Neutron scattering I

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
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The neutron interacts with the atomic nucleus, and not with the electrons as photon does. This has important consequences. The response of neutrons from light atoms such as hydrogen is much higher than for x-rays. Neutrons can easily distinguish atoms of comparable atomic number. For the same wavelength as x-ray, the neutron energy is much lower and comparable to the energy of elementary excitations in matter. Thus neutrons do not only allow the determination of the static average structure of matters, but also the investigation of the dynamic properties of atomic arrangements which are directly related to the physical properties of materials. The neutron has a large penetration depth and the bulk properties of matter can be studied. The neutron carries a magnetic moment which makes it an excellent probe for the determination of the static and dynamical magnetic properties of matters. The charge of neutron is zero. The neutron is a fermion with spin 1/2.

1. de Broglie relation: duality of wave and particle

The kinetic energy of slow neutrons with velocity v is given by

$$E = \frac{1}{2} m v^2$$

where m is the mass of neutron

$$m = 1.674927471(21)\times 10^{-24} \text{ g}$$

The de Broglie wavelength λ of the neutron is defined by

$$\lambda = \frac{h}{p} = \frac{h}{mv}, \qquad \text{(de Broglie relation)}$$

where h is the Planck constant. The wavevector k of the neutron has the magnitude

$$k = \frac{2\pi}{\lambda}.$$

The energy can be expressed by

$$E = \frac{\hbar^2 k^2}{2m}.$$

Here we note that the kinetic energy is related to the temperature T as

$$E = \frac{3}{2} k_B T,$$

using the equipartition theorem since there are 3 degrees of freedom and $\frac{1}{2} k_B T$ for each freedom. The velocity is evaluated as

$$\frac{1}{2} m v_{rms}{}^2 = \frac{3}{2} k_B T,$$

or

$$v_{rms} = \sqrt{\frac{3k_B T}{m}}. \qquad \text{(this velocity is called the root-mean square velocity)}$$

However, we do not use this notation based on the equipartition relation. In the neutron scattering, it is convenient to say that neutron with energy E corresponds to a temperature T;

$$E = \frac{1}{2} m v_{mp}{}^2 = k_B T.$$

The most probable velocity is evaluated as

$$v_{mp} = \sqrt{\frac{2k_B T}{m}}.$$

((**Note-1**)) Using the above relations with $E = k_B T$, we have the following wave-particle relationships.

(a) Energy:

$$E(meV) = 2.07212\ [k(\text{Å}^{-1})]^2$$

from the relation: $E = \frac{\hbar^2 k^2}{2m}$

(b) Wavelength:

$$\lambda(\text{Å}) = \frac{h}{\sqrt{2mE}} = \frac{9.04457}{\sqrt{E(meV)}}$$

$$E(meV) = \left[\frac{9.04457}{\lambda(\text{Å})}\right]^2$$

or

$$\lambda(\text{Å}) = \frac{30.8107}{\sqrt{T(K)}}$$

(c) Wavevector:

$$k(\text{Å}^{-1}) = \frac{2\pi}{\lambda(\text{Å})}.$$

(d) Frequency:

$$\nu(THz) = 0.241799\, E(meV),$$

from the relation; $\nu = \frac{E}{h}$.

(e) Wavenumber:

$$\nu(cm^{-1}) = 33.3565\, \nu(THz)$$

from the relation $\frac{1}{\lambda} = \frac{\nu}{c}$

(f) Velocity:

$$v\left({}^{km}/{}_{s}\right) = 0.629622\, k(\text{Å}^{-1})$$
$$= \frac{3.95603}{\lambda(\text{Å})}$$

from the relation $v = \frac{\hbar}{m} k = \frac{h}{m\lambda}$.

(g) Temperature:

$T(K) = 11.6045\, E(meV)$

from the relation $E = k_B T$

((**Note-2**))
Table from G. Shirane, S.M. Shapiro, and J.M. Tranquada, Neutron Scattering with a Triple Axis Spectrometer (Cambridge, 2004).

Energy	$[\mathrm{meV}] = 2.072k^2[\text{Å}^{-1}]$
Wavelength	$\lambda[\text{Å}] = 9.044/\sqrt{E}[\mathrm{meV}]$
Wave vector	$k[\text{Å}^{-1}] = 2\pi/\lambda[\text{Å}]$
Frequency	$\nu[\mathrm{THz}] = 0.2418E[\mathrm{meV}]$
Wavenumber	$\nu[\mathrm{cm}^{-1}] = \nu[\mathrm{Hz}]/(2.998 \times 10^{10}\ \mathrm{cm/s})$
Velocity	$v[\mathrm{km/s}] = 0.6302\,k[\text{Å}^{-1}]$
Temperature	$T[\mathrm{K}] = 11.605E[\mathrm{meV}]$

((**Note-3**)) **Example**

For T = 300 K;

E = 25.852 meV. λ = 1.779 Å. v = 2.224 km/s

Some useful rules of thumb worth memorizing are

1Å = 81.80 meV, 1 meV = 8.07 cm^{-1} ≈ 0.2418 THz ≈ 11.61 K = 17.3 tesla.

2. Life time of neutron

A free neutron is unstable and undergoes radioactive decay. It is a beta-emitter, decaying spontaneously into a proton, an electron, and an electron anti-neutrino. The life time of the neutron is 886 ± 1 s. The half-life $\tau_{1/2}$, or the time taken for half of the neutrons to decay is

$$\tau_{1/2} = \tau \ln 2 = 614 \text{ s.}$$

At $T = 300$ K, the velocity of neutron is $v = 2.224$ km/s. It takes 45 ms to travel 100 m. So it is safe to assume that a finite life time of the neutron is of no practical significance in a scattering experiment.

3. Magnetic moment

The best available measurement for the value of the magnetic moment of the neutron is

$$\mu_n = -1.91304272(45)\ \mu_N,$$

where μ_N is the nuclear magneton,

$$\mu_N = \frac{e\hbar}{2m_p c} = 5.050783699(31)\times 10^{-24} \text{ emu (=erg/Oe)}$$

4. Maxwell-Boltzmann distribution

We now consider the Boltzmann factor for the kinetic energy of free particles with a mass m. We derive the form of Maxwell-Boltzmann distribution function. The probability of finding the particles between v and $v + dv$ is

$$f(v)dv = \frac{4\pi v^2 dv \exp(-\frac{\beta m v^2}{2})}{\int_0^\infty 4\pi v^2 dv \exp(-\frac{\beta m v^2}{2})}.$$

Here we have

$$\int_0^\infty 4\pi v^2 dv \exp(-\frac{\beta m v^2}{2}) = 4\pi\sqrt{\frac{\pi}{2}}(m\beta)^{-3/2} = (\frac{m\beta}{2\pi})^{-3/2}$$

The Maxwell-Boltzmann distribution function is

$$f(v) = (\frac{m\beta}{2\pi})^{3/2} 4\pi v^2 \exp(-\frac{\beta m v^2}{2})$$
$$= (\frac{m}{2\pi k_B T})^{3/2} 4\pi v^2 \exp(-\frac{m v^2}{2k_B T})$$

where

$$\int_0^\infty f(v)dv = 1$$

The average velocity:

$$\langle v \rangle = \int_0^\infty v f(v)dv = 2\sqrt{\frac{2}{\pi}}(m\beta)^{-1/2} = \sqrt{\frac{8k_B T}{\pi m}}$$

The variance:

$$\langle v^2 \rangle = \int_0^\infty v^2 f(v)dv = \frac{3}{m\beta} = \frac{3k_B T}{m}$$

This can be rewritten as

$$\frac{1}{2}m\langle v^2 \rangle = \frac{3}{2}k_B T$$ (from the equi-partition theorem)

The root-mean square velocity is

$$v_{rms} = \sqrt{\langle v^2 \rangle} = \sqrt{\frac{3k_B T}{m}}.$$

What is the most probable velocity in which $f(v)$ takes a maximum.

$$\frac{df}{dv} = 0$$

$$2v\exp(-\frac{mv^2}{2k_BT})+v^2(-\frac{mv}{k_BT})\exp(-\frac{mv^2}{2k_BT})=0$$

or

$$v_{mp}=\sqrt{\frac{2k_BT}{m}}$$

(most probable velocity)

or

$$\frac{1}{2}mv_{mp}{}^2=k_BT$$

Which can be used conventionally for the neutron scattering.

