Lectures on quantum gases

Lecture 1

Cold Collisions

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Lecture notes:
https://staff.fnwi.uva.nl/j.t.m.walraven/walraven/JookWalraven.htm

outline

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 resonances

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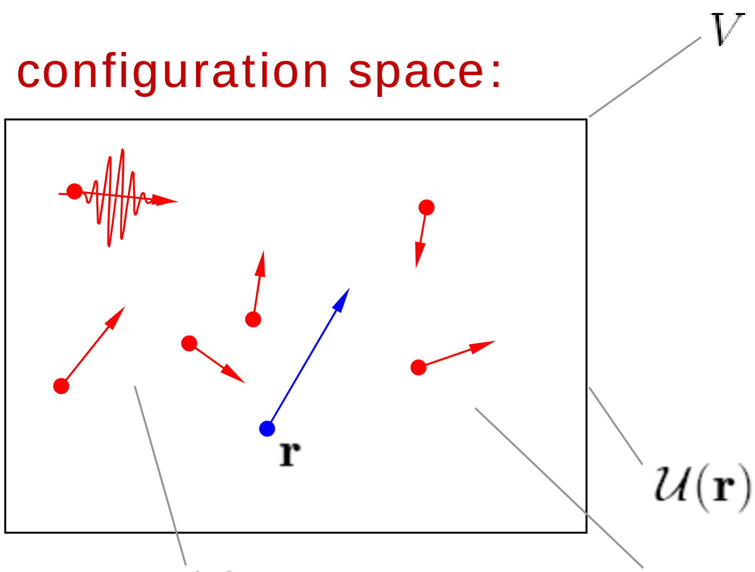
Gas phase and quantum resolution

configuration space:



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

classical particles:

kinetic state

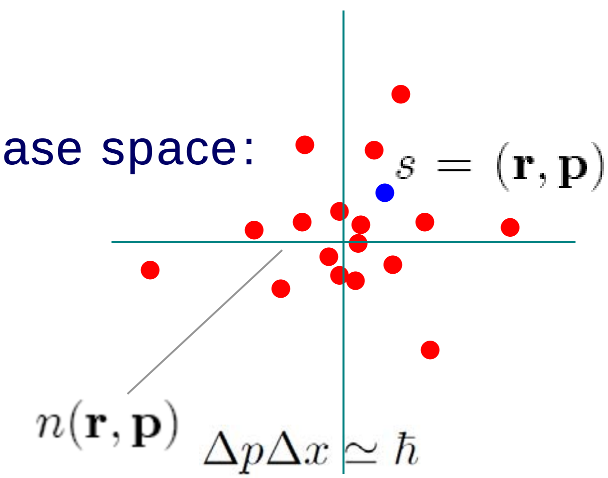
position: $\mathbf{r}$

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

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

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

phase space:



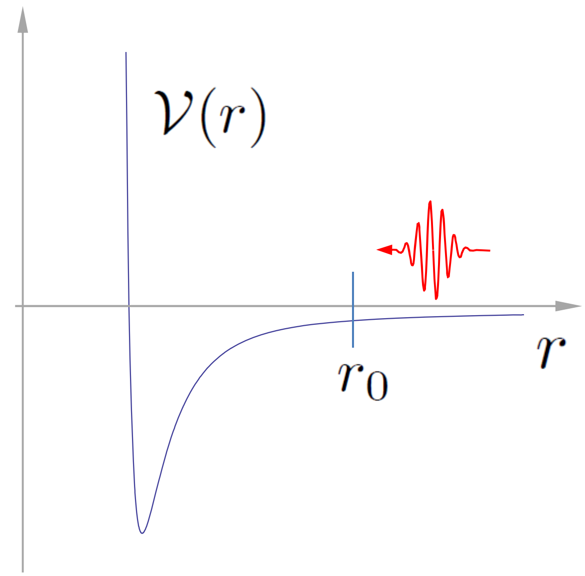
quantum mechanical description ← (quantum resolution limit)

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: $\Lambda \equiv \sqrt{\dfrac{2\pi\hbar^2}{mk_BT}}$

$k \sim 1/\Lambda$

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

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

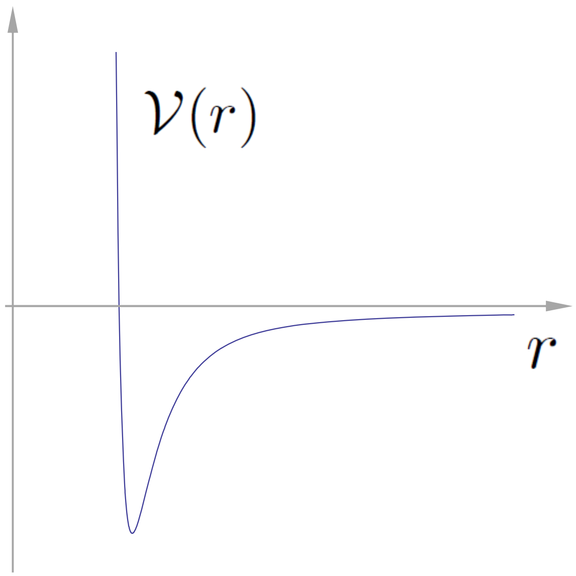
quantum gas: $kr_0 \ll 1$ (degenerate for $n_0\Lambda^3 \gg 1$)

