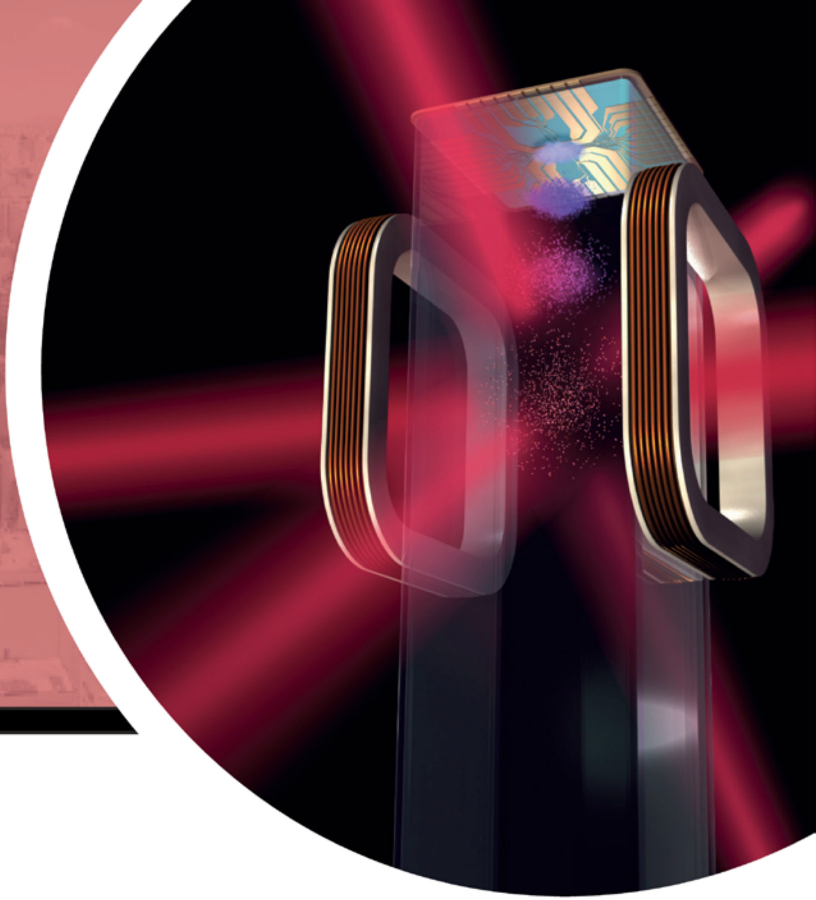
International Centre for Theoretical Physics South American Institute for Fundamental Research

ICTP SAIFR

SCHOOL ON INTERACTION OF LIGHT WITH COLD ATOMS

September 16-27, 2019

at Instituto de Física Teórica - UNESP, São Paulo, Brazil



Collision Phenomena in Quantum Gases

Jook Walraven

University of Amsterdam

FAPESP ICTP unesp IFT - UNESP INSTITUTO DE FÍSICA TEÓRICA

outline

Course of five lectures on collision phenomena in quantum gases

1. Relative motion of interacting particles I
   - model potentials: range, phase shift, scattering length
2. Relative motion of interacting particles II
   - model potentials: effective range and s-wave resonance
   - generalization to arbitrary short-range potentials
3. Scattering of interacting particles
   - scattering amplitude and cross section
   - distinguishable versus identical particles
4. Scattering of particles with internal structure (atoms)
5. Interaction tuning with magnetic Feshbach resonance

Many details given in the lecture notes for ICTP-SAIFR-2019

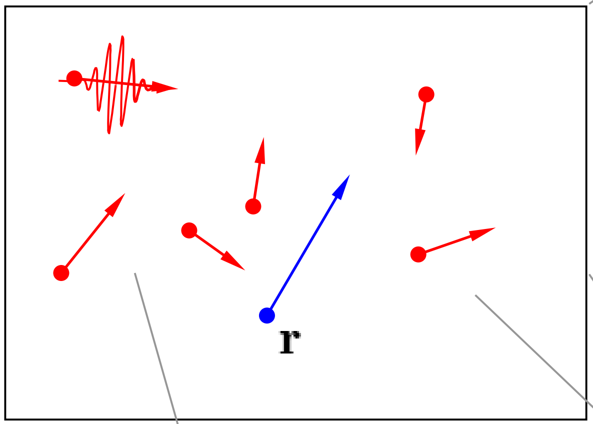
Journal club suggestion: <u>Polaron problem</u>

Seminal paper (theory): P.W. Anderson, INFRARED CATASTROPHE IN FERMI GASES WITH LOCAL SCATTERING POTENTIALS, Phys. Rev. Lett. 18, 1049 (1967)

Polaron formation (expt): M. Cetina et al., ULTRAFAST MANY-BODY INTERFEROMETRY OF IMPURITIES COUPLED TO A FERMI SEA, Science 354 96 (2016)

Gas phase and quantum resolution

configuration space: V



$\mathcal{U}(\mathbf{r})$

density: $n(\mathbf{r})$ temperature: T

classical particles:

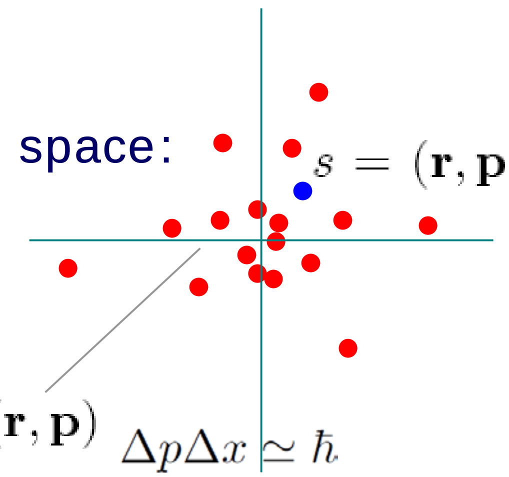
position: $\mathbf{r}$

momentum: $\mathbf{p} = m\mathbf{v}$

$s = (\mathbf{r}, \mathbf{p})$ kinetic state

Gas: $\{\mathbf{r}_i, \mathbf{p}_i\}$ $i \in \{1, \cdots N\}$

phase space:



$n(\mathbf{r}, \mathbf{p})$

quantum mechanical description ← (quantum resolution limit)

