

Lectures on quantum gases

Lecture 3

Scattering of interacting particles

Jook Walraven
University of Amsterdam

Lecture notes:

<https://staff.fnwi.uva.nl/j.t.m.walraven/walraven/JookWalraven.htm>

solutions of RWE for free particles

Free particles: $U(r) \equiv 0$

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

Spherical Bessel differential equation:

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

$\varrho \equiv kr$

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

$$A_l = c_l \cos \eta_l$$

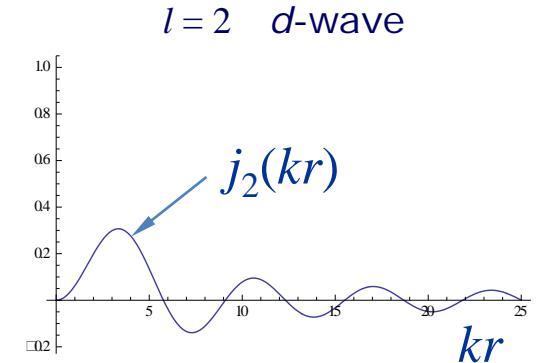
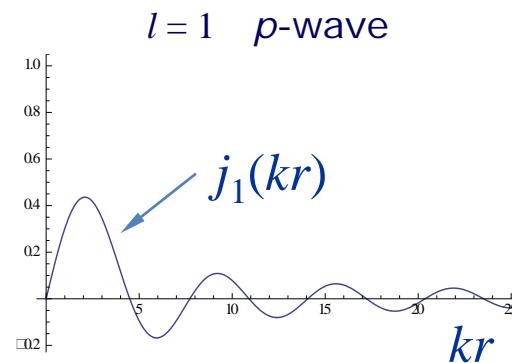
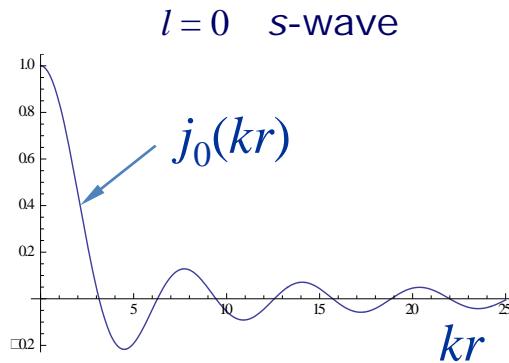
$$B_l = c_l \sin \eta_l$$

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

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

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

spherical Bessel functions



$$R_l(\varrho) = c_l [\cos \eta_l j_l(\varrho) + \sin \eta_l n_l(\varrho)]$$

$$j_l(k, r) \underset{r \rightarrow \infty}{\simeq} \frac{c_l}{kr} \sin(kr - \frac{1}{2}l\pi)$$

$$n_l(k, r) \underset{r \rightarrow \infty}{\simeq} \frac{c_l}{kr} \cos(kr - \frac{1}{2}l\pi)$$

General solution:

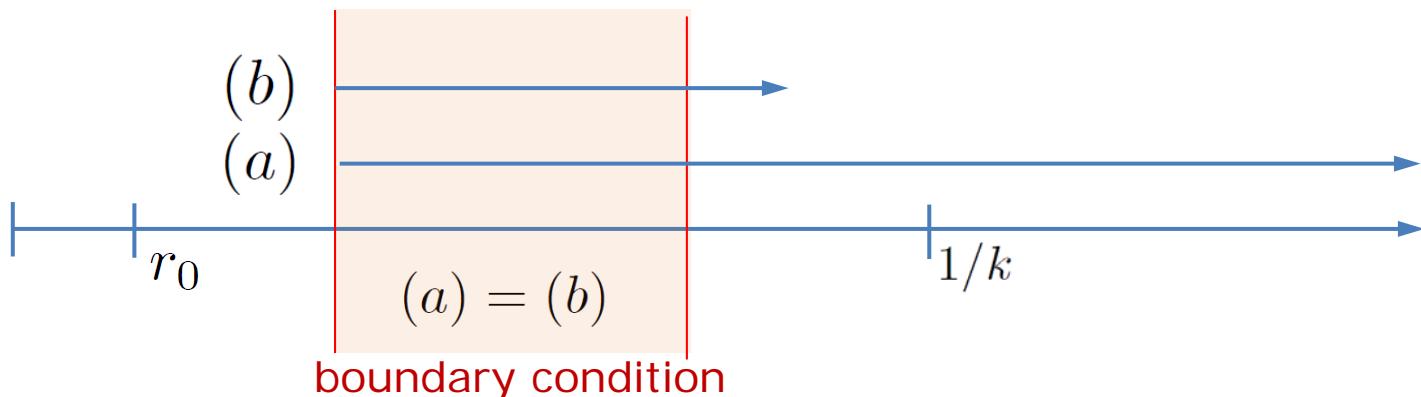
$$R_l(k, r) \underset{r \rightarrow \infty}{\simeq} \frac{c_l}{kr} \sin(kr + \eta_l - \frac{1}{2}l\pi)$$

