - i\varepsilon}}_{\frac{1}{\frac{\hbar^2 q^2}{2m} - E - i\varepsilon}} \underbrace{| \vec{x}' \rangle}$$

$$\underbrace{\langle \vec{q} | \vec{x}' \rangle}_{= \frac{1}{(2\pi)^3} e^{-\vec{q}'\vec{x}'}}$$

$$= G_0(\vec{x}, \vec{x}'; E) = \lim_{\varepsilon \downarrow 0} \int \frac{d^3q}{(2\pi)^3} e^{i(\vec{x} - \vec{x}')\vec{q}} \frac{1}{\frac{\hbar^2 q^2}{2m} - E - i\varepsilon}$$

convergence $\hat{=}$ Feynman $i\varepsilon$ prescription

Lippmann-Schwinger equation in spatial representation:

$$\Psi(\vec{x}) = \underbrace{\phi(\vec{x})}_{\text{plane wave}} + \int d^3x' \, G_0(\vec{x}, \vec{x}'; E) \, V(\vec{x}') \, \Psi(\vec{x}')$$

will be recovered next week from converting the $\overbrace{\text{Schrödinger}}^{\text{time-independent}}$ equation into an equivalent integral equation.

Scattering Theory

$$\left\{ -\frac{\hbar^2}{2m_1}\Delta_{\vec{x}_1} - \frac{\hbar^2}{2m_2}\Delta_{\vec{x}_2} + \underbrace{V^{(int)}(\vec{x}_1, \vec{x}_2)} \right\} \Psi(\vec{x}_1, \vec{x}_2) = E \, \Psi(\vec{x}_1, \vec{x}_2)$$

$= V^{(int)}(\vec{x}_1 - \vec{x}_2)$ interaction potential

collective coordinates:

- center of mass coordinate: $\vec{X} = \frac{m_1 \vec{x}_1 + m_2 \vec{x}_2}{m_1 + m_2}$ $\quad M_{tot} = m_1 + m_2$ total mass

- relative coordinate: $\vec{x} = \vec{x}_1 - \vec{x}_2$ $\quad \frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$ reduced mass

$$\{\underbrace{-\frac{\hbar^2}{2M_{tot}} \Delta_{\vec{X}}}_{\text{dep. } \vec{X}} \underbrace{- \frac{\hbar^2}{2\mu} \Delta_{\vec{x}} + V^{(int)}(\vec{x})}_{\text{dep. on } \vec{x}}\} \Psi(\vec{x}, \vec{X}) = E \, \Psi(\vec{x}, \vec{X})$$

$$\mu = \frac{m_1 \cdot m_2}{m_1 + m_2}$$

separation ansatz: $\Psi(\vec{x}, \vec{X}) = \frac{e^{i\vec{K}\vec{X}}}{(2\pi)^3} \psi(\vec{x})$, $\quad E = \frac{\hbar^2 \vec{K}^2}{2M_{tot}} + \underbrace{\varepsilon}_{= \frac{\hbar^2 \vec{k}^2}{2\mu}}$

$$\{-\frac{\hbar^2}{2\mu} \Delta_{\vec{x}} + \underbrace{V^{(int)}(\vec{x})}_{= v^{(int)}(|\vec{x}|)}\} \psi(\vec{x}) = \underbrace{\varepsilon}_{\geq 0} \psi(\vec{x})$$

≥ 0 for scattering problem

basic assumption

$= v^{(int)}(\underbrace{|\vec{x}|}_{= r})$

isotropy !

Due to assumed isotropy: ~~sph~~ spherical coordination

$$\psi(\vec{x}) = \psi(r, \vartheta, \varphi)$$

$$\Delta_{\vec{x}} = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\vec{L}^2}{r^2 \hbar^2}$$

$\vec{L}^2 \leftarrow$ angular momentum

separation: $\vec{L}^2 Y_{lm}(\vartheta, \varphi) = \hbar^2 l(l+1) Y_{lm}(\vartheta, \varphi)$

$l = 0, 1, 2, 3, \underbrace{\ldots}$; $m = -l, \ldots, +l$

no boundary here in contrast of hydrogen atom

$\psi(r,\vartheta,\varphi) = R_l(r)\, Y_{lm}(\vartheta,\varphi)$; $\varepsilon = \frac{\hbar^2 k^2}{2\mu}$

resulting differential equation for radial part:

$$\left\{ \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} + k^2 - \frac{2\mu}{\hbar^2} v^{(int)}(r) \right\} R_l(r) = 0$$

Free scattering solution: $v^{(int)}(r) \equiv 0$

Here: radial equation far away from localized scattering potential

$\rightarrow$ far-field solution

$$\left\{ \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} + k^2 \right\} R_l(r) = 0$$

