# Oscillator strength

Oscillator strength is a very important parameter in spectroscopy. It is defined in a dimensionless form and gives the probability of absorption or emission of radiation in transitions between energy levels of an atom or a molecule

$$f_{fi} = \frac{2m\omega_{fi}}{3\hbar} |\langle f|\vec{r}|i\rangle|^2 \qquad \omega_{fi} = \frac{E_f - E_i}{\hbar}$$

Where the dipole matrix elements are

$$|\langle f|\vec{r}|i\rangle|^2 \equiv |\langle f|x|i\rangle|^2 + |\langle f|y|i\rangle|^2 + |\langle f|z|i\rangle|^2$$

Oscillator strenghts obey the so-called Thomas-Reiche-Kuhn sum rule

$$\sum_f f_{fi} = 1$$

Obviously $f_{if} < 1$

Ther above sum rule can be derived as follows

$$\langle i|[x, p_x]|i\rangle = i\hbar \quad \leftarrow \text{basic commutator relation}$$

We may write it as

$$\sum_f \langle i|x|f\rangle\langle f|p_x|i\rangle - \langle i|p_x|f\rangle\langle f|x|i\rangle = i\hbar$$

Now, if the Hamiltonian is such that

$$H = \frac{p^2}{2m} + V(\vec{r}) = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(\vec{r})$$ we can

represent $\vec{p}$ as

$$p_x = \frac{im}{\hbar}[H, x]$$

(check: $[x, p_x^2] = [x, p_x]p_x + p_x[x, p_x] = 2i\hbar p_x$ )

Hence, $\langle f|p_x|i\rangle = \frac{im}{\hbar}\langle f|(Hx - xH)|i\rangle$

Because both $|f\rangle$ and $|i\rangle$ are eigenfunctions of $H$ we obtain

$$\langle f|p_x|i\rangle = -\frac{im}{\hbar}(E_i - E_f)\langle f|x|i\rangle$$

or simply

$$\langle f|p_x|i\rangle = +im\omega_{fi}\langle f|x|i\rangle$$

With that

$$\sum_f{}' \langle i|x|f\rangle\langle f|p_x|i\rangle - \langle i|p_x|f\rangle\langle f|x|i\rangle = i\hbar$$

becomes

$$\sum_f{}' [im\omega_{fi}|\langle f|x|i\rangle|^2 + im\omega_{fi}|\langle f|x|i\rangle|^2 = i\hbar$$

or

$$\sum_f \frac{2m\omega_{fi}}{\hbar}|\langle f|x|i\rangle|^2 = 1$$

The same result follows with $x$ replaced by $y$ or $z$. When we combine them we get

$$\sum_f \frac{2m\omega_{fi}}{3\hbar}|\langle f|\vec{r}|i\rangle|^2 = \sum_f f_{fi} = 1$$

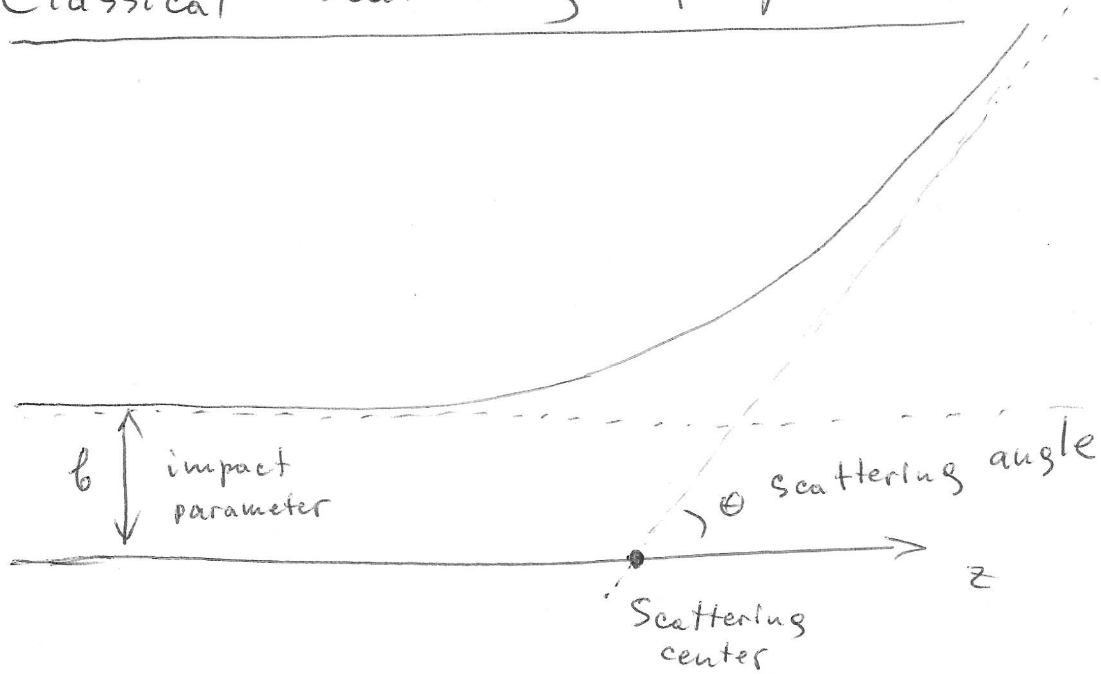
For an atom with $Z$ electrons we make a replacement

