Lectures on quantum gases

Lecture 4

Elastic Collision Phenomena in Quantum Gases

Jook Walraven
University of Amsterdam

Where do we stand?

1. We studied dependence of scattering length on well parameter
2. We found resonant enhancement near the bound state threshold
3. We found universal behavior near the threshold
4. We defined halo states and zero-range potentials
5. We analyzed the energy dependence of the scattering length
6. We introduced the effective range r_e
7. We discussed anomalously large and small scattering lengths
8. We noticed that negative effective ranges did not appear
9. We found r_e to be important only for anomalously large a

Relative motion of interacting particles III

flat-bottom potential

broad s-wave resonances

s-wave resonances

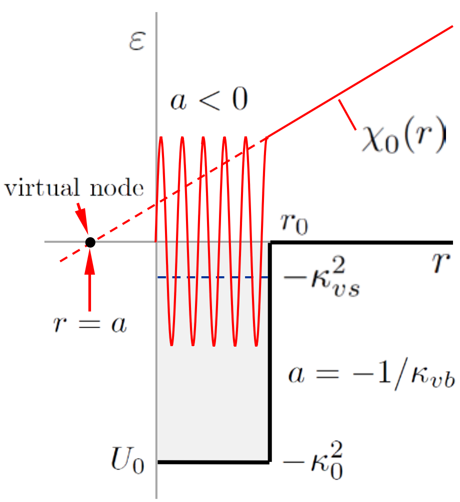
We return to the *energy dependence* of the phase shift

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

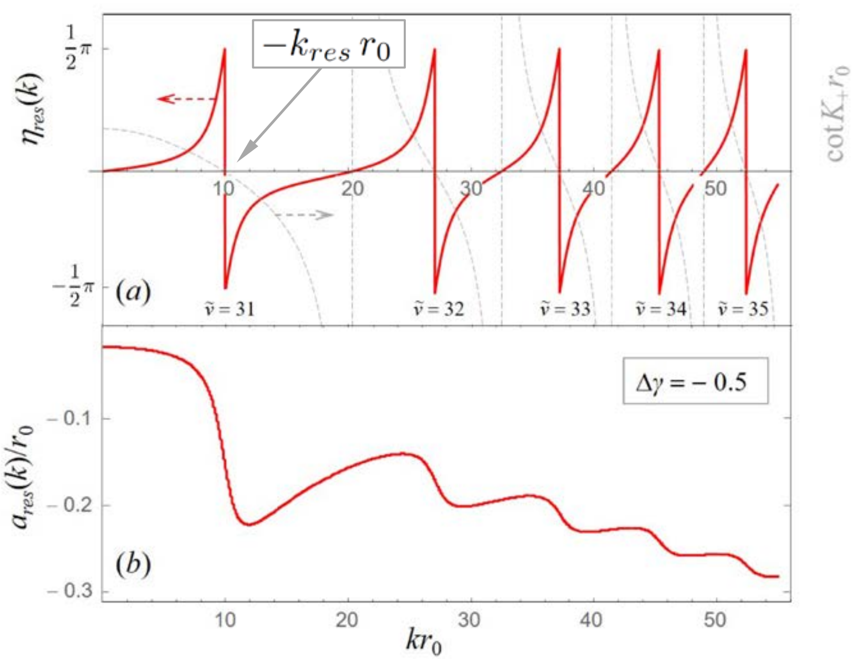
$$a(k) = \underbrace{r_0}_{\text{“background”}} \underbrace{- \frac{1}{k}\arctan\frac{k}{K_+\cot K_+ r_0}}_{\text{“resonant”}}$$

$$K_+^2 = k^2 + \kappa_0^2$$

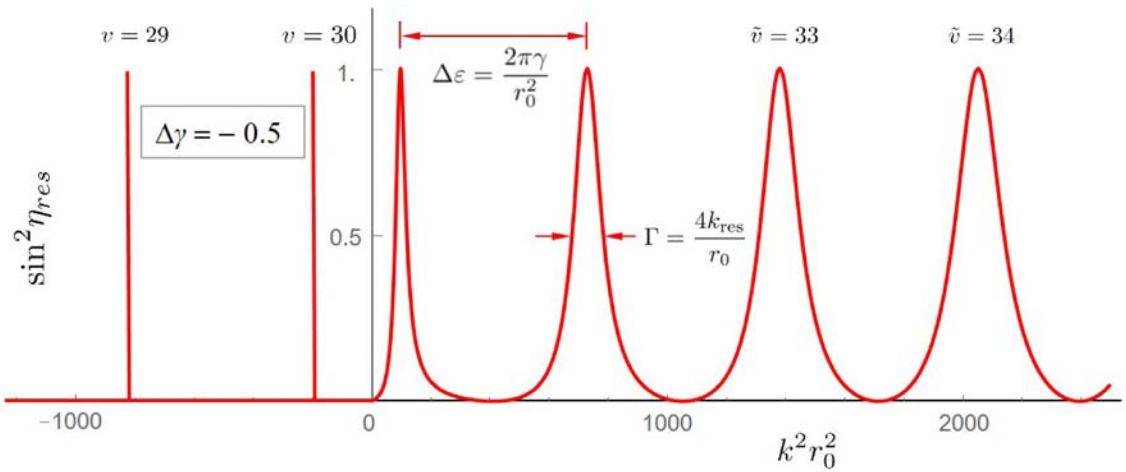
$$a_{res} = a - r_0$$



(virtual level)



Breit-Wigner line shape



Expand about resonance ($\delta k = k - k_{res}$)

