

Lectures on quantum gases

Lecture 3

Significance of the scattering length and scattering properties

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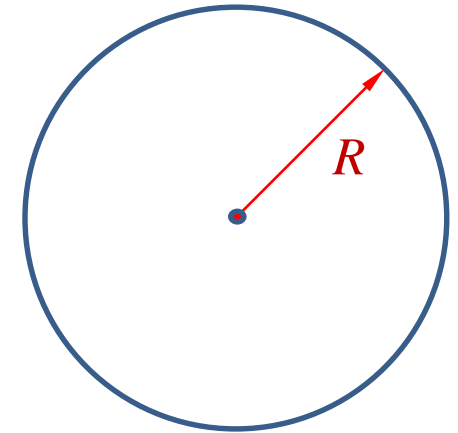
significance of s-wave scattering length

We distinguish between:

- (a) thermodynamic significance
- (b) collisional significance

Thermodynamic significance

particle spherical (macroscopic) box:



(a) without interaction

$$R_0^{(0)}(k_n, r) = \sqrt{\frac{2}{R}} \frac{\sin[k_n r]}{r} \quad k_n = n \frac{\pi}{R}$$

(b) with interaction

$$R_0(k'_n, r) \underset{r > r_0}{=} \sqrt{\frac{2}{R}} \frac{\sin[k'_n r + \eta_0(k'_n)]}{r} \quad k'_n = n \frac{\pi}{R - a}$$

$\eta_0 = -k'_n a$

$$\delta E = \frac{\hbar^2}{2m} (k_n'^2 - k_n^2) \simeq n^2 \frac{\hbar^2}{m} \frac{\pi^2}{R^3} a$$

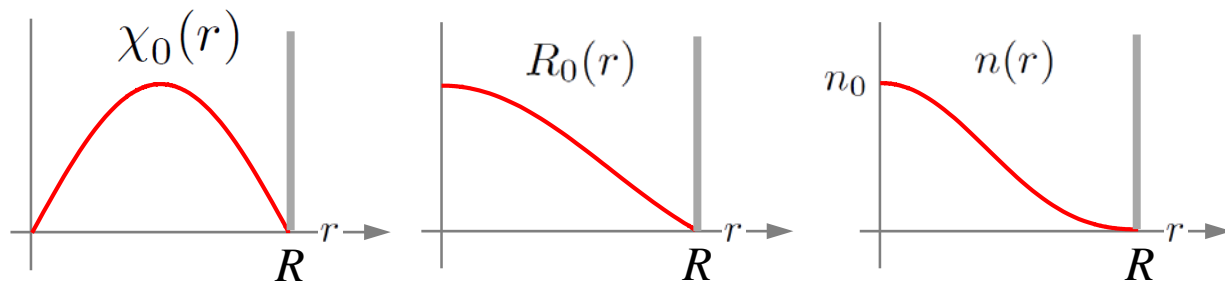
pedestrian view on chemical potential

$$\delta E = \frac{\hbar^2}{2m} (k_n'^2 - k_n^2) \simeq n^2 \frac{\hbar^2 \pi^2}{m R^3} a$$

repulsive for $a > 0$

attractive for $a < 0$

ground state ($n = 0$):



$$1 = \int |\psi_0(\mathbf{r})|^2 d\mathbf{r} = \int n(\mathbf{r}) d\mathbf{r} = n_0 \underbrace{\int \frac{n(\mathbf{r})}{n_0} d\mathbf{r}}_{V_e} \longrightarrow V_e \equiv \frac{N}{n_0} = \frac{2}{\pi} R^3$$

$$\delta E = \frac{4\pi \hbar^2}{m} \frac{a}{V_e}$$

pedestrian view on chemical potential

$$\delta E = \frac{4\pi\hbar^2}{m} \frac{a}{V_e} \rightarrow E = \delta E \frac{N(N-1)}{2} \rightarrow E \simeq \frac{2\pi\hbar^2}{m} a \frac{N^2}{V_e}$$

Chemical potential at $T = 0$:

$$\mu = \frac{\partial E}{\partial N} = \frac{4\pi\hbar^2}{m} a n_0$$

$$\mu = g_0 n_0$$

$$g_0 = \frac{4\pi\hbar^2}{m} a$$

$$\mathcal{V}(\mathbf{r}_1 - \mathbf{r}_2) = g_0 \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

