Last time: 2-particle problem

$\downarrow$ reduction

effective 1-particle problem

$$\left\{ -\frac{\hbar^2}{2\mu}\Delta_{\vec{x}} + \underbrace{V^{(int)}(\vec{x})}_{\text{interaction potential}} \right\} \Psi(\vec{x}) = \overbrace{E}^{= \frac{\hbar^2 k^2}{2\mu}} \Psi(\vec{x})$$

(scattering state)

$m_1 = m_2 = m$

$$\mu = \frac{m_1 \cdot m_2}{m_1 + m_2} \quad \text{(reduced mass)} \quad ; \text{ special case: } \mu = \frac{m}{2}$$

$$\Big\{ \underbrace{\Delta_{\vec{x}}}_{\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\hat{\vec{L}}^2}{r^2 \hbar^2}} + k^2 - \frac{2\mu}{\hbar^2} \underbrace{V^{(int)}(\vec{x})}_{= v^{(int)}(\underbrace{|\vec{x}|}_{= r})} \Big\} \Psi(\vec{x}) = 0 \quad ; \quad \Psi(\vec{x}) = \Psi(r, \vartheta, \varphi)$$

(isotropic)

$$= Y_{lm}(\vartheta, \varphi) \underbrace{R_l(r)}_{\text{depends on } k}$$

square of angular momentum operator

$$\hat{\vec{L}}^2 \, Y_{lm}(\vartheta, \varphi) = \hbar^2 l(l+1) Y_{lm}(\vartheta, \varphi) \quad ; \quad l = 0, 1, 2, \dots$$

$\leftarrow$ no bound.... as no ....

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

7.3 Free Scattering Solutions:

here: consider the radial eq. far away from a localized scattering potential $\Longrightarrow$ far-field solution

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

$\hookrightarrow \rho = rk \quad , \quad R_l(\rho) \hat{=} R_l(kr)$

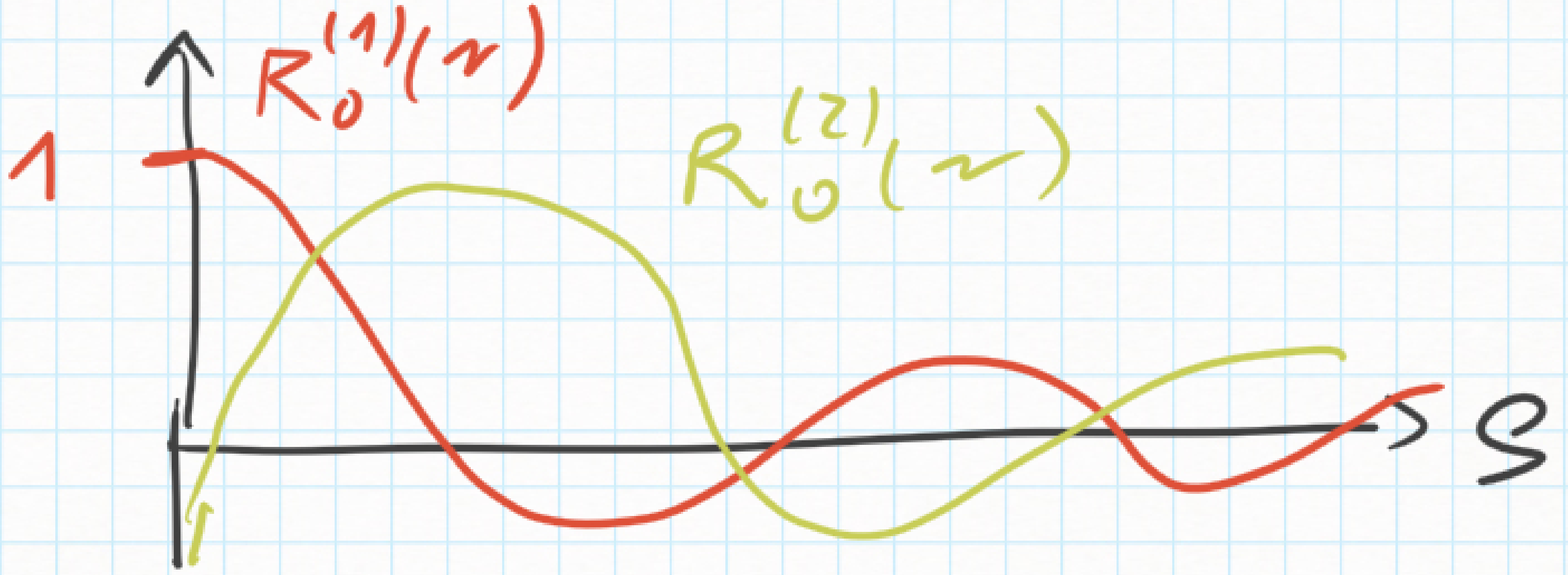
$$\left\{\frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial}{\partial \rho} - \frac{l(l+1)}{\rho^2} + 1\right\} R_l(\rho) = 0 \Longrightarrow 2 \text{ fundamental solutions}$$