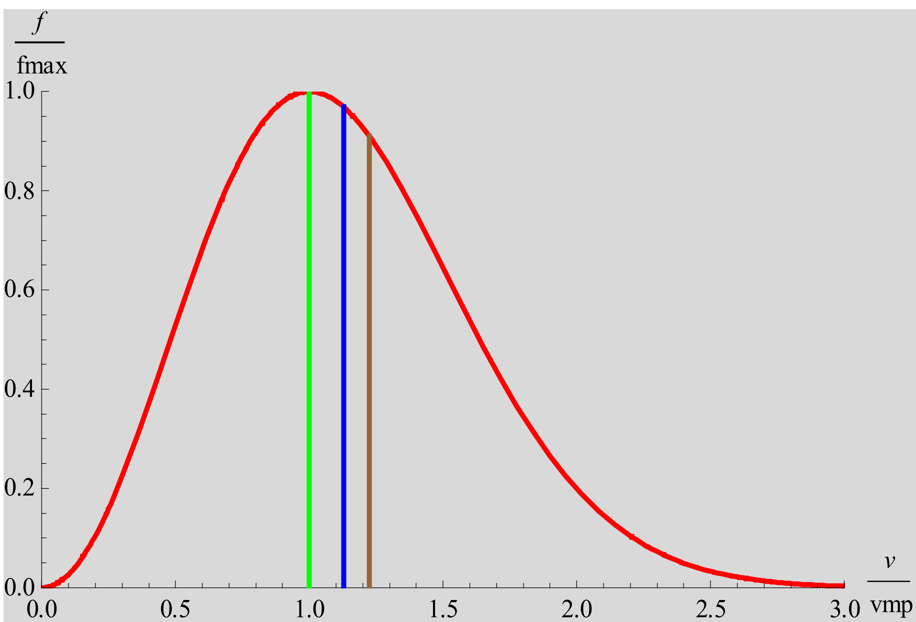


Fig. Plot of the normalized $f(v)/f_{\max}$ as a function of a normalized v/v_{mp}.

Green:	most probable speed	(v_{mp})
Blue:	averaged speed	(v_{avg})
Brown:	root-mean squared speed	(v_{rms})

$$1 < \frac{v_{avg}}{v_{mp}} (= 1.128) < \frac{v_{rms}}{v_{mp}} (= \frac{\sqrt{6}}{2} = 1.225)$$

where

$$v_{mp} = \sqrt{\frac{2k_B T}{m}}, \qquad v_{avg} = \sqrt{\frac{8k_B T}{\pi m}}, \qquad v_{rms} = \sqrt{\frac{3k_B T}{m}}.$$

((**Example**)) Neutron (obeying the Maxwell Boltzmann distribution)

(a) $T = 300$ K (thermal neutron)

$E = \frac{1}{2} m {v_{mp}}^2$=25.852 meV

$\lambda = \frac{h}{m v_{mp}}$ = 1.77885 Å, v_{mp} =2.2239 km/s.

(b) $T = 20$ K (liquid hydrogen or deuterium)

$E = \frac{1}{2} m {v_{mp}}^2$=1.72347 meV

$\lambda = \frac{h}{m v_{mp}}$ = 6.8895 Å, v_{mp} =574.211 m/s.

(c) $T = 2$ K (cold neutron)

$E = \frac{1}{2} m {v_{mp}}^2$=172.347 μeV

$\lambda = \frac{h}{m v_{mp}}$ = 15.405 Å. v_{mp} =256.8 m/s.

(d) $T = 2200$ K (hot neutron)

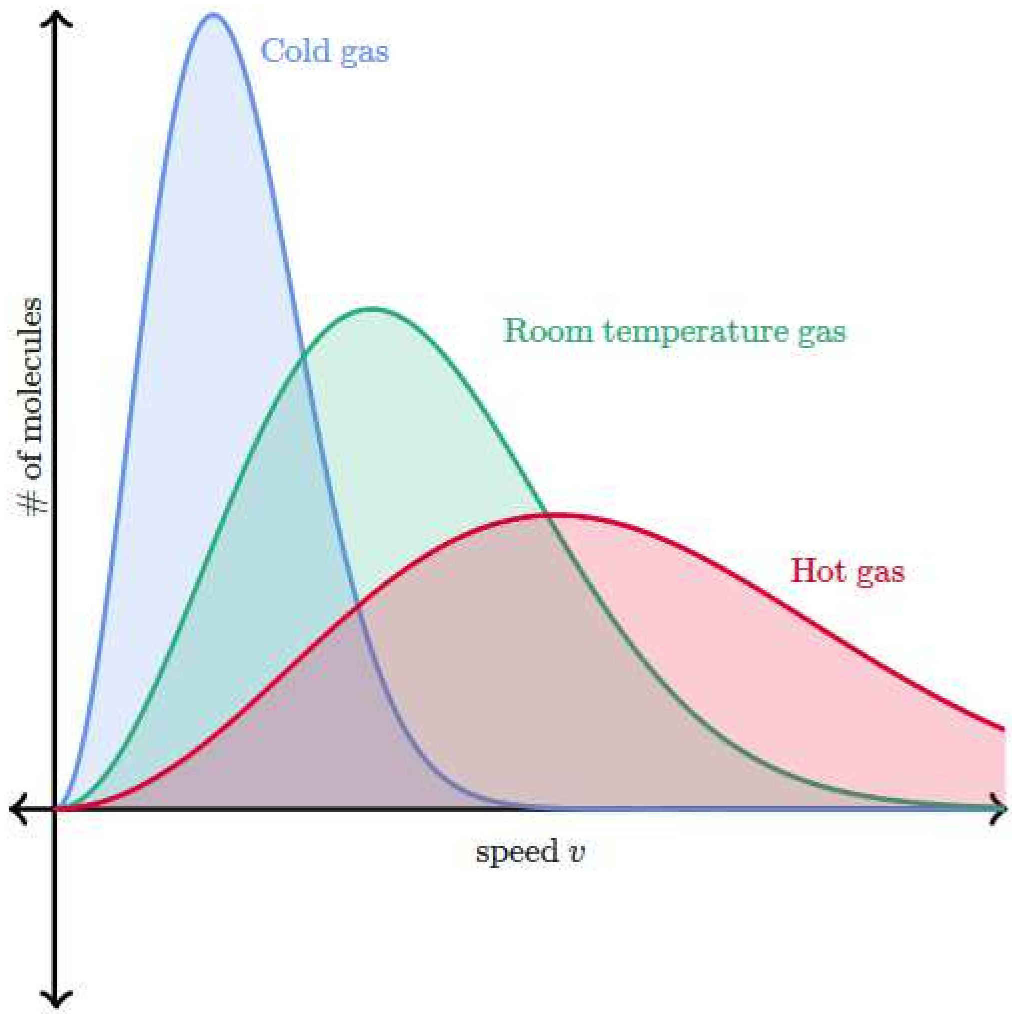
$E = \frac{1}{2} m {v_{mp}}^2$=189.582 meV

$\lambda = \frac{h}{m v_{mp}}$ = 0.6569 Å. v_{mp} =6.022 km/s.

For most reactors designed to produce high thermal neutron flux, the temperature of the moderator is about 300 to 350 K, and the resulting velocity spectrum of the neutrons is suitable for many experiments. However, in some experiments the velocities required for the incident neutrons lie on the low-energy tail of the thermal spectrum, while in other experiments neutrons on the high-energy side are required. It is therefore desirable to be able to change the temperature of the velocity distribution. This is done by placing in the reactor a small amount of moderating material at a different temperature.

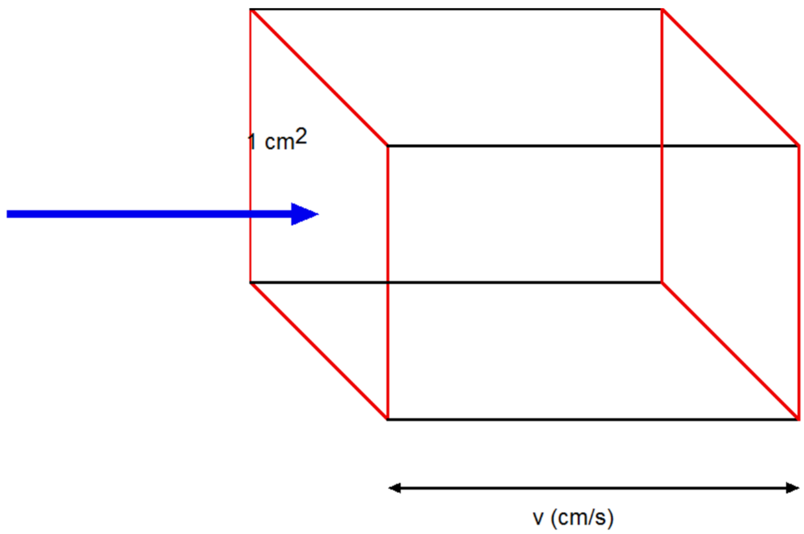
Source	Energy E(meV)	Temperature T (K)	Wavelength λ(Å)
Cold	0.1 – 10	1 – 120	4 – 30
Thermal	5 – 100	60 – 1000	1 - 4
Hot	100 – 500	1000 – 6000	0.4 – 1

Table: Approximate values for the range of energy, temperature, and wavelength for the three types of source in a reactor.