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

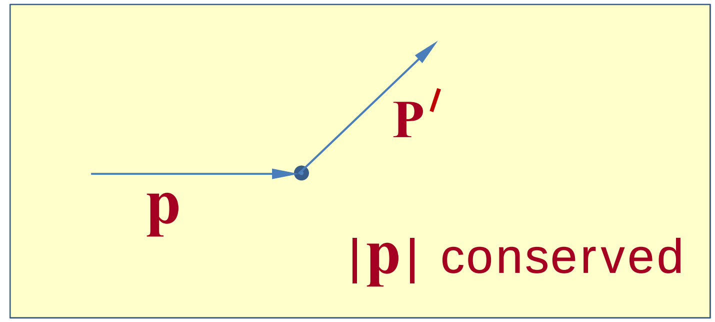
mean free path: $\ell = 1/n\sigma$ →
- $\ell \gg V^{1/3}$ *collisionless*
- $\ell \ll V^{1/3}$ *hydrodynamic (collisional)*

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

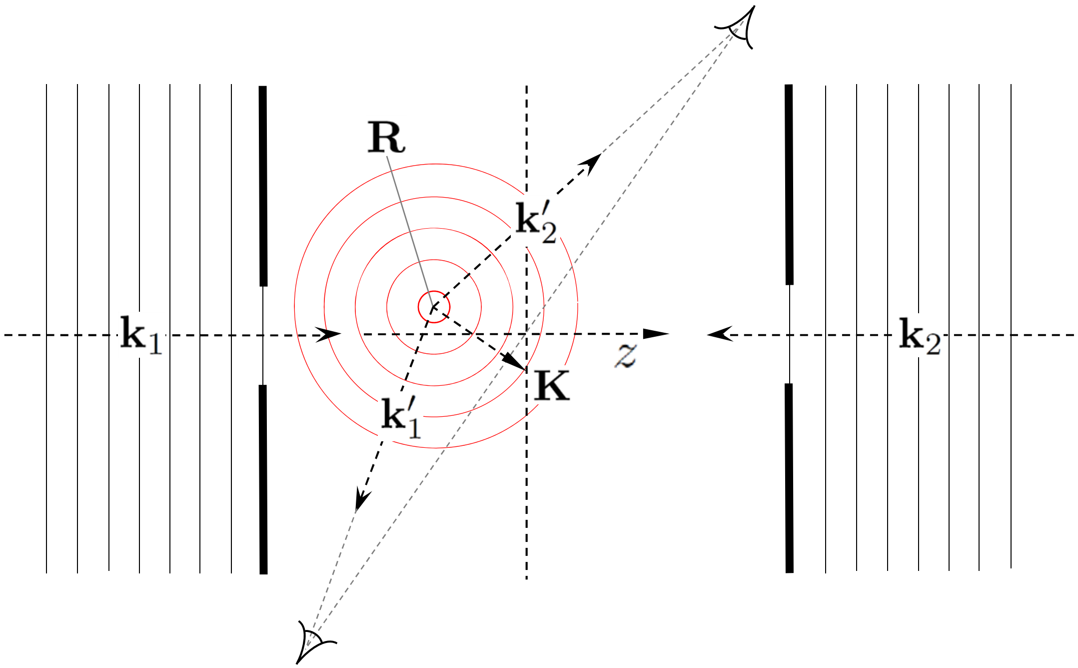
$$E = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} = \frac{P^2}{2M} + \frac{p^2}{2\mu}$$

→ $\dfrac{p^2}{2\mu}$ conserved

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

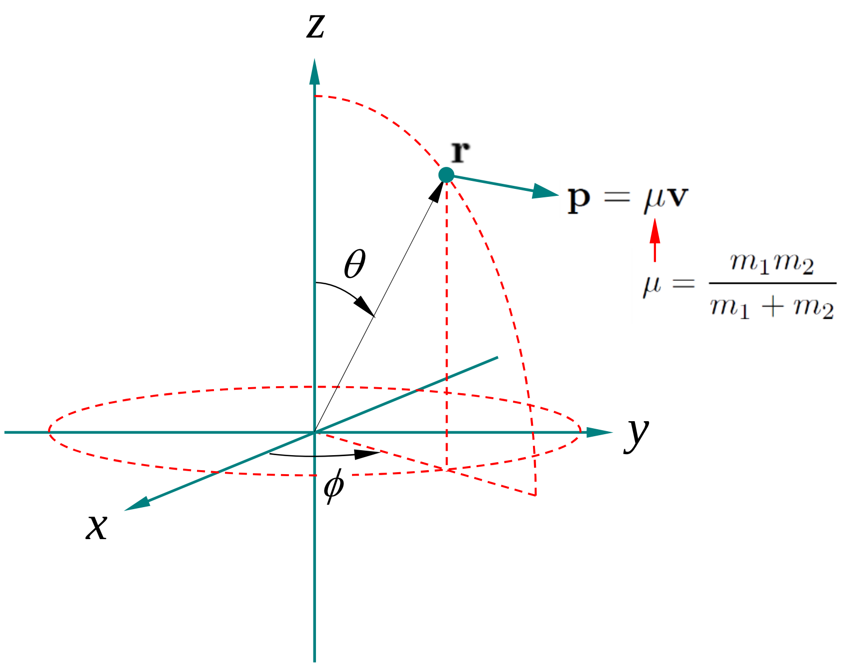
relative momentum: $\mathbf{p} = \mu\mathbf{v}$

