

With the product ansatz  $\psi(\vec{r}) = \phi_l(r) Y_l^m(\theta, \phi)$  this gives the radial Schrödinger equation

$$\left[ -\frac{\hbar^2}{2m} \left( \frac{1}{r} \frac{d^2}{dr^2} r - \frac{l(l+1)}{r^2} \right) + V(r) \right] \phi_l(r) = E \phi_l(r)$$

To simplify the radial derivative we define

$$\underline{\phi_l(r) = \frac{1}{r} u_l(r)}$$

then the free particle with energy  $E = \frac{\hbar^2}{2m} k^2$  satisfies

$$-\frac{\hbar^2}{2m} \left( \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 \right) u_l(r) = 0$$

With the dimensionless spatial coordinate  $\rho = rk$  this finally yields

$$\underline{\left( \frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + 1 \right) u_l(\rho) = 0}$$

We analyze the behavior of solutions for  $\rho \rightarrow 0$  and  $\rho \rightarrow \infty$ , respectively.

$$(i) \underline{\rho \rightarrow 0:} \quad \frac{d^2}{d\rho^2} u_l = \frac{l(l+1)}{\rho^2} u_l$$

$$\underline{\text{Ansatz:}} \quad u_l = \rho^\alpha \Rightarrow u_l'' = \alpha(\alpha-1) \rho^{\alpha-2} =$$

$$= \frac{\alpha(\alpha-1)}{g^2} u_l \Rightarrow \underline{\alpha(\alpha-1) = l(l+1)}$$

This quadratic equation has two solutions:

$$\left. \begin{aligned} \alpha = l+1 &\Rightarrow \underline{\text{regular solution}} & u_l &\sim g^{l+1} \\ \alpha = -l &\Rightarrow \underline{\text{irregular solution}} & u_l &\sim g^{-l} \end{aligned} \right\}$$

$$(ii) \underline{g \rightarrow \infty}: \quad \frac{d^2}{dg^2} u_l = -u_l$$

$$\Rightarrow u_l(g) = A \sin g + B \cos g$$

The full solutions are given in terms of spherical Bessel functions  $j_l, y_l$  as follows:

• regular solutions:

$$u_l = g j_l(g)$$

$$\underline{j_l(g) = g^l \left( -\frac{1}{g} \frac{d}{dg} \right)^l \frac{\sin g}{g}}$$

• irregular solutions:

$$u_l(g) = g y_l(g)$$

Neumann fct.

$$\underline{y_l(g) = -g^l \left( -\frac{1}{g} \frac{d}{dg} \right)^l \frac{\cos g}{g}}$$

To identify the contribution to the asymptote  $\textcircled{5}$  we need to investigate the behavior of the exact solution for  $g \rightarrow \infty$ .

In the regular case we have

$$u_0(g) = \sin g$$

$$\underline{u_1(g)} = g \left\{ g \left( -\frac{1}{g} \frac{d}{dg} \right) \frac{\sin g}{g} \right\} =$$

$$= g \left\{ \frac{1}{g^2} \sin g - \frac{1}{g} \cos g \right\} =$$

$$= \underline{\frac{1}{g} \sin g - \cos g}$$

$$u_2(g) = \underbrace{\frac{2}{g} \left( \frac{1}{g} - \cos g \right) - \frac{1}{g^2} \sin g - \frac{1}{g} \cos g - \sin g}_{\rightarrow 0, g \rightarrow \infty}$$

In general, it can be seen from the definition of  $j_l$  and  $y_l$  that there is always one term where all derivatives act on  $\sin g$  and  $\cos g$ , respectively, and powers of  $g$  cancel:

$$\left. \begin{aligned} j_l(g) &\rightarrow \frac{1}{g} (-1)^l \left( \frac{d}{dg} \right)^l \sin g \\ y_l(g) &\rightarrow \frac{1}{g} (-1)^{l+1} \left( \frac{d}{dg} \right)^l \cos g \end{aligned} \right\} g \rightarrow \infty$$

Each derivative applied to a trigonometric function shifts the phase by  $\pi/2$ :

$$\left. \begin{aligned} \left(\frac{d}{dp}\right)^l \sin p &= \sin\left(p + \frac{l\pi}{2}\right) \\ \left(\frac{d}{dp}\right)^l \cos p &= \cos\left(p + \frac{l\pi}{2}\right) \end{aligned} \right\}$$