regular in origin for $\eta_l \rightarrow 0$

generalization: short-range potentials

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

$$\begin{aligned} r \gg r_0 &\quad \xrightarrow{\hspace{1cm}} \quad R_l'' + \frac{2}{r} R_l' + \left[k^2 - \frac{l(l+1)}{r^2} \right] R_l = 0 \quad \rightarrow (a) \\ kr \ll 1 &\quad \xrightarrow{\hspace{1cm}} \quad R_l'' + \frac{2}{r} R_l' - \frac{l(l+1)}{r^2} R_l = 0 \quad \rightarrow (b) \\ kr_0 \ll kr \ll 1 &\quad \xrightarrow{\hspace{1cm}} \quad r_0 \ll r \ll 1/k \end{aligned}$$



generalization: short-range potentials

$$r \gg r_0 \quad R_l'' + \frac{2}{r} R_l' + \left[k^2 - \frac{l(l+1)}{r^2} \right] R_l = 0 \quad \rightarrow (a)$$

$$kr \ll 1 \quad R_l'' + \frac{2}{r} R_l' - \frac{l(l+1)}{r^2} R_l = 0 \quad \rightarrow (b)$$

$$\begin{aligned} \rightarrow (a) & \xrightarrow{r \gg r_0} R_l(r) = \alpha_l j_l(kr) + \beta_l n_l(kr) \\ kr \ll 1 & \xrightarrow{} = \alpha_l \frac{(kr)^l}{(2l+1)!!} + \beta_l \frac{(2l+1)!!}{(2l+1)} \left(\frac{1}{kr} \right)^{l+1} \end{aligned}$$

$$\rightarrow (b) \xrightarrow{kr \ll 1} R_l(r) = c_{1l} r^l + c_{2l} \left(\frac{1}{r} \right)^{l+1}$$

$$(a) + (b) \xrightarrow{} \begin{cases} \alpha_l = A_l \cos \eta_l \simeq c_{1l} \frac{(2l+1)!!}{k^l} \\ \beta_l = A_l \sin \eta_l \simeq c_{2l} \frac{2l+1}{(2l+1)!!} k^{l+1} \end{cases}$$

generalization: short-range potentials

$$\left. \begin{aligned} \alpha_l &= A_l \cos \eta_l \simeq c_{1l} \frac{(2l+1)!!}{k^l} \\ \beta_l &= A_l \sin \eta_l \simeq c_{2l} \frac{2l+1}{(2l+1)!!} k^{l+1} \end{aligned} \right\} \rightarrow$$

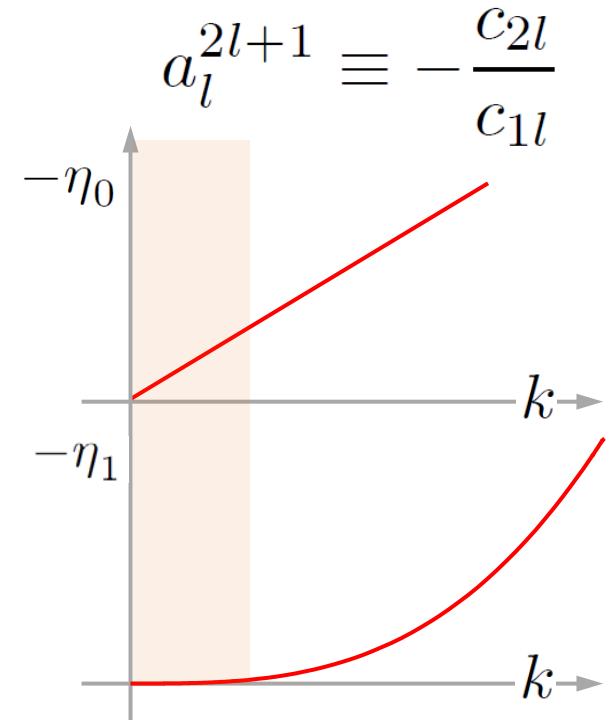
$$\rightarrow \frac{\beta_l}{\alpha_l} = \tan \eta_l \simeq -\frac{2l+1}{[(2l+1)!!]^2} (ka_l)^{2l+1}$$