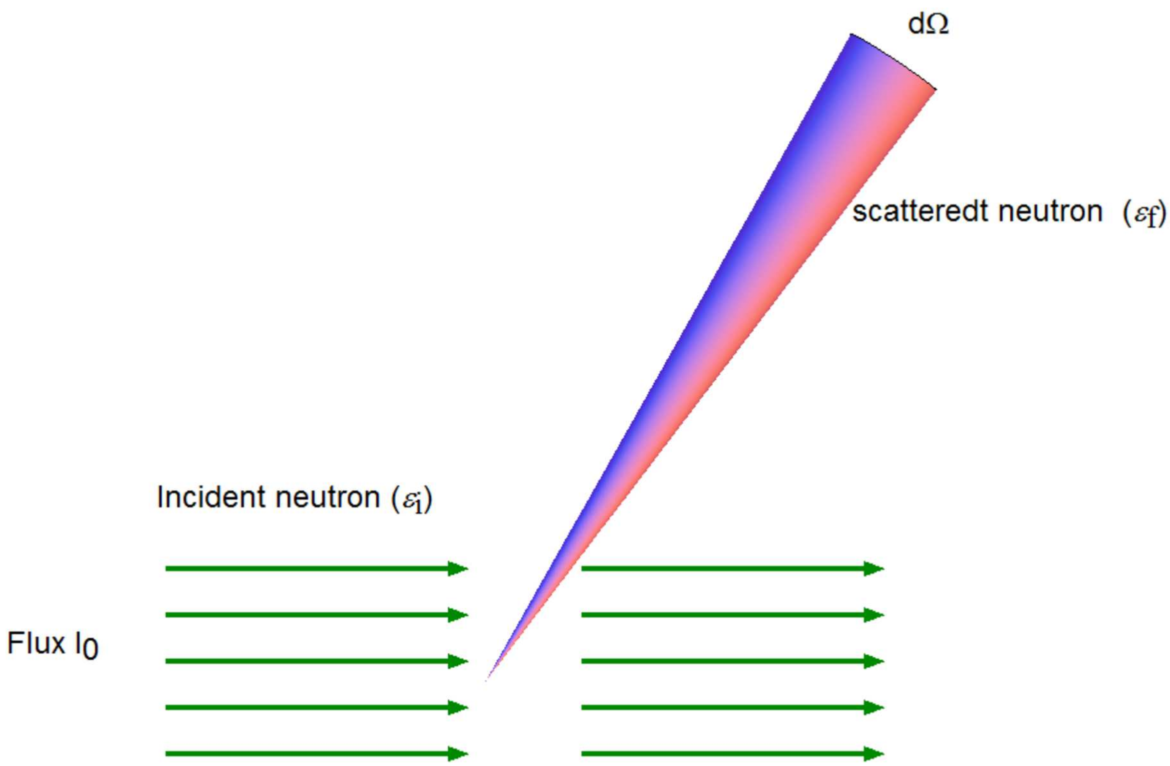
5. Fundamental

Thermal neutron flux



The number of thermal neutrons which pass through a unit area (cm^2) per second.

((**Cross section**))



We assume that the target is sufficiently small that the probability of scattering of a neutron incident on the target is not large.

If the target does scatter some of the incident neutrons, then at a large distance from the target we can detect neutrons that are scattered into a small element of solid angle dΩ with energy ε'.

$$I_0 \frac{d^2\sigma_s}{d\Omega d\varepsilon'} d\Omega d\varepsilon'$$

The number of neutrons per second scattered into solid angle dΩ between ε' and ε' + dε'.

((**Definition**))

$\frac{d^2\sigma_s}{d\Omega d\varepsilon'}$ Partial differential cross section.

Integrating this over dε', we put the number of neutrons per second scattered into solid angle dΩ (regardless of ε') to be

$$I_0 d\Omega \int_0^\infty \frac{d^2\sigma_s}{d\Omega d\varepsilon'} d\varepsilon' = I_0 d\Omega \int_0^\infty \frac{d^2\sigma_s}{d\Omega d\varepsilon'} d\varepsilon' = I_0 d\Omega \frac{d\sigma_s}{d\Omega}$$

$\frac{d\sigma_s}{d\Omega}$: differential cross section

If we now integrate over solid angle, we find that the number of neutrons scattered per second is

$$I_0 \int d\Omega \frac{d\sigma_s}{d\Omega} = I_0 \sigma_s . \quad \text{[number/sec]}$$

since the unit of I_0 is number/(cm^2 sec) and the unit of σ_s is cm^2.

Finally we can write down the number of neutrons per second that have momentum changed in the target as

$$I_0\sigma_t$$

σ_t is the total cross section,

$$\sigma_t = \sigma_a + \sigma_s$$

((**Note**))

$[\sigma]$ = barn.

1 barn = 10^{-28} m^2 = 10^{-24} cm^2.

1 fermi = 10^{-15} m = 10^{-13} cm.

This is about the projected area of an atomic nucleus. If the target consists of many atoms, we can either deal with the cross section for the whole target, or take it per atom or per chemical formula unit.

((**Note**))

σ_s :	transmission
$\dfrac{d\sigma_s}{d\Omega}$;	neutron diffraction, time of flight method
$\dfrac{d\sigma_s}{d\varepsilon}$:	energy spectrum measurement
$\dfrac{d^2\sigma_s}{d\Omega d\varepsilon}$:	inelastic scattering experiment

6. Differential cross section

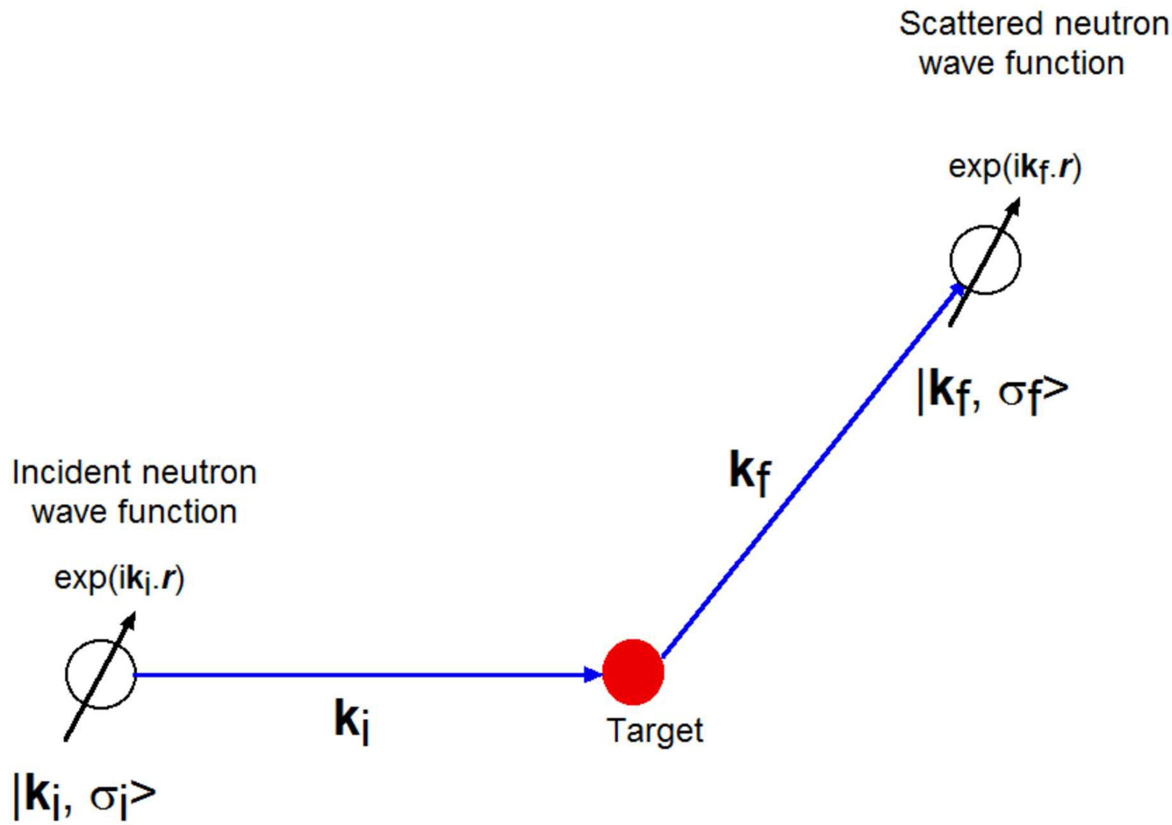


Fig. Scattering of neutron by a target. $\boldsymbol{k}_i = k'$. $\boldsymbol{k}_f = \boldsymbol{k}'$. The scattering vector $Q = \boldsymbol{k}_i - \boldsymbol{k}_f$.