Lecture 1

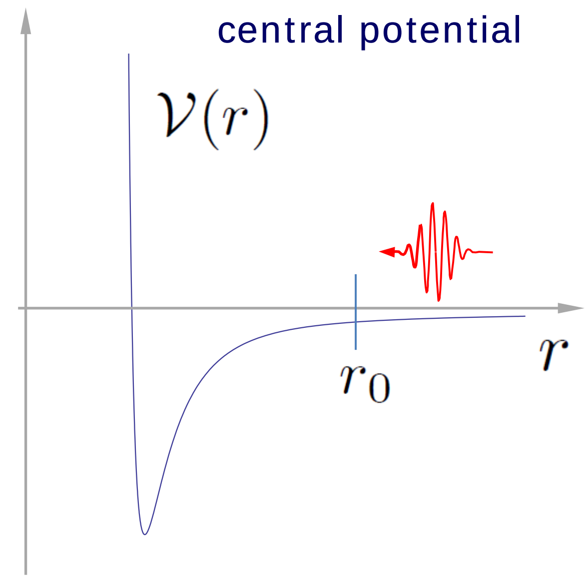
Relative motion of interacting particles

Characteristic lengths and quantum regimes

interaction range: $r_0 \ll n_0^{-1/3} \ll V^{1/3}$

interatomic spacing: (→ $n_0^{-1/3}$)

system size: (→ $V^{1/3}$)



definition quantum regimes:

thermal wavelength: $\Lambda \equiv \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$

$k \sim 1/\Lambda$

$\Lambda \ll r_0 \rightarrow kr_0 \gg 1$ quasi-classical collisions

$\Lambda \gg r_0 \rightarrow kr_0 \ll 1$ ultracold collisions

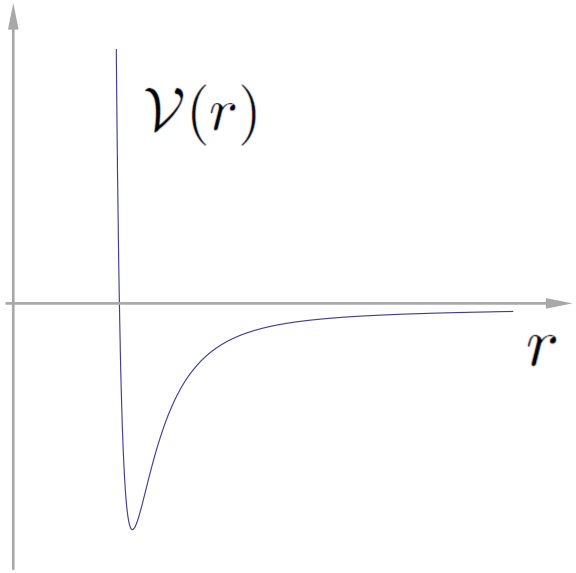
quantum gas: $kr_0 \ll 1$ (degenerate for $n_0\Lambda^3 \gg 1$)

short-range interactions – collisional regimes

only binary interactions: $nr_0^3 \ll 1$ *dilute*

nearly ideal
weakly interacting } $na^3 \ll 1$

s-wave scattering length



cross section: $\sigma \simeq 4\pi a^2$

interaction ranges: r_0, a, r_e, R^*

collision rate: $\tau_c^{-1} = n\bar{v}_r\sigma$

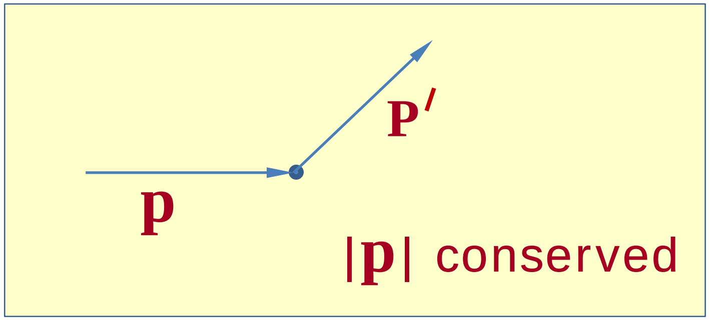
mean free path: $\ell = 1/n\sigma$ → $\ell \gg V^{1/3}$ *collisionless*; $\ell \ll V^{1/3}$ *hydrodynamic (collisional)*

kinematics of binary collision

CM and REL coordinates:

relative position: $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$

relative velocity: $\mathbf{v} = \mathbf{v}_1 - \mathbf{v}_2$



closed system: conserved quantities E and $\mathbf{P}$

no external fields
(kinetic momentum)

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2 \stackrel{\downarrow}{=} m_1\dot{\mathbf{r}}_1 + m_2\dot{\mathbf{r}}_2 = \overbrace{(m_1 + m_2)}^{M}\frac{d}{dt}\overbrace{\frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}}^{\mathbf{R}} = M\,\dot{\mathbf{R}}$$

$\mathbf{P} = M\,\dot{\mathbf{R}}$ conserved

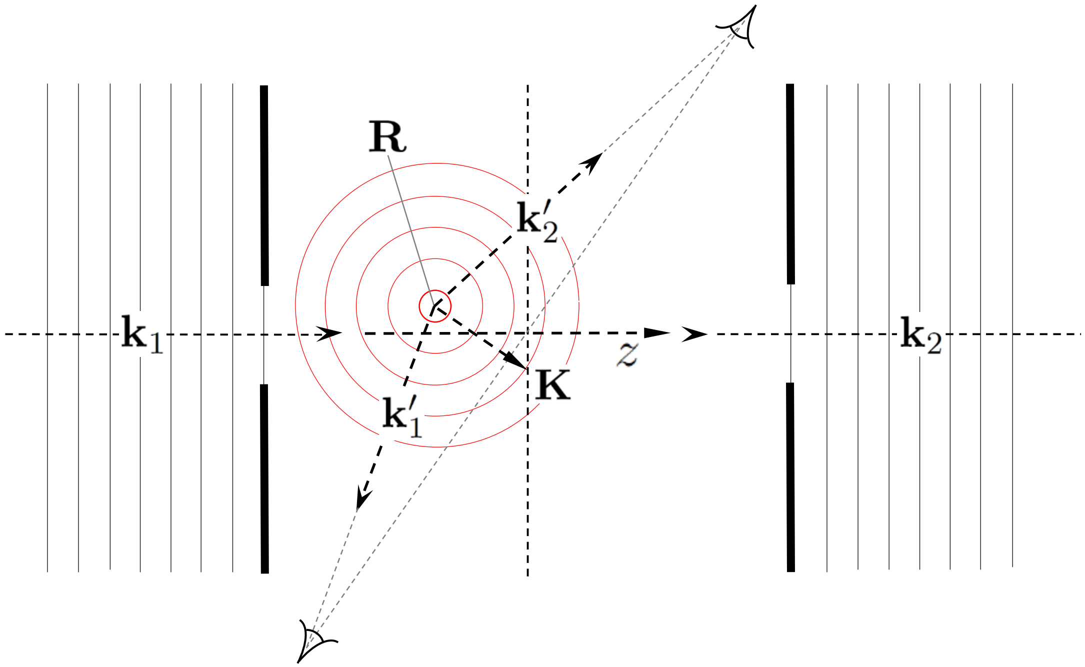
$$E = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} = \frac{P^2}{2M} + \frac{p^2}{2\mu}$$