Quantum limitations



experiments diffraction limited

central potential



Hamiltonian:

potential energy

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

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 r and p_r

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

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

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

radial wave equation:

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

radial wave equation

change to wavenumber notation:

$$\varepsilon = 2\mu E/\hbar^2 \qquad\qquad U(r) = 2\mu \mathcal{V}(r)/\hbar^2$$

radial wave equation:

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

$\varepsilon = k^2$ continuum states $(\varepsilon > 0)$

$\varepsilon = -\kappa^2$ bound states $(\varepsilon < 0)$

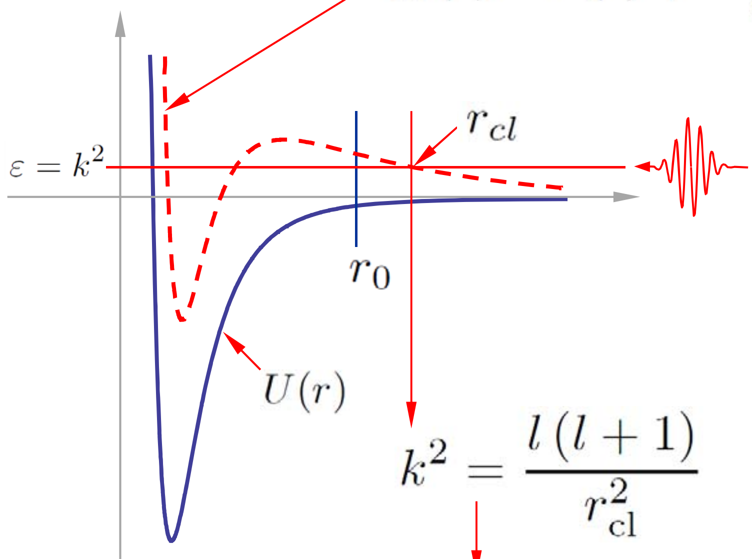
introduce reduced wavefunction: $\chi_l(r) = rR_l(r)$

1D Schrödinger equation:

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

s-wave regime

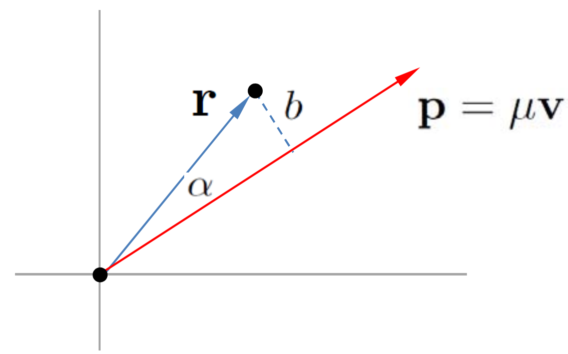
$$U_{\text{eff}}(r) = U(r) + \frac{l(l+1)}{r^2}$$



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

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

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



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

only s-wave collisions

(exception: shape resonances)

RWE for short-range potentials

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

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

$$r \gg 1/k \gg r_0$$

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

General solution: $\chi_l(k,r) \sim \sin(kr + \eta_l - \frac{1}{2}l\pi) \qquad r \gg 1/k \gg r_0$

