Lectures on quantum gases

Lecture 2

Relative motion of interacting particles II

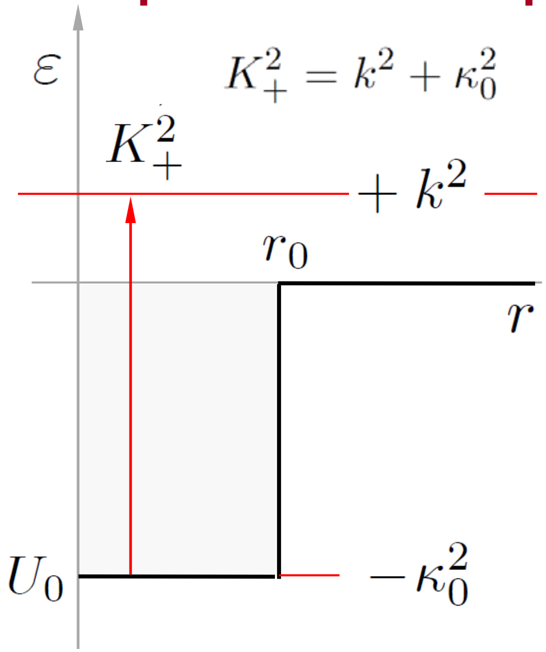
Jook Walraven
University of Amsterdam

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

flat-bottom potential

scattering length - a

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



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

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

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

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

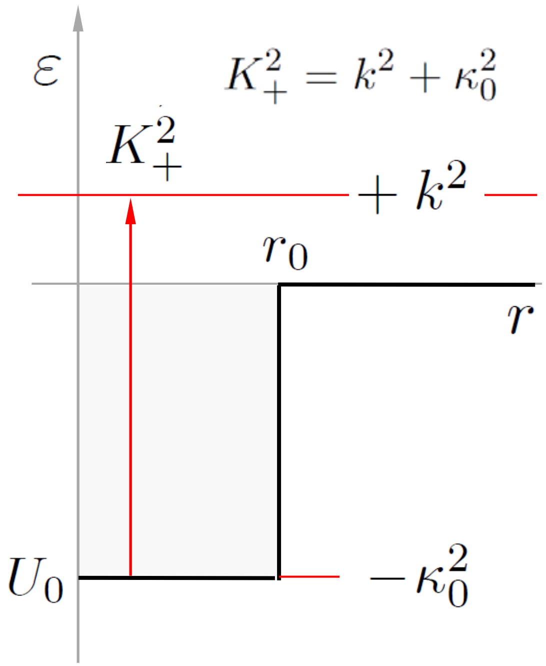
$$\chi_0'' + K_+^2\chi_0 = 0$$
$$\chi_0 = A'\sin(K_+ r + \cancel{\eta_0})$$
$$\chi_0' = K_+ A'\cos(K_+ r)$$