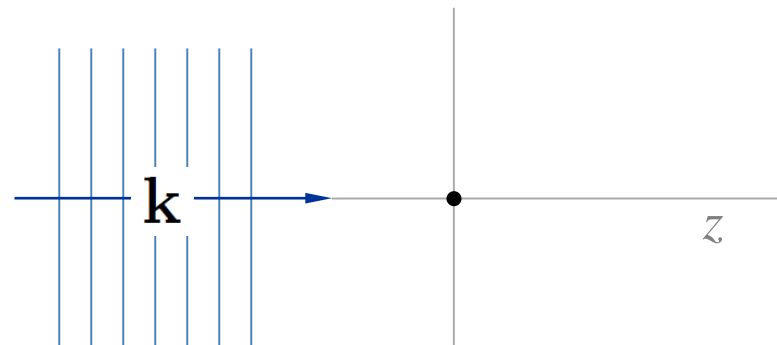
collisional significance: return to RWE

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

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

Example: plane wave in free space

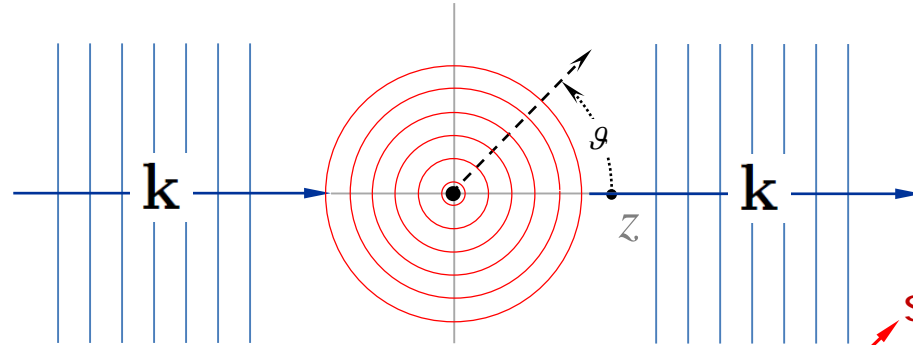
$$R_l(k, r) \rightarrow j_l(kr)$$



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

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

scattering



scattering amplitude

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

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

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

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

scattered wavefunction

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

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

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

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

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

$$e^{i\frac{\pi}{2}} = i$$

scattered wavefunction

create outgoing partial wave:

$$c_l = e^{i\eta_l}$$

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

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

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

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

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

scattered wavefunction

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

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

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

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

forward scattering amplitude

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

partial-wave scattering amplitude

partial wave scattering amplitude

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

$$= k^{-1} e^{i\eta_l} \sin \eta_l \quad (\text{b})$$

$$= \frac{1}{k \cot \eta_l - ik} \quad (\text{c})$$

$$= k^{-1} (\sin \eta_l \cos \eta_l + i \sin^2 \eta_l) \quad (\text{d})$$

partial wave scattering amplitude

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

$$= k^{-1} e^{i\eta_l} \sin \eta_l$$

$$= \frac{1}{k \cot \eta_l - ik}$$

$$= k^{-1} (\sin \eta_l \cos \eta_l + i \sin^2 \eta_l)$$

scattering matrix

(a) $\rightarrow S_l \equiv e^{2i\eta_l} = 1 + 2ikf_l \quad \eta_0 = -ka$

(b) $\rightarrow f_l = \frac{1}{k} e^{i\eta_l} \sin \eta_l \underset{k \rightarrow 0}{\simeq} \frac{1}{k} \sin \eta_l$ $f_0 \underset{k \rightarrow 0}{\simeq} -a$

(c) $\rightarrow f_l = \frac{1}{k} \frac{\tan \eta_l}{1 - i \tan \eta_l} \underset{k \rightarrow 0}{\simeq} \frac{1}{k} \tan \eta_l$

(d) $\rightarrow \text{Im } f_l = \frac{1}{k} \sin^2 \eta_l$

(d) $f(0) = \sum_{l=0}^{\infty} (2l+1) f_l \rightarrow \text{Im } f(0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \sin^2 \eta_l \dots \text{ for later use ...}$

$l < \frac{1}{2}(s-3) \rightarrow \tan \eta_l \underset{k \rightarrow 0}{\simeq} -\frac{2l+1}{[(2l+1)!!]^2} (ka_l)^{2l+1}$