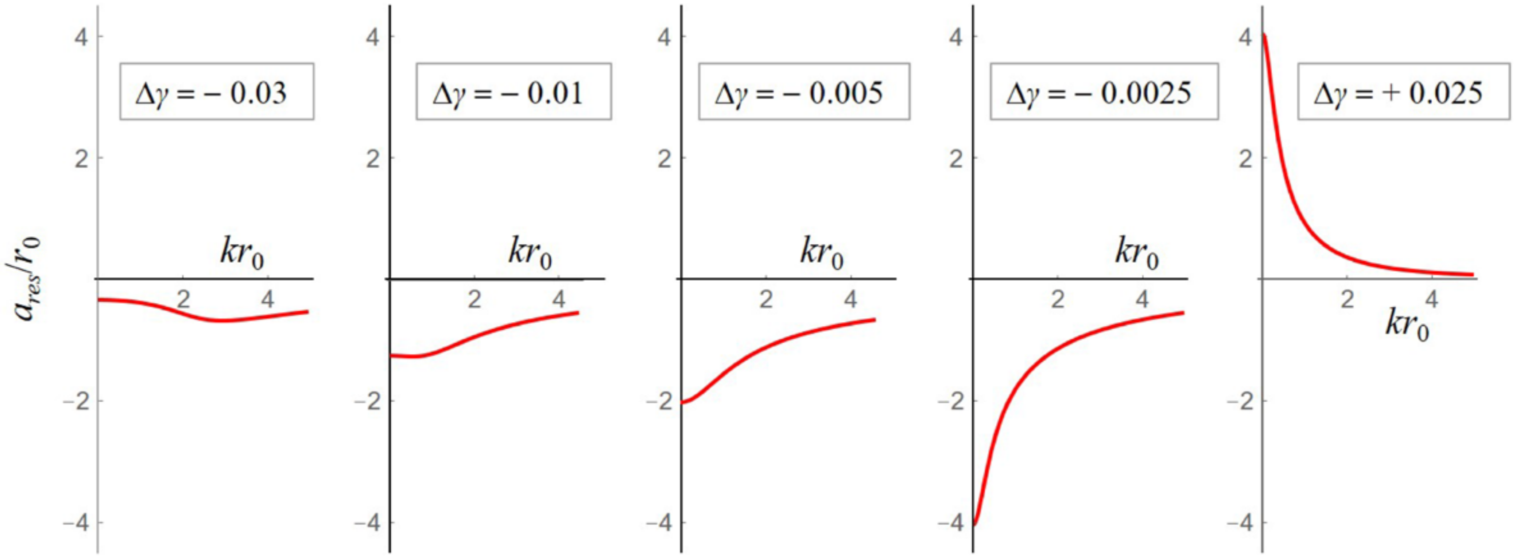
$$\tan\eta_{\rm res} = \frac{k}{K_+ \cot K_+ r_0} \simeq -\frac{1}{\delta k\, r_0} = \frac{-(k+k_{\rm res})}{(k+k_{\rm res})(k-k_{\rm res})r_0} \simeq \frac{-2k_{\rm res}}{(k^2-k_{\rm res}^2)r_0} \equiv -\frac{\Gamma/2}{E-E_{res}}$$

$$\boxed{\sin^2\eta_{\rm res} = \frac{(\Gamma/2)^2}{(E-E_{\rm res})^2+(\Gamma/2)^2}} \qquad \boxed{\Gamma = (\hbar^2/m_r)(2k_{\rm res}/r_0)}$$

(b) $\longrightarrow$ $$\sigma_0 = \frac{4\pi}{k^2}\sin^2\eta_0 \longrightarrow \boxed{\sigma_0 = \frac{4\pi}{k_{\rm res}^2}\frac{(\Gamma/2)^2}{(E-E_{\rm res})^2+(\Gamma/2)^2}}$$

s-wave resonance near threshold

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



$$a(k) \simeq r_0 + \frac{1}{k}\arctan\frac{k}{\kappa}$$

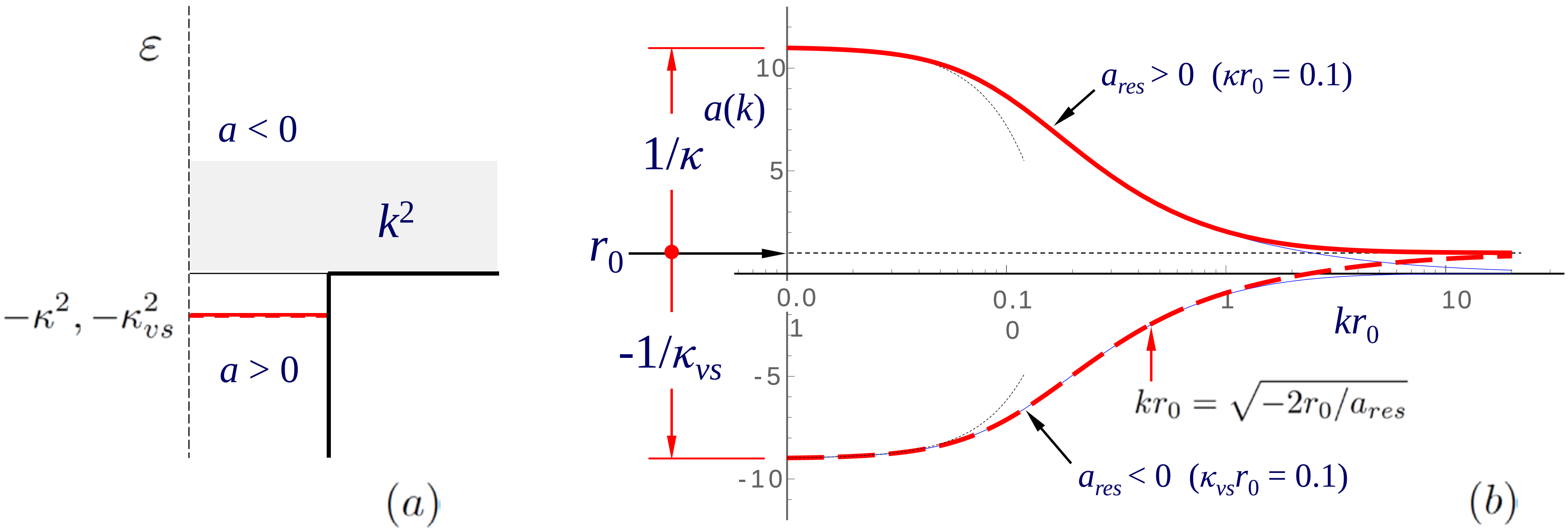
(weakly-bound level)