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

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

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

s-wave scattering length a



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

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

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

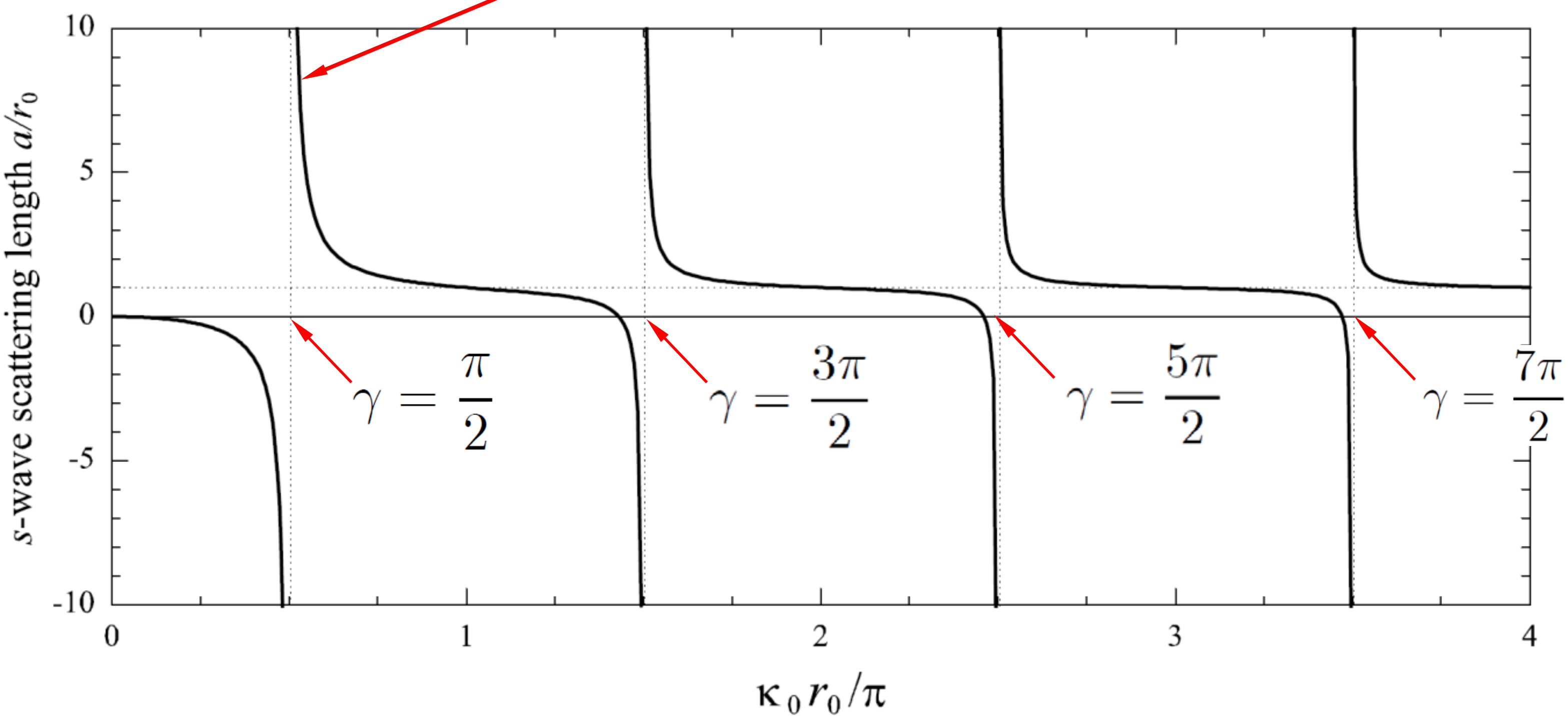
Define scattering length: $a \equiv \lim_{k\to 0} a(k) = -\lim_{k\to 0} \eta_0(k)/k$

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

scattering length a

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

Weakly-bound level:



flat-bottom potential

effective range - r_e

effective range r_e

We now analyze the *energy dependence* of the phase shift

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

"regular" "resonant"

$$\tan(\alpha+\beta) = \frac{\tan\alpha + \tan\beta}{1-\tan\alpha\tan\beta}$$

$$\tan x = x + \tfrac{1}{3}x^3 + \cdots = x(1+\tfrac{1}{3}x^2+\cdots)$$

evaluate phase shift:

$$kr_0\cot\eta_0 = \frac{K_+ r_0\cot K_+ r_0 + k^2 r_0^2 + \cdots}{1-\left(1+\frac{1}{3}k^2r_0^2+\cdots\right)K_+ r_0 \cot K_+ r_0}$$

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

effective range r_e

$$k r_0 \cot \eta_0 = -\frac{1}{1-\tan\gamma/\gamma} + \tfrac{1}{2}k^2 r_0^2 \left(1 - \frac{3\left(1-\tan\gamma/\gamma\right)+\gamma^2}{3\gamma^2\left(1-\tan\gamma/\gamma\right)^2}\right) + \cdots$$

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

r_e : measure for energy dependence of the phase shift

Effective range expansion:

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

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

Two expansions to order k^2:

$$a \neq 0 \qquad k\cot\eta_0 = -\frac{1}{a} + \tfrac{1}{2}k^2 r_0\left(1 - \frac{3ar_0+\gamma^2 r_0^2}{3\gamma^2 a^2}\right) + \cdots$$

$$a \ll r_0 \qquad \frac{1}{k\cot\eta_0} = -a + \tfrac{1}{6}k^2 r_0^3\left[1 - 3\left(a/r_0\right)^2 + \left(3/\gamma^2\right)\left(a/r_0\right)\right] + \cdots$$

effective range r_e – special cases

$$a \neq 0 \qquad k\cot\eta_0 = -\frac{1}{a} + \tfrac{1}{2}k^2 r_0 \left(1 - \frac{3ar_0 + \gamma^2 r_0^2}{3\gamma^2 a^2}\right) + \cdots$$

$$r_e = r_0 \left(1 - \frac{r_0}{\gamma^2 a} - \frac{r_0^2}{3a^2}\right)$$

$a = \pm r_0$ (regular) $\qquad r_e = r_0\left(2/3 \mp 1/\gamma^2\right) \simeq \tfrac{2}{3} r_0$

$$k\cot\eta_0 = \mp\frac{1}{r_0} + \tfrac{1}{3}\cancel{k^2} r_0 + \cdots$$

(k = 0 limit reached)