$\rightarrow$ $\dfrac{p^2}{2\mu}$ conserved

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

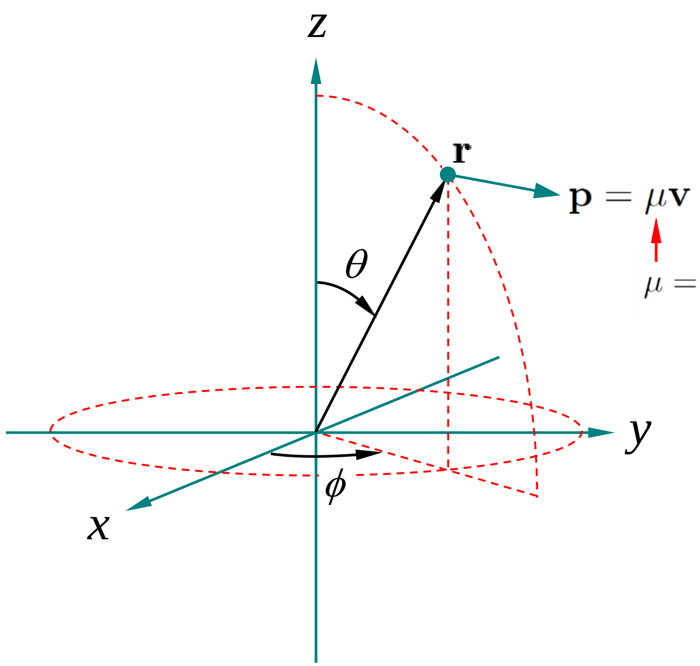
relative momentum: $\mathbf{p} = \mu\mathbf{v}$

Quantum limitations



experiments diffraction limited

central potential



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

potential energy

Hamiltonian:

$$H = \frac{\mathbf{p}^2}{2\mu} + \mathcal{V}(\mathbf{r})$$

central potential: $\mathcal{V}(\mathbf{r}) = \mathcal{V}(r)$

$$\mathbf{p}^2 = (\hat{\mathbf{r}} \cdot \mathbf{p})^2 + (\hat{\mathbf{r}} \times \mathbf{p})^2$$

$$p_r = \hat{\mathbf{r}} \cdot \mathbf{p} \qquad \mathbf{L} = \mathbf{r} \times \mathbf{p}$$

spherical symmetry allows separation of radial and angular motion:

$$H = \frac{1}{2\mu}\left(p_r^2 + \frac{\mathbf{L}^2}{r^2}\right) + \mathcal{V}(r)$$

check solution
for regularity in the origin

$r \neq 0$

Schrödinger equation for the relative motion

$$\left[\frac{1}{2\mu}\left(p_r^2+\frac{\mathbf{L}^2}{r^2}\right)+\mathcal{V}(r)\right]\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

$\mathbf{L}^2, L_z$ commute with each other and with r and p_r

separation of variables: $\psi = R_l(r)Y_l^m(\theta,\phi)$

$$\mathbf{L}^2\, Y_l^m(\theta,\phi)=l(l+1)\hbar^2\, Y_l^m(\theta,\phi)$$
$$L_z\, Y_l^m(\theta,\phi)=m\hbar\, Y_l^m(\theta,\phi).$$

$$\left[\frac{1}{2\mu}\left(p_r^2+\frac{l(l+1)\hbar^2}{r^2}\right)+\mathcal{V}(r)\right]R_l(r)\cancel{Y_l^m(\theta,\phi)}=ER_l(r)\cancel{Y_l^m(\theta,\phi)}$$

radial wave equation:

$$\frac{2\mu}{\hbar^2}\left[\frac{\hbar^2}{2\mu}\left(-\frac{d^2}{dr^2}-\frac{2}{r}\frac{d}{dr}\right)+\underbrace{\frac{l(l+1)\hbar^2}{2\mu r^2}+\mathcal{V}(r)}_{\mathcal{V}_{\text{eff}}(r)}\right]R_l(r)=ER_l(r)$$

radial wave equation

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

we changed to wavenumber notation

$$U(r) = 2\mu\mathcal{V}(r)/\hbar^2 \qquad \varepsilon = 2\mu E/\hbar^2 \begin{cases} \varepsilon = k^2 & \text{continuum states } (\varepsilon > 0) \\ \varepsilon = -\kappa^2 & \text{bound states } (\varepsilon < 0) \end{cases}$$

introduce reduced wavefunction: $\chi_l(r) = rR_l(r)$

1D Schrödinger equation:

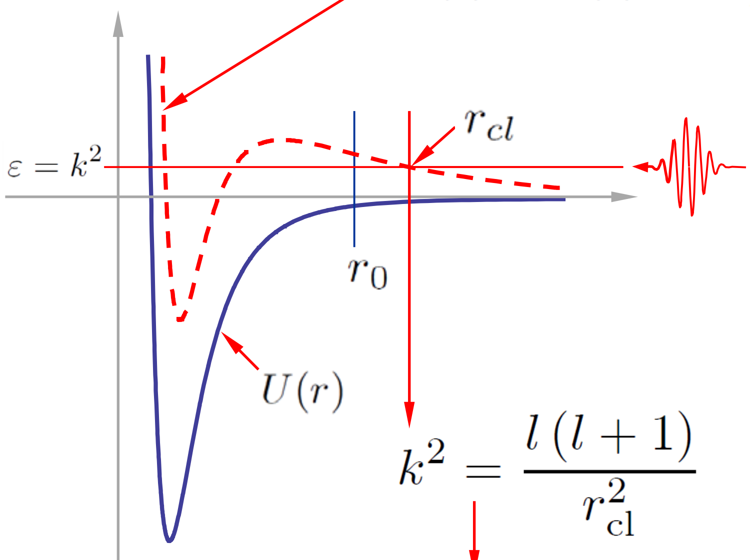
radial wave equation:

$$\frac{2\mu}{\hbar^2}\left[\frac{\hbar^2}{2\mu}\left(-\frac{d^2}{dr^2}\right.\right.$$