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

$\Longrightarrow$ 2 fundamental solutions

$$R_0^{(1)} = \frac{\sin\rho}{\rho} \quad ,$$

$$R_0^{(2)} = -\frac{\cos\rho}{\rho}$$



$R_l(\rho) = \rho^l \chi_l(r)$

$$\left\{\begin{aligned}&\left(\frac{\partial^2}{\partial\rho^2}+\frac{2(l+1)}{\rho}\frac{\partial}{\partial\rho}+1\right)\boxed{\chi_l(\rho)}=0\,; \quad R_l(r)=\underline{\underline{\rho^l}}\,\chi_l(\rho)\\&\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\frac{\partial^2}{\partial\rho^2}+\frac{2(l+1)}{\rho}\frac{\partial}{\partial\rho}+1\right)\chi_l(\rho)=0\end{aligned}\right.$$

$$\Updownarrow$$

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

$$\frac{1}{\rho^2}\left(\cancel{\rho}-\frac{1}{6}\rho^3+\dots\right)-\frac{1}{\rho}\left(\cancel{1}-\frac{1}{2}\rho^2+\dots\right)\sim\rho$$

recursion formula:

<u>spherical Bessel functions</u>

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

convention

$$j_0(\rho)=\frac{\sin\rho}{\rho},\quad j_1(\rho)=\frac{\sin\rho}{\rho^2}-\frac{\cos\rho}{\rho}$$

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

<u>spherical von Neumann functions</u>

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

$$n_0(\rho)=-\frac{\cos\rho}{\rho},\quad n_1(\rho)=-\frac{\cos\rho}{\rho^2}-\frac{\sin\rho}{\rho}$$

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

small arguments:

$$j_\ell(\rho) \approx \frac{\rho^\ell}{(2\ell+1)!!} \quad , \quad n_\ell(\rho) = -\frac{(2\ell-1)!!}{\rho^{\ell+1}} \quad ; \ \rho \downarrow 0$$

$\Rightarrow$ finite at $\rho \downarrow 0$ $\qquad$ $\Rightarrow$ diverge at $\rho \downarrow 0$

large arguments:

$$j_\ell(\rho) \approx \frac{\sin(\rho - \frac{\ell\pi}{2})}{\rho} \qquad n_\ell(\rho) = -\frac{\cos(\rho - \frac{\ell\pi}{2})}{\rho} \quad ; \ \rho \to \infty$$

general solution: superposition principle

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

determined by boundary conditions

localized

far away from interaction potential

$$R_\ell(r) \xrightarrow{r \to \infty} \frac{A_\ell \sin(kr - \ell\pi/2) - B_\ell \cos(kr - \ell\pi/2)}{kr}$$

$$= \frac{C_\ell \sin(kr - \ell\pi/2 + \delta_\ell)}{kr} ;$$

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

phase: $\delta_\ell = -\arctan \frac{B_\ell}{A_\ell}$

$$C_l \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) = C_l \left\{ \sin\left(kr - \frac{l\pi}{2}\right)\cos\delta_l + \cos\left(kr - \frac{l\pi}{2}\right)\sin(\delta_l) \right\}$$

points of constant phase: $kr + \delta_l = \text{const}$

$$\hat{=} A_l \sin\left(kr - \frac{l\pi}{2}\right) - B_l \cos\left(kr - \frac{l\pi}{2}\right)$$

$$\left.\begin{aligned} A_l &= C_l \cos\delta_l \\ B_l &= -C_l \sin\delta_l \end{aligned}\right\} \quad \tan\delta_l = -\frac{B_l}{A_l} \Rightarrow \boxed{\delta_l = -\arctan\frac{B_l}{A_l}}$$