$|a| \gg r_0$ (anomalously large) $\qquad r_e \simeq r_0$

$$k\cot\eta_0 = -\frac{1}{a} + \tfrac{1}{2}k^2 r_0 + \cdots$$

(strongly k dependent)

effective range r_e – special cases

$a \ll r_0$ (anomalously small) $\quad r_e = r_0 \left(1 - \frac{r_0}{\gamma^2 a} - \frac{r_0^2}{3a^2}\right) \simeq -r_0 \frac{r_0^2}{3a^2}$

$$\frac{1}{k\cot\eta_0} = -a + \tfrac{1}{6}k^2 r_0^3 [1 - 3\,(a/r_0)^2 + (3/\gamma^2)\,(a/r_0)] + \cdots$$

$$k\cot\eta_0 = \frac{6}{k^2 r_0^3} + \cdots \qquad (a = 0)$$

(k dependence unimportant)

$$k\cot\eta_0 = \frac{1}{a(k)}$$

Conclusion: effective range important only for $|a| \gg r_0$

examples

nuclear collisions:

proton (uud) I=1/2

neutron (udd) I=1/2

deuteron I=1 bound state $a > 0$ $a = 5.41$ fm $r_e = 1.75$ fm

I=0 excited state $a < 0$ $a = -2.38$ fm $r_e = 2.67$ fm

s-wave regime $kr_0 \ll 1$: 12 orders of magnitude difference in energy

Ultracold atom collisions:

^{133}Cs |4,4> $a = 2400\, a_0$ $r_0 = 100\, a_0$

^{85}Rb |3,3> $a = -369\, a_0$ $r_0 = 83\, a_0$

^{1}H |1,1> $a = 1.22\, a_0$ $r_e = 348\, a_0$

^{88}Sr $a = -2\, a_0$

flat-bottom potential

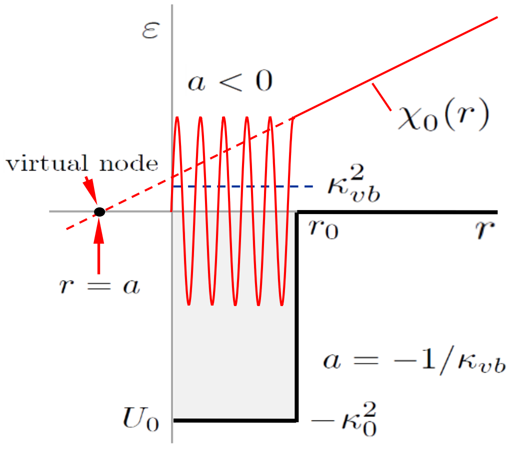
s-wave resonances

s-wave resonances

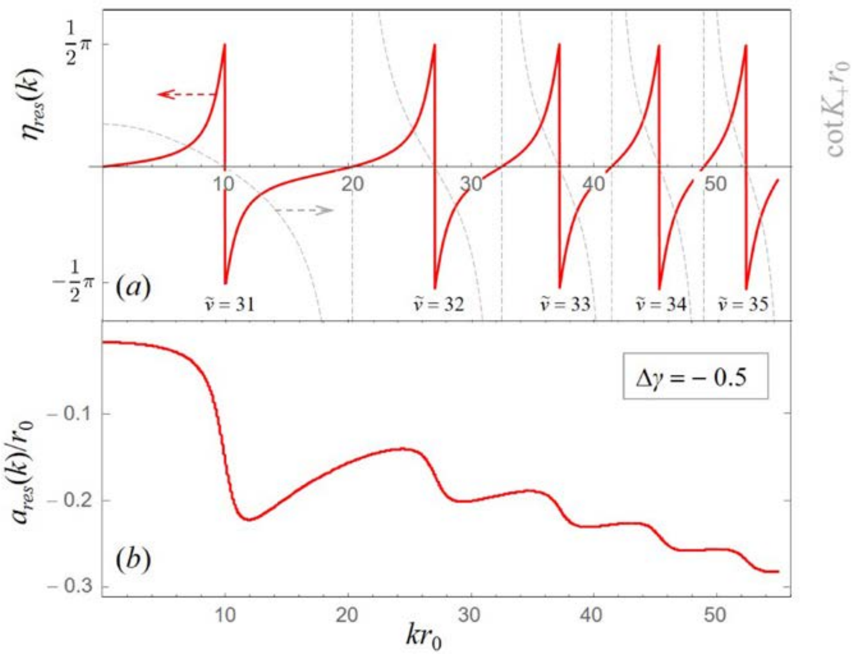
We return to the *energy dependence* of the phase shift

