DCC-LAB 2020

TECHREP-Scattering Cross Section

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This short document discusses the concepts of scattering, scattering cross section and scattered light intensity calculation based on cross section!

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https://docs.google.com/document/d/1QmLpaTMYDGqmnV5jS6Rnv4-kCBtpW4Sew3xY0pk2-yU/edit

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To better view equations, install Equation Editor++ in the Add-ons menu, and activate it.

Introduction

The cross section of an interaction is a very general concept in physics. It represents the equivalent area of an object as seen by another one, for a particular interaction. The simplest case is the collision between two billiard balls: the cross section for the interaction is given by the disk arising from the projected sphere of the target sphere. In this case, the collision is intuitively understood by anyone. But what is the cross-section for other complicated interactions? For instance, we know that two charged particles with the same charge will repel each other, but to the incident particle, what is the "area" of the target particle? How likely are they to collide?

What is Scattering, impact parameter and scattering angle?

We can consider the case of a repulsive central potential. Obviously, the two particles will not orbit each other - they will at most approach each other, before the repulsive potential causes them to move away from each other. This type of behaviour is in fact typically referred to as scattering. [1]

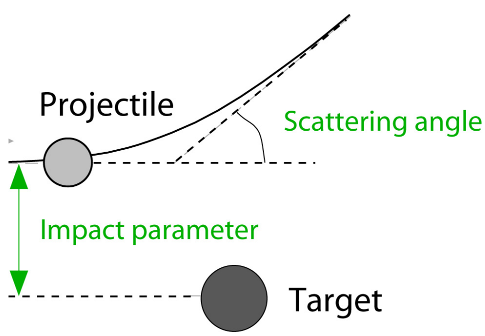

Fig1. A projectile, with impact parameter b, being scattered by a stationary target. After being scattered, the projectile travels off at some angle θ, never to return to the target.[2]

In the case where a collision between two particles conserves total energy, we say the scattering is elastic. The repelling angle of a projectile does not just depend on the energy it carries, but also on the impact parameter. A collision between two particles is typically described in terms of its impact parameter. This is the distance that would be the radius of closest approach, if there were no interaction between the two particles. (Notice that the impact parameter is not the actual distance of closest approach - in the presence of the interaction, the particle will begin to scatter away from the target before it has a chance to reach this distance.)

An outgoing projectile is typically described in terms of its scattering angle, which is the angular distance between its incoming and outgoing velocities. This is illustrated in Figure 1. The scattering angle is taken to range anywhere between zero and π radians. [1]

Total cross section

In most cases, it is impossible to know, for a given scattering event, exactly what the initial impact parameter was. For this reason, most scattering experiments involve firing a large number of particles at a collection of targets, measuring the outgoing angles, and then comparing the results against a set of statistical predictions. [1]

We will start by considering a simple model of scattering, where the potential experienced by the projectile is given by: U(r)=0 \ ,\ r>R \ \ and \ \ U(r)=\infty , \ r<R

$$U(r) = 0\ ,\ r > R\ \ and\ \ U(r) = \infty,\ r < R$$

This type of scattering potential is known as hard sphere scattering, Figure 2.

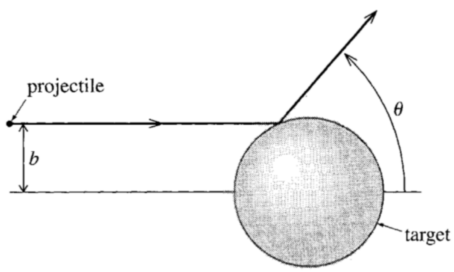

Fig2. An illustration of hard sphere scattering.[1]

The projectile is a point-like mass and the target is a solid sphere of radius R. In this case, if the impact parameter of the incoming particle is larger than R, it will not be deflected at all, and if smaller than R, it may suffer a relatively extreme deflection.

Because the solid sphere has an overall cross-sectional area of $\sigma=\pi R^2$, there is a region of space, with cross-sectional area σ, that projectiles cannot pass through. If the incoming path of a projectile passes through this cross-sectional area, it will be deflected off at some angle. For this reason, we define σ to be the scattering cross section for this potential. [1]

What would happen if we have many targets instead of one? see Figure3.

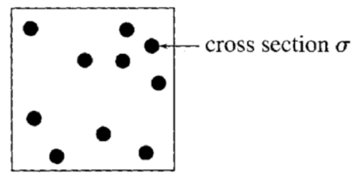

Fig3. A sheet of area A containing many hard sphere targets, each with a scattering cross section σ. [1]

For simplicity, the targets are arranged in a thin, two-dimensional sheet and one scattering event only will involve one target: there is no secondary scattering event after the first scattering event.