$f_1 \underset{k \rightarrow 0}{\simeq} -a_1 \frac{1}{3} k^2 a_1^2$

$l > \frac{1}{2}(s-3) \rightarrow \sin \eta_l \underset{k \rightarrow 0}{\simeq} \kappa_c^2 r_c^2 \frac{3\pi(2l+3-s)!!}{(2l+5)!!} (kr_c)^{s-2}$

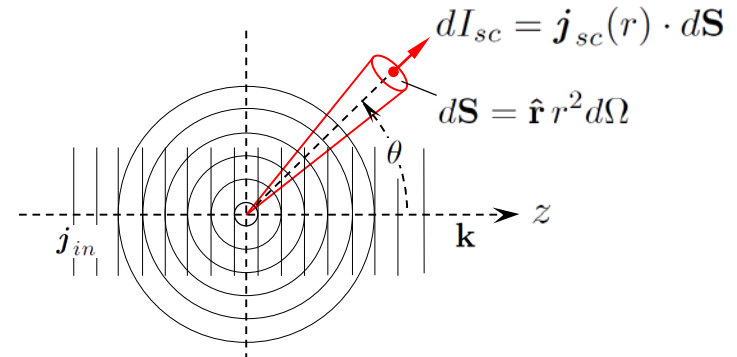
$s = 6 \quad l = 2 \quad f_2 \underset{k \rightarrow 0}{\simeq} \frac{1}{k} \sin \eta_2$

$f_2 \underset{k \rightarrow 0}{\simeq} r_c \frac{1}{100} k^3 r_c^3 \kappa_c^2 r_c^2$

$\mathcal{V}(r) = -\frac{C_s}{r^s}$

differential cross section

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



Current density incident wave:

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

Current density scattered wave

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

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

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

$$\uparrow$$

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

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

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

cross sections

Partial cross section:

$$d\sigma(\theta, \phi) = |f(\theta)|^2 d\Omega$$

$$d\sigma(\theta) = 2\pi \sin\theta |f(\theta)|^2 d\theta$$

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

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

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

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

Total cross section:

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

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

$$\sigma = \int_0^\pi 2\pi \sin\theta |f(\theta)|^2 d\theta$$

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \eta_l$$

unitarity and optical theorem

$$\sigma_0 = \frac{4\pi}{k^2} \sin^2 \eta_0 \xrightarrow{k \rightarrow 0} \boxed{\sigma = 4\pi a^2}$$

$\eta_0 = -ka$
↓

What happens to cross section when a diverges?

$$\sigma_l \leq \frac{4\pi}{k^2} (2l + 1) \leftarrow \text{unitary limit}$$

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \eta_l$$

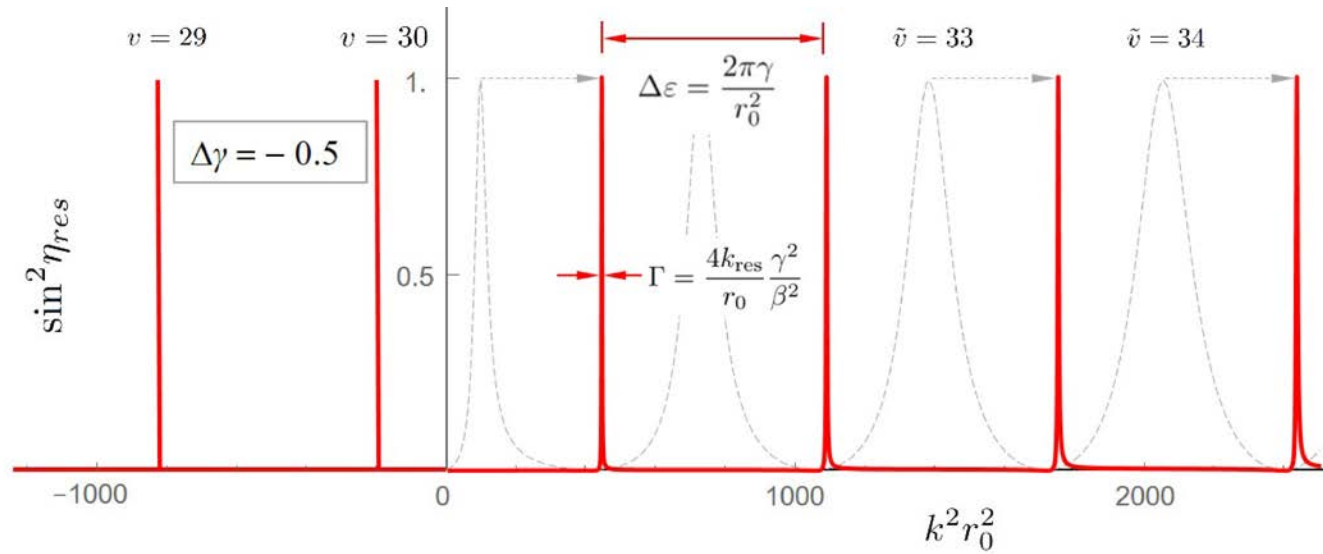
recall ...