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

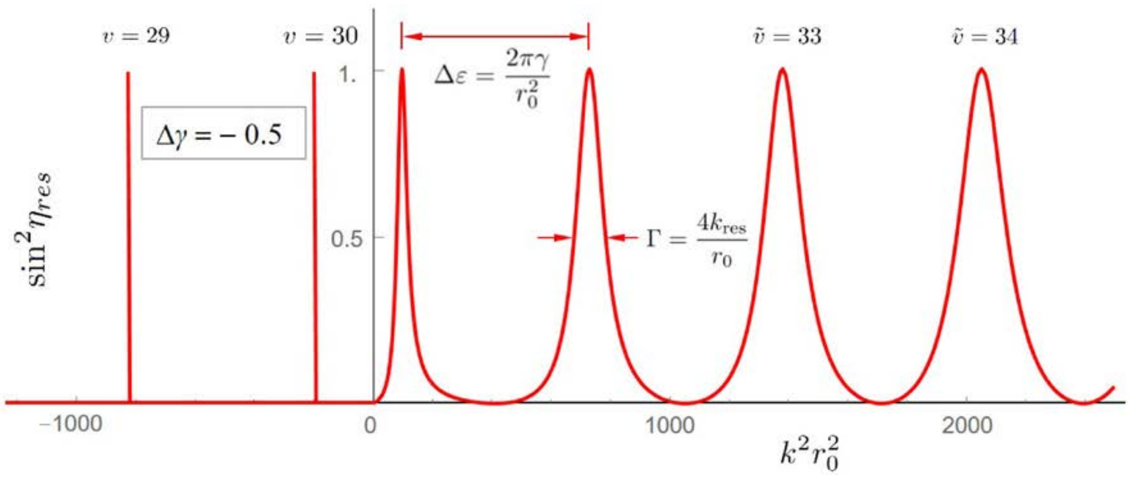
$$K_+^2 = k^2 + \kappa_0^2$$



virtual level



Breit-Wigner line shape



Expand about resonance ($k \simeq k_{\rm res}$) $\Gamma/2 = 2k_{\rm res}/r_0$

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

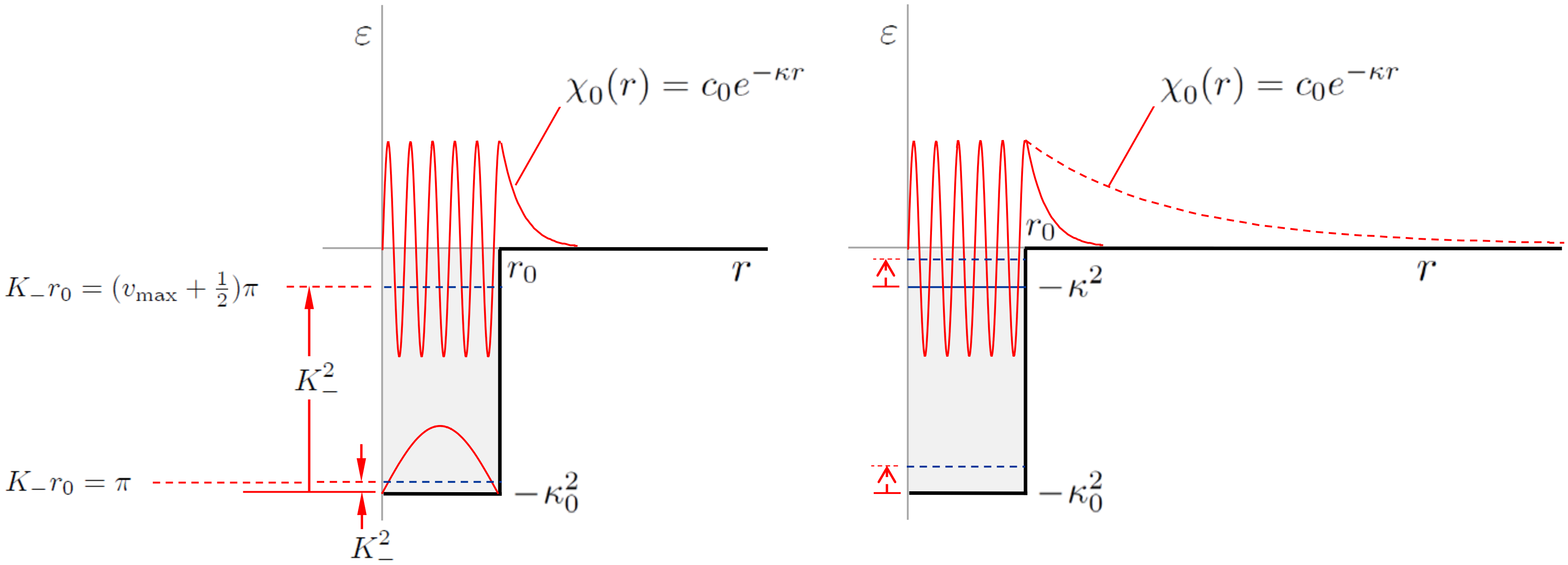
$$\boxed{\sin^2\eta_{\rm res} = \frac{(\Gamma/2)^2}{(\varepsilon - \varepsilon_{\rm res})^2 + (\Gamma/2)^2}}$$