If we describe the density of targets by the quantity n_{tar}, then the total number of targets in the sheet is given by An_{tar} , where A is the area under consideration.

For any given projectile that is randomly fired at the target assembly, the probability that it will hit one of the spheres and scatter is given by the total cross-sectional area of all of the targets, divided by the total area of the assembly, so that: p=\frac{An_{tar}\sigma}{A}=n_{tar}\sigma

$$p = \frac{An_{tar}\sigma}{A} = n_{tar}\sigma$$

If we now imagine that the number of incident projectiles incident on the sheet is N_{inc}, then statistically speaking, the number of scattered particles, N_{sc}, should be given by:

N_{sc}=PN_{inc}=N_{inc}n_{tar} \sigma

$$N_{sc} = PN_{inc} = N_{inc}n_{tar}\sigma$$

In this regard, it is possible to measure whether or not a given projectile was scattered. The above formula then allows us to experimentally determine the scattering cross section, by knowing the density of targets, the number of incident particles, and the number of scattered particles. [1]

What is the Differential Cross Section?

Let’s consider the motion of a single projectile striking the target with impact parameter b. This is indicated in Figure 4. In this simple model, it is relatively straight-forward to determine the scattering angle as a function of the impact parameter. We make use of the fact that the angle of incidence on the surface of the sphere must be the same as the angle of reflection, with respect to the surface tangent of the sphere. [1]

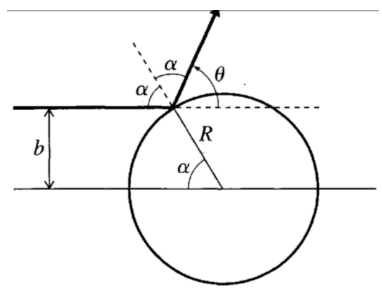

Fig 4. The motion of a projectile which strikes a hard sphere with impact parameter b.[1]

As a result, we have b=R\sin\alpha \ \ \ \ \ and \ \ \ \ \ \pi=\theta+2\alpha

$$b = R\sin\alpha \qquad and \qquad \pi = \theta + 2\alpha$$

Finally: b=R\sin(\frac{\pi}{2}-\frac{\theta}{2})=R\cos(\frac{\theta}{2})

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

So scattering angle is: \theta=2\arccos(\frac{b}{R})

$$\theta = 2\arccos(\frac{b}{R})$$

To find the range of impact parameter b:

In order to achieve a scattering by particles that scatter only in a small range of angles, $d\theta$, what range of db is needed? [1]

b+db=R\cos(\frac{\theta}{2})-\frac{R}{2}\sin(\frac{\theta}{2})d\theta

$$b + db = R\cos(\frac{\theta}{2}) - \frac{R}{2}\sin(\frac{\theta}{2})d\theta$$

So, increasing the scattering angle by an amount $d\theta$, the impact parameter should be increased by db: db=-\frac{R}{2}\sin\frac{\theta}{2}d\theta

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

So db as the amount of "infinitesimal cross section" which determines the area within which a particle's path would need to pass in order for it to scatter into a range of angles $d\theta$.

If we consider multiple projectiles coming in along multiple paths, then we should consider all azimuthal incoming angles around the central scattering axis. This idea is illustrated in Figure 5. In this case, the infinitesimal amount of scattering area is not db, but rather: d\sigma=2\pi bdb

$$d\sigma = 2\pi b db$$

Then: \int d\sigma=- \pi R^2 \int_0 ^\pi \sin(\frac{\theta}{2})\cos(\frac{\theta}{2})d\theta=-\pi R^2

$$\int d\sigma = -\pi R^2 \int_0^\pi \sin(\frac{\theta}{2}) \cos(\frac{\theta}{2}) d\theta = -\pi R^2$$

Aside from a minus sign, this is simply the total cross section for scattering by the hard sphere.