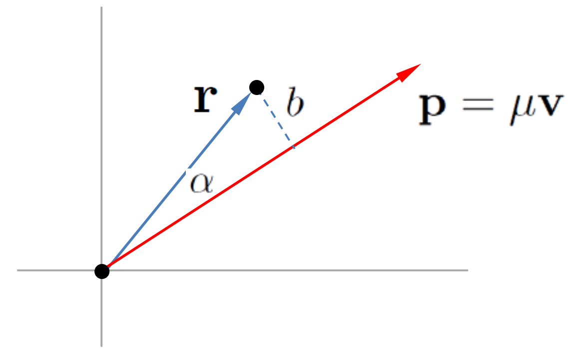
$$\chi_l'' + [\varepsilon - U(r) - \frac{l(l+1)}{r^2}]\chi_l = 0 R_l(r)$$

s-wave regime

$$U_{\text{eff}}(r) = U(r) + \frac{l(l+1)}{r^2}$$



$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \qquad L = p \overbrace{r \sin\alpha}^{b}$$



$$k^2 = \frac{l\,(l+1)}{r_{\text{cl}}^2} \qquad l \neq 0$$

$$kr_0 = \sqrt{l(l+1)}\,\frac{r_0}{r_{cl}} \ll 1 \quad \rightarrow \quad \boxed{r_0 \ll r_{cl}}$$

conclusion: for $kr_0 \ll 1$ no collisions with l > 0

only s-wave collisions

(exception: quasi-bound states in continuum/shape resonances)

RWE for short-range potentials

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

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

$r \gg r_0$

$\varrho \equiv kr$

Spherical Bessel differential equation

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

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

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

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

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

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

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

In the far field the distortion is gone but <u>a phase shift remains</u>

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 $U(r) = 0$

↓

$$\chi_0'' + k^2\chi_0 = 0$$

General solution:

$$R_0 = c_0 \frac{\sin(kr + \eta_0)}{kr}$$

regular only for $\eta_0 = 0$

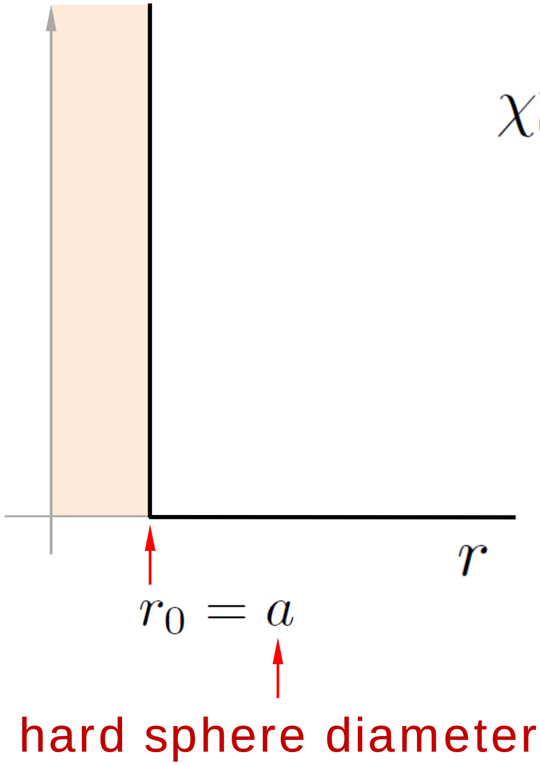
↓

Conclusion: free particle – no phase shift

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: $R_0(a) = 0$

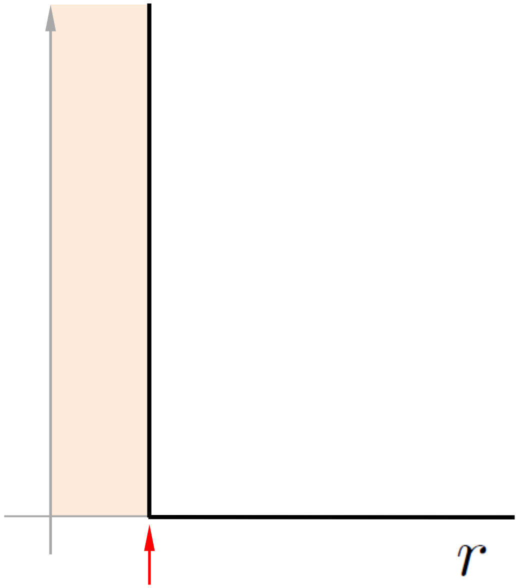
$$\sin(ka + \eta_0) = 0$$

$$\eta_0 = -ka$$

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

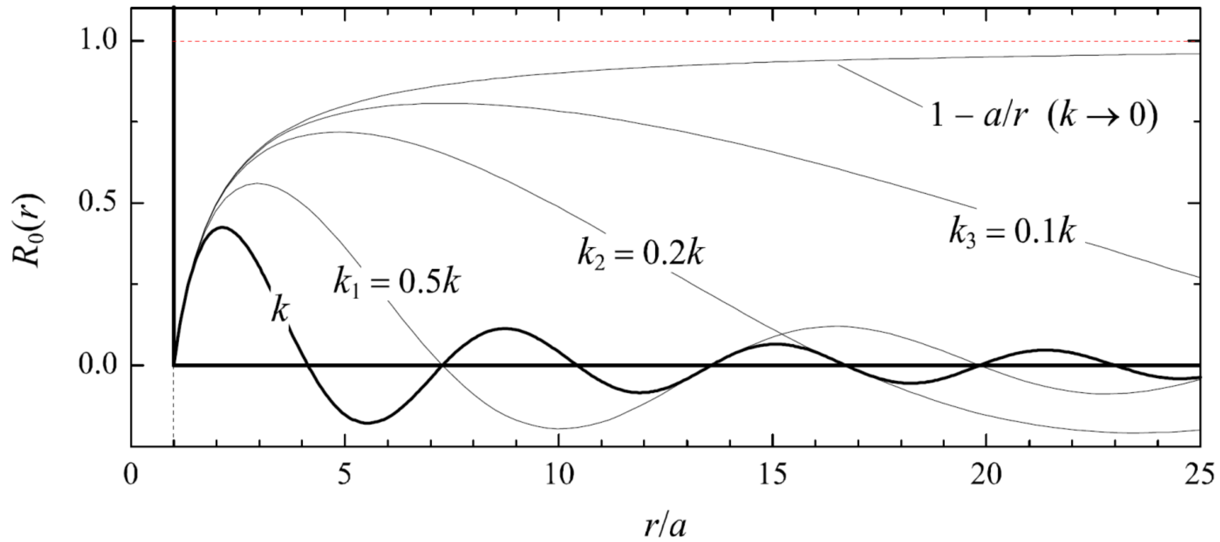
$$R_0(r) = \frac{1}{kr}\sin[k(r-a)]$$

hard sphere potential for $l = 0$



$r_0 = a$

hard sphere diameter

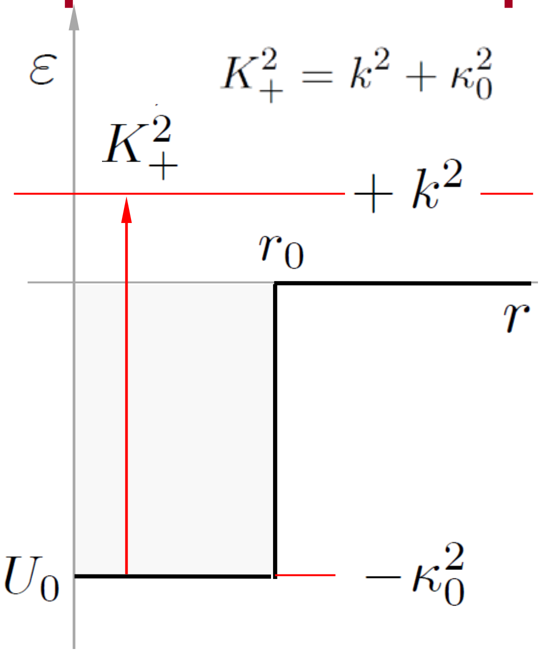


$$R_0(r) = \frac{1}{kr}\sin[k(r-a)] \underset{k\to 0}{\simeq} 1 - \frac{a}{r}$$

flat-bottom potential

scattering length - a

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



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

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

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

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

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

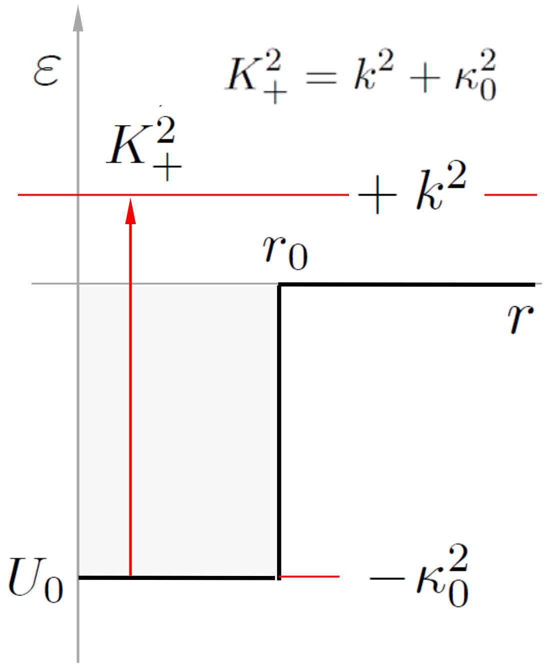
boundary condition: $\chi_0(r)$ and $\chi_0'(r)$ continuous at $r = r_0$

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

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

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

s-wave scattering length a

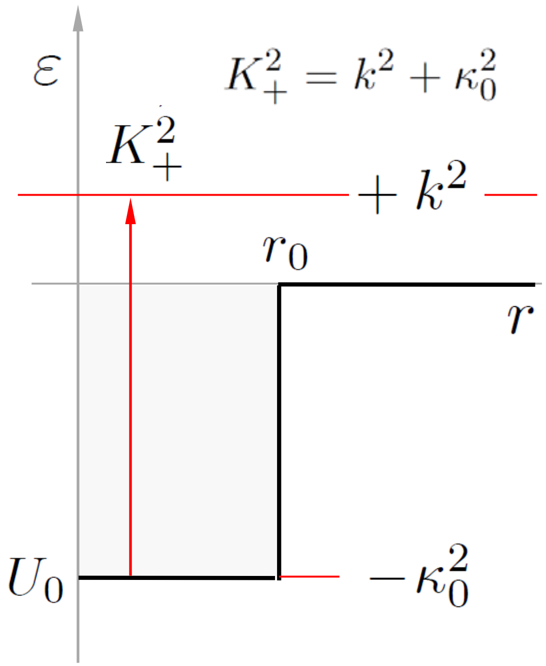


$$\eta_0(k) = -kr_0 + \arctan \frac{k}{K_+ \cot K_+ r_0}$$

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:

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

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

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

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

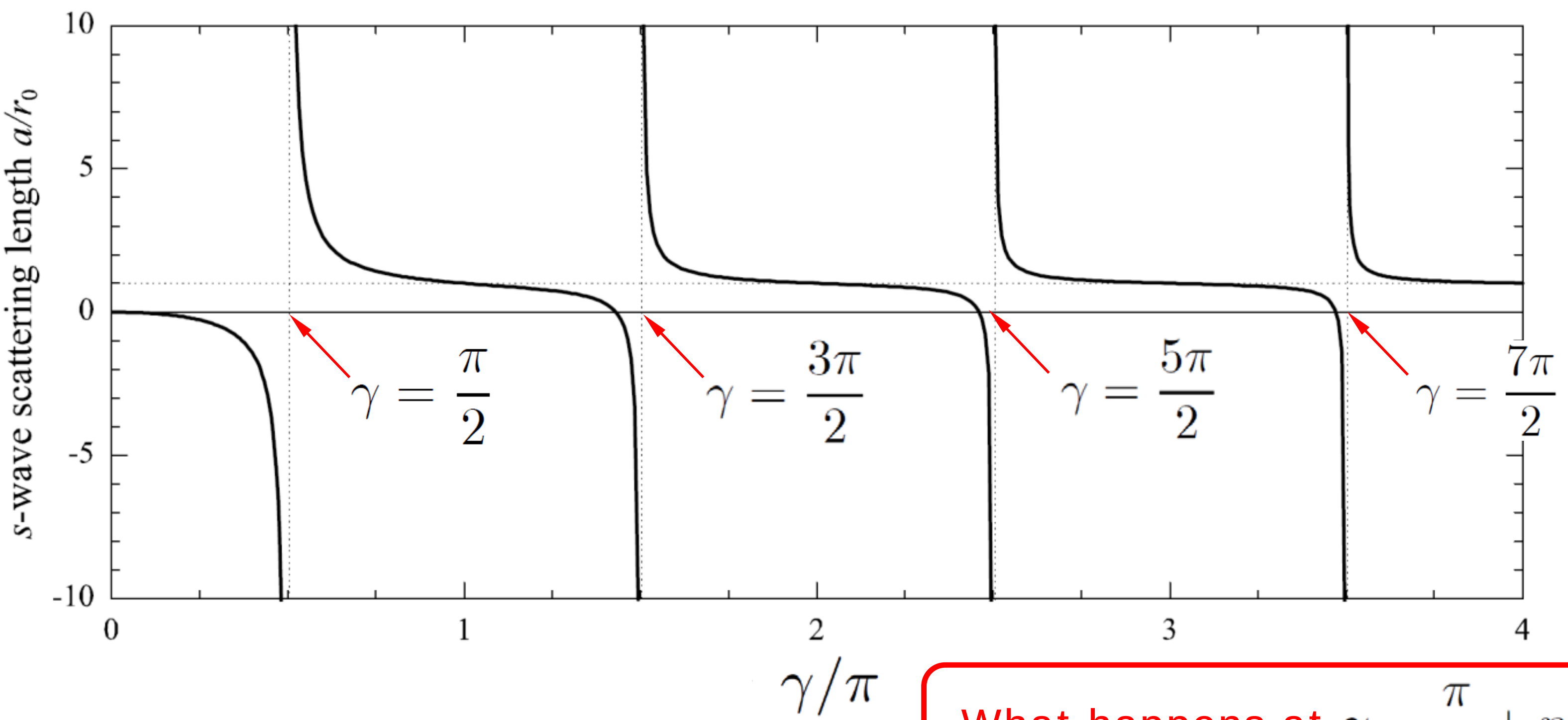
$$\rightarrow\quad a = r_0 - \frac{r_0}{\kappa_0 r_0 \cot \kappa_0 r_0} \quad\rightarrow\quad \kappa_0 \cot \kappa_0 r_0 = \frac{1}{r_0 - a}$$