$$\langle f|\vec{r}|i\rangle \Longrightarrow \langle f|\sum_{i=1}^{Z}\vec{r}_i|i\rangle$$

and then

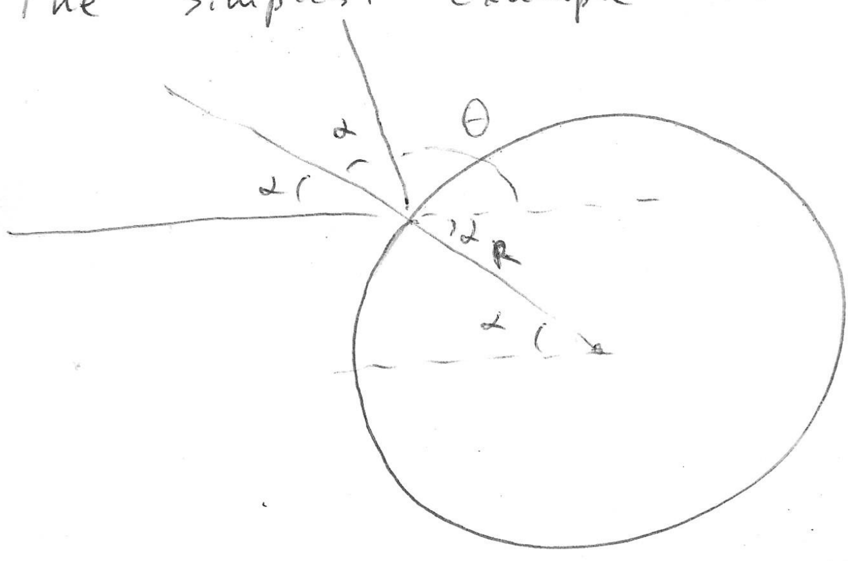
$$\sum_f{}' f_{fi} = Z$$

# Classical scattering of particles




Let us consider a particle incident on some scattering center. The particle has some initial energy, $E$, and impact parameter, $b$. Eventually it scatters at some scattering angle $\theta$. For simplicity we will assume that the target's potential is spherically symmetric. Then the trajectory lies in a single plain. Our task is to compute $\theta$ given $b$.

The simplest example is a hard-sphere potential




$$b = R\sin\alpha$$

$$\theta = \pi - 2\alpha$$

$$b = R\sin\left(\frac{\pi}{2} - \frac{\theta}{2}\right) = R\cos\frac{\theta}{2}$$