$$l = 0 \rightarrow \tan \eta_0 \stackrel{ka \ll 1}{\simeq} -ka$$

$$l = 1 \rightarrow \tan \eta_1 \stackrel{ka_1 \ll 1}{\simeq} -\frac{1}{3}(ka_1)^3$$

But ...

$$\boxed{\mathcal{V}(r) = -\frac{C_s}{r^s} \rightarrow l < \frac{1}{2}(s-3)}$$



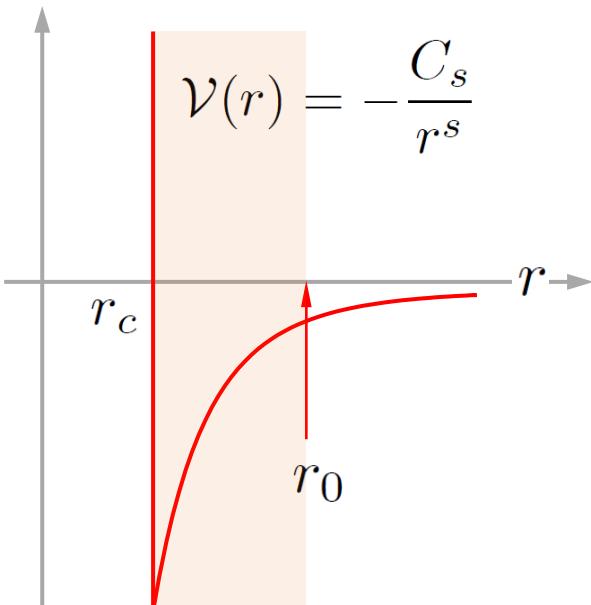
power-law potentials

Short range r_0 can only be defined for $l < \frac{1}{2}(s - 3)$

$$l = 0 \rightarrow s > 2l + 3 = 3$$

Van der Waals potential: $s = 6 \rightarrow l < 1.5 \rightarrow l = 0, 1$

Let us analyze the case of power-law potentials:



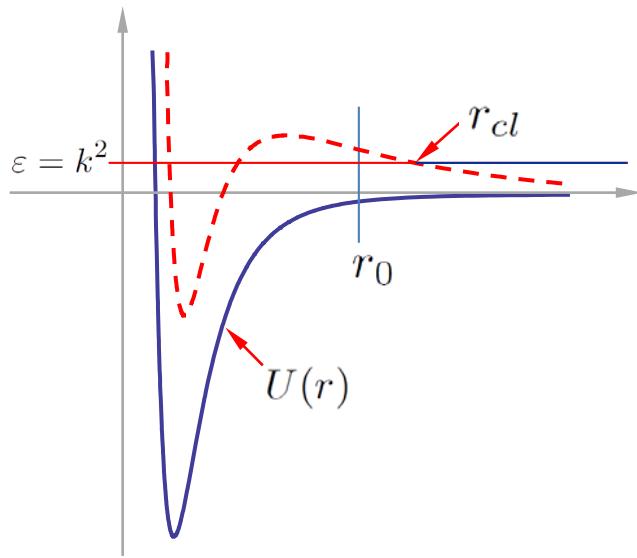
range: heuristic argument

range exist if $E_{\text{conf}} > E_{\text{pot}}$

$$\frac{\hbar^2}{2\mu r_0^2} > \frac{C_s}{r_0^s}$$

$$r_0^{s-2} \simeq 2\mu C_s / \hbar^2 \xrightarrow{s=6} r_0 \simeq [2\mu C_6 / \hbar^2]^{1/4}$$

s-wave regime



phase shift for power-law potentials:

$$l < \frac{1}{2}(s - 3)$$

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

$$l > \frac{1}{2}(s - 3)$$

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

without derivation

full solution of RWE

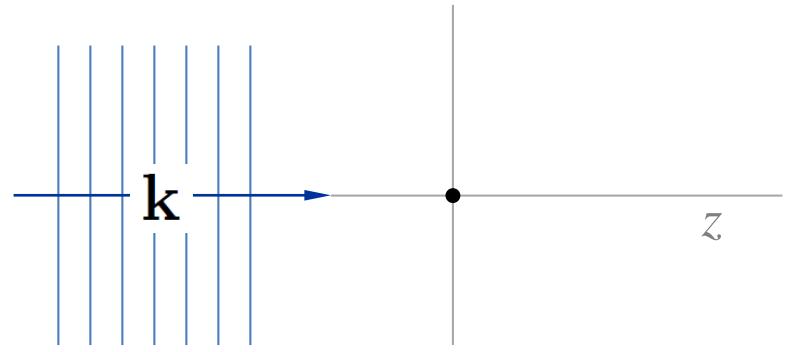
$$\psi_{lm}(\mathbf{r}) = c_{lm} R_l(k, r) Y_l^m(\theta, \phi)$$

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

Example: plane wave in free space

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

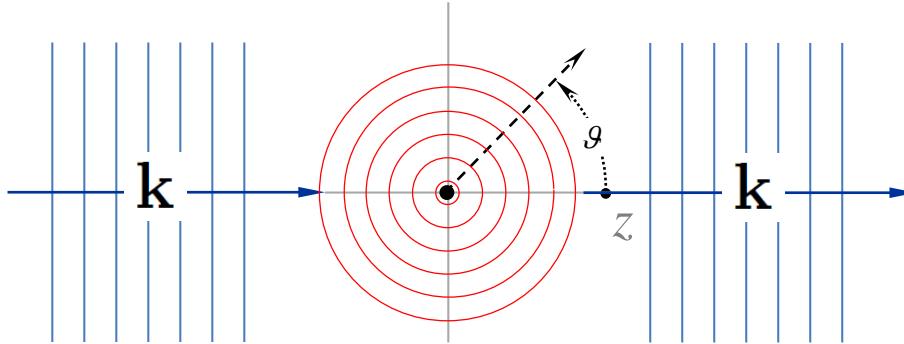
$$\sin(kr + \eta_l - \frac{1}{2}l\pi) \rightarrow \sin(kr - \frac{1}{2}l\pi)$$



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

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

scattering



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

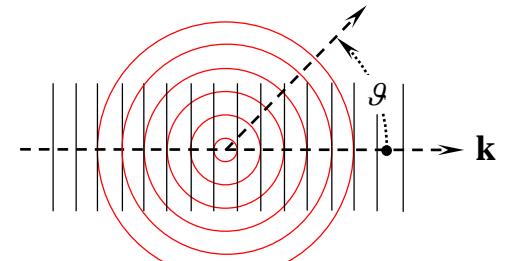
$$e^{ikz} = \sum_{l=0}^{\infty} (2l+1)i^l j_l(kr) P_l(\cos \theta)$$

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

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

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

scattered wavefunction



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

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

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

$$\begin{aligned} Q_l(k, r) &\underset{r \rightarrow \infty}{\simeq} \frac{1}{kr} \left[c_l \sin(kr + \eta_l - \frac{1}{2}l\pi) - \sin(kr - \frac{1}{2}l\pi) \right] \\ &\underset{r \rightarrow \infty}{\simeq} \frac{1}{2ikr} [i^{-l} e^{ikr} e^{i\eta_l} c_l - i^l e^{-ikr} e^{-i\eta_l} c_l - i^{-l} e^{ikr} + i^l e^{-ikr}] \end{aligned}$$

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

scattered wavefunction

create outgoing partial wave:

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

$$\underset{r \rightarrow \infty}{\underset{\sim}{=}} \frac{1}{2ikr} i^{-l} (e^{ikr} e^{2i\eta_l} - i^{2l} e^{-ikr} - e^{ikr} + i^{2l} e^{-ikr})$$