$$a(k) \simeq r_0 - \frac{1}{k}\arctan\frac{k}{\kappa_{vs}}$$

(virtual level)

s-wave resonance near threshold

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

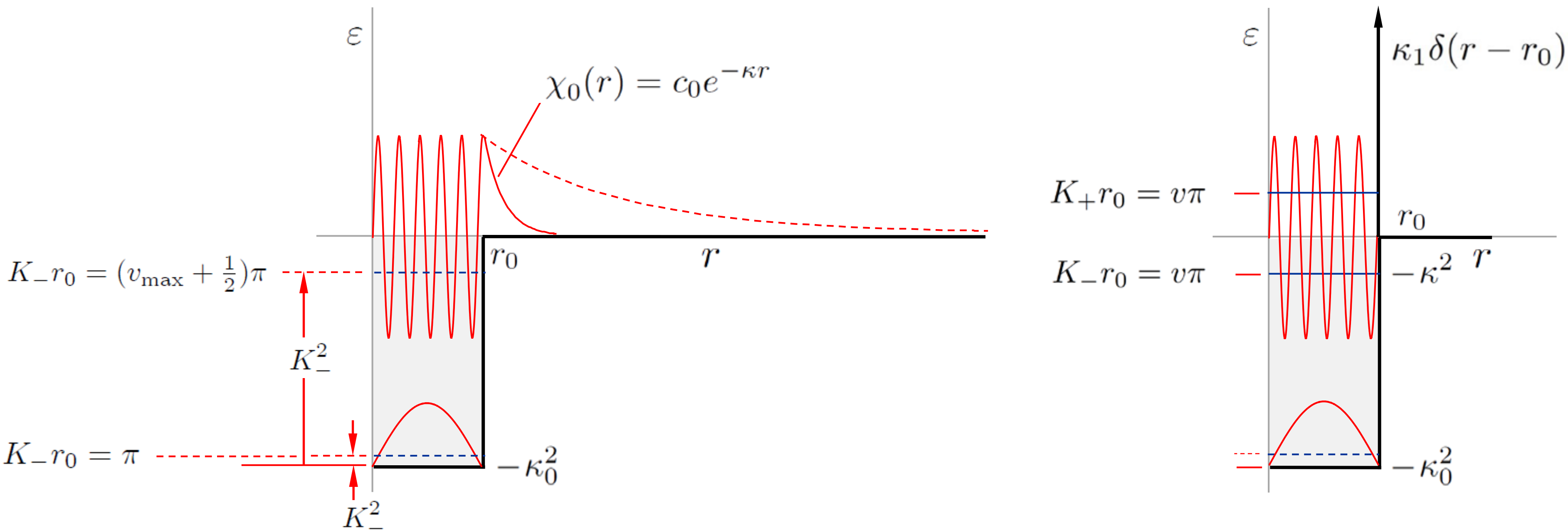


Conclusion: scattering length approximation valid for $\boxed{\begin{array}{l} k \ll \kappa \\ k \ll \kappa_{vs} \end{array}}$

from halo state to narrow resonance

Bound states ($\varepsilon < 0$):