Define well parameter: $\gamma \equiv \kappa_0 r_0$ $\rightarrow$ $a = r_0\left(1 - \tan\gamma/\gamma\right)$

s-wave scattering length a

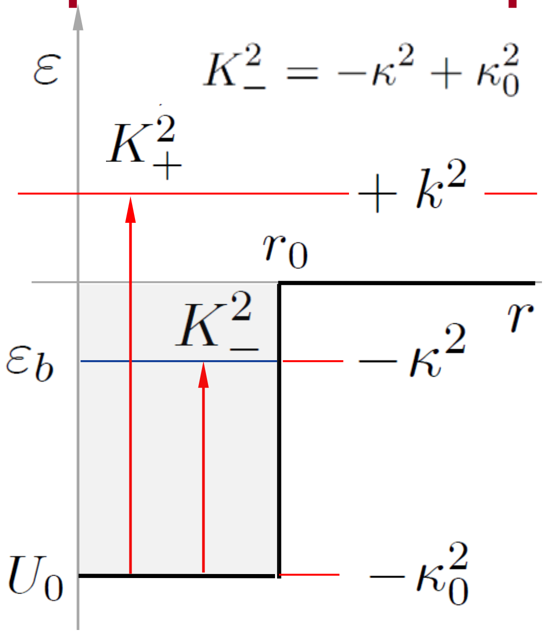
well parameter

$$a = r_0 \left(1 - \tan\gamma/\gamma\right) \qquad \gamma \equiv \kappa_0 r_0$$



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

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



$\chi_0'' + \left[-\kappa^2 - U_0\right] R_l = 0$

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

$$\chi_0'' - \kappa^2 \chi_0 = 0$$

$$\chi_0 = A e^{-\kappa r} \qquad (\kappa > 0) \text{ normalization}$$

$$\chi_0' = -\kappa A e^{-\kappa r}$$

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

$$\chi_0'' + K_-^2 \chi_0 = 0$$

$$\chi_0 = A' \sin(K_- r + \eta_0')$$

$$\chi_0' = K_- A' \cos(K_- r)$$

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

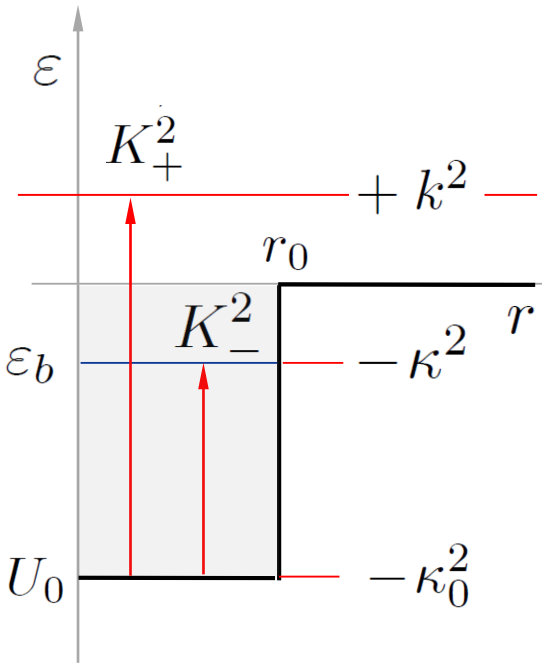
$$\underbrace{\chi_0'/\chi_0|_{r=r_0} = K_- \cot K_- r_0}_{r \leq r_0} = \underbrace{-\kappa}_{r > r_0}$$

Bethe-Peierls boundary condition

$$K_-^2 = \kappa_0^2 - \kappa^2 \xrightarrow[\kappa \to 0]{} K_- \to \kappa_0 \longrightarrow \chi_0'/\chi_0|_{r=r_0} = \kappa_0 \cot \kappa_0 r_0 = 0 \text{ for } \kappa \to 0$$

Conclusion: next bound state appears for $\gamma = \frac{\pi}{2} + n\pi$

universal behavior near threshold



Continuum state near threshold:

$$\varepsilon > 0 \quad (k \to 0) \quad \kappa_0 \cot \kappa_0 r_0 = \frac{1}{r_0 - a} \simeq -\frac{1}{a}$$

Bound state near threshold:

$$\varepsilon < 0 \quad (\kappa \to 0) \quad \kappa_0 \cot \kappa_0 r_0 = -\kappa \qquad (\kappa > 0)$$

$$\rightarrow \boxed{a = \frac{1}{\kappa}} \rightarrow \boxed{a > 0 \quad \text{for} \quad \kappa \to 0}$$

Universal dependence of binding energy on scattering length:

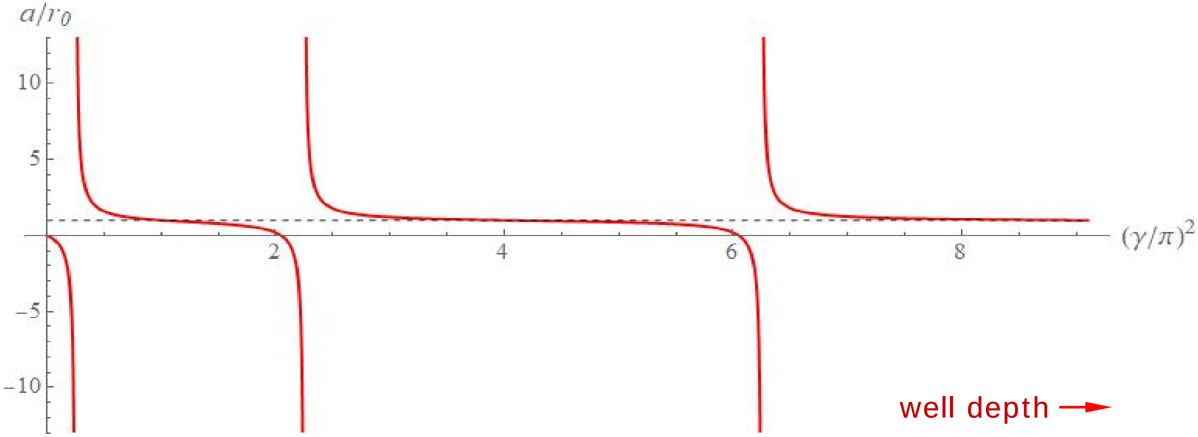
$$\varepsilon = -\kappa^2 = -\frac{1}{a^2} \rightarrow \boxed{E_b = -\frac{\hbar^2}{2\mu}\frac{1}{a^2}}$$