$|\mathbf{k},\sigma\rangle$: initial state of neutron

$|\mathbf{k}',\sigma'\rangle$: final state of neutron

where

$\boldsymbol{k}$: neutron wave vector
σ: spin state

The target is initially in quantum state $|\lambda\rangle$ and after the scattering event is in quantum state $|\lambda'\rangle$.

m: mass of the neutron
V: interaction potential between the neutron and the target.

E_λ: energy of the target in state $|\lambda\rangle$.

The first order Born approximation is given by

$$\frac{d^2\sigma_s}{d\Omega d\varepsilon'} = \frac{k'}{k}(\frac{m}{2\pi\hbar^2})|\langle\mathbf{k}'\sigma'\lambda'|V|\mathbf{k}\sigma\lambda\rangle|^2\delta(E_\lambda - E_{\lambda'} + \varepsilon - \varepsilon')$$

from the quantum mechanics (see the Appendix)

7. Nuclear elastic scattering

For nuclear scattering, we describe the interaction potential by a quantity known as the Fermi pseudopotential

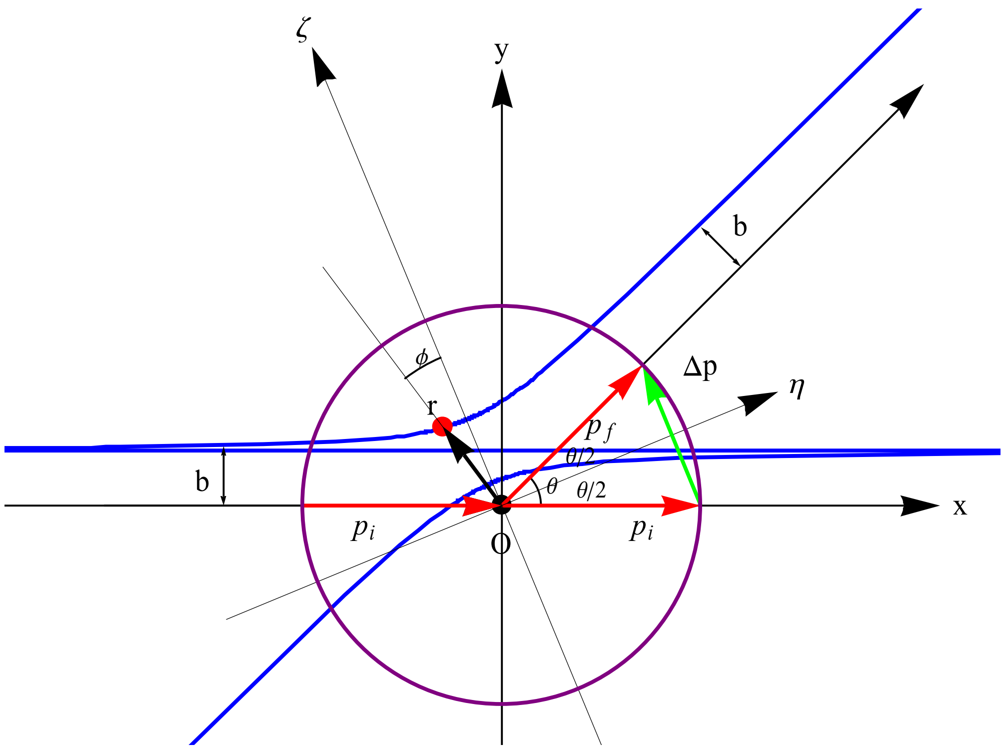


Fig. The distance over which the nuclear force extends (10^{-12} cm). The wavelength of the neutron is $\lambda = 10^{-8}$ cm. The target is located at the origin.

$$V = \frac{2\pi\hbar^2}{m} b\delta(\mathbf{r} - \mathbf{R}),$$

where b is the scattering length. It is typically found to be of the order of 10 fm.

((**Note**))

The Fermi pseudopotential cannot be the correct interaction potential, since the interaction is not actually infinite anywhere. However, the nuclear size and range of the nuclear force are so small compared with the wavelength of a thermal neutron that the delta function pseudopotential gives an excellent representation of the actual scattering.

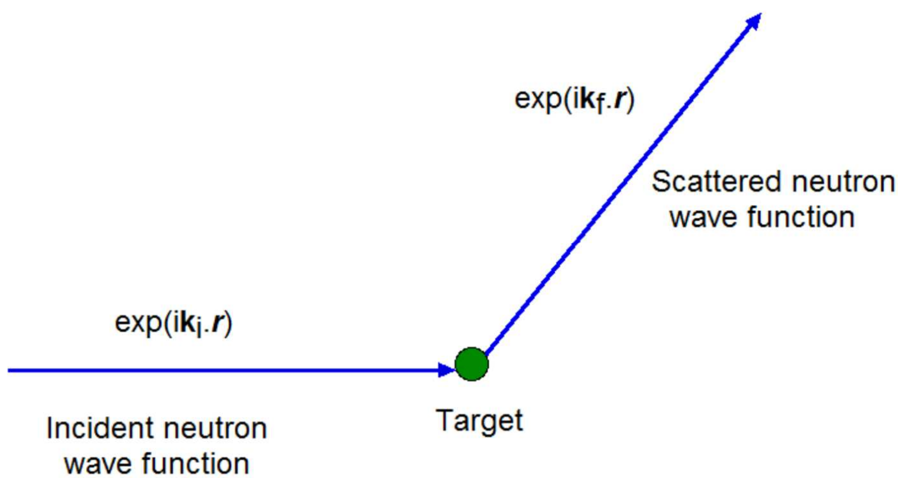


Fig. Schematic diagram for the neutron scattering, $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$. $\boldsymbol{k}_\mathrm{i} = \boldsymbol{k}$. $\boldsymbol{k}_\mathrm{f} = \boldsymbol{k}'$.

$\boldsymbol{Q}$ is the scattering wave vector.

$$\mathbf{Q} = \mathbf{k} - \mathbf{k}'$$

The matrix element is given by

$$\langle \mathbf{k}'|V|\mathbf{k}\rangle = \frac{2\pi\hbar^2}{m} b \int d\mathbf{r} e^{-i\mathbf{k}'\cdot\mathbf{r}} \delta(\mathbf{r} - \mathbf{R}) e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{2\pi\hbar^2}{m} b e^{i\mathbf{Q}\cdot\mathbf{R}}$$

where $\hbar\mathbf{Q}$ is the momentum transfer in the scattering event. We assume that the scattering is from an assembly of fixed nuclei at the position $\boldsymbol{R}_j$ that have scattering length b_j. We will further assume that this scattering length is independent of the neutron state $|\sigma\rangle$.

$$\langle\lambda'|\sum_j b_j e^{i\mathbf{Q}\cdot\mathbf{R}_j}|\lambda\rangle = \sum_j b_j \langle\lambda'|e^{i\mathbf{Q}\cdot\mathbf{R}_j}|\lambda\rangle = \sum_j b_j F_j$$

