Lectures on quantum gases

Lecture 2

Elastic Collision Phenomena in Quantum Gases

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Relative motion of interacting particles I

1. We defined what we mean by ultracold – characteristic lengths
2. Short-range interactions - collisional regimes
3. Separation into CM and REL coordinates
4. We derived the radial wave equation
5. We defined the s-wave regime
6. We identified the phase shift as the central quantity of interest

free particle motion for $l = 0$

$$\chi_l'' + \left[k^2 - U(r) - \frac{l(l+1)}{r^2}\right]\chi_l = 0$$

$l = 0$ and $U(r) = 0$

$$\boxed{\chi_0'' + k^2\chi_0 = 0}$$

General solution: $\boxed{R_0(r) = \frac{\chi_0(r)}{r} = c_0\frac{\sin(kr + \eta_0)}{kr}}$

regular only for $\eta_0 = 0$

Conclusion: free particle – no phase shift

$$R_0(r) = c_0\frac{\sin(kr)}{kr} = c_0 j_0(kr)$$

RWE for short-range potentials

For $U(r) \neq 0$ the radial waves are *distorted*

$$R_l'' + \frac{2}{r} R_l' + \left[k^2 - \cancel{U(r)} - \frac{l(l+1)}{r^2} \right] R_l = 0$$

$r \gg r_0$

$\varrho \equiv kr$

Spherical Bessel differential equation

(free particles)

$$R_l'' + \frac{2}{\varrho} R_l' + \left[1 - \frac{l(l+1)}{\varrho^2} \right] R_l = 0$$

General solution: $R_l(\varrho) = A_l j_l(\varrho) + B_l n_l(\varrho)$

$$\{A_l,\, B_l\} \to \{c_l,\, \eta_l\}$$

$$A_l = c_l \cos \eta_l$$
$$B_l = c_l \sin \eta_l$$

$$\eta_l = \arctan B_l / A_l$$

General solution: $R_l(\varrho) = c_l \left[\cos \eta_l \, j_l(\varrho) + \sin \eta_l \, n_l(\varrho) \right]$

$$\boxed{R_l(k,r) \underset{r \to \infty}{\simeq} \frac{c_l}{kr} \sin(kr + \eta_l - \tfrac{1}{2} l \pi)}$$

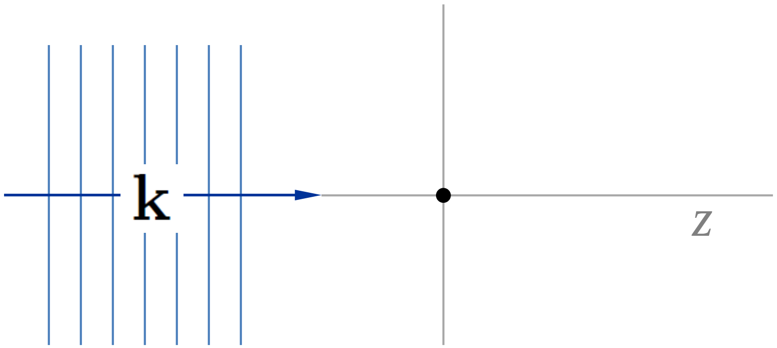
In the far field the distortion is gone but a phase shift remains

full solution

$$\psi_{lm}(\mathbf{r}) = c_{lm} R_l(k,r) Y_l^m(\theta,\phi)$$

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} c_{lm} R_l(k,r) Y_l^m(\theta,\phi)$$