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

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

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

scattered wavefunction

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

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

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

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

forward scattering amplitude

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

partial-wave scattering amplitude

partial wave scattering amplitude

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

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

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

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

intermezzo

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

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

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

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

scattering matrix

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

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

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

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

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

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

$$f_0 \underset{k \rightarrow 0}{\simeq} -a$$

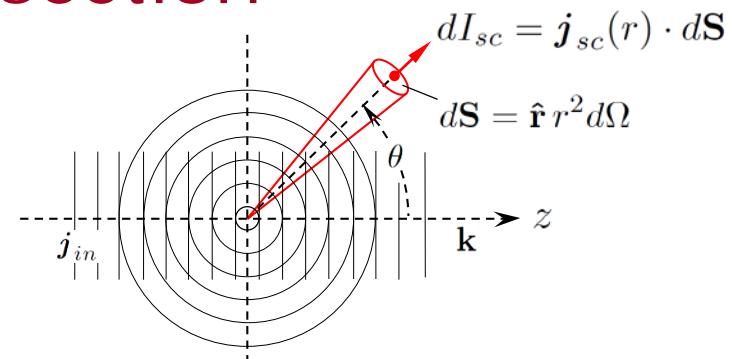
$$f_1 \underset{k \rightarrow 0}{\simeq} -a_1 \frac{1}{3} k^2 a_1^2$$

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

$$s = 6 \quad l = 2 \quad f_2 \underset{k \rightarrow 0}{\simeq} \frac{1}{k} \sin \eta_2 \quad \left. \right\} \rightarrow f_2 \underset{k \rightarrow 0}{\simeq} r_c \frac{1}{100} k^3 r_c^3 \kappa_c^2 r_c^2$$

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 $d\Omega$):

$$dI_{sc} = \mathbf{j}_{sc}(r) \cdot d\mathbf{S} = v |f(\theta)|^2 d\Omega \quad d\sigma(\theta, \phi) = \frac{dI_{sc}(\theta, \phi)}{j_{in}} = |f(\theta)|^2 d\Omega$$

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

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

cross sections

Differential cross section:

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

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

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

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

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

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

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

Total cross section:

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

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

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

optical theorem

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

What happens to cross section when a diverges?

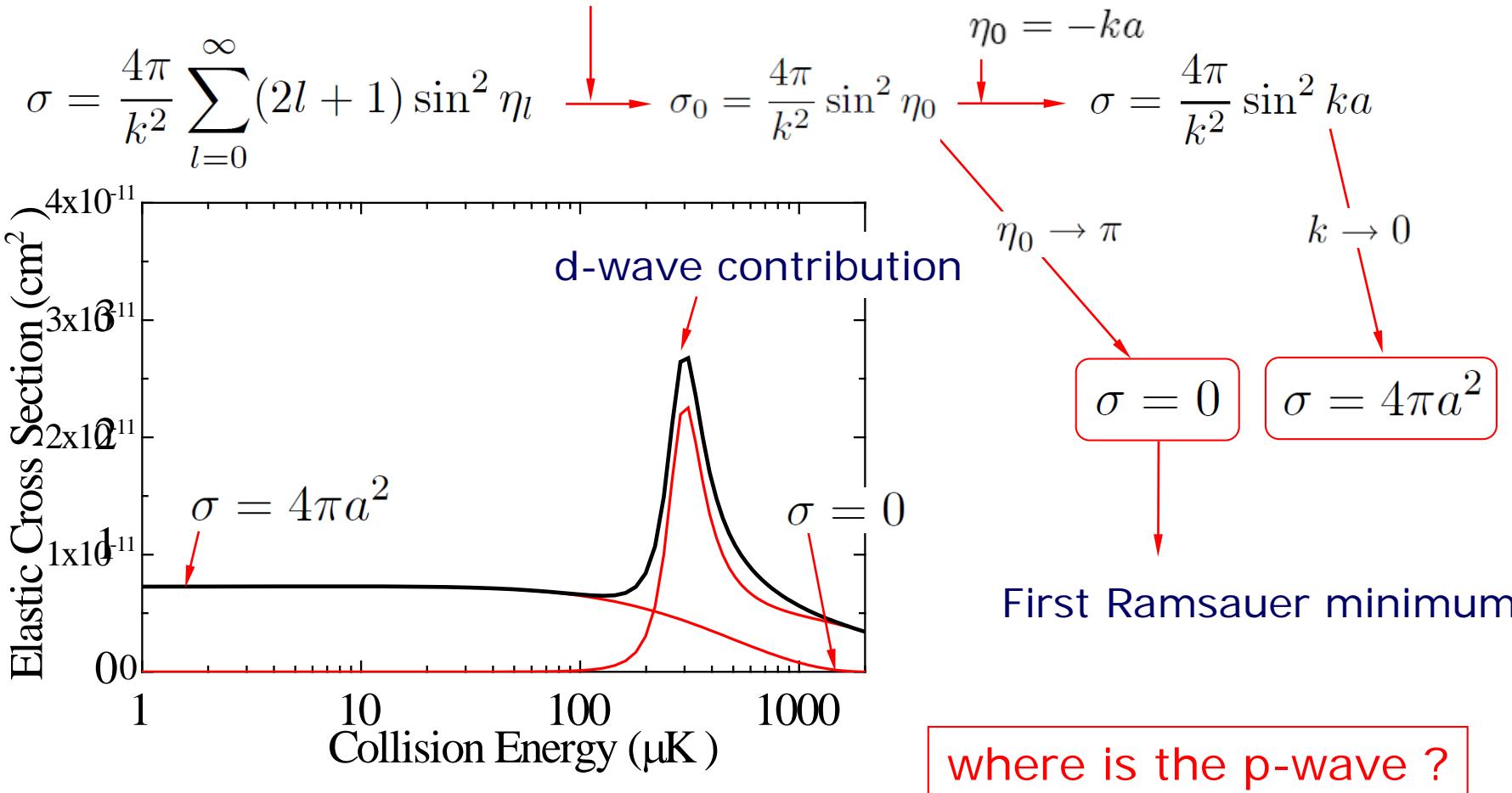
unitarity limit: $\sigma_l \leq \frac{4\pi}{k^2} (2l + 1)$