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

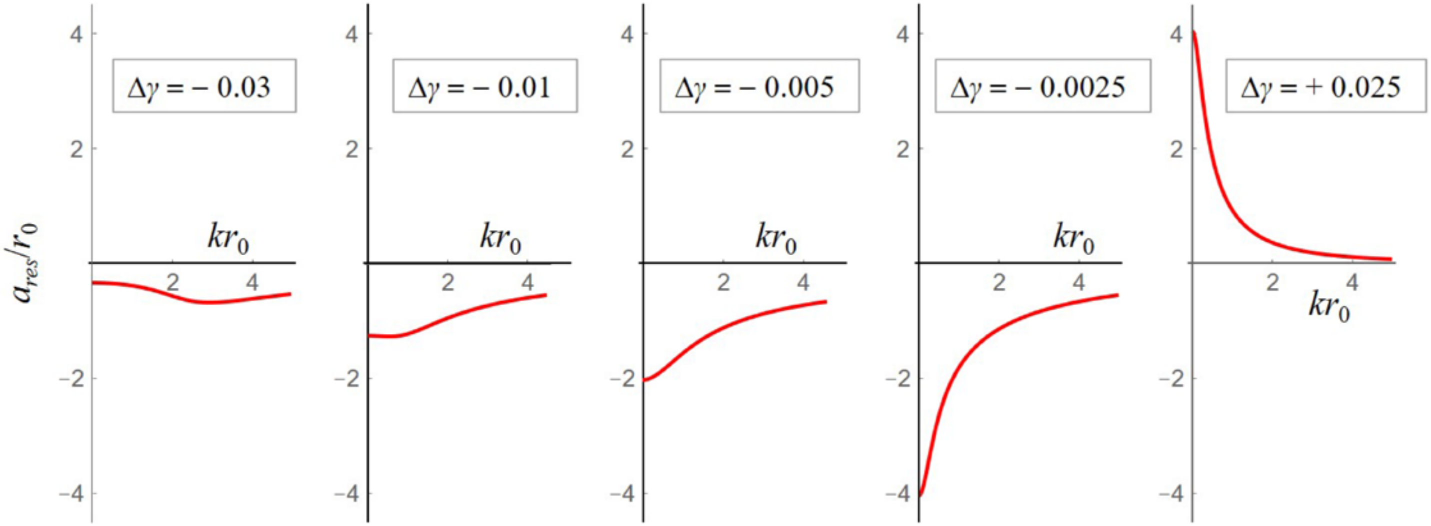
strange molecule: large probability to find the atoms *outside* the classical turning point



s-wave resonance near threshold

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

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



$$\text{for } K_+ \simeq \kappa_0 \simeq K_- \longrightarrow \kappa_0 \cot\kappa_0 r_0 = -\kappa$$

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

weakly-bound state

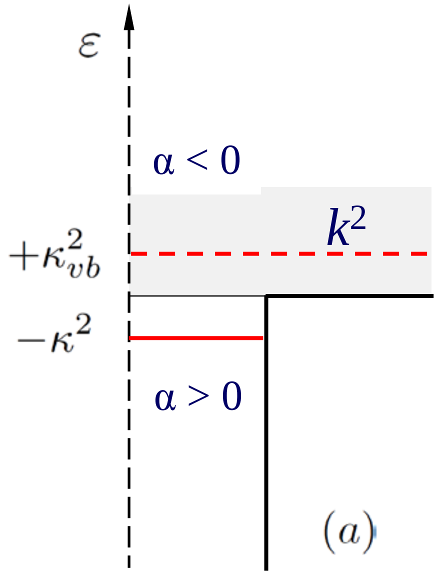
$$a(k) \simeq r_0 - \frac{1}{k}\arctan\frac{k}{\kappa_{vb}}$$