Example: plane wave in free space

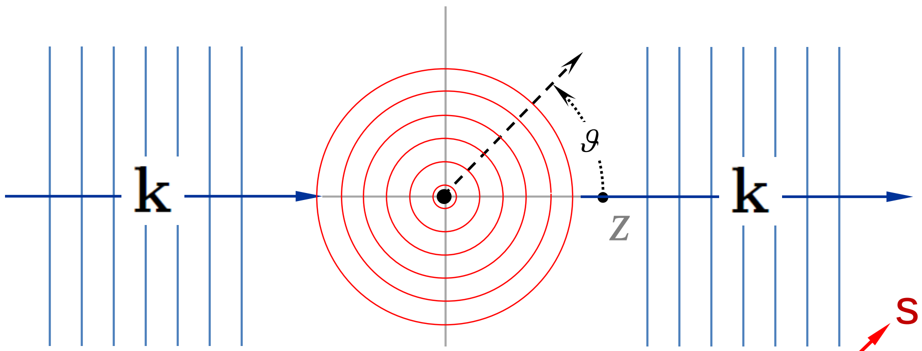


$$R_l(k,r) \rightarrow j_l(kr)$$

$$Y_l^m(\theta,\phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\phi}$$

$$\boxed{e^{ikz} = \sum_{l=0}^{\infty} \underbrace{(2l+1)i^l}_{c_l} j_l(kr) P_l(\cos\theta)}$$

scattering



scattering amplitude

$$\boxed{\psi = \psi_{in} + \psi_{sc} \underset{r\to\infty}{\simeq} e^{ikz} + f(\theta)\frac{e^{ikr}}{r}}$$

$$\psi = \sum_{l=0}^{\infty}(2l+1)i^l c_l R_l(k,r)P_l(\cos\theta) \qquad e^{ikz} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(\cos\theta)$$

$$\psi - \psi_{in} = \psi_{sc} = \sum_{l=0}^{\infty}(2l+1)i^l Q_l(k,r)P_l(\cos\theta)$$

$$Q_l(k,r) \equiv c_l R_l(k,r) - j_l(kr)$$

scattered wavefunction

$$\psi - \psi_{in} = \psi_{sc} = \sum_{l=0}^{\infty} (2l+1) i^l Q_l(k,r) P_l(\cos\theta)$$

$$Q_l(k,r) \equiv c_l R_l(k,r) - j_l(kr)$$

scattered wavefunction

$$\psi - \psi_{in} = \psi_{sc} = \sum_{l=0}^{\infty} (2l+1) i^l Q_l(k,r) P_l(\cos\theta)$$

$$Q_l(k,r) \equiv c_l R_l(k,r) - j_l(kr)$$

$$Q_l(k,r) \underset{r\to\infty}{\simeq} \frac{1}{kr}\left[c_l \sin(kr + \eta_l - \frac{1}{2}l\pi) - \sin(kr - \frac{1}{2}l\pi)\right]$$

$$\underset{r\to\infty}{\simeq} \frac{1}{2ikr}\left[i^{-l}e^{ikr}e^{i\eta_l}c_l - i^l e^{-ikr}e^{-i\eta_l}c_l - i^{-l}e^{ikr} + i^l e^{-ikr}\right]$$

$$\boxed{\sin x = \frac{e^{ix} - e^{-ix}}{2i}} \quad \boxed{e^{i\frac{\pi}{2}} = i}$$

scattered wavefunction

create outgoing partial wave: $c_l = e^{i\eta_l}$

$$Q_l(k,r) \underset{r\to\infty}{\simeq} \frac{1}{2ikr}\left(i^{-l}e^{ikr}e^{i\eta_l}c_l - i^l e^{-ikr}e^{-i\eta_l}c_l - i^{-l}e^{ikr} + i^l e^{-ikr}\right)$$

$$\underset{r\to\infty}{\simeq} \frac{1}{2ikr}i^{-l}\left(e^{ikr}e^{2i\eta_l} - \cancel{i^{2l}e^{-ikr}} - e^{ikr} + \cancel{i^{2l}e^{-ikr}}\right)$$

$$\underset{r\to\infty}{\simeq} \frac{e^{ikr}}{2ikr}i^{-l}\left(e^{2i\eta_l} - 1\right)$$

$$\psi_{sc} = \sum_{l=0}^{\infty}(2l+1)i^l Q_l(k,r)P_l(\cos\theta)$$

$$\psi_{sc} = \frac{e^{ikr}}{r}\sum_{l=0}^{\infty}(2l+1)\frac{1}{2ik}\left(e^{2i\eta_l}-1\right)P_l(\cos\theta)$$