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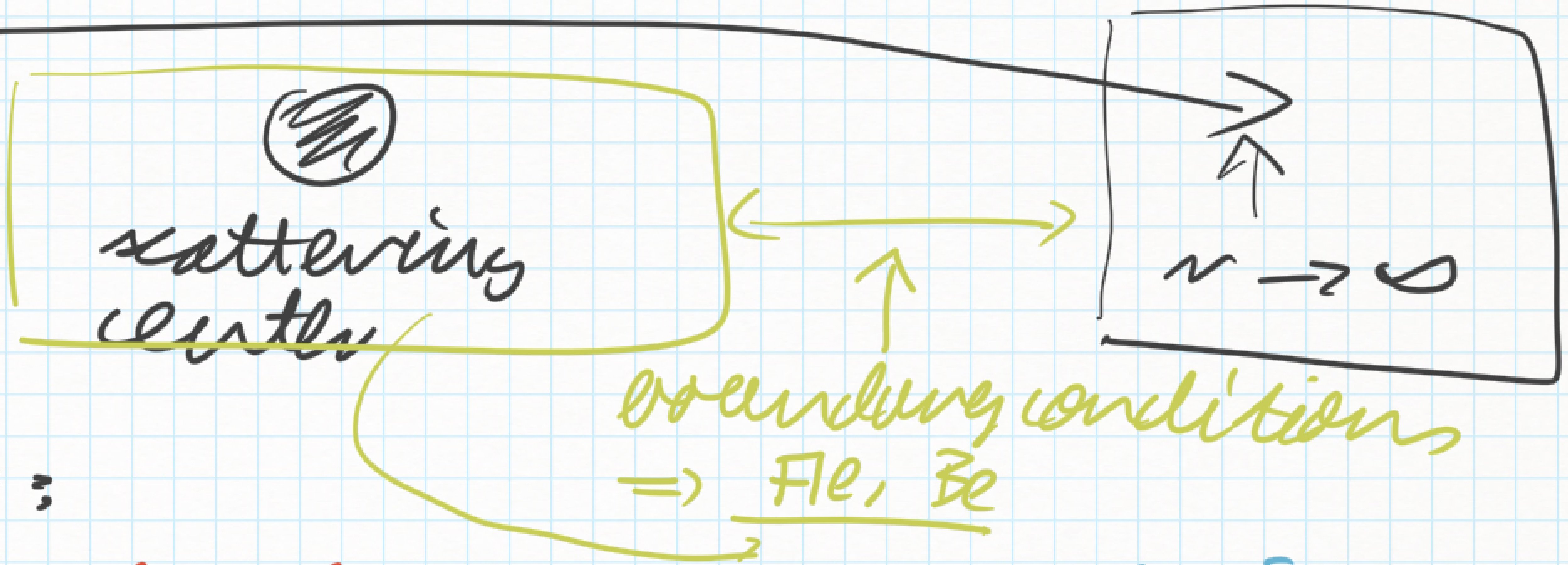
so for: $V^{(int)}(r) = 0$