Thus the Hankel functions  $h_l^{(1,2)}(p)$  defined by

$$\left. \begin{aligned} h_l^{(1)}(p) &= j_l(p) + i y_l(p) \\ h_l^{(2)}(p) &= j_l(p) - i y_l(p) \end{aligned} \right\} \text{ have the asymptotic behavior}$$

$$\begin{aligned} \underline{h_l^{(1)}(p)} &\approx \frac{1}{p} \underbrace{(-1)^l}_{(e^{i\pi})^l} \underbrace{\left(\sin\left(p + \frac{l\pi}{2}\right) - i \cos\left(p + \frac{l\pi}{2}\right)\right)}_{= \frac{1}{i} e^{i\left(p + \frac{l\pi}{2}\right)}} \\ &= \underline{\frac{1}{pi} e^{i\left(p - \frac{l\pi}{2}\right)}} \end{aligned}$$

Thus these solutions have the form of a outgoing spherical wave

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Similarly  $h_e^{(2)}(\rho) \approx \frac{i}{\rho} e^{-i(\rho - \frac{\pi}{2})}$ .

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## b) Scattering phases

In the following we assume that the potential is of strictly finite range, i.e.

$$V(r) = 0 \quad \text{for } r > R$$

Then the total wave function

$$\psi(\vec{r}) = e^{ikz} + \psi_s(\vec{r}) \quad (A=1)$$

is a solution of the free particle Schrödinger equation with asymptotics  $\textcircled{S}$ , i.e.

$$\textcircled{S'} \quad \underline{\psi_s(\vec{r}) \approx f(\theta, \phi) \frac{e^{ikr}}{r}, \quad r \rightarrow \infty}$$

The most general expansion of  $\psi_s$  is

$$\psi_s(\vec{r}) = \sum_{l,m} \phi_l(r) Y_l^m(\theta, \phi)$$

However, because of the radial symmetry of the potential there cannot be any dependence on  $\phi$ , i.e. only terms with  $\underline{m=0}$  contribute:

$$\begin{aligned} \underline{\psi_s(\vec{r})} &= \sum_l \phi_l(r) Y_l^0(\theta) = \\ &= \sum_l \phi_l(r) \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \theta) \end{aligned}$$

where  $P_l(x) = 2^{-l} (l!)^{-1} \left( \frac{d}{dx} \right)^l (x^2-1)^l$

are Legendre polynomials defined on  $(-1, 1)$ .

To satisfy the boundary condition  $(5')$  the  $\phi_l$  have to be proportional to  $h_l^{(1)}$ :

$$\psi_s(\vec{r}) = \sum_l i^l \left( \frac{2l+1}{2} \right) a_l h_l^{(1)}(kr) P_l(\cos \theta)$$

For  $|\vec{r}| \rightarrow \infty$   $h_l^{(1)} \approx \frac{1}{ikr} e^{i(kr - \frac{l\pi}{2})}$

$$\begin{aligned} &= \left( \frac{1}{i} e^{-i\frac{\pi}{2}l} \right) \frac{e^{ikr}}{kr} \\ &= \left( \frac{1}{i} \right)^{l+1} \end{aligned}$$

$$\begin{aligned} \Rightarrow \psi_s(\vec{r}) &\xrightarrow{r \rightarrow \infty} \left[ \frac{1}{2ik} \sum_l (2l+1) a_l P_l(\cos \theta) \right] \frac{e^{ikr}}{r} \\ &= f(\theta) \end{aligned}$$

The form of the expansion coefficients becomes clear by considering the representation of the incoming plane wave in terms of spherical harmonics:

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


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### Rayleigh formula

With this the full wave function becomes

$$\begin{aligned} \underline{\psi(\vec{r})} &= e^{ikz} + \psi_s(\vec{r}) = \\ &= \sum_{l=0}^{\infty} (2l+1) i^l P_l(\cos \theta) \left[ j_l(kr) + \frac{a_l}{2} h_l^{(1)}(kr) \right] \end{aligned}$$