The differential cross-section for the elastic scattering from an assembly of fixed nuclei in the system $\frac{d\sigma}{d\Omega}$ can be given by

$$\frac{d\sigma}{d\Omega} = \left|\langle\lambda'|\sum_j b_j e^{i\mathbf{Q}\cdot\mathbf{R}_j}|\lambda\rangle\right|^2 = \sum_{j,l} b_j b_l F_j F_l^*$$

where we assume b to be real and

$$F_j = \langle\lambda'|e^{i\mathbf{Q}\cdot\mathbf{R}_j}|\lambda\rangle$$

It will normally be the case that the *isotopic distribution* is random, so that, if the nuclear spins have *random orientation*, then the value of the scattering length b_j at the j-th site will not be correlated with l.

$$\begin{aligned}\sum_{j,l} b_j b_l F_j F_l^* &= \sum_j b_j^2 F_j F_j^* + \sum_{j\neq l} b_j b_l F_j F_l^* \\ &= \sum_j \langle b^2\rangle F_j F_j^* + \sum_{j\neq l} \langle b\rangle^2 F_j F_l^*\end{aligned} \quad (1)$$

where < > indicates the mean value. If j and j' refer to different sites ($j \neq j'$) and there is no correlation between the values of b_j and $b_{j'}$ we can write

$$\langle b_j b_{j'}\rangle = \langle b_j\rangle\,\langle b_{j'}\rangle = \langle b\rangle^2$$

Note that

$$\langle b\rangle = \sum_j p_j b_j, \qquad \langle b^2\rangle = \sum_j p_j {b_j}^2$$

with

$$\sum_j p_j = 1,$$

where p_j denotes the probability that a nucleus has the scattering length b_j. Thus Eq.(1) can be rewritten as

$$\frac{d\sigma}{d\Omega} = \sum_{j,l} b_j b_l F_j F_l^* = \langle b\rangle^2 \sum_{j,l} F_j F_l^* + (\langle b^2\rangle - \langle b\rangle^2) \sum_j F_j F_j^*$$

The first term is a coherent term, while the second term is an incoherent term. The scattering can be divided into two parts; coherent scattering and incoherent scattering. If the cross sections for these parts are σ_c and σ_i, then for a single fixed atom,

$$\sigma_c = 4\pi\langle b\rangle^2,$$

$$\sigma_i = 4\pi(\langle b^2\rangle - \langle b\rangle^2)$$

and

$$\sigma_s = \sigma_c + \sigma_i$$

The coherent scattering is the scattering the same system (same nuclei with the same positions and motions) would give if all the scattering lengths were equal to <*b*>. The incoherence scattering is the term we must add to this to obtain the scattering due to the actual system. Physically the incoherent scattering arises from the random distribution of the deviations of the scattering lengths from their mean value.

((From G.L. Squires, Thermal Neutron Scattering, Cambridge University Press, 19768)

Table Values of σ_{coh} and σ_{inc}

Element or nuclide	Z	σ_{coh}	σ_{inc}
^1H	1	1.8	80.2

^{2}H	1	5.6	2.0
C	6	5.6	0.0
O	8	4.2	0.0
Mg	12	3.6	0.1
Al	13	1.5	0.0
V	23	0.02	5.0
Fe	26	11.5	0.4
Co	27	1.0	5.2
Ni	28	13.4	5.0
Cu	29	7.5	0.5
Zn	30	4.1	0.1

To simplify matters, we drop the operator formalism, since the atomic positions $\boldsymbol{R}_\mathrm{j}$ are fixed. Note that

$$F_j = e^{i\boldsymbol{Q}\cdot\boldsymbol{R}_\mathrm{j}}, \quad F_j^* = e^{-i\boldsymbol{Q}\cdot\boldsymbol{R}_j}$$

Thus we have

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{coh} + \left(\frac{d\sigma}{d\Omega}\right)_{inc}$$

with

$$\left(\frac{d\sigma}{d\Omega}\right)_{coh} = \langle b\rangle^2 \sum_{j,l} F_j F_l^* = \langle b\rangle^2 \sum_{j,l} e^{i\boldsymbol{Q}\cdot(\boldsymbol{R}_\mathrm{j}-\boldsymbol{R}_l)}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{inc} = (\langle b^2\rangle - \langle b\rangle^2) \sum_{j} F_j F_j^* = N(\langle b^2\rangle - \langle b\rangle^2)$$

The incoherent elastic scattering is isotropic and yields a constant background. On the other hand, the coherent elastic scattering provides the information about the mutual arrangement of the atoms due to the phase factor. The coherent elastic scattering is rewritten as

$$\left(\frac{d\sigma}{d\Omega}\right)_{coh} = N_0\langle b\rangle^2 \sum_{j} e^{i\boldsymbol{Q}\cdot\boldsymbol{R}_\mathrm{j}} = N_0\langle b\rangle^2 \frac{(2\pi)^3}{v_0} \sum_{G} \delta(\boldsymbol{Q}-\boldsymbol{G})$$

leading to the Bragg reflection. Note that N_0 is the number of unit cells and v_0 is the volume of unit cell.

9. Structure factor for simple liquid

We discuss the formulation of $S(\boldsymbol{Q})$ for liquid, using the number density $\rho_N(\boldsymbol{r})$

$$S(\boldsymbol{Q}) = \frac{1}{N}\langle\sum_{j,l} e^{i\boldsymbol{Q}\cdot(\boldsymbol{R}_{\mathrm{j}}-\boldsymbol{R}_l)}\rangle_{ensemble} = \frac{1}{N}\langle\left|\int d\boldsymbol{r}e^{i\boldsymbol{Q}\cdot\boldsymbol{r}}\rho_N(\boldsymbol{r})\right|^2\rangle$$

We use the relation

$$\sum_j e^{i\boldsymbol{Q}\cdot\boldsymbol{R}_{\mathrm{j}}} = \int d\boldsymbol{r}e^{i\boldsymbol{Q}\cdot\boldsymbol{r}}\sum_j \delta(\boldsymbol{r}-\boldsymbol{R}_{\mathrm{j}}) = \int d\boldsymbol{r}e^{i\boldsymbol{Q}\cdot\boldsymbol{r}}\rho_N(\boldsymbol{r})$$

where $\rho_N(\boldsymbol{r})$ is the nuclear number density

$$\rho_N(\boldsymbol{r}) = \sum_j \delta(\boldsymbol{r}-\boldsymbol{R}_{\mathrm{j}})$$

The structure factor for thye simple liquid is given by

$$S(\boldsymbol{Q}) = \frac{1}{N}\int d\boldsymbol{r}\int d\boldsymbol{r}' e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\langle\rho(\boldsymbol{r})\rho(\boldsymbol{r}')\rangle$$

This can be rewritten as

$$S(\boldsymbol{Q}) = \frac{1}{N}\int d\boldsymbol{r}\int d\boldsymbol{R}e^{i\boldsymbol{Q}\cdot\boldsymbol{R}}\langle\rho(\boldsymbol{r})\rho(\boldsymbol{r}-\boldsymbol{R})\rangle$$

10. Structure factor for solid

For systems with more than one atom per unit cell, we define the position vector of the atoms as

$$\boldsymbol{R_j} = \boldsymbol{R_{j0}} + \boldsymbol{r}_s$$

with $\boldsymbol{R}_{j0}$ and $\boldsymbol{r}_s$ being the position vectors of the *j*-th unit cell and of the *s*-th atom in the unit cell, respectively.

$$\left(\frac{d\sigma}{d\Omega}\right)_{coh} = N_0 \langle b \rangle^2 \sum_{j,j'} e^{i\boldsymbol{Q}\cdot(\boldsymbol{R}_{\mathrm{j}}-\boldsymbol{R}_{\mathrm{j'}})} \sum_{s,s'} b_s b_{s'} e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}_{\mathrm{s}}-\boldsymbol{r}_{\mathrm{s'}})}$$

Using the relation

$$\sum_{s,s'} b_s b_{s'} e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}_{\mathrm{s}}-\boldsymbol{r}_{\mathrm{s'}})} = |S(\boldsymbol{Q})|^2$$

where $S(\boldsymbol{Q})$ is the structure factor,

$$S(\boldsymbol{Q}) = \sum_{s} b_s e^{i\boldsymbol{Q}\cdot\boldsymbol{r}_{\mathrm{s}}}$$

The expression for the coherent elastic neutron cross section is

$$\left(\frac{d\sigma}{d\Omega}\right)_{coh} = N_0 \frac{(2\pi)^3}{v_0} |S(\boldsymbol{Q})|^2 \exp[-2W(\boldsymbol{Q})] \sum_{G} \delta(\boldsymbol{Q}-\boldsymbol{G})$$

Where $\exp[-2W(\boldsymbol{Q})]$ is the Debye-Waller factor that accounts for thermal motion of atoms,

$$2W(\boldsymbol{Q}) = \frac{1}{3} Q^2 \langle u^2 \rangle$$

and $\langle u^2 \rangle$ is the measured squared displacements of atoms.