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

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 $\eta_0 = 0$

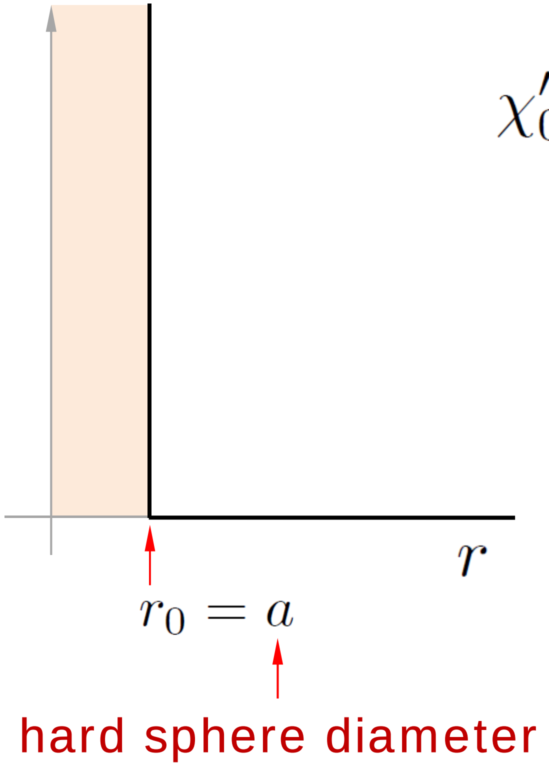
↓

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: $R_0(a) = 0$

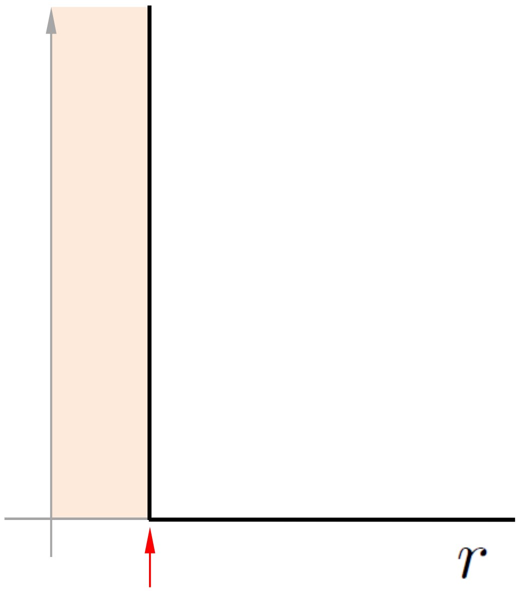
$$\sin(ka + \eta_0) = 0$$

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

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

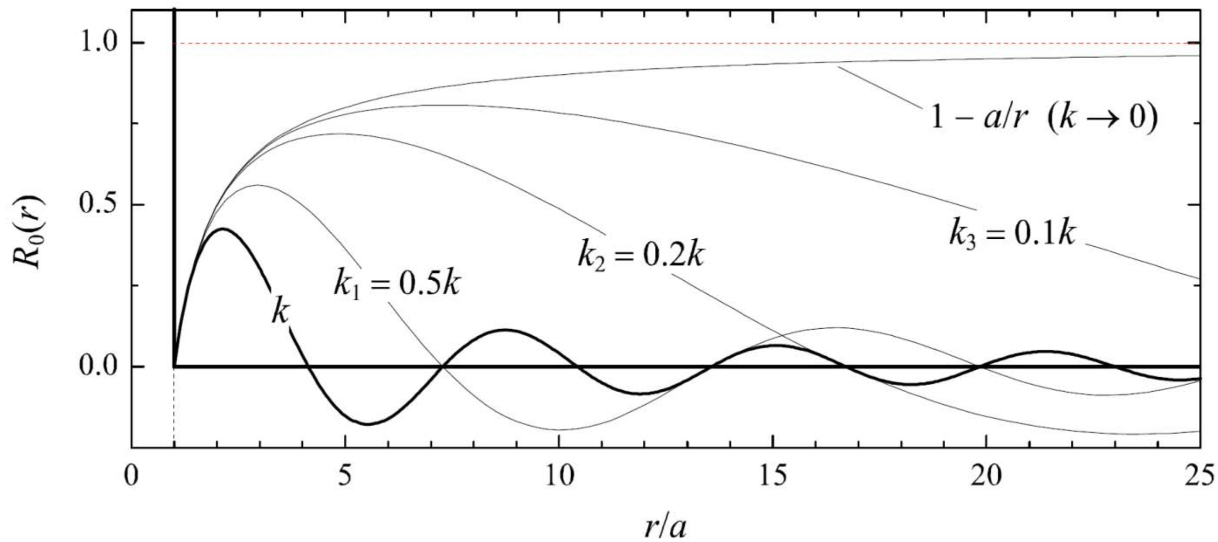
$$R_0(r) = \frac{1}{kr}\sin[k(r-a)]$$

hard sphere potential for $l = 0$



$r_0 = a$

hard sphere diameter

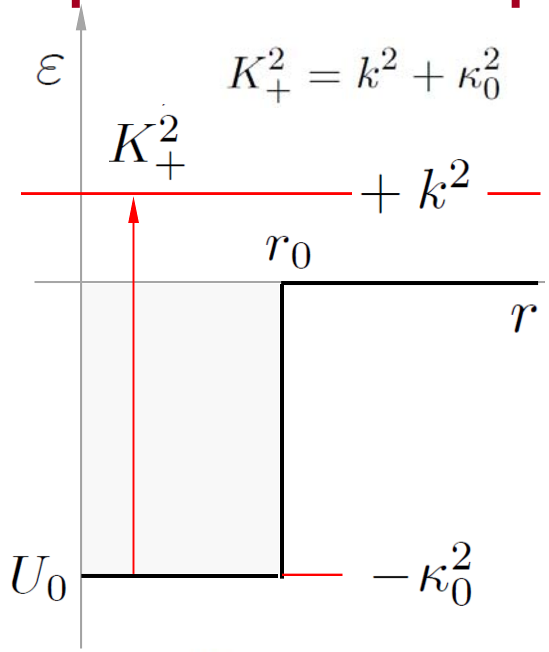


$$R_0(r) = \frac{1}{kr}\sin[k(r-a)] \underset{k\to 0}{\simeq} 1 - \frac{a}{r}$$

flat-bottom potential

scattering length - a

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



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

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

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

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

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

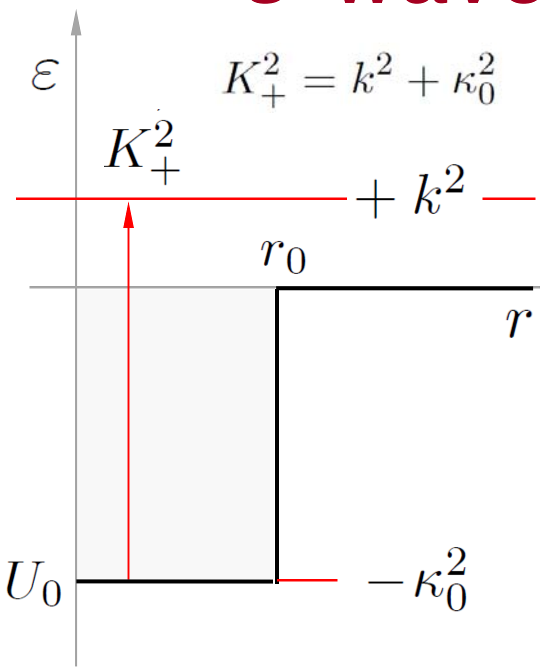
boundary condition: $\chi_0(r)$ and $\chi_0'(r)$ continuous at $r = r_0$