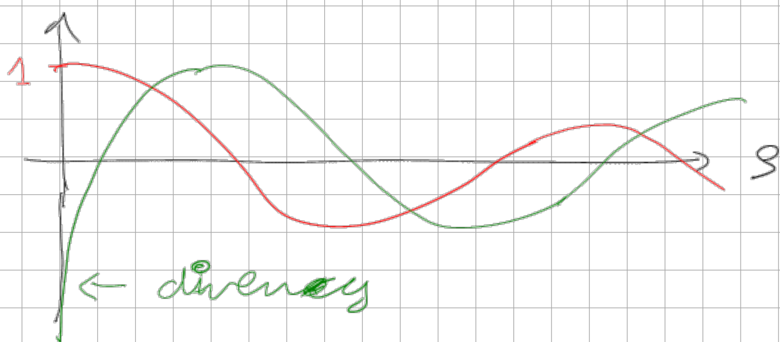
dimensionless radius: $\rho = rk$, $R_l(\rho) \hat{=} R_l(kr)$

$$\left\{ \frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial}{\partial \rho} - \frac{l(l+1)}{\rho^2} + 1 \right\} R_l(\rho) = 0$$

$\rightarrow$ two fundamental solutions:

$l = 0$: s-wave
$$\left\{ \frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial}{\partial \rho} + 1 \right\} R_0(\rho) = 0$$

$$\boxed{\begin{aligned} R_0^{(1)}(\rho) &= \frac{\sin\rho}{\rho} \\ R_0^{(2)}(\rho) &= -\frac{\cos\rho}{\rho} \end{aligned}}$$



general l: $\quad R_l(\rho) = \underline{\rho^l}\, \chi_l(\rho)$

$$\left(\frac{\partial^2}{\partial\rho^2} + \frac{2(l+1)}{\rho}\frac{\partial}{\partial\rho} + 1\right)\chi_l(\rho) = 0 \qquad \Big|\ \boxed{\frac{1}{\rho}\frac{\partial}{\partial\rho}}$$

$$\left(\frac{\partial^2}{\partial\rho^2} + \frac{2(l+2)}{\rho}\frac{\partial}{\partial\rho} + 1\right)\underbrace{\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\right)\chi_l(\rho)}_{=:\ \chi_{l+1}(\rho)} = 0$$

recursion formula

spherical Bessel functions

$$j_l(\rho) = -(-\rho)^l\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\right)^l \frac{\sin\rho}{\rho}$$

$$j_0(\rho) = \frac{\sin\rho}{\rho}$$

$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}$$

$$j_2(\rho) = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin\rho - \frac{3}{\rho^2}\cos\rho$$

spherical von Neumann functions

$$n_l(\rho) = -(-\rho)^l\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\right)^l \frac{\cos\rho}{\rho}$$

$$n_0(\rho) = -\frac{\cos\rho}{\rho}$$

$$n_1(\rho) = -\frac{\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho}$$

$$n_2(\rho) = \left(-\frac{3}{\rho^3} + \frac{1}{\rho}\right)\cos\rho - \frac{3}{\rho^2}\sin\rho$$

small argument:

$$j_l(\rho) \approx \frac{\rho^l}{(2l+1)!!}\ ; \quad \rho \downarrow 0 \qquad\qquad n_l(\rho) = -\frac{(2l-1)!!}{\rho^{l+1}}\ ; \quad \rho\downarrow 0$$

finite at $\rho \downarrow 0$ $\qquad\qquad$ diverges at $\rho\downarrow 0$

large arguments:

$$j_l(\rho) \approx \frac{\sin\left(\rho - \frac{l\pi}{2}\right)}{\rho}\ ; \quad \rho\to\infty \qquad\qquad n_l(\rho) = -\frac{\cos\left(\rho - \frac{l\pi}{2}\right)}{\rho}\ ; \quad \rho\to\infty$$