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



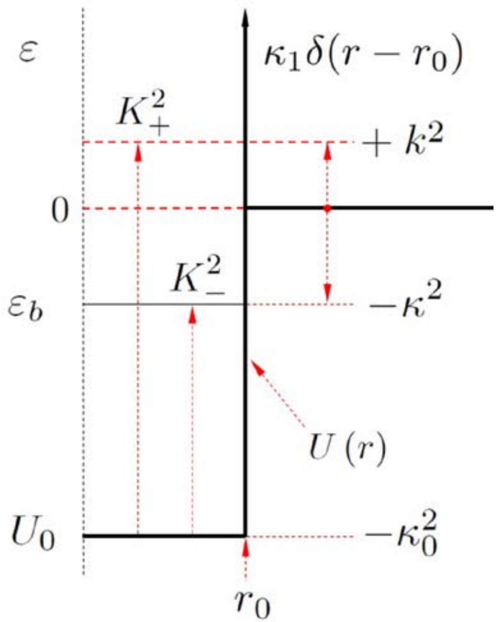
‘open’ channel

‘closed’ channel

screened flat-bottom potential

narrow *s*-wave resonances

screened flat-bottom potential



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

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

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

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

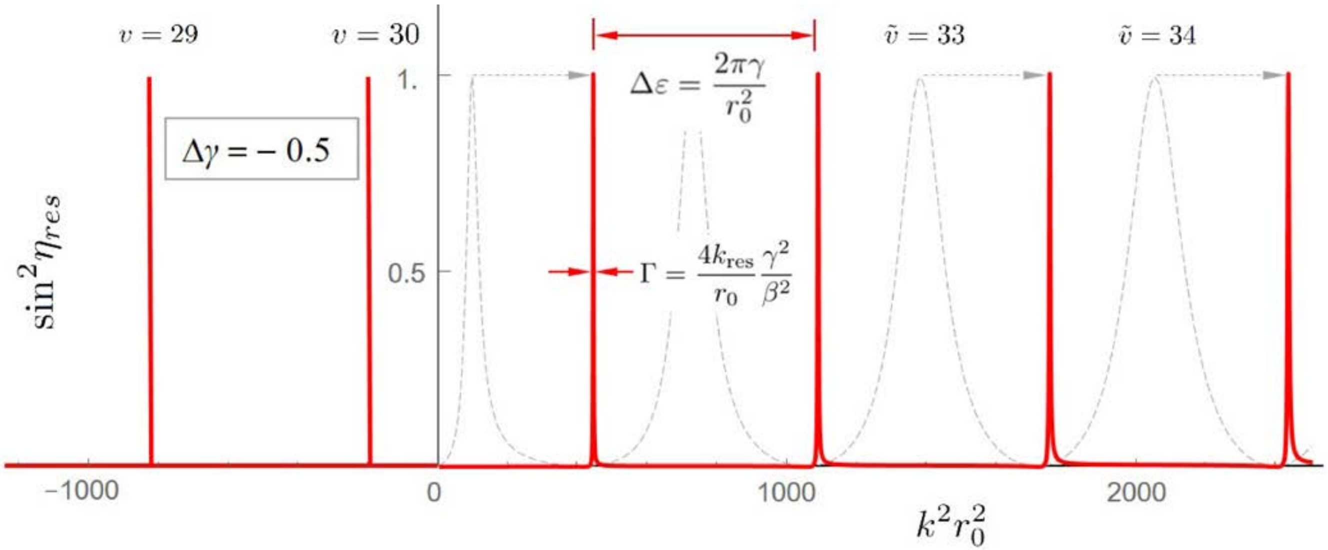
$$\chi_0'' + K_+^2\chi_0 = 0$$
$$\chi_0 = A'\sin(K_+ r + \cancel{\eta_0})$$
$$\chi_0' = K_+ A'\cos(K_+ r)$$

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

$$\chi_0'/\chi_0|_{r=r_0} = \underbrace{K_+\cot K_+ r_0}_{r<r_0} = \underbrace{k\cot(kr_0+\eta_0) + \kappa_1}_{r>r_0}$$

Barrier parameter: $\beta \equiv \kappa_1 r_0$ $\longrightarrow$ $\boxed{a(k) = r_0 - \frac{1}{k}\arctan\left(\frac{kr_0}{K_+ r_0\cot K_+ r_0 - \beta}\right)}$

screened flat-bottom potential



Expand about resonance ($\delta k = k - k_{res}$)

$$\tan\eta_{\rm res} = \frac{k}{K_+\cot K_+ r_0 - \kappa_1} \simeq -\frac{1}{\delta k\, r_0}\frac{\kappa_1^2}{\kappa_0^2} = \frac{-(k+k_{\rm res})}{(k^2-k_{\rm res}^2)r_0}\frac{\kappa_1^2}{\kappa_0^2} \simeq \frac{-\Gamma/2}{E-E_{\rm res}}$$

$$\boxed{\sin^2\eta_{\rm res} = \frac{(\Gamma/2)^2}{(E-E_{\rm res})^2+(\Gamma/2)^2}}$$

$$\boxed{\Gamma = (\hbar^2/m_r)(2k_{\rm res}/R^*)}$$

$$\boxed{R^* = \tfrac{1}{2}r_0(\kappa_1/\kappa_0)^2}$$

effective range r_e

We analyze the energy dependence of a resonance <u>near threshold</u>

$$\eta_0(k) = \underbrace{-kr_0}_{\text{“regular”}} + \underbrace{\arctan\left(\frac{kr_0}{K_+r_0\cot K_+r_0 - \beta}\right)}_{\text{“resonant”}}$$

evaluate phase shift:

$$k\cot\eta_0 = \frac{(K_+\cot K_+r_0 - \kappa_1) + k^2r_0 + \cdots}{1 - r_0\left(1 + \frac{1}{3}k^2r_0^2 + \cdots\right)(K_+\cot K_+r_0 - \kappa_1)}$$

$$K_+^2 = k^2 + \kappa_0^2 \longrightarrow K_+r_0 = \kappa_0 r_0[1 + k^2/\kappa_0^2]^{1/2} = \gamma + \tfrac{1}{2}k^2r_0^2/\gamma + \cdots$$

$$\boxed{a = r_0\left(1 - \tan\gamma/\gamma\right)}$$

effective range r_e

Effective range expansion: r_e : measure for energy dependence of the phase shift

$$\boxed{k\cot\eta_0 = -\frac{1}{a} + \tfrac{1}{2}k^2 r_e + \cdots}$$

effective range: $$r_e = r_0\left(1 - \frac{3ar_0 + \gamma^2 r_0^2 - 3\beta(a^2 - r_0^2) + 3\beta^2(a-r_0)^2}{3a^2\gamma^2}\right)$$

broad resonance – open channel ($r_e > 0$ for large $|a|$):

$$\kappa_1 \to 0 \quad \longrightarrow \quad r_e = r_0\left(1 - \frac{3ar_0 + \gamma^2 r_0^2}{3a^2\gamma^2}\right) = r_0\left(1 - \frac{r_0}{a\gamma^2} - \frac{r_0^2}{3a^2}\right)$$

narrow resonance – closed ($r_e < 0$ for large $|a|$):

$$\kappa_1^2 \gg \kappa_0^2 \quad \longrightarrow \quad r_e \simeq -r_0\frac{\kappa_1^2}{\kappa_0^2}\frac{(a-r_0)^2}{a^2} = -r_0\frac{\kappa_1^2}{\kappa_0^2}\left(1 - 2\frac{r_0}{a} + \frac{r_0^2}{a^2}\right)$$