$$\text{Im } f(0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \eta_l$$

$$\boxed{\sigma = \frac{4\pi}{k} \text{Im } f(0)}$$

↑
optical theorem

screened flat-bottom potential



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

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

near threshold:

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

$$R^* = -\frac{1}{2}r_e \simeq \frac{1}{2}r_0 \frac{\beta^2}{\gamma^2}$$

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

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

screened flat-bottom potential

Breit-Wigner s-wave resonances:

$$\sin^2 \eta_{\text{res}} = \frac{(\Gamma/2)^2}{(E - E_{\text{res}})^2 + (\Gamma/2)^2} \quad \Gamma = (\hbar^2/m_r)(2k_{\text{res}}/R^*)$$

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

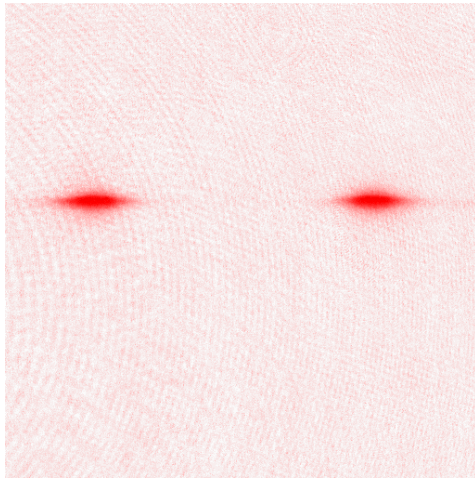
s-wave resonance near threshold:

$$k \cot \eta_0 = -\frac{1}{a} - k^2 R^* \quad R^* = -\frac{1}{2}r_e \simeq \frac{1}{2}r_0 \frac{\beta^2}{\gamma^2}$$

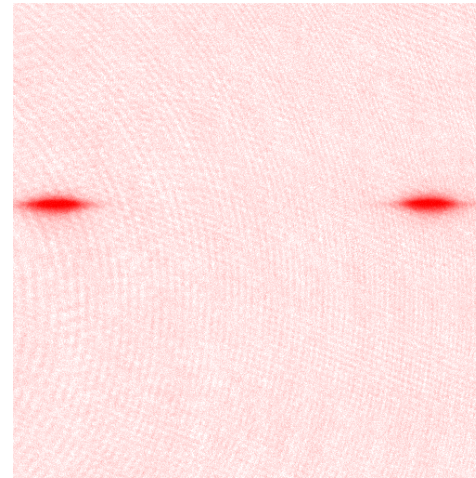
(c) $\left\{ \begin{array}{l} f_0 = \frac{1}{k \cot \eta_0 - ik} \rightarrow f_0 = \frac{-1}{1/a + R^* k^2 + ik} \\ \sigma_0 = 4\pi \frac{1}{k^2 \cot^2 \eta_0 + k^2} \rightarrow \sigma_0 = 4\pi a^2 \frac{1}{1 + k^2 a^2 (1 + 2R^*/a) + \dots} \\ \sigma_0 = 4\pi a^2 \frac{1}{1 + k^2 a^2 (1 - r_e/a) + \dots} \end{array} \right.$