For  $r \rightarrow \infty$

$$j_l(kr) + \frac{a_l}{2} h_l^{(1)}(kr) \rightarrow \frac{1}{kr} \left[ \underbrace{(-1)^l \sin(kr + \frac{\pi l}{2})}_{\sin(kr - \frac{\pi l}{2})} + \frac{a_l}{2i} e^{i(kr - \frac{\pi l}{2})} \right]$$

$$= \frac{1}{2ikr} \left[ e^{i(kr - \frac{\pi l}{2})} - e^{-i(kr - \frac{\pi l}{2})} + a_l e^{i(kr - \frac{\pi l}{2})} \right] =$$

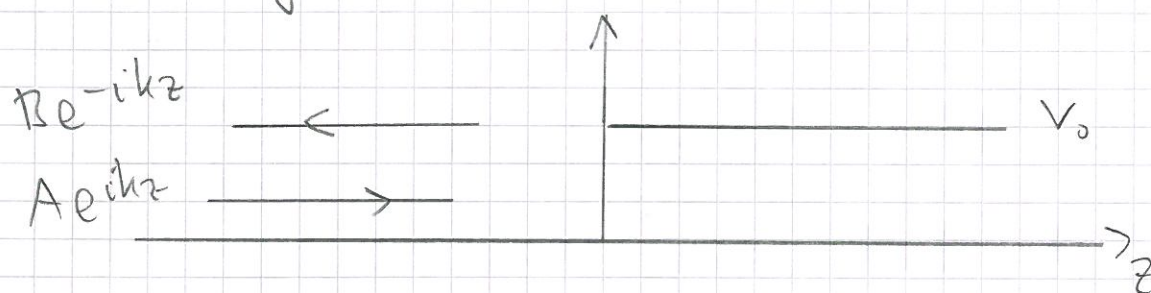
$$= \frac{i}{2kr} \left[ \underbrace{e^{-i(kr - \frac{\pi l}{2})}}_{\text{incoming}} - \underbrace{(1+a_l) e^{i(kr - \frac{\pi l}{2})}}_{\text{outgoing spherical wave}} \right]$$

$\overset{= S_l}{\text{outgoing spherical wave}}$

$S_l$  is called the "scattering matrix", which is diagonal in this case. Because of probability conservation  $|S_l|^2 = 1$ , which implies that

$$\underline{S_l = e^{2i\delta_l}} \quad \text{with the scattering phases } \delta_l \in [-\pi/2, \pi/2].$$

Analogy to one-dimensional scattering:



Then for  $E < V_0$   $|A|^2 = |B|^2$ , but the reflected wave function has a different phase:

$$\underline{B = e^{2i\delta} A}$$

The terms in the decomposition of  $\psi(\vec{r})$  are called partial waves, and the scattering phase  $\delta_l$  completely characterizes the scattering of the  $l$ -th partial wave.

### c) Scattering amplitude and cross section

The scattering amplitude is given in terms of the scattering phases as

$$\underline{f(\theta)} = \frac{1}{2ik} \sum_l (2l+1) (e^{2i\delta_l} - 1) P_l(\cos\theta) =$$

$$= \underline{\frac{1}{k} \sum_l (2l+1) e^{i\delta_l} \sin(\delta_l) P_l(\cos\theta)}$$

and the differential cross section is  $\frac{d\sigma}{d\Omega} = |f(\theta)|^2$ .

Thus the total cross section is

$$\sigma_{\text{tot}} = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta |f(\theta)|^2 =$$

$$= \frac{2\pi}{k^2} \sum_l \sum_{l'} (2l+1)(2l'+1) e^{i(\delta_l - \delta_{l'})} \sin(\delta_l) \sin(\delta_{l'}) \times$$

$$\times \int_0^{\pi} d\theta \sin\theta P_l(\cos\theta) P_{l'}(\cos\theta)$$

$$= \int_{-1}^1 d(\cos\theta) P_l(\cos\theta) P_{l'}(\cos\theta) =$$

$$= \frac{2}{2l+1} \delta_{ll'} \quad \text{orthogonality relation}$$

$$\Rightarrow \sigma_{\text{tot}} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