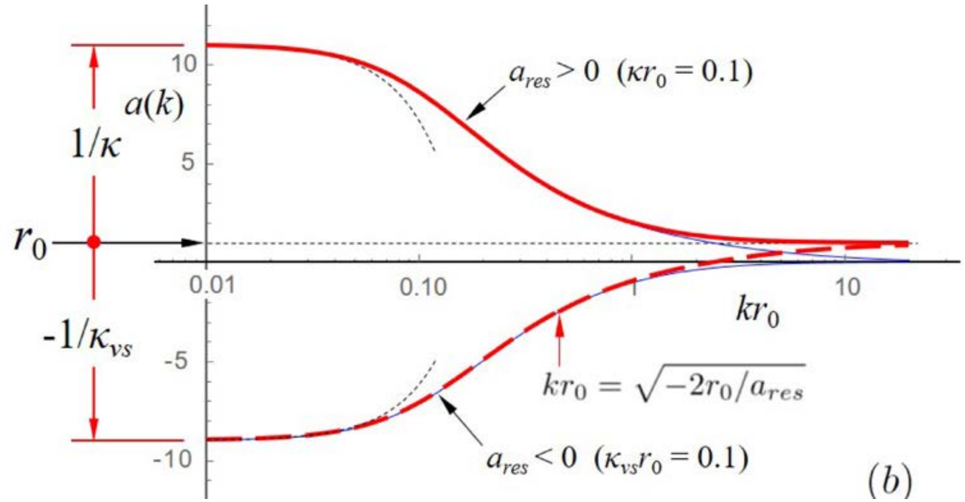
virtual state

s-wave resonance near threshold

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

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



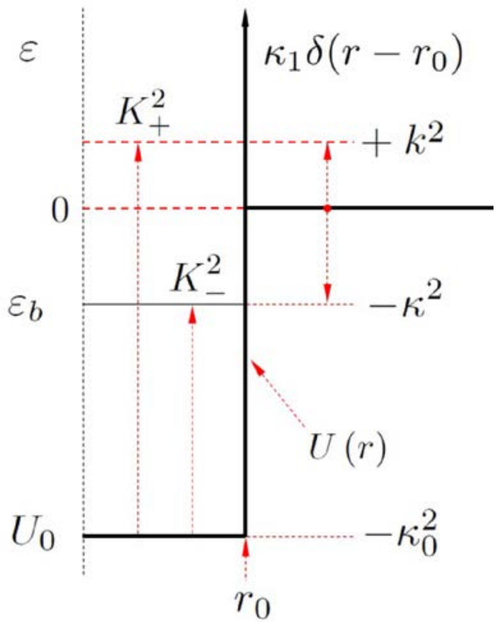


Conclusion: scattering length approximation valid for $\boxed{\begin{array}{l} k \ll \kappa \\ k \ll \kappa_{vb} \end{array}}$

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 $r = r_0$

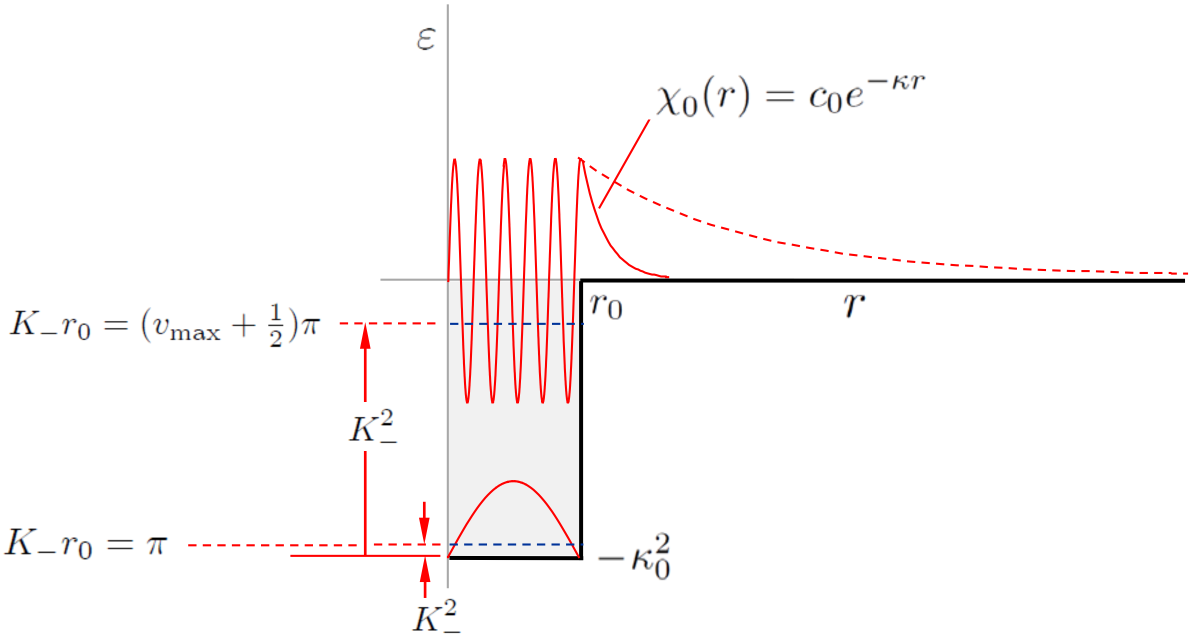
$$\chi_0'/\chi_0|_{r=r_0} = \underbrace{K_+\cot K_+ r_0}_{r<r_0} = \underbrace{k\cot(kr_0+\eta_0)}_{r>r_0} + \kappa_1$$