collisions of ultracold atoms

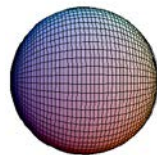
$$E_c/k_B = 138 \mu\text{K}$$



$$E_c/k_B = 1230 \mu\text{K}$$

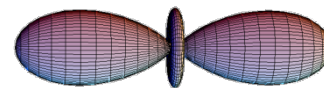


~1mm



$Y_0^0(\mathbf{q})$
s-wave

$^{87}\text{Rb} \left| F = 2, m_F = 2 \right\rangle$

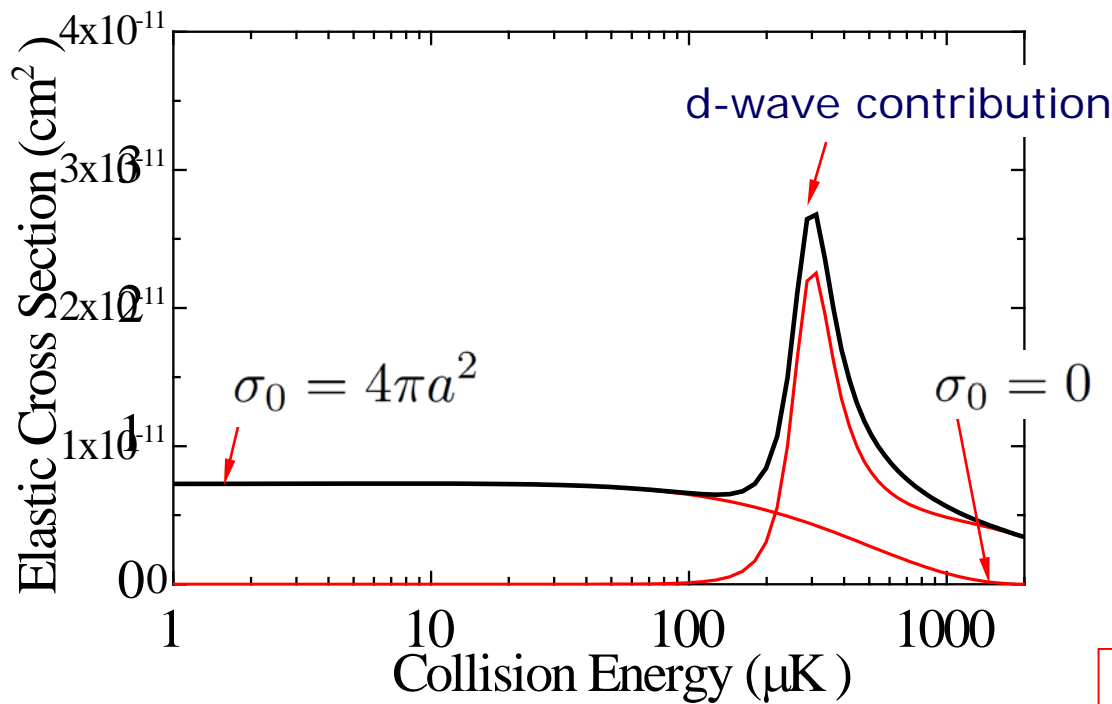


$Y_2^0(\mathbf{q})$
d-wave

properties of elastic cross section

s-wave scattering (low-energy limit)

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \eta_l \quad \xrightarrow{\text{red arrow}} \quad \sigma_0 = \frac{4\pi}{k^2} \sin^2 \eta_0 \quad \xrightarrow{\eta_0 = -ka} \quad \sigma_0 = \frac{4\pi}{k^2} \sin^2 ka$$



$\eta_0 \rightarrow \pi$

$k \rightarrow 0$

$$\sigma_0 = 0$$

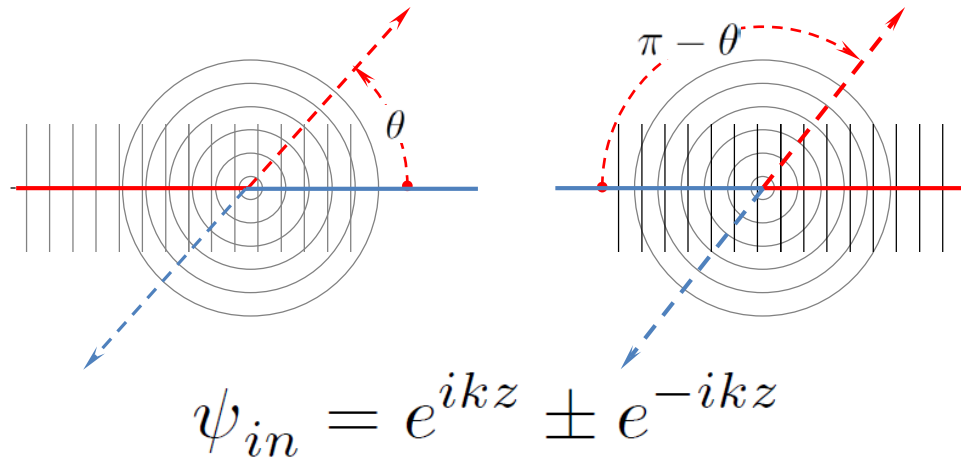
$$\sigma_0 = 4\pi a^2$$

First Ramsauer minimum

where is the p-wave ?