Resonance-width parameter R^*

$$k\cot\eta_0 = -\frac{1}{a} + \tfrac{1}{2}k^2 r_e + \cdots$$

narrow resonance – 'closed' channel ($r_e < 0$ for large $|a|$):

$$\kappa_1^2 \gg \kappa_0^2 \;\longrightarrow\; r_e \simeq -r_0 \frac{\kappa_1^2}{\kappa_0^2}\left(1 - 2\frac{r_0}{a} + \frac{r_0^2}{a^2}\right) \simeq -2R^*$$

$$R^* = -\tfrac{1}{2}r_e \simeq \tfrac{1}{2}r_0(\kappa_1/\kappa_0)^2$$

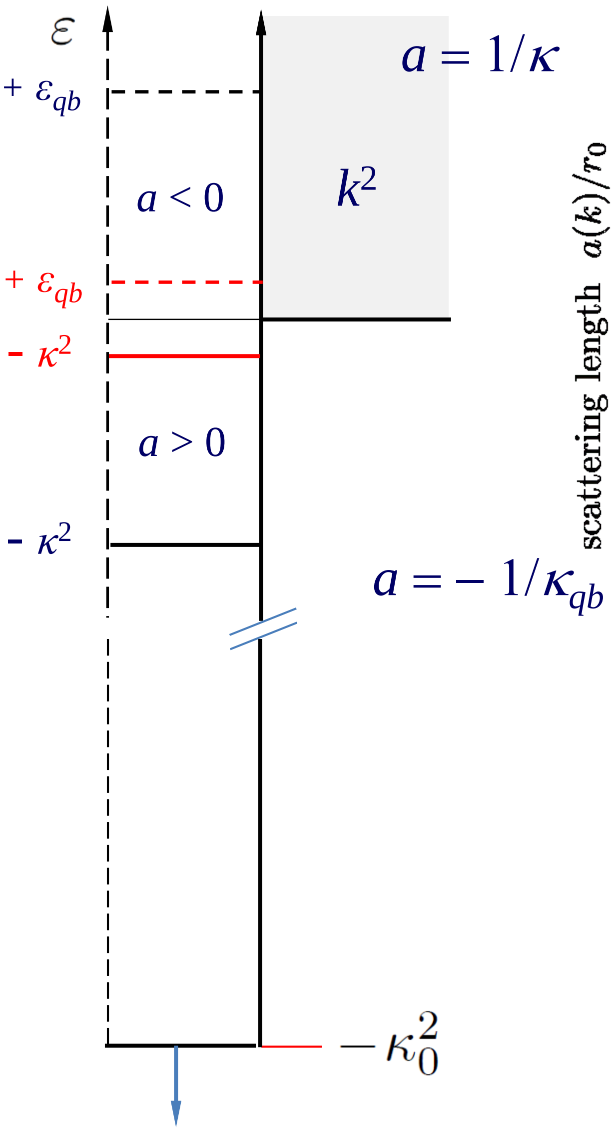
positive

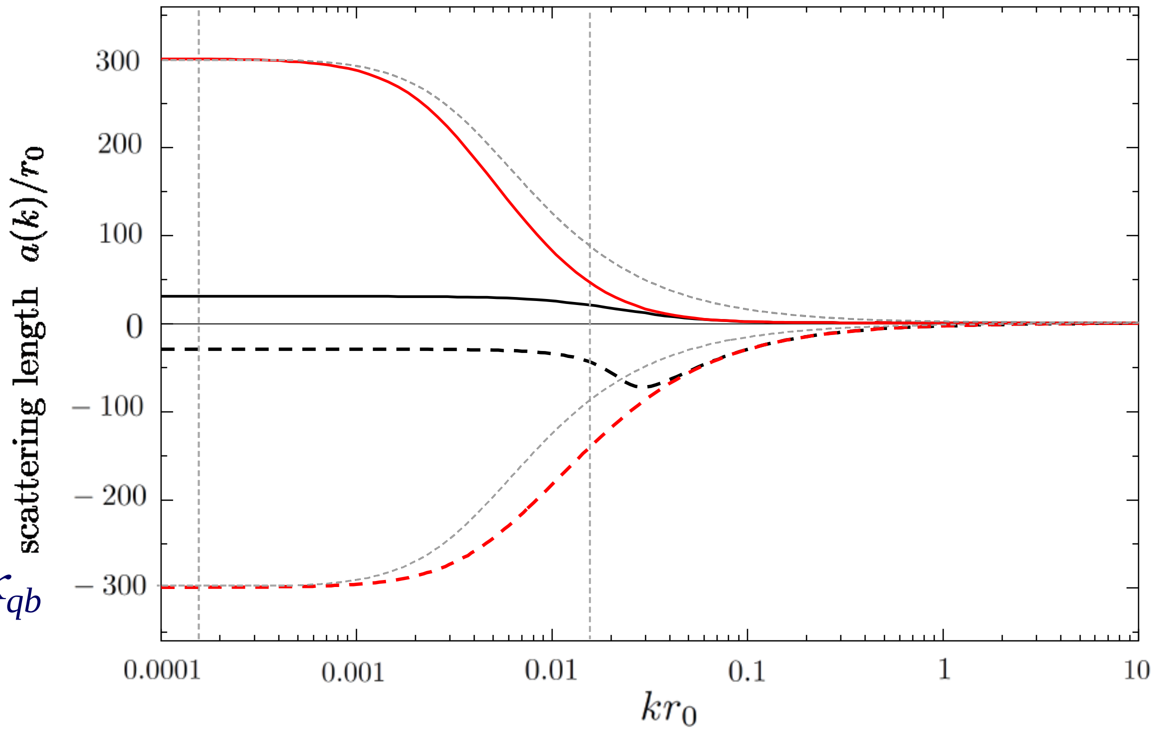
$$\boxed{k\cot\eta_0 = -\frac{1}{a} - k^2 R^*}$$

strong barrier – weak coupling – narrow resonance – closed channel $R^* >> r_0$

weak barrier – strong coupling – broad resonance – open channel $R^* << r_0$

narrow resonance near threshold





$$a(k) = r_0 - \frac{1}{k} \arctan\left(\frac{kr_0}{K_+ r_0 \cot K_+ r_0 - \beta} \right)$$

$$K_+^2 = k^2 + \kappa_0^2$$

particles with internal structure
(scattering of atoms)

Schrödinger equation

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

thus far: fixed potential

What happens if we add internal structure?