now: $V^{(int)}(r) \neq 0$, localized

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

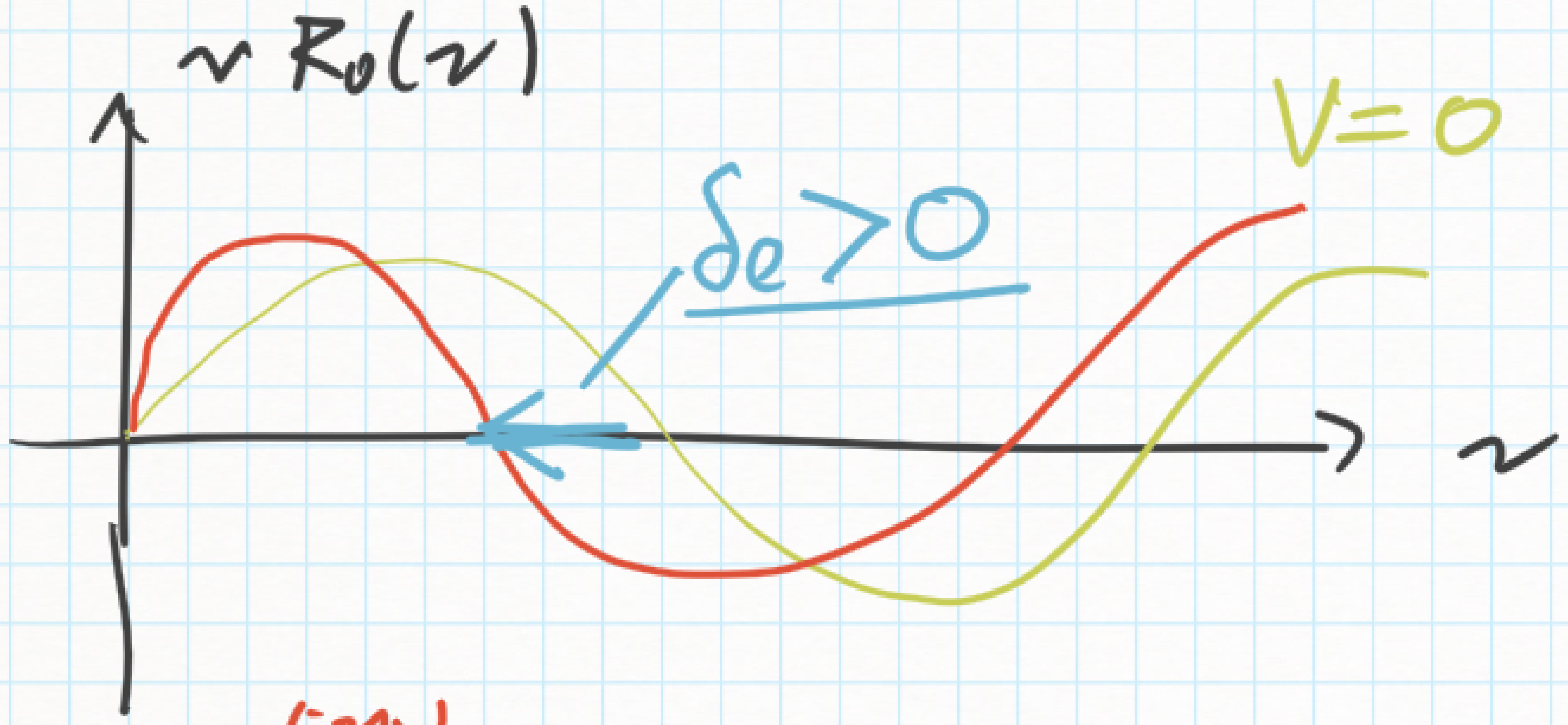


repulsive scattering potential: wave function is pushed away

attractive " " : is shifted towards interaction center

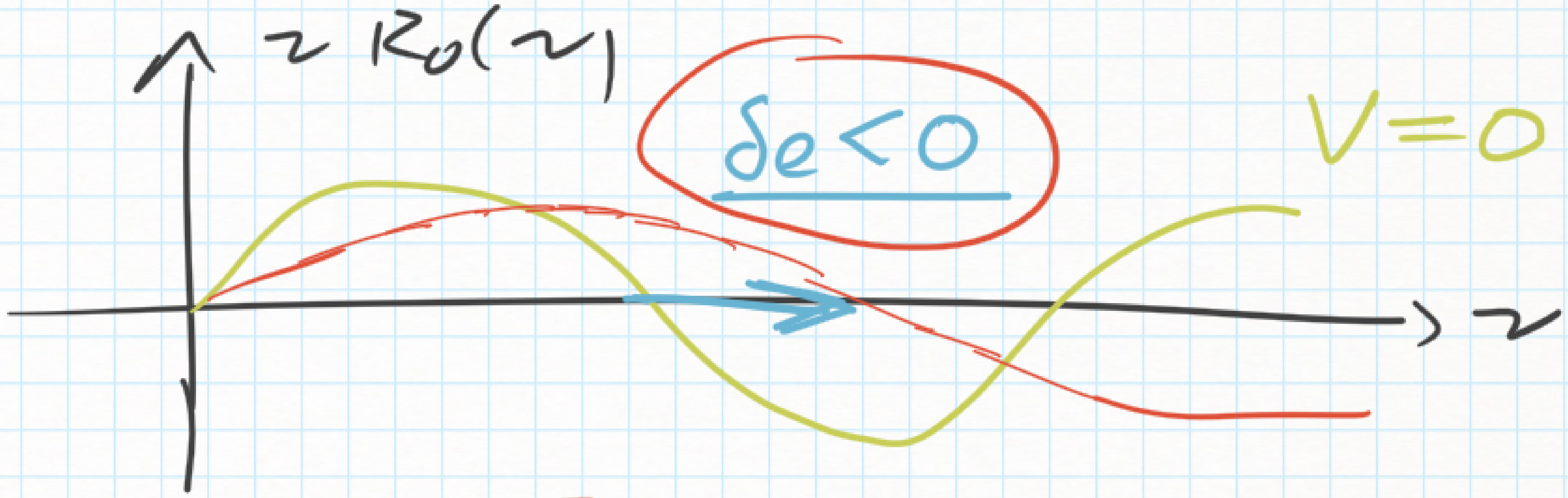
$V^{(int)} > 0 \;\hat{=}\; \delta_l < 0$