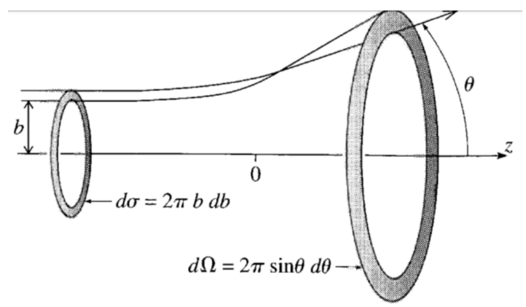

Fig5. The scattering of multiple projectiles off of a hard sphere, all with an impact parameter which lies between b and b + db. [1]

In the previous formula: The result for b as a function of the scattering angle θ did not depend on the angle around the central scattering axis. If we refer to this angle around the axis as ϕ, then we can say that the infinitesimal amount of scattering cross section dσ required to scatter into some direction is independent of ϕ. [1]

But sometimes our result for the required impact parameter as a function of b may depend on both angles θ and ϕ. This requires us to extend our notion of an infinitesimal range of angles to the more general concept of solid angle, which is illustrated in Figure 6. [1]

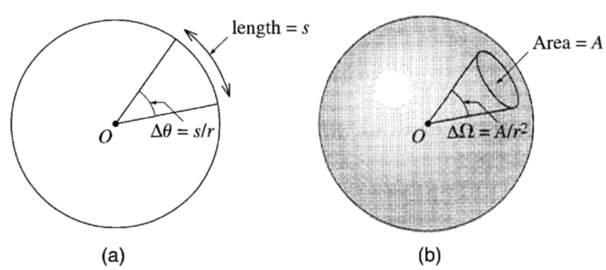

Fig6. a.) The definition of an angle in two dimensions. b.) The definition of solid angle in three dimensions. [1]

In two dimensions, the angular difference between two points on a circle can be defined as:

\Delta \theta=\frac{s}{r}

$$\Delta\theta = \frac{s}{r}$$

and for three dimensional: \Delta \Omega=\frac{A}{r^2}

$$\Delta\Omega = \frac{A}{r^2}$$

Notice: The unit of solid angle is the steradian, as opposed to the radian which describes regular angles.

In a spherical coordinate system[1], the differential volume element is given by:

$$dV = r^2 \sin\theta d\theta dr d\phi$$

so that the infinitesimal amount of area on the surface of a sphere with radius r is given by:

dA=\frac{dV}{dr}=r^2 \sin\theta d\theta d\phi

$$dA = \frac{dV}{dr} = r^2 \sin\theta d\theta d\phi$$

Thus, the infinitesimal amount of solid angle in a given direction in spherical coordinates is given by: d\Omega=\frac{dA}{r^2}=\sin\theta d\theta d\phi

$$d\Omega = \frac{dA}{r^2} = \sin\theta d\theta d\phi$$

Because we cannot measure every scattering angle, the differential cross section gives us more detail on how the scattering is going on.[3]

The incident particles within an infinitesimal cross-sectional area $d\sigma$ will scatter into a corresponding infinitesimal solid angle $d\Omega$. The ratio of these, is called the "differential scattering cross-section".[4] D(\theta)=\frac{d\sigma}{d\Omega}

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

We also know that: (according to the figure7) d\Omega=\frac{dA}{r^2}=\sin\theta d\theta d\phi \ \ \ \ and \ \ \ \ d\sigma=bdbd\phi

$$d\Omega = \frac{dA}{r^2} = \sin\theta d\theta d\phi \quad and \quad d\sigma = bdbd\phi$$

Therefore:

D(\theta)=\frac{d\sigma}{d\Omega}=\frac{b}{\sin \theta} |\frac{db}{d\theta}|

$$D(\theta) = \frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}|\frac{db}{d\theta}|$$

The total scattering cross-section is the integral of D over all angles,

\sigma=\int d\Omega D(\theta)

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

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[1] The differential volume element is dV = dx dy dz. To go to spherical coordinates, we use the Jacobian dV

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

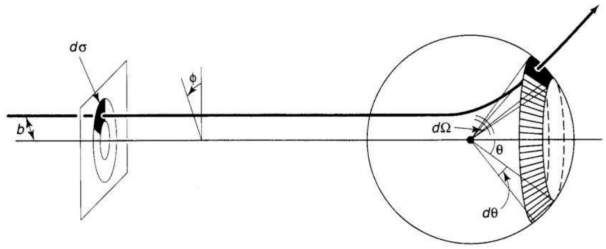

Fig7. Particles incident in the area dσ scatter into the solid angle /dΩ.[2]

Scattered light intensity calculation based on cross section:

In very general terms, there is scattering when light is incident on a particle. The probability of occurring such an event depends on the scattering cross section σ which is the imaginary surface corresponding to the possible interaction with the particle. [5]