First we recapitulate:

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

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

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

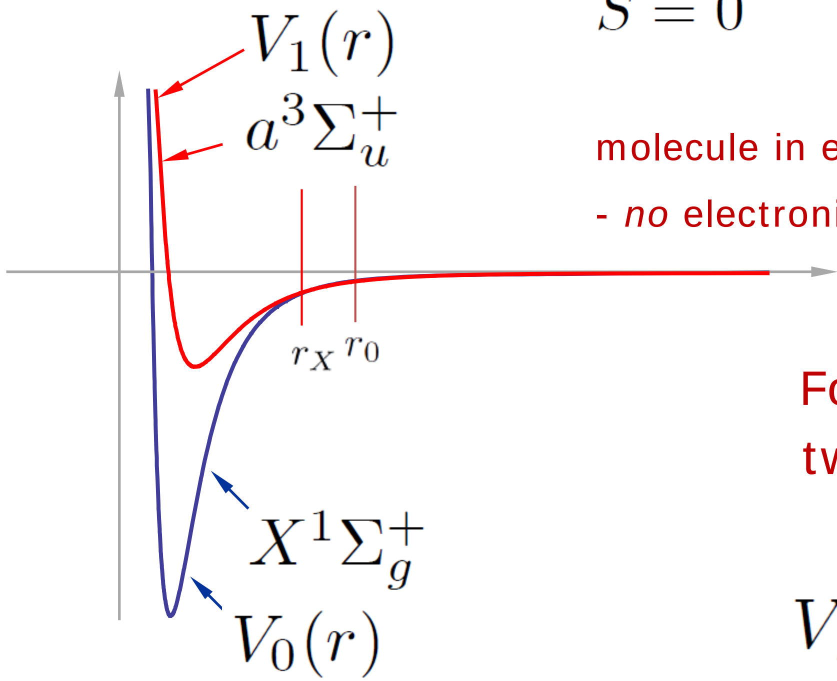
$$\left[\frac{\hbar^2}{2\mu}\left(-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr}\right) + \underbrace{\frac{l(l+1)\hbar^2}{2\mu r^2} + \mathcal{V}(r)}_{\mathcal{V}_{\text{eff}}(r)}\right] R_l(r) = E R_l(r)$$

good for systems like helium

Interactions between alkali atoms

$\mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2$

$S = 0$ $\qquad$ $S = 1$



molecule in electronic ground state

- *no* electronic angular momentum: $\Lambda = 0$

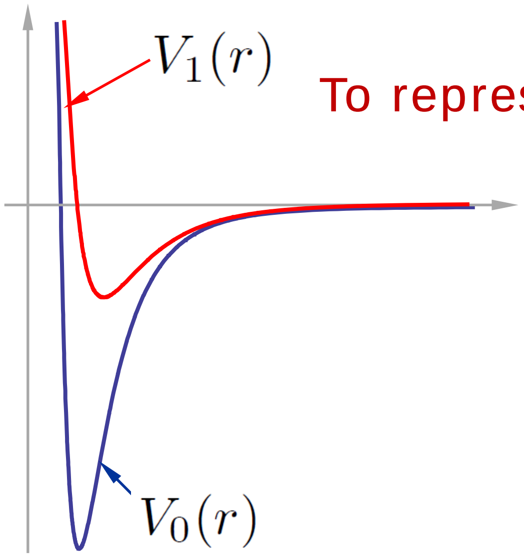
For two ground-state alkali atoms
two (not more than two) potentials

$$V_S(r) \longrightarrow \begin{cases} S = 1 & V_1(r) \quad \text{triplet} \\ S = 0 & V_0(r) \quad \text{singlet} \end{cases}$$

Conclusion: exchange determines interatomic interaction

To solve Schrödinger equation
we turn to the basis: $|\psi\rangle = |R_l\rangle |l m_l; \psi_e\rangle \, |S, M_S\rangle$

Interactions between alkali atoms



To represent exchange we construct a *spin hamiltonian*:

$$\mathcal{V}(r) = V_D(r) + J(r)\mathbf{s}_1 \cdot \mathbf{s}_2$$

$$J(r) = V_1(r) - V_0(r)$$

$$V_D(r) = \tfrac{1}{4}[V_0(r) + 3V_1(r)]$$

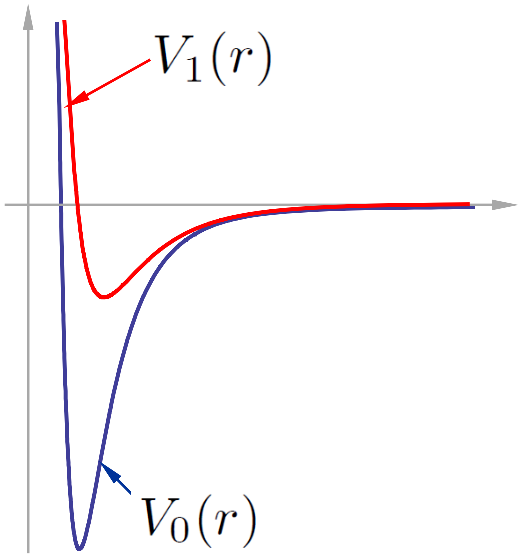
$$\boxed{\mathbf{s}_1 \cdot \mathbf{s}_2 = \tfrac{1}{2}\left(\mathbf{S}^2 - \mathbf{s}_1^2 - \mathbf{s}_2^2\right)}$$

Properties of operator $\mathcal{V}(r)$:

$$\left.\begin{aligned} \mathcal{V}(r)\,|0,0\rangle &= V_0(r)\,|0,0\rangle \\ \mathcal{V}(r)\,|1,M_S\rangle &= V_1(r)\,|1,M_S\rangle \end{aligned}\right\} \longrightarrow \mathcal{V}(r)\,|S,M_S\rangle = V_S(r)\,|S,M_S\rangle$$