On the other hand, because  $P_l(1) = 1 \quad \forall l$ ,

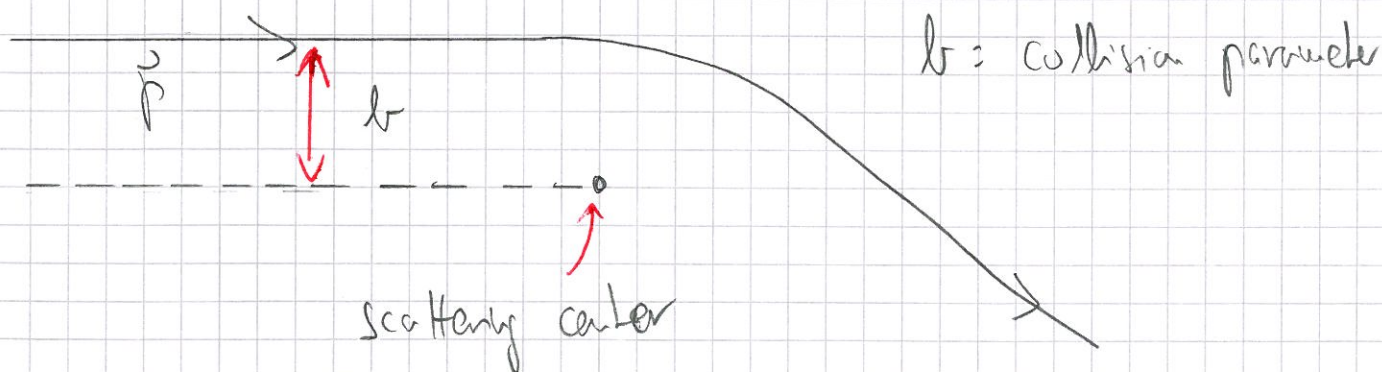
$$f(0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l} \sin \delta_l =$$

$$= \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \left( \cos(\delta_l) \sin(\delta_l) + \underline{i \sin^2 \delta_l} \right)$$

$$\Rightarrow \underline{\text{Im } f(0) = \frac{k}{4\pi} \sigma_{\text{tot}}} \quad \underline{\text{optical theorem}}$$

which is a consequence of probability conservation  
(exercise 13.1)

To obtain a general bound on  $\sigma_{\text{tot}}$  we  
involve a classical picture of the scattering process:



$$\Rightarrow \text{angular momentum of the particle is } \underline{L = bp}$$

$$\Rightarrow l = \frac{b p}{\hbar} = \underline{b k} \Rightarrow b = l/k$$

If the range of the potential is  $R$ , then no scattering occurs for  $b > R$

$$\Rightarrow \underline{l \leq l_{\max} = kR} \quad \text{contribute to the sum over } l.$$

$$\Rightarrow \underline{\sigma_{\text{tot}}} = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l \leq$$

$$\leq \frac{4\pi}{k^2} \sum_{l=0}^{l_{\max}} (2l+1) = \frac{4\pi}{k^2} \left( 2 \cdot \frac{l_{\max}(l_{\max}+1)}{2} + l_{\max} \right)$$

$$= \frac{4\pi}{k^2} (l_{\max}^2 + 2l_{\max}) \approx \underline{4\pi R^2 = 4\sigma_{\text{geom}}}$$

for  $l_{\max} \gg 1$ , where  $\sigma_{\text{geom}} = \pi R^2$  is the expected geometric cross section.

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## 5° Hard sphere scattering

For the hard sphere potential

$$V(r) = \begin{cases} 0 & r > R \\ \infty & r \leq R \end{cases}$$

the radial wave functions have to vanish at  $r = R$ :

$$j_\ell(kR) + \frac{a_\ell}{2} h_\ell^{(1)}(kR) = 0 \quad \forall \ell$$

$$= \frac{1}{2} \{ h_\ell^{(1)}(kR) + h_\ell^{(2)}(kR) + a_\ell h_\ell^{(1)}(kR) \}$$

$$= \frac{1}{2} \{ \underbrace{(1 + a_\ell)}_{= e^{2i\delta_\ell}} h_\ell^{(1)}(kR) + h_\ell^{(2)}(kR) \} =$$

$$= \frac{1}{2} e^{i\delta_\ell} \{ \underbrace{e^{i\delta_\ell} h_\ell^{(1)}(kR) + e^{-i\delta_\ell} h_\ell^{(2)}(kR)}_{= 2 \operatorname{Re}(h_\ell^{(1)}(kR) e^{i\delta_\ell})} \}$$