binding energy versus well parameter

$$\chi_0'/\chi_0|_{r=r_0} = K_- \cot K_- r_0 = -\kappa$$

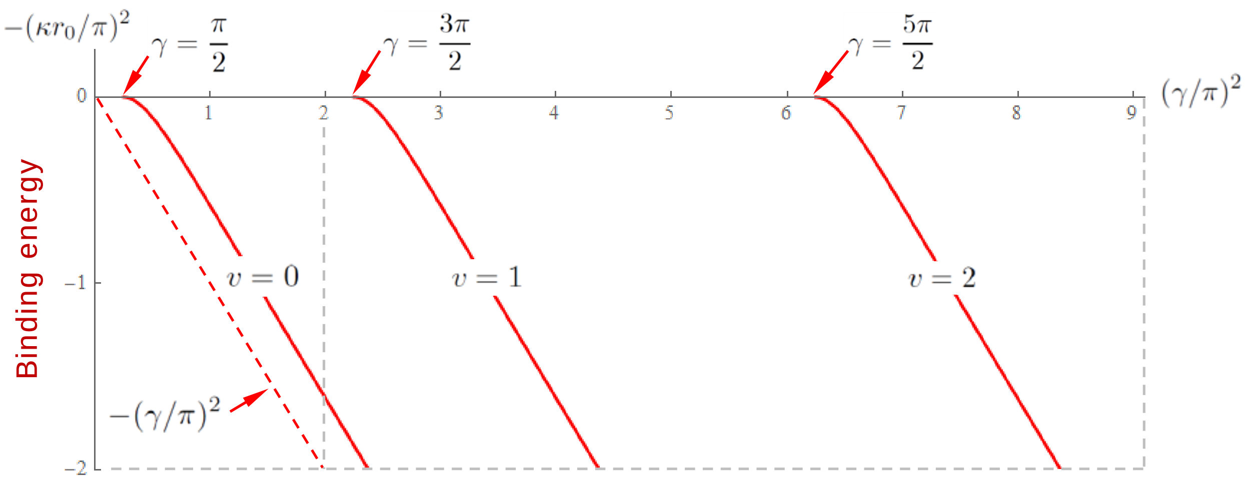
$$K_-^2 = -\kappa^2 + \kappa_0^2$$

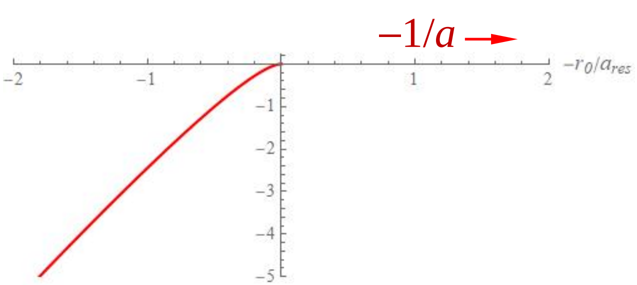
well parameter: $\gamma \equiv \kappa_0 r_0$



well depth →

$$E_b = -\frac{\hbar^2}{2\mu}\frac{1}{a^2}$$





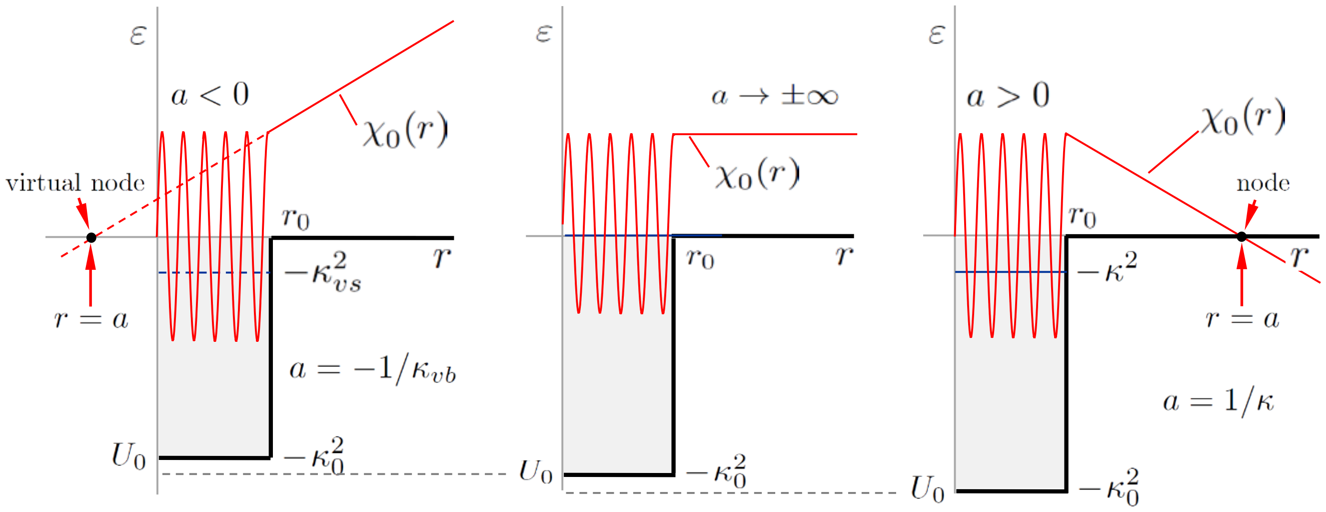
Binding energy

scattering length a

Continuum states ($\varepsilon > 0$):

$$\eta_0 = -ka$$

$$\chi_0(r) = \sin(kr + \eta_0) = \sin[k(r-a)] \underset{k\to 0}{\simeq} k(r-a)$$