$r \le r_0 \qquad\qquad r > r_0$

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

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

s-wave scattering length *a*



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

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

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

Change parameters:

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

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

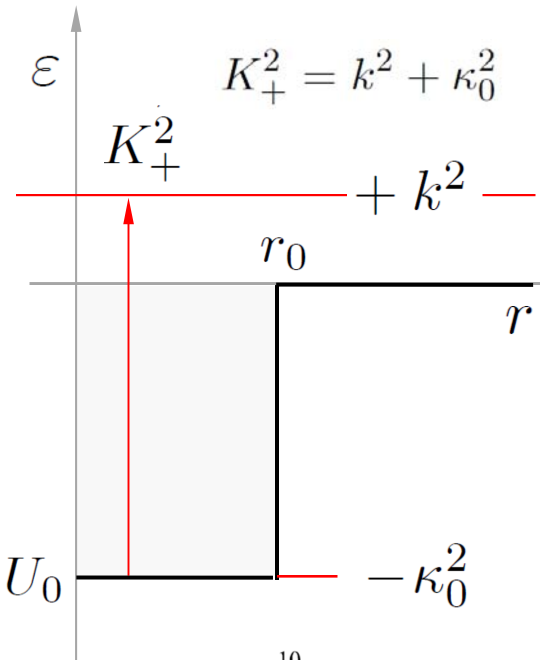
Define scattering length: $a \equiv \lim_{k\to 0} a(k) = -\lim_{k\to 0} \eta_0(k)/k$

$k \to 0$, $K_+^2 = k^2 + \kappa_0^2$ → $K_+ \to \kappa_0$

$K_+ \to \kappa_0$ → $$a = r_0 - \frac{1}{k} \arctan \frac{k}{\kappa_0 \cot \kappa_0 r_0}$$ $\xrightarrow{k\to 0}$

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

s-wave scattering length a

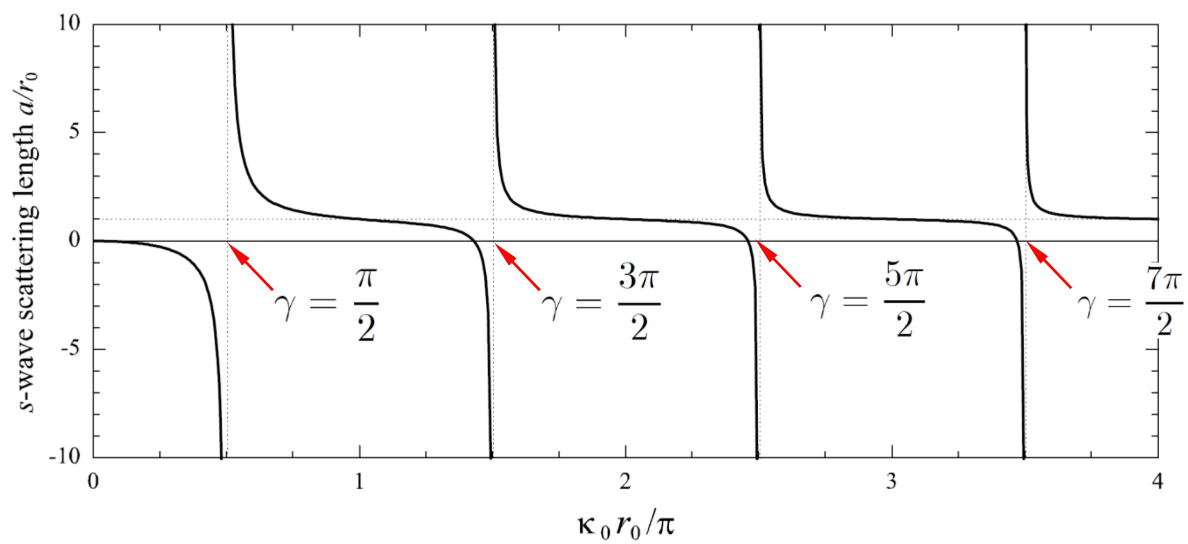


$$\kappa_0 \cot \kappa_0 r_0 = \frac{1}{r_0 - a}$$

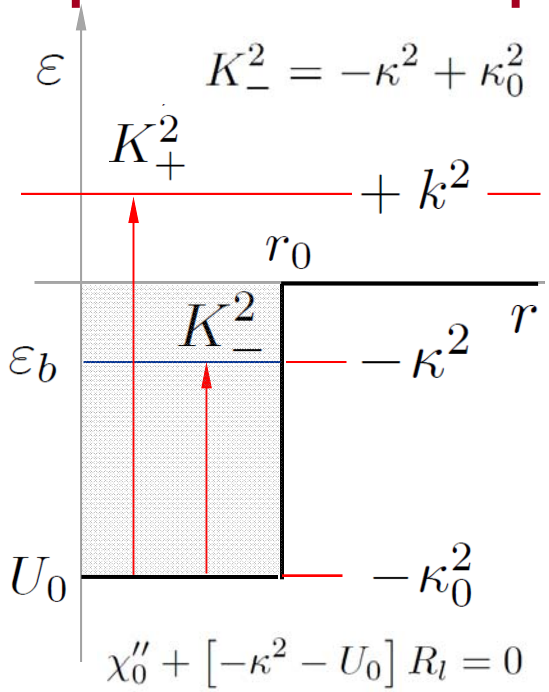
Define well parameter: $\gamma \equiv \kappa_0 r_0$