$$= 2 \operatorname{Re}(h_\ell^{(1)}(kR) e^{i\delta_\ell}) =$$

$$= \underline{2 \{ j_\ell(kR) \cos(\delta_\ell) - y_\ell(kR) \sin(\delta_\ell) \}}$$

because  $(h_\ell^{(2)})^* = h_\ell^{(1)}$ . Thus the scattering phases are given by

$$\underline{\tan(\delta_\ell) = \frac{j_\ell(kR)}{y_\ell(kR)}}$$

a) Low energy scattering

Recall that  $j_l(p) \sim p^l$ ,  $y_l(p) \sim p^{-(l+1)}$   
 for  $p \rightarrow 0$

$$\Rightarrow \frac{j_l(kR)}{y_l(kR)} \sim (kR)^{2l+1}, \quad kR \rightarrow 0$$

The dominant contribution to the scattering cross section comes from  $l=0$ , where

$$\frac{j_0(kR)}{y_0(kR)} = -\tan(\delta_0) \Rightarrow \underline{\delta_0 \approx -kR}$$

This motivates to introduce the scattering length

$$\underline{a = -\lim_{k \rightarrow 0} \frac{\delta_0(k)}{k}}$$

which in this case is equal to  $R$ .

Taking into account only the  $l=0$  term, the scattering amplitude is

$$f(\theta) = \frac{1}{k} e^{i\delta_0} \underbrace{\sin(\delta_0) P_0(\cos\theta)}_{=1} = \frac{1}{k} e^{i\delta_0} \sin(\delta_0)$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = |f|^2 = \frac{1}{k^2} \sin^2(\delta_0) \approx \frac{\delta_0^2}{k^2} = \underline{R^2}$$

Scattering is isotropic, and the total

Cross section is

$$\underline{\sigma_{tot} = 4\pi \frac{d\sigma}{d\Omega} = 4\pi R^2}$$

Also note that

$$\underline{I_{in}(\theta) = \frac{1}{k} \sin^2(\delta_0) = \frac{k}{4\pi} \sigma_{tot}}$$

as required by the optical theorem

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### b) High energy scattering

As discussed above, the total cross section is

$$\underline{\sigma_{tot} \approx \frac{4\pi}{k^2} \sum_{l=0}^{l_{max}} (2l+1) \sin^2(\delta_l)} \quad \text{with } \underline{l_{max} = kR} \gg 1$$

For the hard sphere

$$\begin{aligned} \underline{\sin^2(\delta_l)} &= \frac{\sin^2(\delta_l)}{\sin^2(\delta_l) + \cos^2(\delta_l)} = \frac{\tan^2(\delta_l)}{1 + \tan^2(\delta_l)} = \\ &= \frac{(j_l/y_l)^2}{1 + (j_l/y_l)^2} = \underline{\frac{j_l^2(kR)}{j_l^2(kR) + y_l^2(kR)}} \end{aligned}$$

Moreover

$$\left. \begin{aligned} j_l(\rho) &\approx (-1)^l \frac{1}{\rho} \sin\left(\rho - \frac{l\pi}{2}\right) \\ y_l(\rho) &\approx (-1)^{l+1} \frac{1}{\rho} \cos\left(\rho - \frac{l\pi}{2}\right) \end{aligned} \right\} \text{ for } \rho \rightarrow \infty$$

$$\Rightarrow \underline{\sin^2(\delta_l) \cong \sin^2\left(kR - \frac{l\pi}{2}\right)}$$

This implies that

$$\begin{aligned} \underline{\sin^2(\delta_l) + \sin^2(\delta_{l+1})} &= \sin^2\left(kR - \frac{l\pi}{2}\right) + \\ &+ \sin^2\left(kR - \frac{l\pi}{2} - \frac{\pi}{2}\right) = \underline{1} \\ &= \cos^2\left(kR - \frac{l\pi}{2}\right) \end{aligned}$$

independent of  $l$ . Thus  $\sin^2(\delta_l)$  can be replaced by  $\frac{1}{2}$  in the sum and