scattered wavefunction

$$\psi(r,\theta) \underset{r\to\infty}{\sim} e^{ikz} + \underbrace{f(\theta)e^{ikr}/r}$$

$$\psi_{sc} = \frac{e^{ikr}}{r} \underbrace{\sum_{l=0}^{\infty}(2l+1)\frac{1}{2ik}\left(e^{2i\eta_l}-1\right)P_l(\cos\theta)}$$

$$\boxed{f(\theta) = \sum_{l=0}^{\infty}(2l+1)f_l P_l(\cos\theta)}$$

$$f(0) = \sum_{l=0}^{\infty}(2l+1)f_l$$

forward scattering amplitude

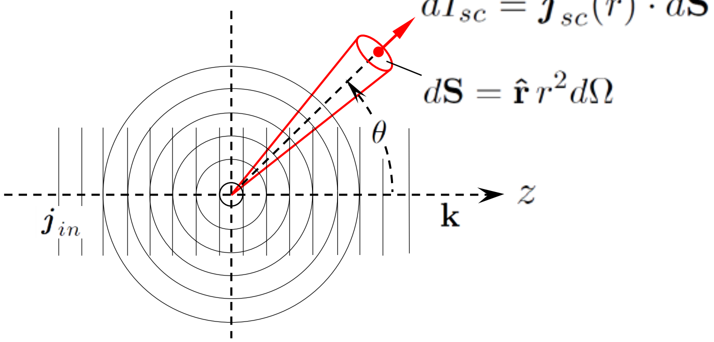
$$f_l = \frac{1}{2ik}(e^{2i\eta_l}-1)$$

partial-wave scattering amplitude

partial wave scattering amplitude

$$\begin{aligned} f_l &= \frac{1}{2ik}\left(e^{2i\eta_l} - 1\right) && \text{(a)} \\ &= k^{-1} e^{i\eta_l} \sin\eta_l && \text{(b)} \\ &= \frac{1}{k\cot\eta_l - ik} && \text{(c)} \\ &= k^{-1}\left(\sin\eta_l \cos\eta_l + i\sin^2\eta_l\right) && \text{(d)} \end{aligned}$$

differential cross section



$$\psi = \psi_{in} + \psi_{sc} \underset{r \to \infty}{\simeq} e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$$

Current density incident wave:

$$\boldsymbol{j}_{in} = \frac{i\hbar}{2\mu}\left(\psi_{in}\boldsymbol{\nabla}\psi_{in}^* - \psi_{in}^*\boldsymbol{\nabla}\psi_{in}\right) = \hat{\mathbf{z}}\frac{i\hbar}{2\mu}(-2ik) = \frac{\hbar\mathbf{k}_z}{\mu} = \mathbf{v}_z$$

Current density scattered wave

$$\boldsymbol{j}_{sc} = \frac{i\hbar}{2\mu}\left(\psi_{sc}\boldsymbol{\nabla}\psi_{sc}^* - \psi_{sc}^*\boldsymbol{\nabla}\psi_{sc}\right) = \frac{|f(\theta)|^2}{r^2}\frac{\hbar\mathbf{k}_r}{\mu} = \frac{|f(\theta)|^2}{r^2}\mathbf{v}_r$$

Current scattered through surface $d\mathbf{S}$ (into solid angle $d\boldsymbol{\Omega}$):

$$dI_{sc} = \boldsymbol{j}_{sc}(r) \cdot d\mathbf{S} = v\,|f(\theta)|^2\, d\Omega$$

$$d\mathbf{S} = \hat{\mathbf{r}}\, r^2 d\Omega$$

$$d\sigma(\theta, \phi) = \frac{dI_{sc}(\theta, \phi)}{j_{in}} = |f(\theta)|^2\, d\Omega$$

$$\boxed{\frac{d\sigma(\theta, \phi)}{d\Omega} = |f(\theta)|^2}$$

cross sections

Partial cross section:

$$\boxed{d\sigma\left(\theta,\phi\right) = \left|f\left(\theta\right)\right|^{2} d\Omega} \longrightarrow d\sigma(\theta) = 2\pi \sin\theta \left|f\left(\theta\right)\right|^{2} d\theta$$