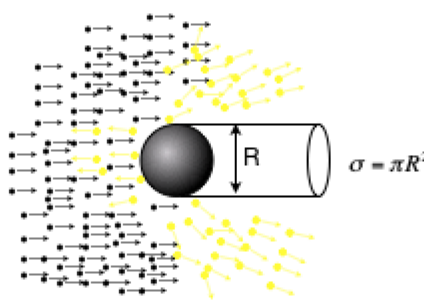

Fig8. Illustration of cross section for a solid particle on which small solid particles are incident. The incident particles that their trajectories are modified are drawn in yellow and in fact, these particles are scattered. [5]

If we want to calculate the light distribution as a function of the scattering angle, we must calculate the differential cross section or the phase function.

If we know the amount of photons per unit area per second I, (i.e. the irradiance of a laser), we can calculate the total amount of photons per second W, that will be scattered by a single particle simply by:

$$W = I\sigma$$

If there is a collection of particles with an effective cross-section σ_i arranged in a thin layer of thickness dz, as long as the concentration remains low, the total light that will scatter (integrated in all directions) will be

Scattering Cross Section

dW=\sum_i^{ }I\sigma_i=I\sum_i^{ }\sigma_i=I\rho \sigma dV

$$dW = \sum_i I\sigma_i = I\sum_i \sigma_i = I\rho\sigma dV$$

Where ρ is the particle density per volume and σ is the effective cross section of a single particle. Knowing that the incident light intensity I can be rewritten as $I=\frac{W}{A}$ where W is the number of photons incident per second on the surface A, we obtain:

\frac{dW}{W}=\sigma \rho dz

$$\frac{dW}{W} = \sigma\rho dz$$

On the other hand, If the cross section gives the probability of interaction between a wave and a single particle, then it can be used to calculate the scattering coefficient μs, which represents the number of collisions per distance travelled. A simple calculation can show that if we have a particle density of ρ and cross-section σ, the scattering coefficient μs will be:

\mu_s=\rho \sigma

$$\mu_s = \rho\sigma$$

So, \frac{dW}{W}=\mu_s dz

$$\frac{dW}{W} = \mu_s dz$$

We know that $\frac{dW}{W}$ is the fraction of incident photons that are scattered in the volume dV. It can therefore be interpreted as the probability dP that a photon is scattered by propagating over a distance dZ:

dP=\mu_s dz

$$dP = \mu_s dz$$

Where the scattered intensity is given by:

dI=IdP=I \mu_s dz

$$dI = IdP = I\mu_s dz$$

And therefore:

I=I_0 e^{-\mu_sz}

$$I = I_0 e^{-\mu_s z}$$

The light intensity will also decay as a consequence of absorption. This is characterised by the absorption coefficient μ_a. The attenuation processes act independently of each other and so their separate contributions can be added together. The variation of the intensity with z is therefore given by: [5] I=I_0 e^{-(\mu_s+\mu_a)z}

Scattering Cross Section

$$I = I_0 e^{-(\mu_s+\mu_a)z}$$

References

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[5]. Optique des tissus by Prof. Daniel Côté, dccote@cervo.ulaval.ca and Prof. Simon Rainville, Simon.Rainville@phy.ulaval.ca

[6] Cheng, Ji-Xin, and Xiaoliang Sunney Xie. 2016. *Coherent Raman Scattering Microscopy*. CRC Press.

Proposed enhancement:

Classical explanation of Raman cross-section [6]

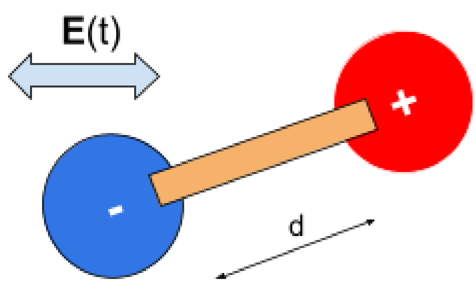
The way the cross-section is defined, as the effective area, is really just a geometric analogy that is simple and that is enough to be workable. As mentioned earlier, it was approximated as a radius R where the potential was infinite. However, it can be demonstrated that the cross section is directly related not to the geometric size, but to the change of polarizability of the dipolar molecule/bond according to a certain mode of vibration of the nuclei.