$$\underline{\sigma_{\text{tot}}} \approx \frac{2\pi}{k^2} \sum_{l=0}^{l_{\text{max}}} (2l+1) = \frac{2\pi}{k^2} (l_{\text{max}}^2 + 2l_{\text{max}})$$

$$\approx \underline{2\pi R^2} \quad \text{for } kR \gg 1.$$

$$= 2 \sigma_{\text{geom.}}$$

On the other hand the limit

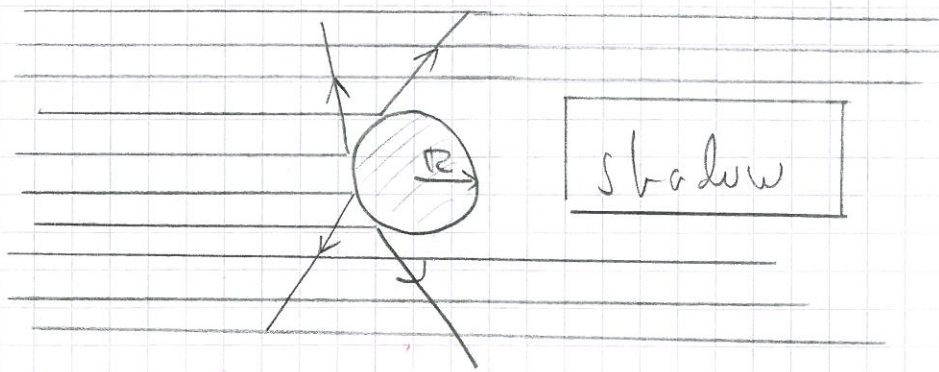
$$kR = \frac{p}{\hbar} R \rightarrow \infty$$

can also be understood as a classical limit ( $\hbar \rightarrow 0$ ) at fixed momentum  $p$ , and therefore one would expect

$$\sigma_{\text{tot}} \rightarrow \sigma_{\text{geom}} = \pi R^2.$$

Where does the factor 2 come from?

- Classically a shadow would form behind the target:



- In the wave picture the shadow has to be created by destructive interference with the incoming wave  $e^{ikz}$ , which is present also behind the target.
- The interfering wave is part of the scattered wave function  $\psi_s$ . It is focused in the forward direction and its integrated flux is  $\pi R^2$ .

For a formal treatment we write

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \underbrace{e^{i\delta_l} \sin(\delta_l)} P_l(\cos \theta)$$

$$= \frac{1}{2i} (e^{2i\delta_l} - 1)$$

$$= \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) e^{2i\delta_l} P_l(\cos \theta) +$$

$f_{\text{refl}}$

$$+ \frac{i}{2k} \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta)$$

$= f_{\text{shadow}}$

The contribution from the first part to the total cross section is

$$\begin{aligned}
 \underline{\sigma_{\text{tot}}^{\text{refl}}} &= 2\pi \int_{-1}^1 d(\cos\theta) \underbrace{|\underline{f_{\text{refl}}}(\theta)|^2}_{\substack{\text{Legendre} \\ \text{polynomials}}} \\
 &= \frac{1}{4k^2} \sum_{l,l'} (2l+1)(2l'+1) e^{2i(\delta_l - \delta_{l'})} P_l(\cos\theta) P_{l'}(\cos\theta) \\
 &= \frac{\pi}{2k^2} \sum_{l=0}^{l_{\text{max}}} 2 \cdot (2l+1) \approx \frac{\pi l_{\text{max}}^2}{k^2} = \underline{\pi R^2}
 \end{aligned}$$

because of the orthogonality of the Legendre polynomials,

$$\int_{-1}^1 dx P_l(x) P_{l'}(x) = \frac{2}{2l+1} \delta_{l,l'}$$

The second contribution  $\underline{f_{\text{shadow}}}$  is purely imaginary and focused in the forward direction, because all terms are in phase and maximal at  $\theta=0$ .

Further consideration shows that

$$2\pi \int_{-1}^1 d(\cos\theta) |f_{\text{shadow}}(\theta)|^2 \approx \pi R^2 = \sigma_{\text{tot}}^{\text{shadow}}$$

$$\text{and } \sigma_{\text{tot}} = \sigma_{\text{tot}}^{\text{refl}} + \sigma_{\text{tot}}^{\text{shadow}}$$