$$d\Omega = \sin\theta d\theta d\phi$$

$$f\left(\theta\right) = \sum_{l=0}^{\infty}(2l+1) f_l P_l(\cos\theta)$$

(b) $\longrightarrow f_l = \frac{1}{k} e^{i\eta_l} \sin\eta_l$

$$d\sigma(\theta) = \frac{2\pi}{k^2} \sum_{l,l'=0}^{\infty} (2l+1)(2l'+1) e^{i(\eta_l - \eta_{l'})} \sin\eta_l \sin\eta_{l'} P_l(\cos\theta) P_{l'}(\cos\theta) \sin\theta d\theta$$

$$\int_0^{\pi} \left[P_l(\cos\theta)\right]^2 \sin\theta d\theta = \frac{2}{2l+1}$$

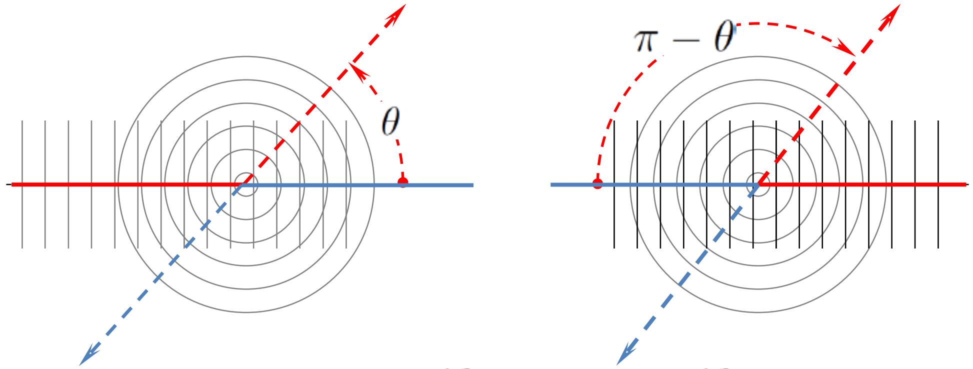
$$\sigma = 4\pi \sum_{l=0}^{\infty}(2l+1)|f_l|^2 \equiv \sum_{l=0}^{\infty} \sigma_l$$

Total cross section:

$$\boxed{\sigma = \int_0^{\pi} 2\pi \sin\theta \left|f\left(\theta\right)\right|^{2} d\theta} \longrightarrow \boxed{\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty}(2l+1)\sin^2\eta_l}$$

Identical particles

Identical particles



$$\psi_{in} = e^{ikz} \pm e^{-ikz}$$

Bosons: symmetric under exchange

Fermions: antisymmetric under exchange

$$\psi_{sc} \underset{r\to\infty}{\simeq} [f(\theta) \pm f(\pi - \theta)]e^{ikr}/r$$

$$\psi \underset{r\to\infty}{\simeq} (e^{ikz} \pm e^{-ikz}) + [f(\theta) \pm f(\pi - \theta)]e^{ikr}/r$$

Identical particles

$$e^{ikz} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta)$$

$$e^{-ikz} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(-\cos\theta)$$

$$P_l(-u) = (-1)^l P_l(u)$$

$$\rightarrow \quad e^{-ikz} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) (-1)^l P_l(\cos\theta)$$

$$\psi_{in} = e^{ikz} \pm e^{-ikz} = 2 \sum_{l=\substack{even \\ odd}}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta)$$

Conclusion: Bosons *even* partial waves; fermions *odd* partial waves

quantum statistical properties of cross section

Bosons (even partial waves): s-wave scattering

$$\sigma = \frac{8\pi}{k^2} \sum_{l=\text{even}} (2l+1)\sin^2\eta_l \longrightarrow \sigma = \sum_{l=\text{even}} \sigma_l \longrightarrow \sigma_0 = \frac{8\pi}{k^2}\sin^2\eta_0$$