general solution: superposition principle

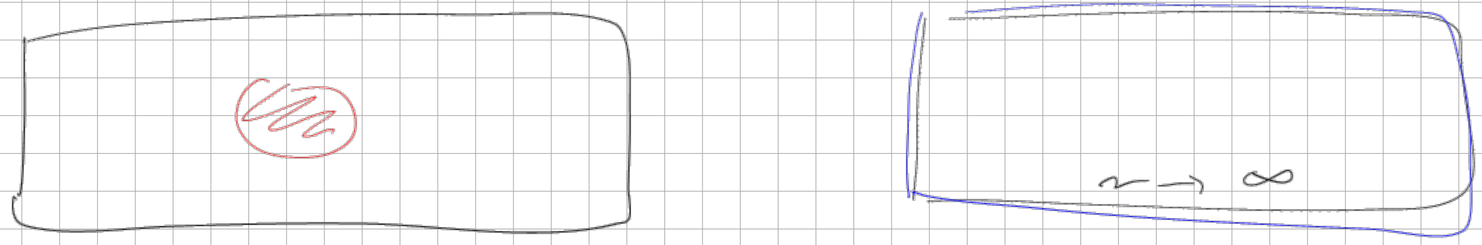
$$R_\ell(r) = A_\ell\, j_\ell(kr) + B_\ell\, n_\ell(kr)$$

determined by boundary conditions

$$R_\ell(r) \xrightarrow{r\to\infty} \frac{A_\ell \sin(\rho - \frac{\ell\pi}{2}) - B_\ell \cos(\rho - \frac{\ell\pi}{2})}{kr} = \frac{C_\ell \sin(kr - \frac{\ell\pi}{2} + \delta_\ell)}{kr}$$

$$C_\ell = \sqrt{A_\ell^2 + B_\ell^2}$$

$$\boxed{\delta_\ell = -\arctan\frac{B_\ell}{A_\ell} \quad \text{phase shift}}$$



scattering center

far away from scattering center

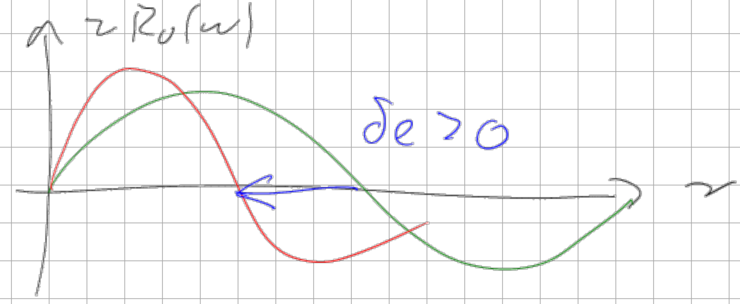
Qualitative result: phase shift δ_ℓ far away from scattering center is affected by $v^{(int)}(r)$:

repulsive scattering potential $v^{(int)}(r) > 0$ $\Rightarrow$ wave function is pushed out $\quad \delta_\ell < 0$

$v^{(int)}(r) < 0$ **attractive** $\Rightarrow$ wave function is pushed in $\quad \delta_\ell > 0$

$v^{(int)}(r) > 0$

repulsive



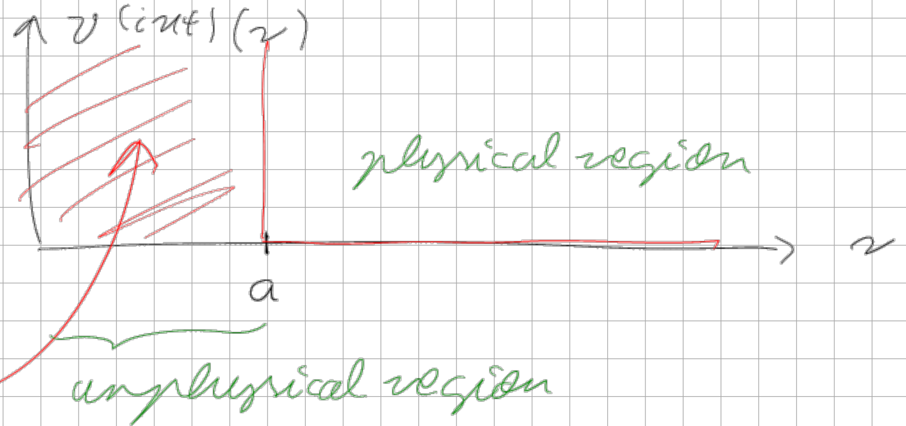
$v^{(int)}(r) < 0$

attractive

Without any calculation we have obtained a qualitative result

Hard spheres:

$$v^{(int)}(r) = \begin{cases} 0 & ; \ r > a \\ \underbrace{\infty}_{\text{forbidden region}} & ; \ 0 \le r \le \underbrace{a}_{\text{radius of sphere}} \end{cases}$$



$$R_\ell(r) = \begin{cases} A_\ell \, j_\ell(kr) + B_\ell \, n_\ell(kr) & ; \ r > a \\ 0 & ; \ 0 \le r \le a \end{cases}$$

boundary condition: continuous at $r = a$

$$0 = A_\ell\, j_\ell(ka) + B_\ell\, n_\ell(ka) \Rightarrow A_\ell = D_\ell\, n_\ell(ka), \quad B_\ell = -D_\ell\, j_\ell(ka)$$

$$C_\ell = \sqrt{A_\ell^2 + B_\ell^2} = D_\ell \sqrt{n_\ell^2(ka) + j_\ell^2(ka)}$$