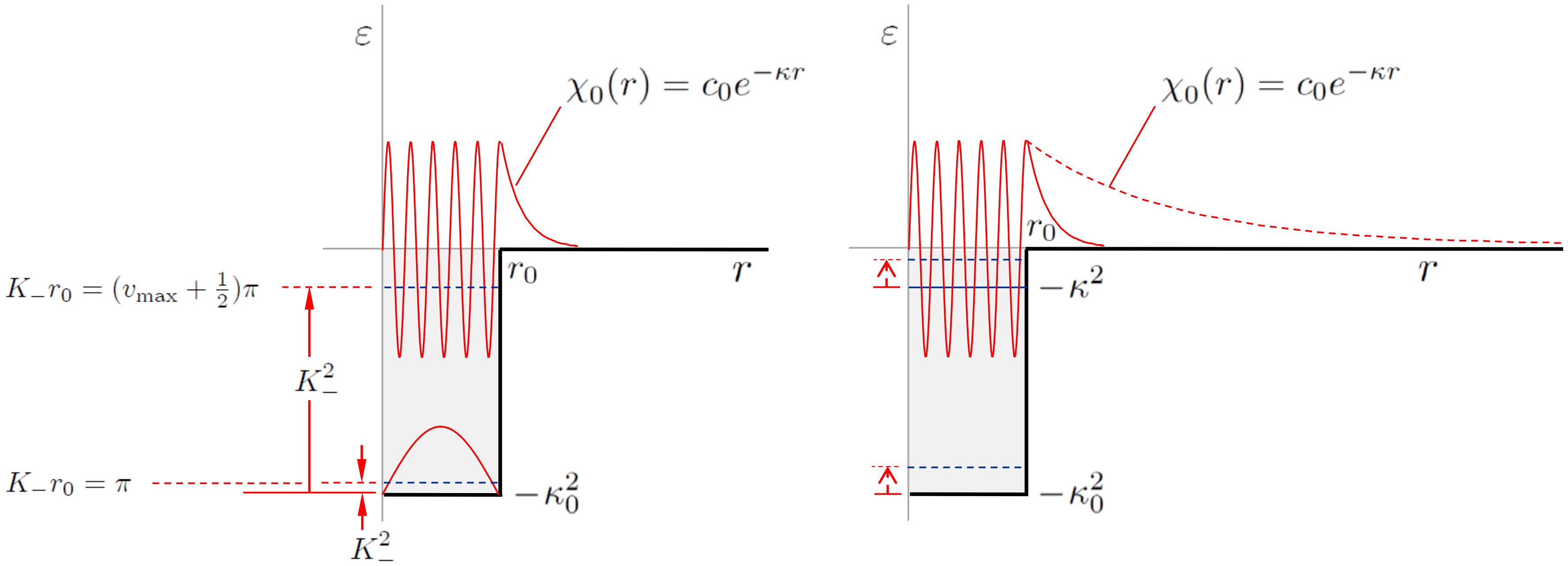
halo states

Bound states ($\varepsilon < 0$):

$$\chi_0 = A e^{-\kappa r}$$
$$\kappa r_0 \ll 1$$

→ universal bound states: halo states

strange molecule: large probability to find the atoms *outside* the classical turning point

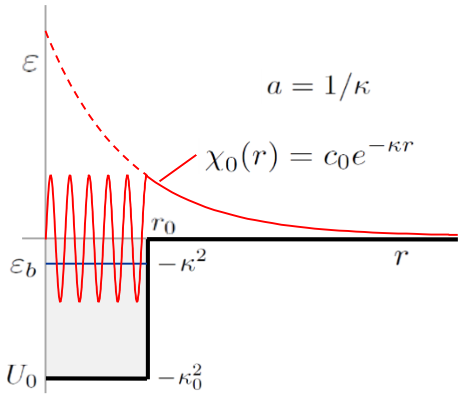


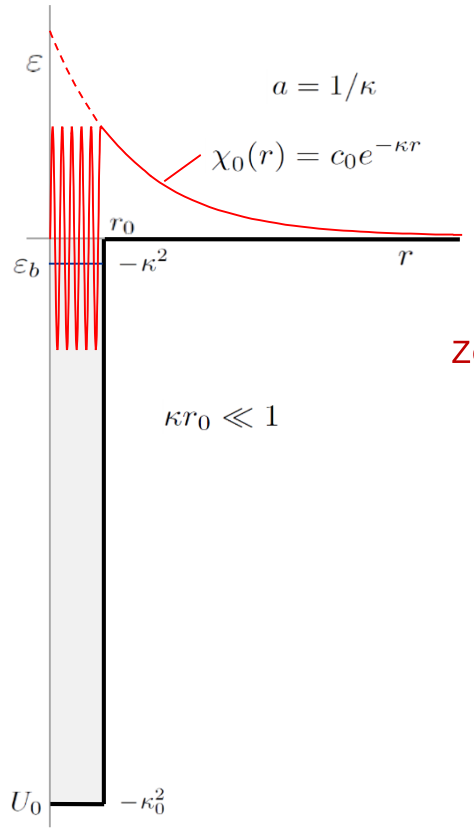
halo states

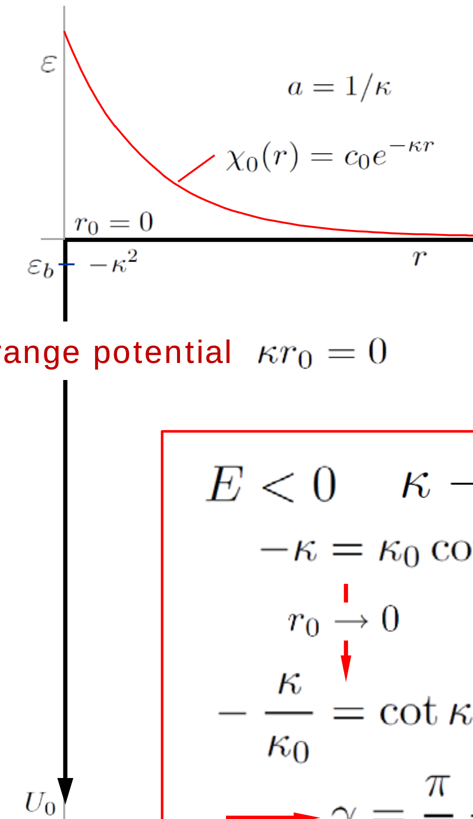
Bound states ($\varepsilon < 0$):

$$\chi_0 = Ae^{-\kappa r}$$
$$\kappa r_0 \ll 1$$

→ universal bound states: halo states







$$E < 0 \quad \kappa \to 0$$
$$-\kappa = \kappa_0 \cot \kappa_0 r_0$$
$$r_0 \to 0$$
$$-\frac{\kappa}{\kappa_0} = \cot \kappa_0 r_0 \to 0$$
$$\to \gamma = \frac{\pi}{2} + n\pi$$

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 derived the partial wave expansion
7. We identified the phase shift as the central quantity of interest
8. We studied the phase shift for hard spheres
9. We studied the phase shift for spherical square wells
10. We defined the scattering length
11. We studied its dependence on the well parameter
12. We found universal behavior near the bound state threshold
13. We defined halo states and zero-range potentials