Fermions (odd partial waves): no s-wave scattering

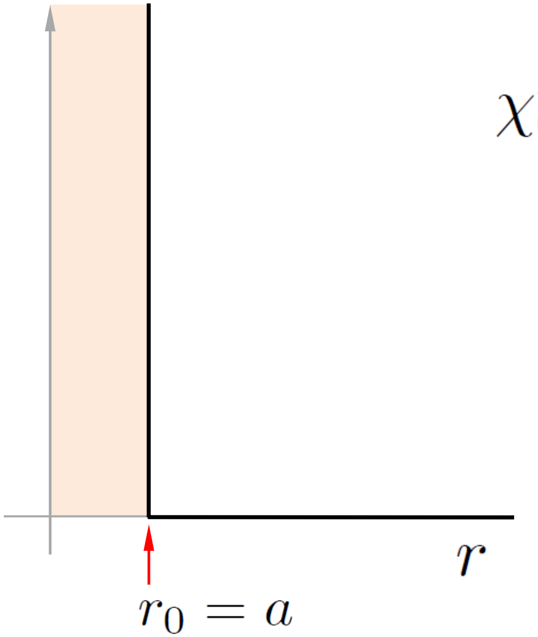
$$\sigma = \frac{8\pi}{k^2} \sum_{l=\text{odd}} (2l+1)\sin^2\eta_l \longrightarrow \sigma = \sum_{l=\text{odd}} \sigma_l \longrightarrow \sigma_0 = 0$$