$$a = r_0\,(1 - \tan\gamma/\gamma)$$

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



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



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

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

normalization

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

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

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

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

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

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

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

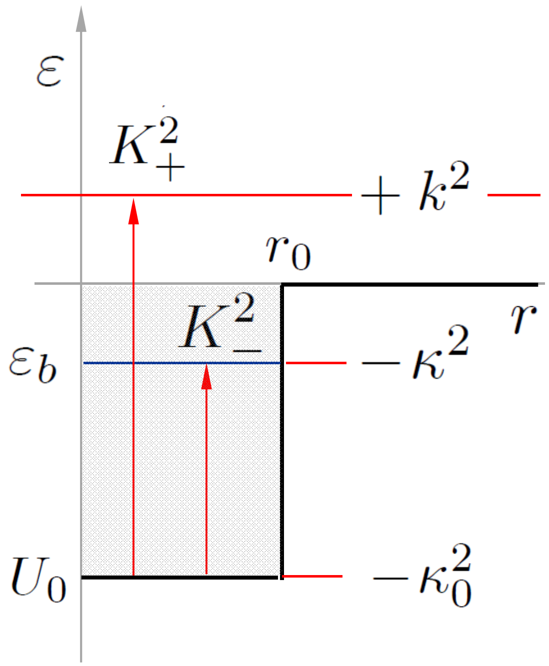
$$\underbrace{\chi_0'/\chi_0|_{r=r_0} = K_- \cot K_- r_0}_{r \le r_0} = \underbrace{-\kappa}_{r > r_0}$$

Bethe-Peierls boundary condition

$$\left.\begin{matrix} \kappa \to 0 \\ K_-^2 = \kappa_0^2 - \kappa^2 \end{matrix}\right] \rightarrow K_- \to \kappa_0 \longrightarrow \chi_0'/\chi_0|_{r=r_0} = \kappa_0 \cot \kappa_0 r_0 = 0 \text{ for } \kappa \to 0$$

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

universal behavior near threshold



Almost-bound level:

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

Weakly-bound level:

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

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

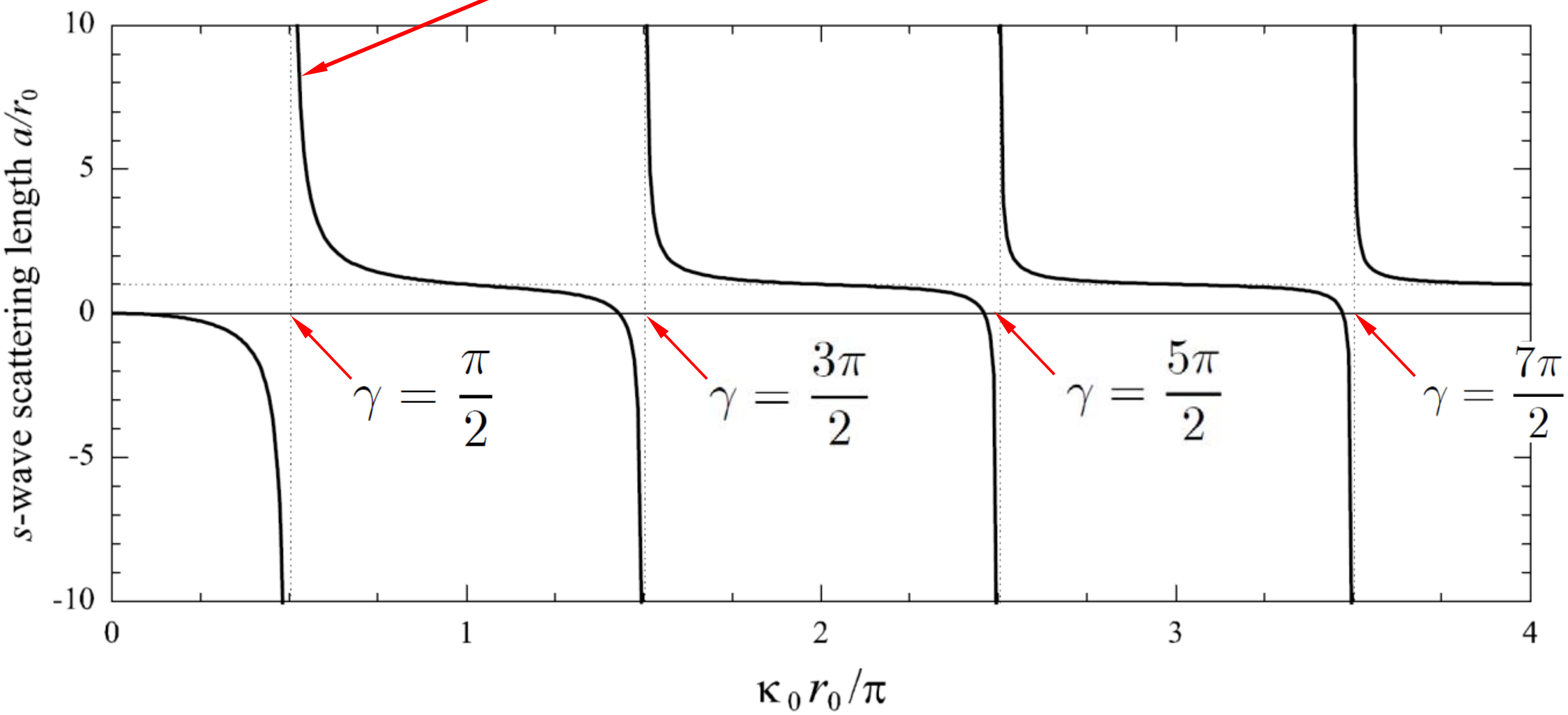
Universal dependence of binding energy on scattering length:

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

scattering length a

$$a > 0 \quad \text{for} \quad \kappa \to 0 \quad (\kappa > 0)$$

Weakly-bound level:

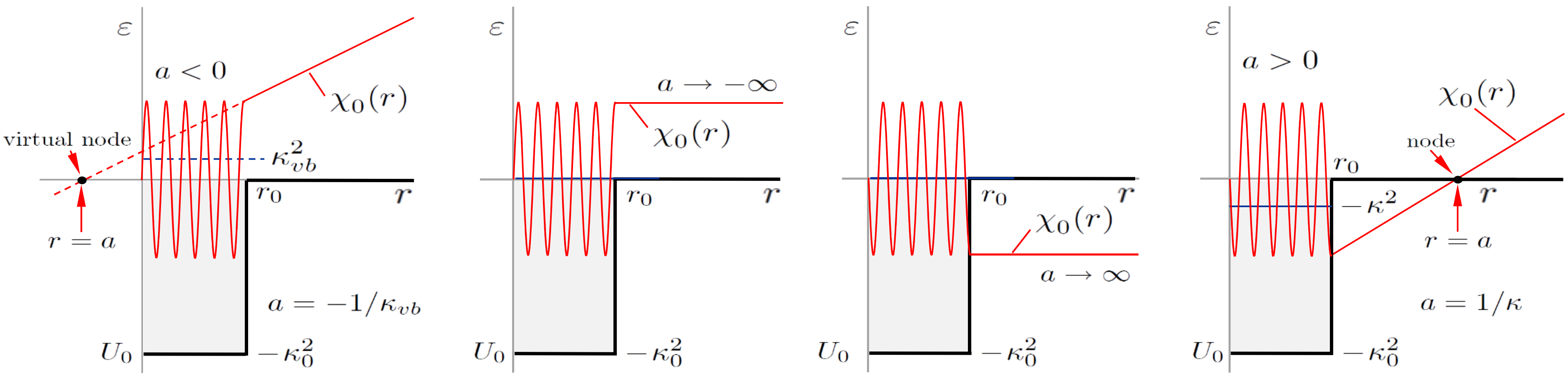


scattering length *a*

Continuum states ($\varepsilon > 0$):

$$\eta_0 = -ka$$

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



virtual level

resonant level

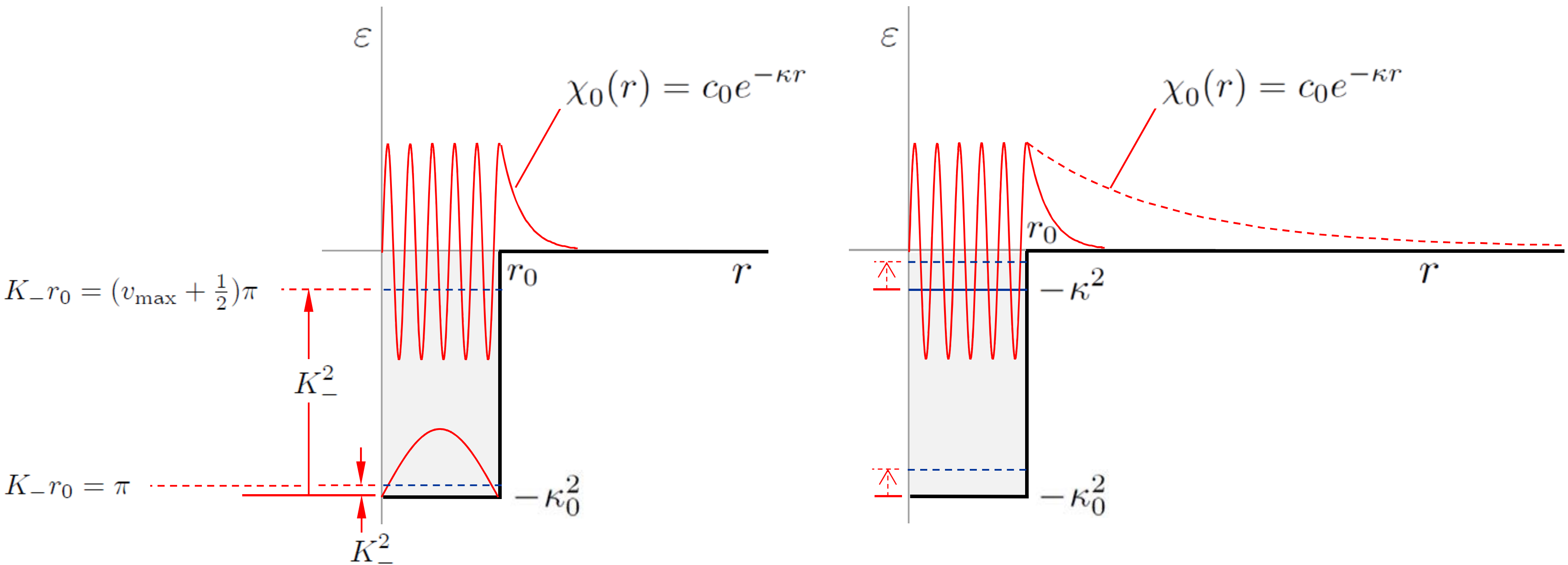
weakly-bound level

halo states

Bound states ($\varepsilon < 0$):