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

Interactions between alkali atoms



Let us add magnetic field:

$$\mathcal{H}_Z = \gamma_e \mathbf{s}_1 \cdot \mathbf{B} + \gamma_e \mathbf{s}_2 \cdot \mathbf{B} = \gamma_e \mathbf{S} \cdot \mathbf{B} = \gamma_e B\, S_z$$

$$\gamma_e = g_s \mu_B / \hbar$$

$$\Delta E_Z = g_s \mu_B B M_S$$

$M_S = m_{s_1} + m_{s_2}$ is good quantum number

$$\boxed{\mathbf{s}_1 \cdot \mathbf{s}_2 = \tfrac{1}{2}\left(\mathbf{S}^2 - \mathbf{s}_1^2 - \mathbf{s}_2^2\right)}$$

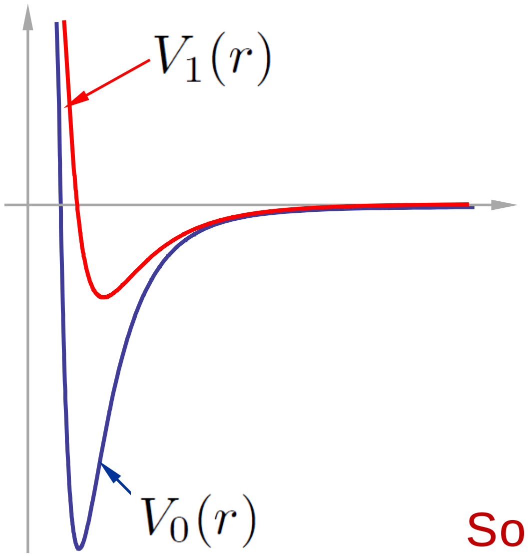
$$\boxed{\mathbf{s}_1 \cdot \mathbf{s}_2 = s_{1z} s_{2z} + \tfrac{1}{2}\left(s_1^+ s_2^- + s_1^- s_2^+\right)}$$

Hamiltonian including spin Zeeman term:

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

good basis states: $|\psi\rangle = |R_l^S\rangle |l, m_l\rangle |S, M_S\rangle$

Interactions between alkali atoms



Hamiltonian including spin Zeeman term:

$$\mathcal{V}(r) = V_D(r) + J(r)\mathbf{s}_1 \cdot \mathbf{s}_2$$

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

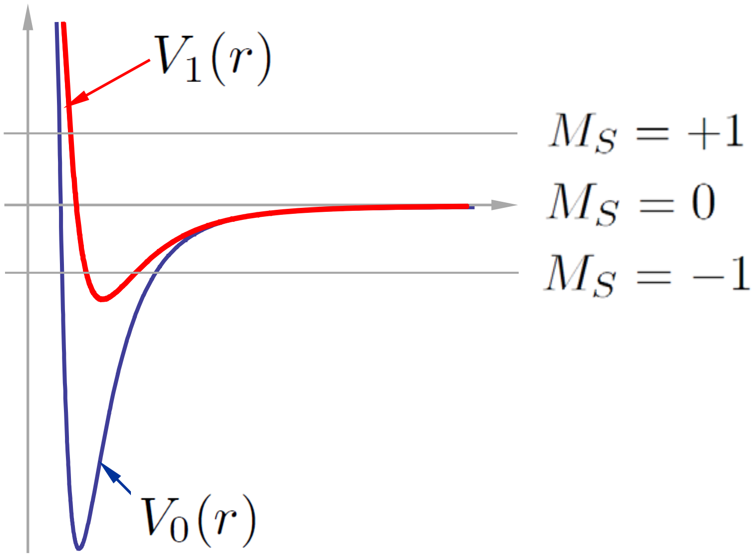
good basis states: $|\psi\rangle = |R_{v,l}^S\rangle |S, M_S\rangle |l, m_l\rangle$

Solve radial wave equation for given l, S and M_S:

$$R''_{S,l} + \frac{2}{r} R'_{S,l} + \left[\varepsilon - U_{S,l}(r)\right] R_{S,l} = 0$$

$$U_{S,l}(r) = U_S(r) + \frac{l\,(l+1)}{r^2} + \frac{2\mu}{\hbar^2}\gamma_e B\, M_S$$

Interactions between alkali atoms

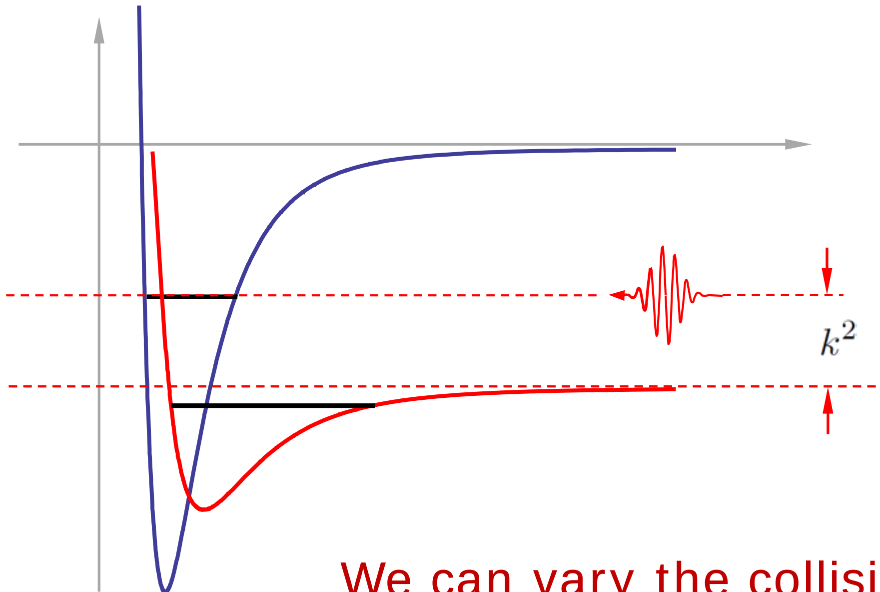


magnetic field lifts degeneracy of triplet potential

$$U_{S,l}(r) = U_S(r) + \frac{l\,(l+1)}{r^2} + \frac{2\mu}{\hbar^2}\gamma_e B\, M_S$$