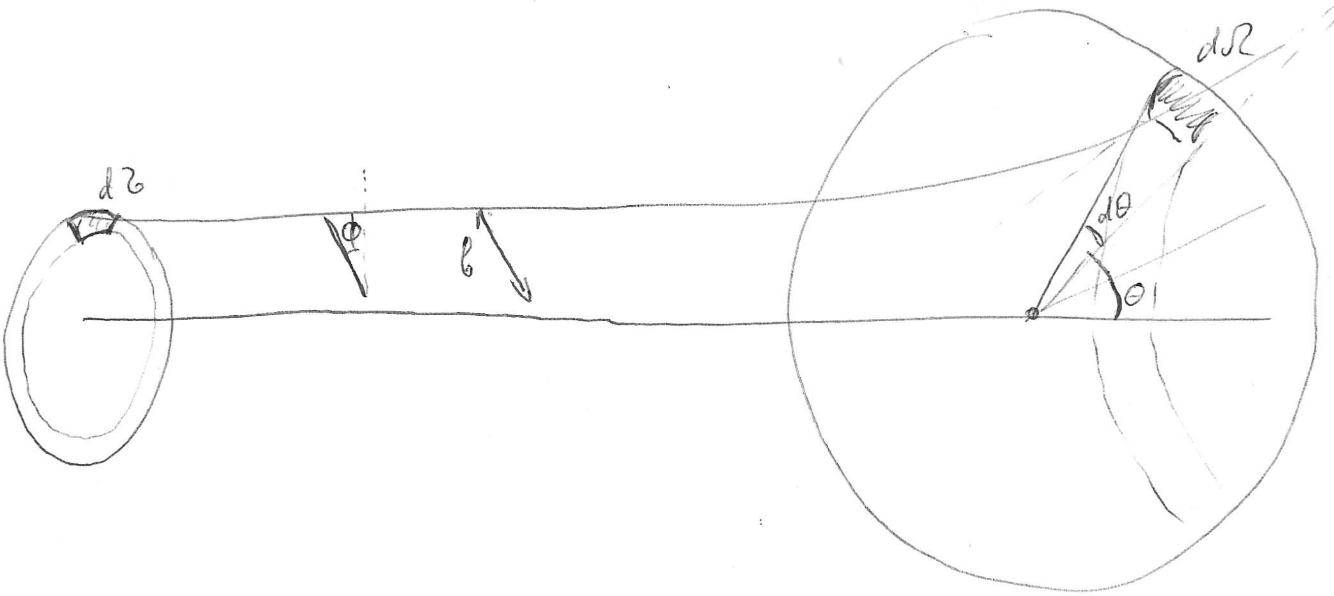
$$\theta = \begin{cases} 2\arccos\frac{b}{R}, & b < R \\ 0, & b \geq R \end{cases}$$

# Differential cross section

$$D(\theta) = \frac{d\sigma}{d\Omega}$$

$d\sigma$ – crossectional area

$d\Omega$ – solid angle




$$d\sigma = D(\theta)\, d\Omega$$

$$d\sigma = b\, db\, d\phi \qquad d\Omega = \sin\theta\, d\theta\, d\phi$$

$$D(\theta) = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

For a hard sphere

$$\frac{db}{d\theta} = -\frac{1}{2} R \sin\frac{\theta}{2}$$

and $$D(\theta) = \frac{R\cos\frac{\theta}{2}}{\sin\theta}\left(\frac{R\sin\frac{\theta}{2}}{2}\right) = \frac{R^2}{4}$$

The total cross-section is the integral of $D(\theta)$ over all solid angles:

$$\sigma \equiv \int D(\theta)\, d\Omega$$

For a hard sphere $\sigma = \frac{R^2}{4}\int d\Omega = \pi R^2$

If we have a beam of incident particles with uniform intensity (luminocity)

$\mathcal{L}$ - # particles per unit area per unit time

then the number of particles going through area $d\sigma$ (and scattered into solid angle $d\Omega$) per unit time is

$$dN = \mathcal{L}\, d\sigma = \mathcal{L}\, D(\theta)\, d\Omega$$

So

$$D(\theta) = \frac{1}{\mathcal{L}} \frac{dN}{d\Omega}$$

This is taken as the definition of the differential cross section because it makes reference only to quantities easily measured in the experiment.

As a model to practice let us consider a Coulomb system of charges $q_1$ and $q_2$ and masses $m_1 = m$ and $M_2 = \text{infinity}$.

Conservation of energy gives $E = \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\varphi}^2) + V(r)$

where $V(r) = \frac{q_1 q_2}{4\pi\varepsilon_0} \frac{1}{r}$

Conservation of angular momentum: $L = m r^2 \dot{\varphi}$ So $\dot{\varphi} = \frac{L}{mr^2}$

$$\dot{r}^2 + \frac{L^2}{mr^2} = \frac{2}{m}(E - V)$$

let $u \equiv \frac{1}{r}$ then

$$\dot{r} = \frac{dr}{dt} = \frac{dr}{du}\frac{du}{d\phi}\frac{d\varphi}{dt} =$$

$$= -\frac{1}{u^2}\frac{du}{d\varphi}\frac{L}{m}u^2 = -\frac{L}{m}\frac{du}{d\varphi}$$