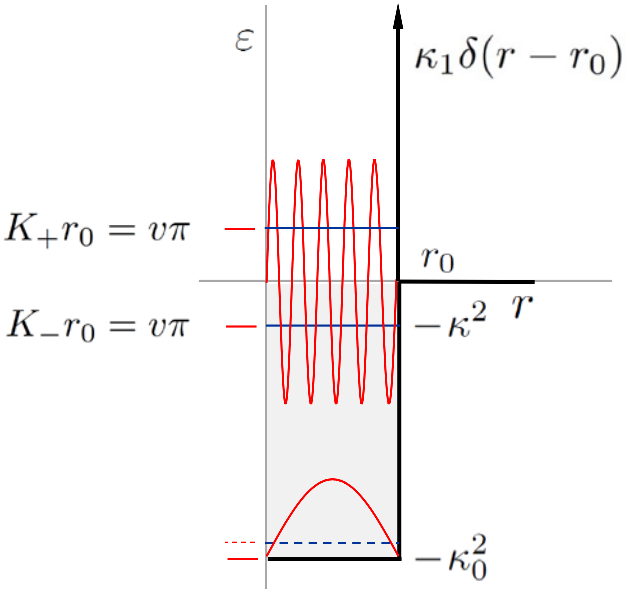
Barrier parameter: $\beta \equiv \kappa_1 r_0 \rightarrow$ $\boxed{a(k) = r_0 - \frac{1}{k}\arctan\left(\frac{kr_0}{K_+ r_0\cot K_+ r_0 - \beta}\right)}$

from halo state to narrow resonance

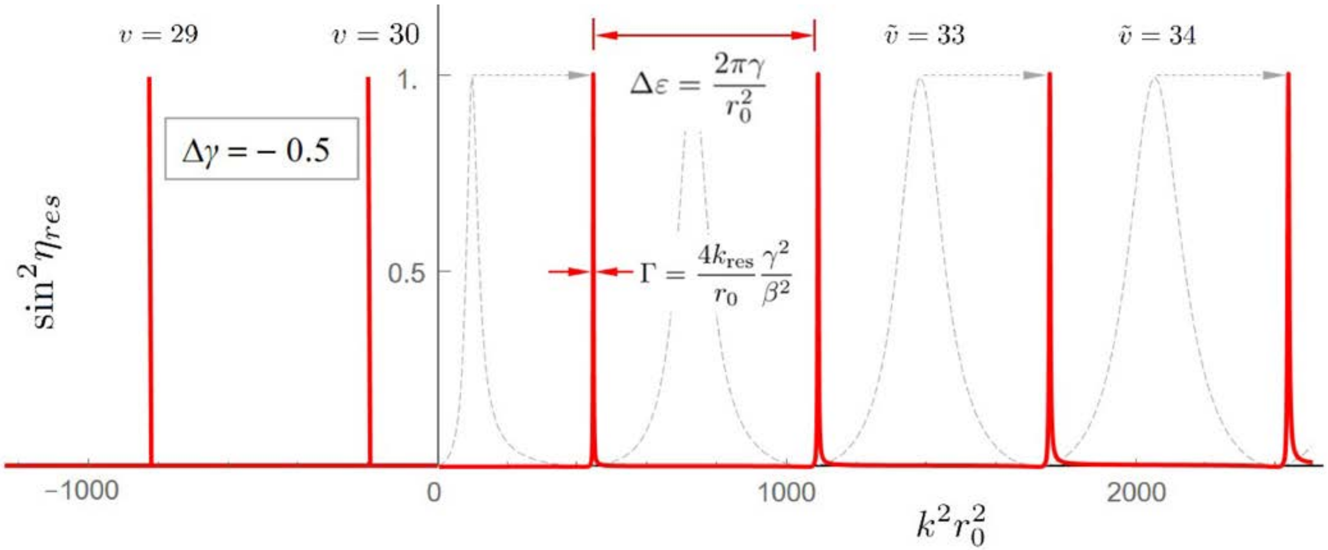
Bound states ($\varepsilon < 0$):

$$\chi_0 = Ae^{-\kappa r}$$





screened flat-bottom potential



New notation: expand about resonance ($k \simeq k_{\rm res}$)

$$\tan\eta_{\rm res} = \frac{k}{K_+ \cot K_+ r_0 - \kappa_1} \simeq \frac{-\Gamma/2}{\varepsilon - \varepsilon_{\rm res}} \qquad \Gamma/2 = (2k_{\rm res}/r_0)\frac{\gamma^2}{\beta^2} = 2k_{\rm res}/R^*$$