Relative motion of interacting particles II

hard-sphere potential

Interaction range - r_0

hard sphere potential for $l = 0$



$$\chi_0'' + \left[k^2 - U(r)\right]\chi_0 = 0$$

$$r > r_0 \qquad \chi_0'' + k^2\chi_0 = 0$$

solution: $R_0(r) = \dfrac{1}{kr}\sin(kr + \eta_0)$

boundary condition: $R_0(a) = 0$

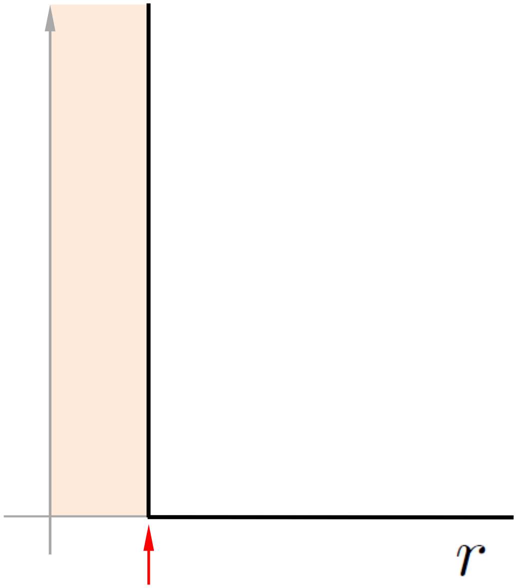
$$\sin(ka + \eta_0) = 0$$

$$\boxed{\eta_0 = -ka}$$

$$\{A_0,\, B_0\} \rightarrow \{c_0,\, \eta_0\} \rightarrow \{c_0,\, a\}$$

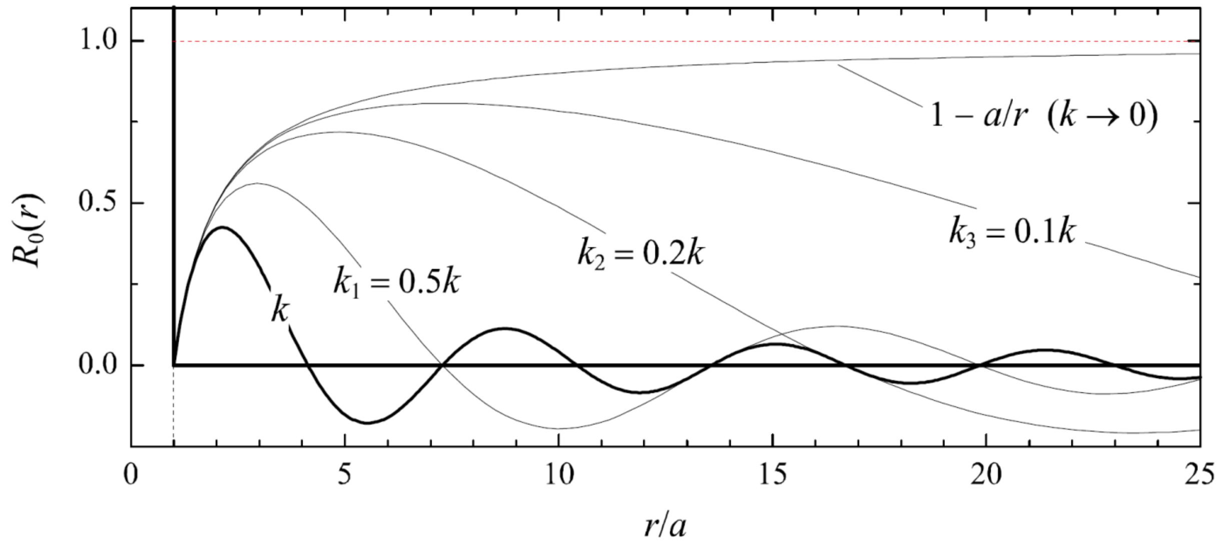
$$R_0(r) = \frac{1}{kr}\sin[k(r-a)]$$

hard sphere potential for $l = 0$



$r_0 = a$

hard sphere diameter

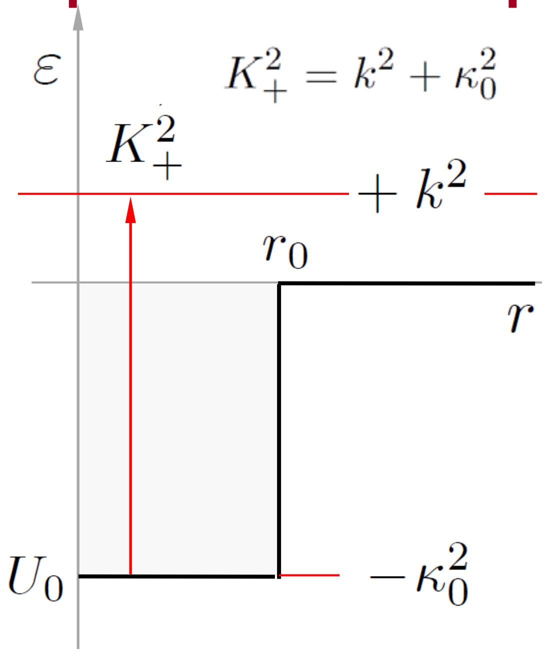


$$\boxed{R_0(r) = \frac{1}{kr}\sin[k(r-a)] \underset{k\to 0}{\simeq} 1 - \frac{a}{r}}$$

flat-bottom potential

scattering length - a

spherical square well for $l = 0$ and $\varepsilon > 0$



$$\chi_0'' + \left[k^2 - U(r)\right]\chi_0 = 0$$

$r > r_0 \quad U_0(r) = 0$

$$\chi_0'' + k^2\chi_0 = 0$$
$$\chi_0 = A\sin(kr + \eta_0)$$
$$\chi_0' = kA\cos(kr + \eta_0)$$

$r \leq r_0 \quad U_0(r) = -\kappa_0^2$

$$\chi_0'' + K_+^2\chi_0 = 0$$
$$\chi_0 = A'\sin(K_+r + \cancel{\eta_0})$$
$$\chi_0' = K_+A'\cos(K_+r)$$