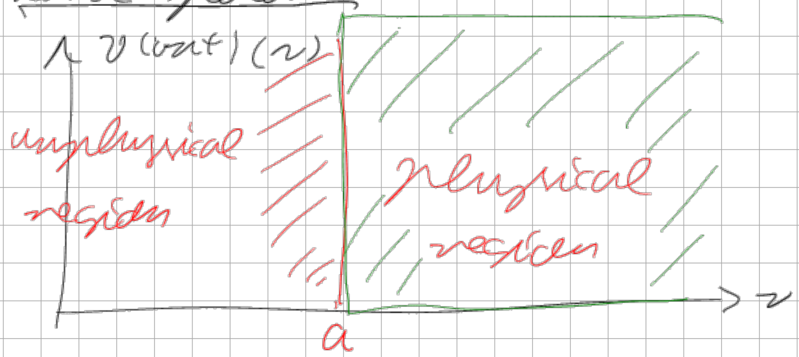
$$\delta_\ell = -\arctan \frac{B_\ell}{A_\ell} = \arctan \frac{j_\ell(ka)}{n_\ell(ka)} = -\frac{(2\ell+1)(ka)^{2\ell+1}}{[(2\ell+1)!!]^2}$$

small energies ≙ small $k = \sqrt{\frac{2\mu E}{\hbar^2}}$: $ka \ll 1$

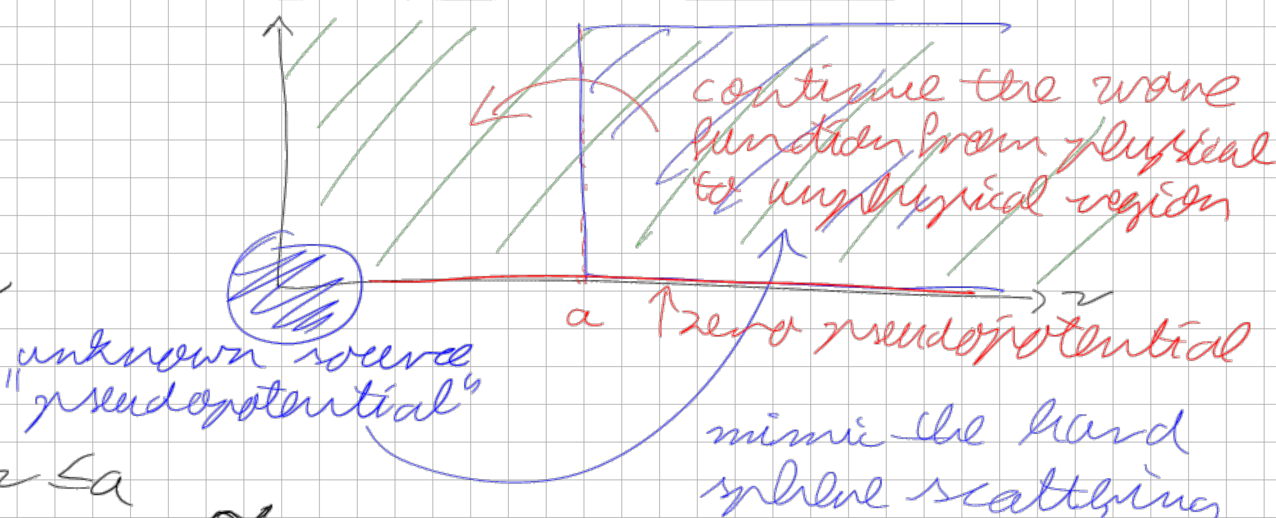
must be because hard sphere scattering is repulsive

$\Rightarrow$ largest phase shift occurs for $\ell = 0$ ≙ s-wave scattering

Hard sphere



Pseudopotential method



$$R_0(r) = \begin{cases} 0 & ; \ 0 \le r \le a \\ A_0\, j_0(kr) + B_0\, n_0(kr) & ; \ r > a \end{cases}$$

$$\tilde{R}_0(r) = A_0\, j_0(kr) + B_0\, n_0(kr); \quad r > 0$$

Goal for next time: find out pseudopotential

$$\tilde{v}^{(int)}(r) = \underbrace{\frac{\hbar^2}{2\mu} 4\pi}_{a} \frac{\tan ka}{k}\, \delta(\vec{x})\, \underbrace{\frac{\partial}{\partial r}\left[r \ \cdot \ \right]}$$