This makes it possible to shift the triplet potential with respect to the singlet potential

Feshbach resonance

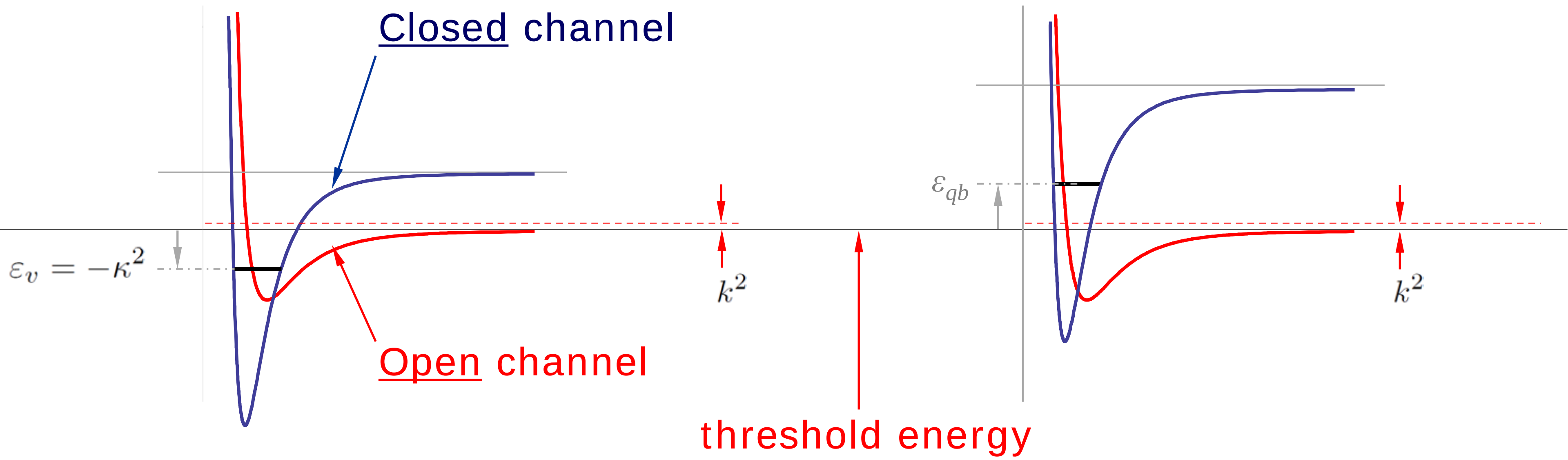


We can <u>vary</u> the collision energy to be resonant with a bound state in a closed channel

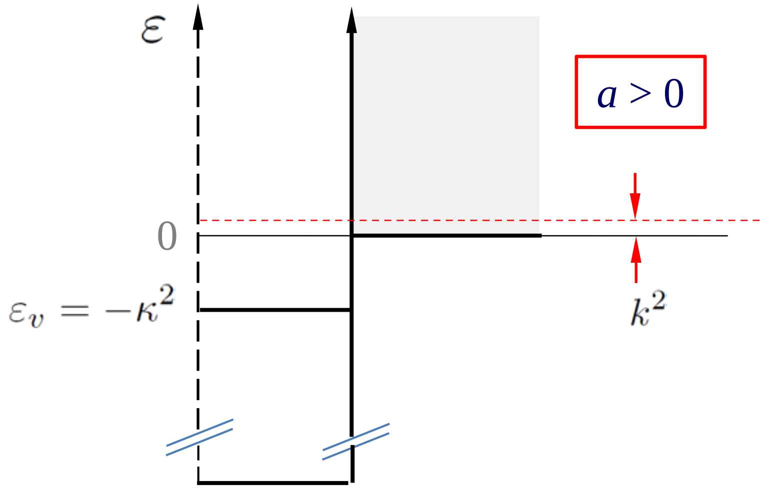
Any weak singlet-triplet coupling induces a scattering resonance in the open channel: Feshbach resonance

With cold alkali atoms we can tune to a Feshbach resonance at arbitrary, <u>fixed</u> (low) collisional energy by varying the magnetic field: Zeeman tuning

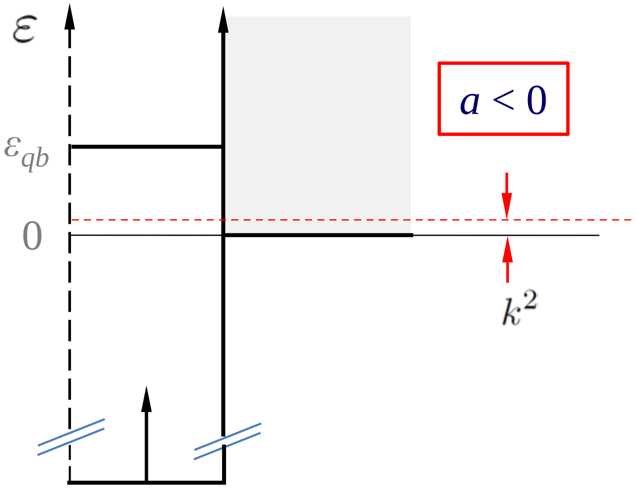
some nomenclature



Closed channel: below threshold



Closed channel: above threshold



particles with internal structure

1. We analyzed s-wave resonances
2. We noticed that negative effective ranges did not appear
3. We introduced a tunnel barrier
4. We found that for a weak tunnel coupling $r_e < 0$
5. We introduced the width parameter R^* to discriminate between broad and narrow s-wave resonances
6. We introduced atoms with spin
7. We found triplet and singlet potentials
8. We introduced the Feshbach problem