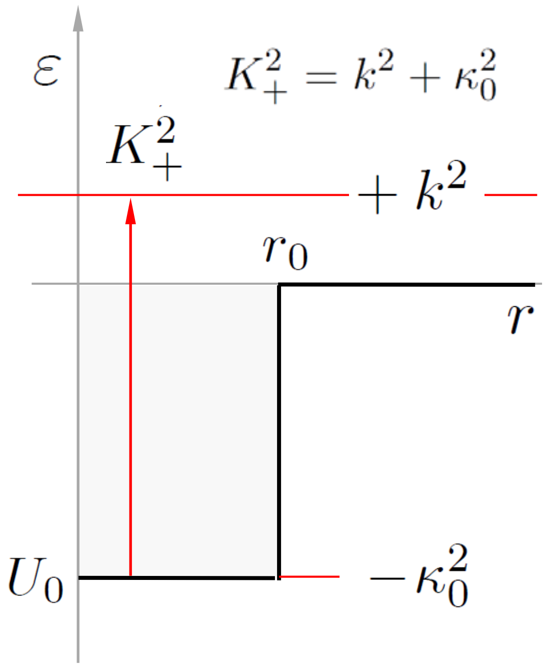
boundary condition: $\chi_0(r)$ and $\chi_0'(r)$ continuous at $r = r_0$

$r \leq r_0 \qquad\qquad r > r_0$

$$\chi_0'/\chi_0|_{r=r_0} = K_+\cot K_+r_0 = k\cot(kr_0 + \eta_0)$$

$$\tan(kr_0 + \eta_0) = \frac{k}{K_+\cot K_+r_0} \rightarrow \boxed{\eta_0(k) = -kr_0 + \arctan\frac{k}{K_+\cot K_+r_0}}$$

s-wave scattering length a

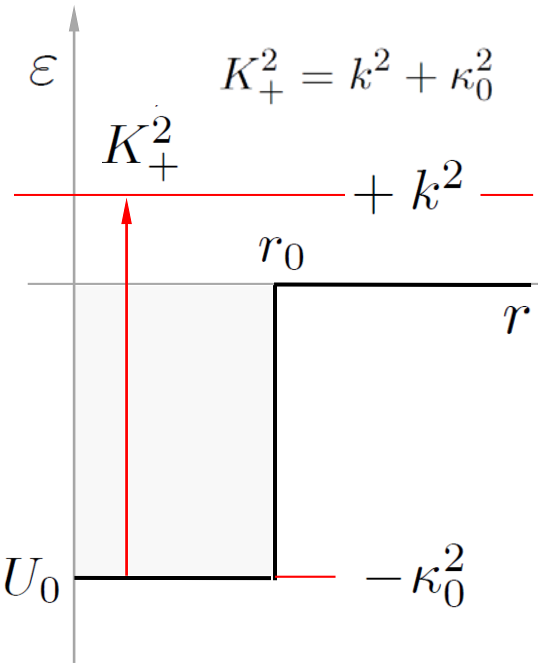


$$\eta_0(k) = -kr_0 + \arctan \frac{k}{K_+ \cot K_+ r_0}$$

Remember the hard sphere result:

$$\boxed{\eta_0 = -ka}$$

s-wave scattering length *a*



$$\eta_0(k) = -kr_0 + \arctan\frac{k}{K_+ \cot K_+ r_0}$$

Introduce *effective hard sphere diameter* $a(k)$

$$\eta_0(k) \equiv -k a(k)$$

We changed parameters:

$$\{A_0,\, B_0\} \to \{A,\, \eta_0\} \to \{A,\, a\}$$

$$\boxed{a(k) = r_0 - \frac{1}{k}\arctan\frac{k}{K_+ \cot K_+ r_0}}$$

Define scattering length: $a \equiv \lim_{k\to 0} a(k) = -\lim_{k\to 0} \eta_0(k)/k$