Identical atoms

Identical atoms



Bosons: symmetric under exchange

Fermions: antisymmetric under exchange

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

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

Identical atoms

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

$$e^{-ikz} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(-\cos \theta) \left. \vphantom{\sum_{l=0}^{\infty}} \right\} \begin{array}{l} P_l(-u) = (-1)^l P_l(u) \end{array}$$

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

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

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

statistical properties of elastic cross section

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

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

Bosons (even partial waves): s-wave scattering

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

elastic cross section for identical bosons

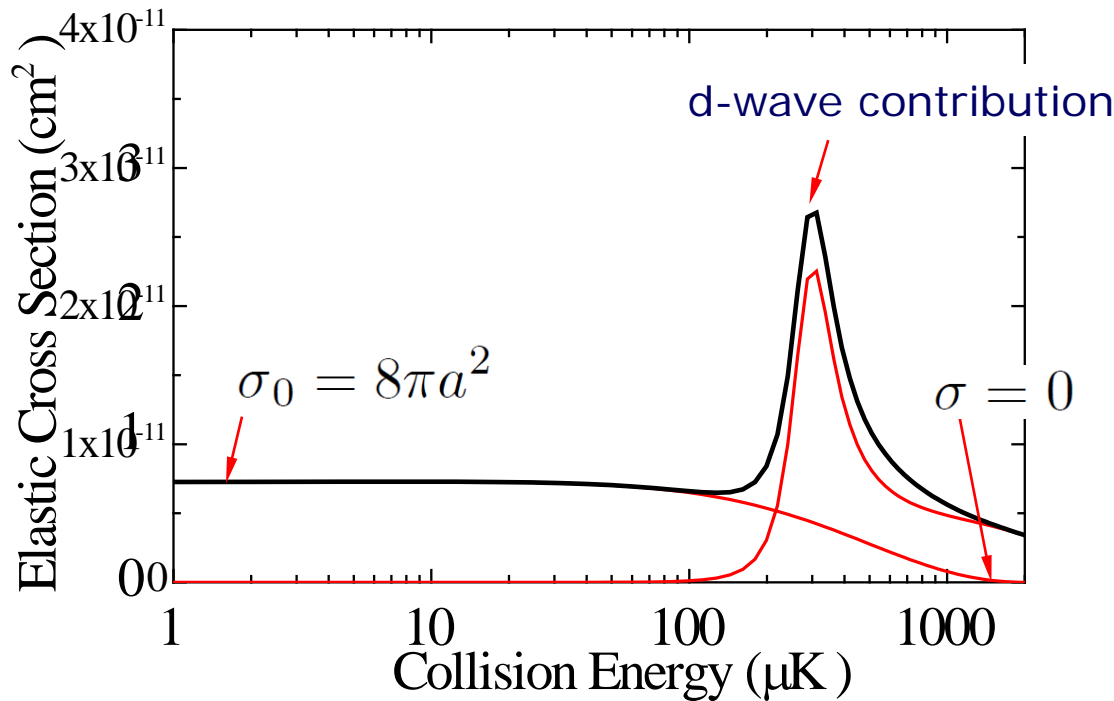
$$\sigma_l = \frac{8\pi}{k^2} \sum_{l=\text{even}} (2l+1) \sin^2 \eta_l \longrightarrow \sigma_0 = \frac{8\pi}{k^2} \sin^2 \eta_0 \xrightarrow{\eta_0 = -ka} \sigma_0 = \frac{8\pi}{k^2} \sin^2 ka$$

$$\eta_0 \rightarrow \pi$$

$$k \rightarrow 0$$

$$\sigma = 0$$

$$\sigma_0 = 8\pi a^2$$



First Ramsauer minimum

NO p-wave !

Scattering of interacting particles

1. We distinguished between the thermodynamic and collisional significance of the scattering length
2. We found limitations to the existence of a potential “range”
3. We introduced the partial-wave expansion
4. We determined the scattering amplitude (4 expressions for f_l)
5. We pointed to limitations of the range concept
6. We introduced the differential and total (elastic) cross section
7. We expressed the cross section in terms of the phase shifts
8. We discussed the unitary limit and the optical theorem
9. We demonstrated elastic scattering for Rb-atoms
10. We missed the p-waves
11. We found the effect of quantum statistics on the cross section