$$\left. \begin{aligned} \sigma &= \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \eta_l \\ \text{Im } f(0) &= \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \eta_l \end{aligned} \right\} \xrightarrow{\quad} \boxed{\sigma = \frac{4\pi}{k} \text{Im } f(0)}$$

optical theorem

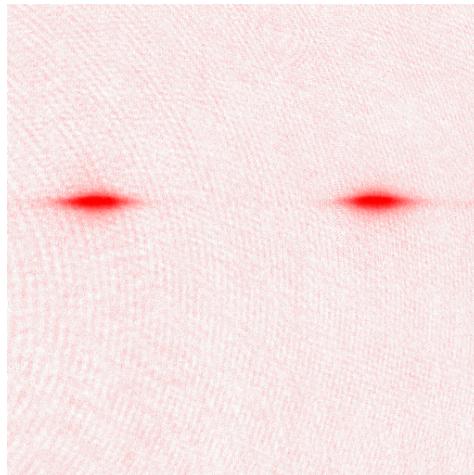
properties of elastic cross section

s-wave scattering (low-energy limit)

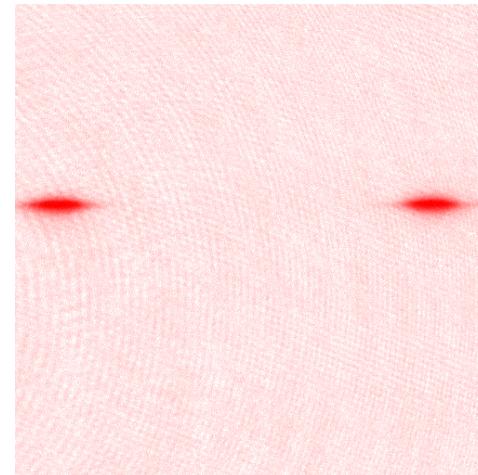


collisions of ultracold atoms

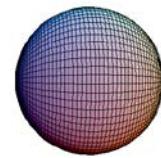
$$E_c/k_B = 138 \mu\text{K}$$



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



↔ ~1mm →



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

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



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

Scattering of interacting particles

1. We generalized the discussion to arbitrary short-range potentials
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 introduced the differential and total (elastic) cross section
6. We expressed the cross section in terms of the phase shifts
7. We discussed the unitarity limit and the optical theorem
8. We demonstrated elastic scattering for Rb-atoms