11. Inelastic neutron scattering: van Hove expression for the nuclear scattering

In inelastic neutron scattering experiments the energy transfer $\hbar\omega$ may be positive and negative, corresponding to neutron energy-loss and energy-gain processes, respectively. The partial differential cross section is given by

$$\frac{d^2\sigma_s}{d\Omega d\varepsilon'} = \frac{k'}{k} N b^2 S(\mathbf{Q},\omega),$$

where

$$S(\mathbf{Q},\omega)=\frac{1}{N}\sum_{\lambda}P_{\lambda}\sum_{\lambda'}\left|\langle\lambda'|\sum_{j}e^{i\mathbf{Q}\cdot\mathbf{R}_j}|\lambda\rangle\right|^2\delta(E_{\lambda}-E_{\lambda'}+\hbar\omega)$$

and

$$\hbar\omega=\varepsilon-\varepsilon',$$

Using the relation for the Dirac delta function,

$$\delta(E_{\lambda}-E_{\lambda'}+\hbar\omega)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dte^{\frac{i}{\hbar}(-E_{\lambda}+E_{\lambda'}-\hbar\omega)t}$$

we get

$$\begin{aligned}S(\mathbf{Q},\omega)&=\frac{1}{2\pi\hbar N}\int_{-\infty}^{\infty}e^{\frac{i}{\hbar}(-E_{\lambda}+E_{\lambda'}-\hbar\omega)t}dt\sum_{\lambda}P_{\lambda}\sum_{\lambda'}\left|\langle\lambda'|\sum_{j}e^{i\mathbf{Q}\cdot\mathbf{R}_j}|\lambda\rangle\right|^2\\&=\frac{1}{2\pi\hbar N}\int_{-\infty}^{\infty}d\tau e^{\frac{i}{\hbar}(-E_{\lambda}+E_{\lambda'}-\hbar\omega)t}\sum_{\lambda}P_{\lambda}\sum_{\lambda'}\langle\lambda'|\sum_{l}e^{i\mathbf{Q}\cdot\mathbf{R}_l}|\lambda\rangle^*\langle\lambda'|\sum_{j}e^{i\mathbf{Q}\cdot\mathbf{R}_j}|\lambda\rangle\\&=\frac{1}{2\pi\hbar N}\sum_{\lambda}P_{\lambda}\sum_{\lambda'}\int_{-\infty}^{\infty}d\tau e^{-i\omega t}\sum_{j,l}\langle\lambda|e^{-i\mathbf{Q}\cdot\mathbf{R}_l}|\lambda'\rangle\langle\lambda'|e^{\frac{i}{\hbar}E_{\lambda'}t}e^{i\mathbf{Q}\cdot\mathbf{R}_j}e^{-\frac{i}{\hbar}E_{\lambda}t}|\lambda\rangle\end{aligned}$$

Here we note that

$$\langle\lambda'|e^{\frac{i}{\hbar}E_{\lambda'}t}e^{i\mathbf{Q}\cdot\mathbf{R}_j}e^{-\frac{i}{\hbar}E_{\lambda}t}|\lambda\rangle=\langle\lambda'|e^{\frac{i}{\hbar}Ht}e^{i\mathbf{Q}\cdot\mathbf{R}_j}e^{-\frac{i}{\hbar}Ht}|\lambda\rangle$$

We use the Heisenberg representation

$$\langle\lambda'|e^{\frac{i}{\hbar}Ht}e^{i\mathbf{Q}\cdot\mathbf{R}_j}e^{-\frac{i}{\hbar}Ht}|\lambda\rangle=\langle\lambda'|e^{i\mathbf{Q}\cdot\mathbf{R}_j(t)}|\lambda\rangle$$

Then we have

$$S(\mathbf{Q},\omega)=\frac{1}{2\pi\hbar N}\sum_{\lambda}P_{\lambda}\sum_{\lambda'}\int_{-\infty}^{\infty}d\tau e^{-i\omega t}\sum_{j,l}\langle\lambda|e^{-i\mathbf{Q}\cdot\mathbf{R}_l}|\lambda'\rangle\langle\lambda'|e^{i\mathbf{Q}\cdot\mathbf{R}_j(t)}|\lambda\rangle$$

Noting that

$$\sum_{\lambda'}|\lambda'\rangle\langle\lambda'|=1$$

and

$$\langle O\rangle=\sum_{\lambda}P_{\lambda}\langle\lambda|O|\lambda\rangle$$

(O is any operator).

The final expression can be derived by

$$S(\mathbf{Q},\omega)=\frac{1}{2\pi\hbar N}\int_{-\infty}^{\infty}dte^{-i\omega t}\sum_{j,l}\left\langle e^{-i\mathbf{Q}\cdot\hat{\mathbf{R}}_l}e^{i\mathbf{Q}\cdot\hat{\mathbf{R}}_j(t)}\right\rangle \qquad \text{(van Hove)}$$

This expresses the cross section as the temporal Fourier transform of a correlation function between the position vector of the l-th atoms at $t = 0$ and the j-th atom at time t.

$$\hat{\rho}(\mathbf{r},t)=\sum_j\delta(r-\hat{\mathbf{R}}_j(t)).$$

We introduce the Fourier tranform as

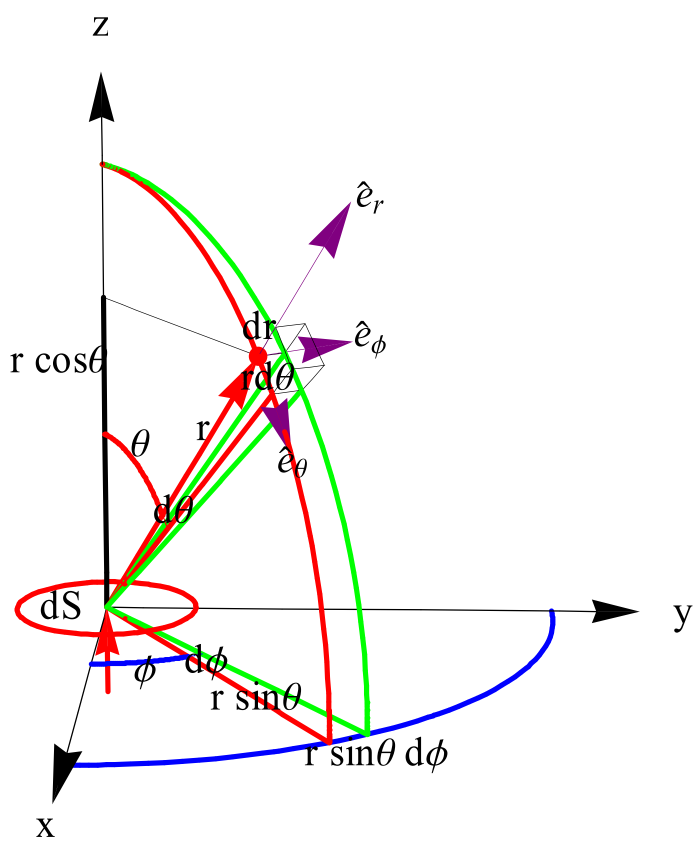
$$\begin{aligned}\hat{\rho}_{\mathbf{Q}}(t)&=\int d\mathbf{r}e^{-i\mathbf{Q}\cdot\mathbf{r}}\hat{\rho}(\mathbf{r},t)\\&=\int d\mathbf{r}e^{i\mathbf{Q}\cdot\mathbf{r}}\sum_j\delta(\mathbf{r}-\hat{\mathbf{R}}_j(t))\\&=\sum_j e^{-i\mathbf{Q}\cdot\hat{\mathbf{R}}_j(t)\cdot}\end{aligned}$$

Then we have

$$S(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar N}\int_{-\infty}^{\infty} dt e^{-i\omega t}\left\langle \hat{\rho}_{\mathbf{Q}}(0)\hat{\rho}_{-\mathbf{Q}}(t)\right\rangle$$

which shows that S($\boldsymbol{Q}$, ω) can be expressed in terms of a density-density correlation function.

$$\begin{aligned}\int_{-\infty}^{\infty} S(\mathbf{Q},\omega)d\omega &= \frac{1}{2\pi\hbar N}\int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} d\omega e^{-i\omega t}\left\langle \hat{\rho}_{\mathbf{Q}}(0)\hat{\rho}_{-\mathbf{Q}}(t)\right\rangle \\ &= \frac{1}{\hbar N}\int_{-\infty}^{\infty} dt\delta(t)\left\langle \hat{\rho}_{\mathbf{Q}}(0)\hat{\rho}_{-\mathbf{Q}}(t)\right\rangle \\ &= \frac{1}{\hbar N}\left\langle \hat{\rho}_{\mathbf{Q}}(0)\hat{\rho}_{-\mathbf{Q}}(0)\right\rangle\end{aligned}$$



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APPENDIX: Born approximation

1. Green's function in scattering theory

We start with the original Schrödinger equation.