$V^{(int)} < 0 \;\hat{=}\; \delta_l > 0$



$V^{(int)} < 0$

attraction



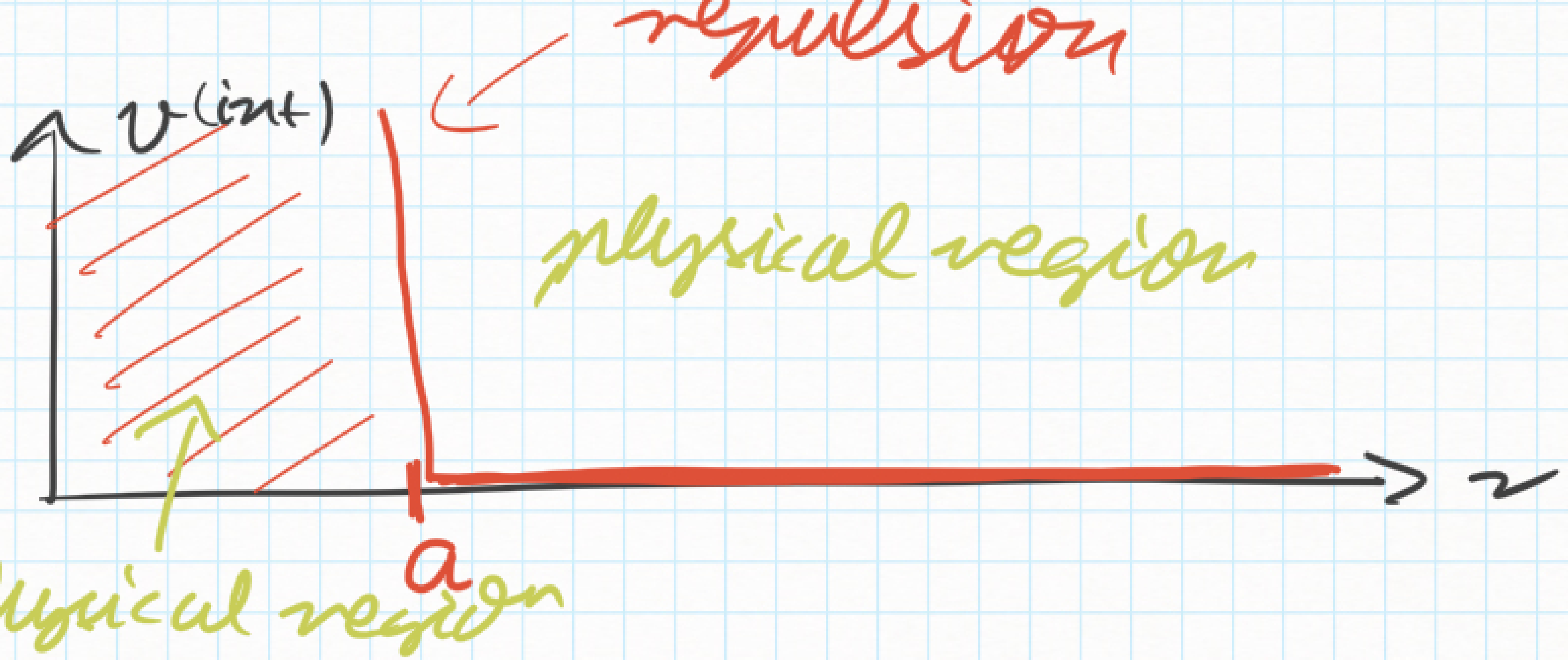
$V^{(int)} > 0$

repulsion

Without any calculation we have obtained already a qualitative inside

7.4 Hard ~~Balls~~ Spheres:

$$v^{(int)}(r) = \begin{cases} 0; & r>a \\ \infty; & 0\le r<a \end{cases}$$



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

boundary condition: continuous at $r = a$

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

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

small argument expansions for j_ℓ, n_ℓ

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

small energies $\hat{=}$ small k $\hat{=}$ small a $\Rightarrow$ $ka \ll 1$

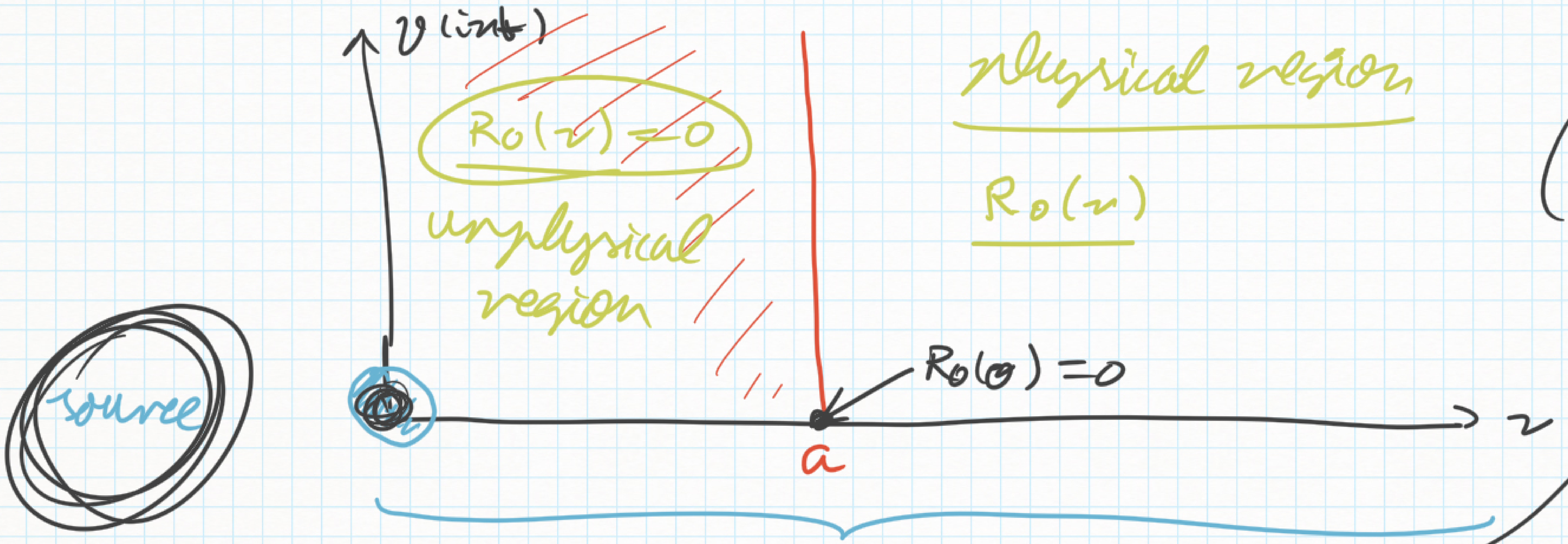
factorial: $\ell! = 1 \cdot 2 \cdot 3 \cdot 4 \cdot 5 \cdot \ldots \ldots$ product of integers

double factorial $\ell!! = 1 \cdot 3 \cdot 5 \cdot \ldots$ product of odd integers

small energies $\Rightarrow$ $ka \ll 1$ $\Rightarrow$ $\ell = 0$ scattering channel is most important

$\Rightarrow$ s-wave scattering

7.5 Pseudopotential Method:



$$\tilde{R}_0(r) = \begin{cases} R_0(r) & ; \; r > a \\ \tilde{R}_0(r) & ; \; 0 \le r \le a \end{cases}$$

$$\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + k^2\right)\tilde{R}_0(r) = 0$$

$$\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + k^2 - \frac{2\mu}{\hbar^2}V^{(int)}(r)\right)\tilde{R}_0(r) = 0$$

Which source at $r=0$ allows us to describe hard sphere problem