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

effective range r_e

We now analyze the *energy dependence* of the phase shift

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

evaluate phase shift:

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

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

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

effective range r_e

r_e : measure for energy dependence of the phase shift

Effective range expansion:

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

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 ($r_e > 0$ for large $|a|$):

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

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

$$|\beta| \to \infty \quad \rightarrow \quad r_e \simeq -r_0\frac{\beta^2}{\gamma^2}\frac{(a-r_0)^2}{a^2} = -r_0\frac{\beta^2}{\gamma^2}\left(1 - 2\frac{r_0}{a} + \frac{r_0^2}{a^2}\right)$$

Resonance-width parameter R^*

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

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

$$|\beta| \to \infty \quad \longrightarrow \quad r_e \simeq -r_0 \frac{\beta^2}{\gamma^2} \frac{(a-r_0)^2}{a^2} = -r_0 \frac{\beta^2}{\gamma^2} \left(1 - 2\frac{r_0}{a} + \frac{r_0^2}{a^2}\right)$$

define <u>positive</u> width parameter: $R^* = -\tfrac{1}{2} r_e \simeq r_0 \dfrac{\beta^2}{\gamma^2}$

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

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

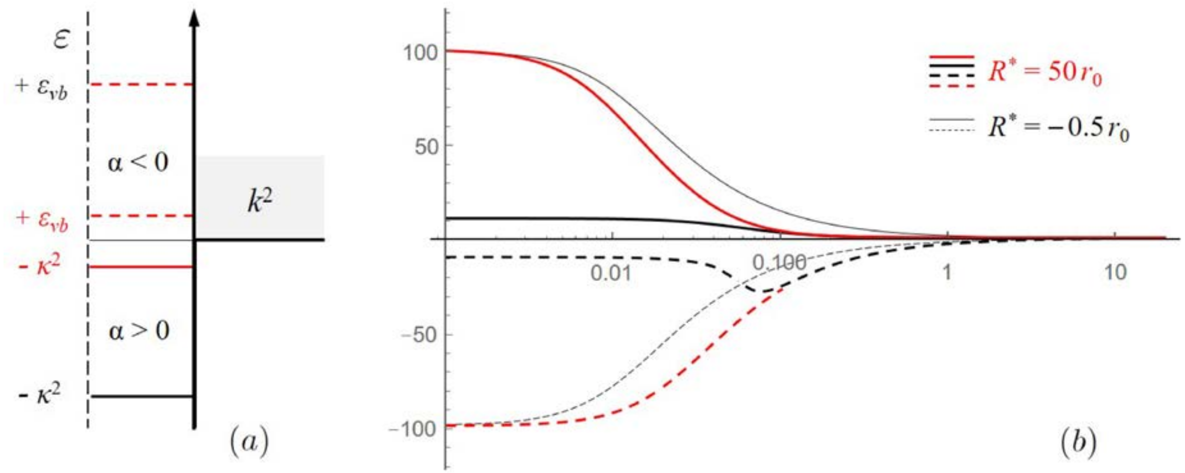
weak barrier – strong coupling – broad resonance $R^* << r_0$

resonance near threshold

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

$$a = \frac{1}{\kappa}$$

$$a = -\frac{1}{\kappa_{vb}}$$



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

$$\Gamma/2 = k_{\rm res}/R^*$$

weakly bound level:

$$k \cot \eta_0 = -\kappa - (k^2 + \kappa^2)R^*$$

$$\tan \eta_0 = \frac{-k}{\kappa + (k^2+\kappa^2)R^*}$$

Relative motion of interacting particles II

1. We analyzed the energy dependence of the scattering length
2. We introduced the effective range r_e
3. We analyzed when the effective range is important
4. We discussed anomanously large and small scattering lengths
5. We analyzed s-wave resonances
6. We noticed that negative effective ranges did not appear
7. We introduced a tunnel barrier
8. We found that for a weak tunnel coupling $r_e < 0$
9. We introduced the width parameter R* to discriminate between broad and narrow s-wave resonances