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\boldsymbol{r}) + V(\boldsymbol{r})\psi(\boldsymbol{r}) = E_k\psi(\boldsymbol{r}),$$

or

$$(\nabla^2 + \frac{2\mu}{\hbar^2}E_k)\psi(\boldsymbol{r}) = \frac{2\mu}{\hbar^2}V(\boldsymbol{r})\psi(\boldsymbol{r}).$$

under the potential energy $V(\boldsymbol{r})$. We assume that

$$E = E_k = \frac{\hbar^2}{2\mu}k^2,$$

We put

$$f(\boldsymbol{r}) = -\frac{2\mu}{\hbar^2}V(\boldsymbol{r})\psi(\boldsymbol{r}),$$

Using the operator

$$L_{\mathbf{r}} = \nabla^2 + k^2.$$

we have the differential equation

$$L_{\boldsymbol{r}}\psi(\boldsymbol{r}) = (\nabla^2 + k^2)\psi(\boldsymbol{r}) = -f(\boldsymbol{r}).$$

Suppose that there exists a Green's function $G(\boldsymbol{r})$ such that

$$(\nabla_{\boldsymbol{r}}{}^2 + k^2)G^{(+)}(\boldsymbol{r},\boldsymbol{r}') = -\delta(\boldsymbol{r}-\boldsymbol{r}'),$$

with

$$G^{(+)}(\boldsymbol{r},\boldsymbol{r}') = \frac{\exp(ik|\boldsymbol{r}-\boldsymbol{r}'|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} \qquad \text{(Green function)}$$

We will discuss about the derivation of this Green function later. Then $\psi(\mathbf{r})$ is formally given by

$$\psi^{(+)}(\boldsymbol{r}) = \phi(\boldsymbol{r}) + \int d\boldsymbol{r}' G^{(+)}(\boldsymbol{r},\boldsymbol{r}') f(\boldsymbol{r}') = \phi(\boldsymbol{r}) - \frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' \frac{\exp(ik|\boldsymbol{r}-\boldsymbol{r}'|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} V(\boldsymbol{r}')\psi^{(+)}(\boldsymbol{r}')$$

,

where $\phi(\mathbf{r})$ is a solution of the homogeneous equation satisfying

$$(\nabla^2 + k^2)\phi(\boldsymbol{r}) = 0,$$

or

$$\phi(\boldsymbol{r}) = \langle r|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}), \qquad \text{(plane wave, } \boldsymbol{k} \text{ is continuous)}$$

with

$$k = |\boldsymbol{k}|$$

Note that

$$\begin{aligned}(\nabla^2 + k^2)\psi(\boldsymbol{r}) &= (\nabla^2 + k^2)\phi(\boldsymbol{r}) + \int d\boldsymbol{r}'(\nabla^2 + k^2)G^{(+)}(\boldsymbol{r},\boldsymbol{r}')f(\boldsymbol{r}') \\ &= -\int d\boldsymbol{r}'\delta(\boldsymbol{r}-\boldsymbol{r}')f(\boldsymbol{r}') \\ &= -f(\boldsymbol{r})\end{aligned}$$

2. Born approximation

We start with

$$\psi^{(+)}(\boldsymbol{r}) = \phi(\boldsymbol{r}) - \frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' \frac{\exp(ik|\boldsymbol{r}-\boldsymbol{r}'|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} V(\boldsymbol{r}')\psi^{(+)}(\boldsymbol{r}'),$$

$$\phi(\boldsymbol{r}) = \langle r|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}), \qquad \text{(plane wave).}$$

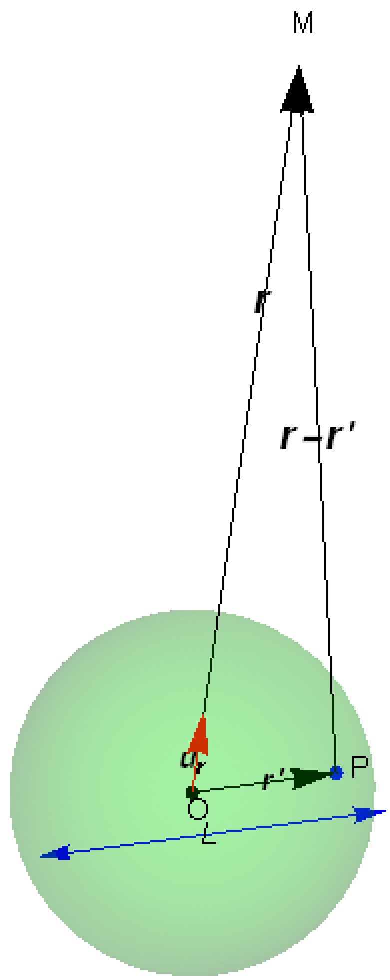


Fig. Vectors ***r*** and ***r***' in calculation of scattering amplitude in the first Born approximation

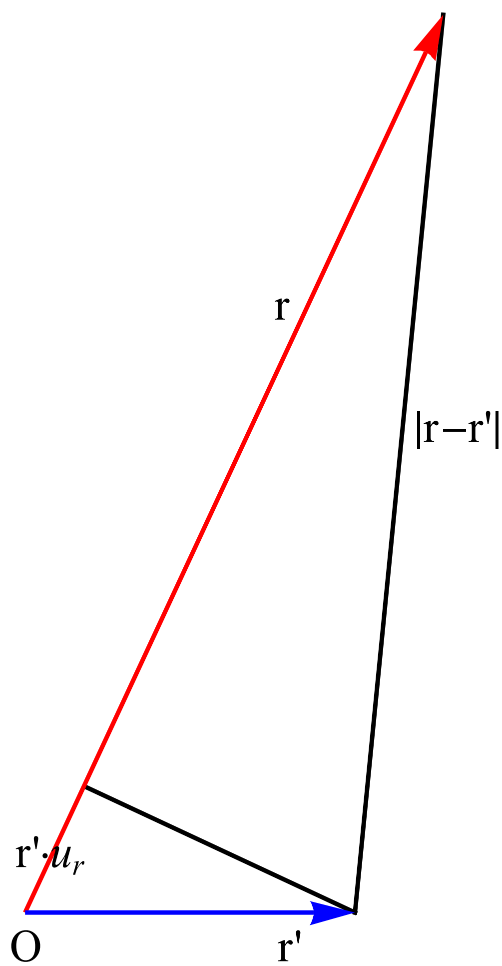


Fig. $\boldsymbol{u}_r = \boldsymbol{e}_r$

Here we consider the case of $\psi^{(+)}(r)$

$$|\boldsymbol{r} - \boldsymbol{r}'| \approx r - \boldsymbol{r}'\cdot\boldsymbol{e}_r$$

$$\boldsymbol{k}' = k\boldsymbol{e}_r$$

$$e^{ik|\boldsymbol{r}-\boldsymbol{r}'|} \approx e^{ik(r-\boldsymbol{r}'\cdot\boldsymbol{e}_r)} = e^{ikr}e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}$$ for large r.