To describe the effects of nuclear motions, we describe the dipole moment μ of a bond/molecule, as such:

$$\mu(t) = \alpha(t)E(t)$$

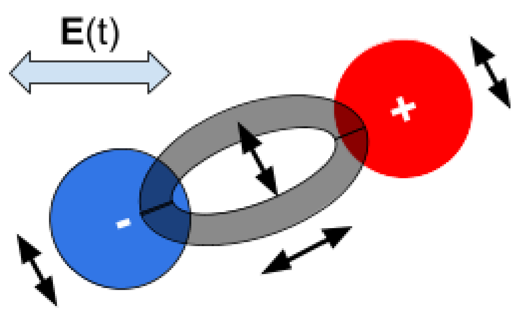
Where α is the polarizability assuming non resonant conditions of the electronic levels and E the incident electric field. The polarizability is usually defined as $\alpha = p/E$, p being the dipole moment, which is defined as $p = q \cdot d$, q being the charge and d the distance between them.

Imagine a dipole made out of 2 charged copper balls with a stiff wood stick linking the two. Imagine there is also an oscillation field $E(t)$ driving the dipole back and forth.



The polarizability of this dipole is a constant; it will always experience the same torque no matter the frequency because the distance between the charges is fixed, thus the polarizability is fixed.

Imagine now the same dipole, but linked by a soft rubber band



It is evident that under some frequency/intensity of the incident electric field, this dipole is going to experience some unusual vibrations and motions. The distance will vary in really complex ways. Thus, the polarizability will change with time $\alpha(t)$ because p will change with time.

Now, let's imagine that the charges are actually electronics clouds, so that the actual dipole is really more a function of charge density probability, this becomes very complicated. We could however propose that these complex variations are only due to the vibrations modes between the nucleii (The position Q of the nuclei which would have an influence on the cloud's position). We could than expand the polarizability as a taylor series

$$\alpha(t) = \alpha_0 + \frac{\partial \alpha}{\partial Q}_0 \cdot Q(t) + ...$$

Where Q is the nuclear position with respect to time.
So to modelize a nuclear/bond vibration, we can model it as a simple sinusoidal wave.

$$Q(t) = Q_0 \cos(\omega_{vib} t + \phi) = Q_0 \left(e^{i(\omega_{vib} t + \phi)} + e^{i(\omega_{vib} t + \phi)}\right)$$

If we plug this equation in the dipole moment equation, we get the following:

$$\mu(t) = \alpha_0 A e^{-i\omega_1 t} + A\left(\frac{\delta\alpha}{\delta Q}\right)_0 Q_0 \left\{e^{-i(\omega_1 - \omega_v)t + i\phi} + e^{-i(\omega_1 + \omega_v)t - i\phi}\right\} + \mathrm{c.C}$$

The first term is the oscillation of the dipole moment at the same frequency than the incoming field (Rayleigh scattering!), which is ω_1. The second term shows an oscillation at $\omega_1 - \omega_v$ and $\omega_1 + \omega_v$, which really represent the Stokes and antiStokes vibrations.

The electric field radiated by a dipole is

$$E(\omega_s) = \frac{\omega_s^2}{4\pi\epsilon_0 c^2} |\mu(\omega_s)| \frac{e^{ikr}}{r} \sin\theta$$

where

k is the wave vector of the radiated field
c is the speed of light
θ is the angle relative to the dipole axis
r is the distance from the dipole location to the observation point
$|\mu(\omega_s)|$ is the amplitude of the dipole oscillation at ω_s

The Poynting vector is described by

$$S(\omega_s) = \frac{\epsilon_0 c}{2} |E(\omega_s)|^2$$

And integrating the poynting vector on the whole sphere, it is possible to calculate the intensity of the radiated energy from the dipole as

$$I(\omega_s) = \frac{\omega_s^4}{12\pi\epsilon_0 c^3} Q_0^2 |A|^2 \left|\frac{\delta\alpha}{\delta Q}\right|^2$$

From [6], the definition of the intensity according to the cross section is

$$I(\omega_s) = Nz\sigma(\omega_s)I_0$$

From these 2 equations, we can see that A^2 is just I_0and that the actual cross-section is actually linearly dependant to (da/dq)^2. Thus, the cross section is, in reality related to the rate of change of the polarizability of the molecule/bond and is very dependant on the Raman frequency of emission (dependant to the power 4).

To summarize, the geometrical cross section is a conceptual approach to what the efficient area of action is for a given molecule regarding the Raman signal, but this cross section efficiency is actually dependant of the frequency of Raman signal and of the rate of change of polarizability as a function of the position of the nucleus squared. This is however, not a real picture, since at this level, many quantum processes are involved.

Quantum explanation of Raman cross-section