$$\left.\begin{array}{r}\chi_0 = Ae^{-\kappa r} \\ \kappa r_0 \ll 1\end{array}\right] \rightarrow$$ universal bound states: halo states

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

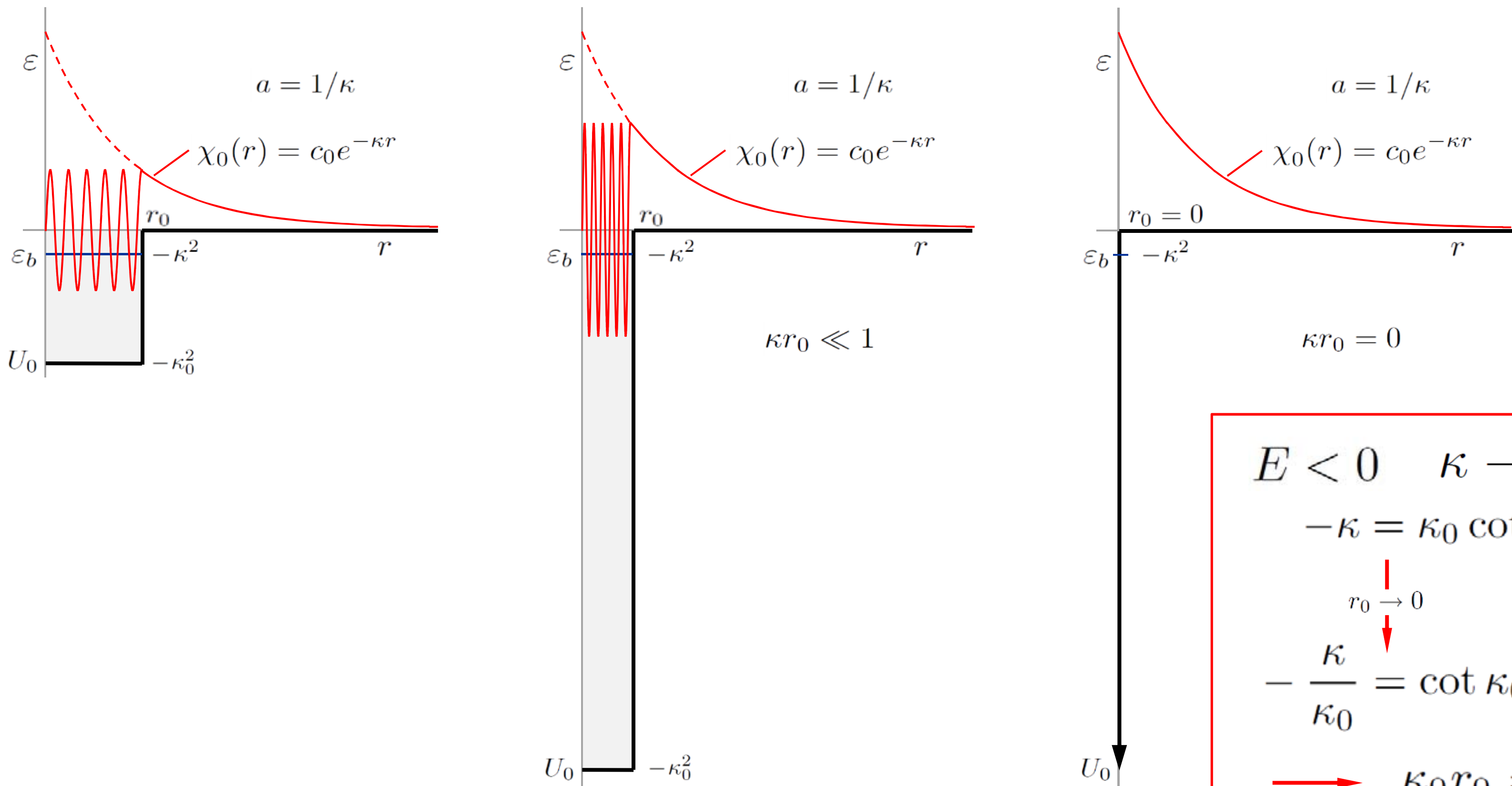


halo states

Bound states ($\varepsilon < 0$):

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

→ universal bound states: halo states



$$E < 0 \quad \kappa \to 0$$

$$-\kappa = \kappa_0 \cot \kappa_0 r_0$$

$\downarrow$ $r_0 \to 0$

$$-\frac{\kappa}{\kappa_0} = \cot \kappa_0 r_0 \to 0$$

→ $\kappa_0 r_0 = \pi/2$

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