$$K_+^2 = k^2 + \kappa_0^2 \xrightarrow[k\to 0]{} K_+ \to \kappa_0$$

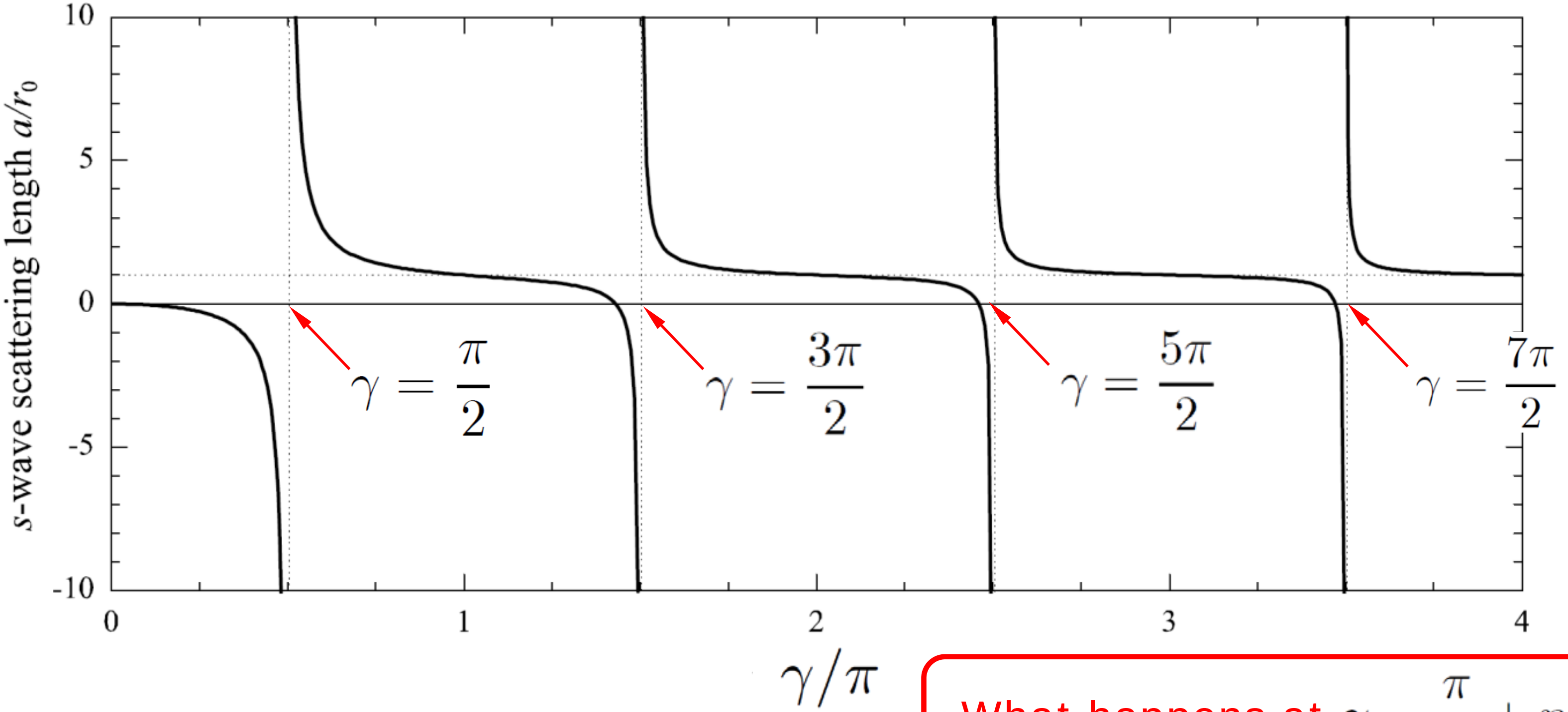
$$\longrightarrow \quad a = r_0 - \frac{r_0}{\kappa_0 r_0 \cot \kappa_0 r_0} \quad \longrightarrow \quad \boxed{\kappa_0 \cot \kappa_0 r_0 = \frac{1}{r_0 - a}}$$

Define well parameter: $\gamma \equiv \kappa_0 r_0 \quad \longrightarrow \quad \boxed{a = r_0\left(1 - \tan\gamma/\gamma\right)}$

s-wave scattering length a

well parameter

$$\boxed{a = r_0\,(1 - \tan\gamma/\gamma)} \qquad \gamma \equiv \kappa_0 r_0$$



What happens at $\gamma = \frac{\pi}{2} + n\pi$?

Where do we stand?

1. We identified the phase shift as the central quantity for scattering
2. We determined the scattering amplitude (4 expressions for f_l)
3. We derived the differential and total cross sections
4. We identified the role of quantum statistics
5. We studied the phase shift for hard spheres
6. We studied the phase shift for spherical square wells
7. We defined the scattering length
8. We studied its dependence on the well parameter