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} \approx \frac{1}{r}$$

Then we have

$$\psi^{(+)}(r) = \frac{1}{(2\pi)^{3/2}}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) - \frac{2\mu}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\psi^{(+)}(\boldsymbol{r}')$$

or

$$\psi^{(+)}(r) = \frac{1}{(2\pi)^{3/2}}[e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{ikr}}{r}f(\boldsymbol{k}',\boldsymbol{k})]$$

The first term denotes the original plane wave in the propagation direction $\boldsymbol{k}$. The second term denotes the outgoing spherical wave with amplitude, $f(\boldsymbol{k}',\boldsymbol{k})$,

$$f(\boldsymbol{k}',\boldsymbol{k}) = -\frac{1}{4\pi}(2\pi)^{3/2}\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\psi^{(+)}(\boldsymbol{r}') .$$

The first Born approximation:

$$\begin{aligned} f(\boldsymbol{k}',\boldsymbol{k}) &= -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')e^{i\boldsymbol{k}\cdot\boldsymbol{r}'} \\ &= -\frac{\mu}{2\pi\hbar^2}\int d\boldsymbol{r}' V(\boldsymbol{r}')e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}'} \end{aligned}$$

when $\psi^{(+)}(r)$ is approximated by

$$\psi^{(+)}(r) \approx \frac{1}{(2\pi)^{3/2}}e^{i\mathbf{k}\cdot\mathbf{r}} .$$

Note that $f(\boldsymbol{k}',\boldsymbol{k})$ is the Fourier transform of the potential energy with the wave vector $\boldsymbol{Q}$; the scattering vector;

$$\boldsymbol{Q} = \boldsymbol{k}' - \boldsymbol{k} .$$

Formally $f(\boldsymbol{k}',\boldsymbol{k})$ can be rewritten as

$$\begin{aligned} f(\boldsymbol{k}',\boldsymbol{k}) &= -\frac{\mu}{2\pi\hbar^2}(2\pi)^3\langle\boldsymbol{k}'|\hat{V}|\boldsymbol{k}\rangle \\ &= -\frac{4\pi^2\mu}{\hbar^2}\langle\boldsymbol{k}'|\hat{V}|\boldsymbol{k}\rangle \end{aligned}$$

where

$$\langle \boldsymbol{k}'|\hat{V}|\boldsymbol{k}\rangle = \int d^3\boldsymbol{r}\langle \boldsymbol{k}'|\boldsymbol{r}\rangle V(\boldsymbol{r})\langle \boldsymbol{r}|\boldsymbol{k}\rangle$$
$$= \frac{1}{(2\pi)^3}\int d^3\boldsymbol{r} e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} V(\boldsymbol{r})$$

with

$$\langle \boldsymbol{r}|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})$$

((**Forward scattering**))

Suppose that $\boldsymbol{k}' = \boldsymbol{k}$ ($\boldsymbol{Q} = 0$). Then we have

$$f(0) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}\cdot\boldsymbol{r}'} V(\boldsymbol{r}') e^{i\boldsymbol{k}\cdot\boldsymbol{r}'}$$
$$= -\frac{\mu}{2\pi\hbar^2}\int d\boldsymbol{r}' V(\boldsymbol{r}')$$

Suppose that the attractive potential is a type of square-well

$$V(r) = \begin{cases} -V_0 & r < R \\ 0 & r > R \end{cases}$$

Then we have

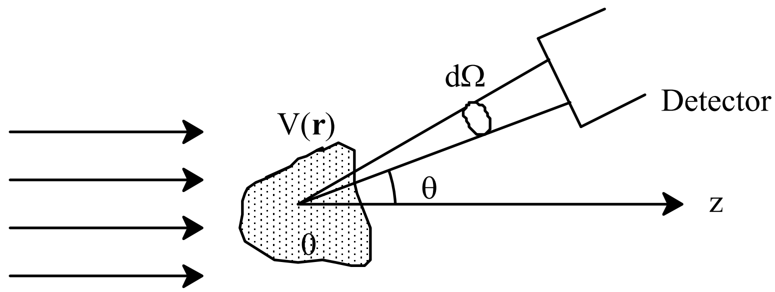
$$f(0) = \frac{2}{3}\frac{\mu V_0}{\hbar^2}R^3 \approx \frac{\mu V_0}{\hbar^2}R^3$$

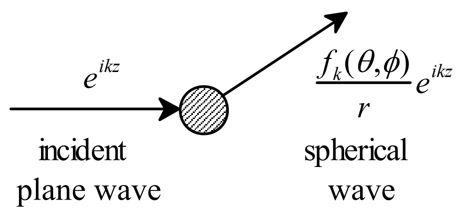
The total cross section (which is isotropic) is obtained as

$$\sigma = 4\pi|f(0)|^2 = 4\pi\left(\frac{\mu V_0}{\hbar^2}R^3\right)^2.$$

The units of $f(0)$ is cm, and the units of σ is cm^2.

3. Differential cross section





We define the differential cross section $\frac{d\sigma}{d\Omega}$ as the number of particles per unit time scattered into an element of solid angle $d\Omega$ divided by the incident flux of particles.

The probability flux associated with a wave function

$$\phi_k(\boldsymbol{r}) = \langle \boldsymbol{r}|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \frac{1}{(2\pi)^{3/2}}e^{ikz},$$

is obtained as

$$N_z = J_z = \frac{\hbar}{2\mu i}[\phi_k^*(\boldsymbol{r})\frac{\partial}{\partial z}\phi_k(\boldsymbol{r}) - \phi_k(\boldsymbol{r})\frac{\partial}{\partial z}\phi_k^*(\boldsymbol{r})] = \frac{1}{(2\pi)^3}\frac{\hbar k}{\mu} = \frac{v}{(2\pi)^3}$$

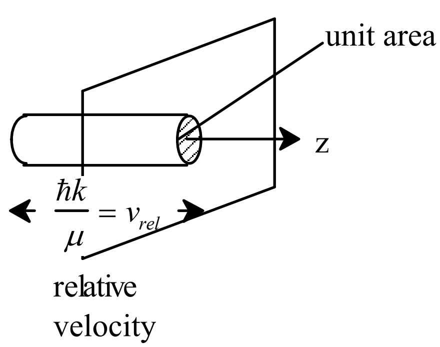


Fig.

$$\text{volume} = \frac{\hbar k}{\mu} \times 1$$

$\left| e^{ikz} \right|^2 = 1$ means that there is one particle per unit volume. J_z is the probability flow (probability per unit area per unit time) of the incident beam crossing a unit surface perpendicular to OZ

The probability flux associated with the scattered wave function

$$\chi_r = \frac{1}{(2\pi)^{3/2}} \frac{e^{ikr}}{r} f(\theta) \qquad \text{(spherical wave)}$$

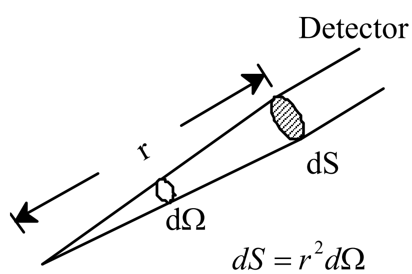
is

$$J_r = \frac{\hbar}{2\mu i}(\chi_r^* \frac{\partial}{\partial r}\chi_r - \chi_r \frac{\partial}{\partial r}\chi_r^*) = \frac{1}{(2\pi)^3} \frac{\hbar k}{\mu} \frac{\left| f(\theta) \right|^2}{r^2}$$

$$dA = r^2 d\Omega$$

$$\Delta N = J_r dA = \frac{v}{(2\pi)^3} \frac{\left| f(\theta) \right|^2}{r^2} r^2 d\Omega = \frac{v}{(2\pi)^3} \left| f(\theta) \right|^2 d\Omega$$

where J_r is the probability flow (probability per unit area per unit time)



The differential cross section

$$\frac{d\sigma}{d\Omega} d\Omega = \frac{\Delta N}{N_z} = \left| f(\theta) \right|^2 d\Omega$$

or

$$\frac{\partial\sigma}{\partial\Omega} = \left|f(\theta)\right|^2.$$

First-order Born amplitude:

$$\begin{aligned} f(\boldsymbol{k}',\boldsymbol{k}) &= -\frac{1}{4\pi}(2\pi)^3\frac{2\mu}{\hbar^2}\langle\boldsymbol{k}'|V|\boldsymbol{k}\rangle \\ &= -\frac{\mu}{2\pi\hbar^2}\int d^3\boldsymbol{r}' e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}V(\boldsymbol{r}'), \\ &= -\frac{\mu}{2\pi\hbar^2}\int d^3\boldsymbol{r}' e^{-i\boldsymbol{Q}\cdot\boldsymbol{r}}V(\boldsymbol{r}') \end{aligned}$$

which is the Fourier transform of the potential with respect to $\boldsymbol{Q}$, where

$\boldsymbol{Q} = \boldsymbol{k}'-\boldsymbol{k}$: scattering wave vector.

$|\boldsymbol{Q}| = Q = 2k\sin\frac{\theta}{2}$ for the elastic scattering.

The Ewald sphere is given by this figure. Note that the scattering angle is θ here. In the case of x-ray and neutron diffraction, we use the scattering angle 2θ, instead of θ.

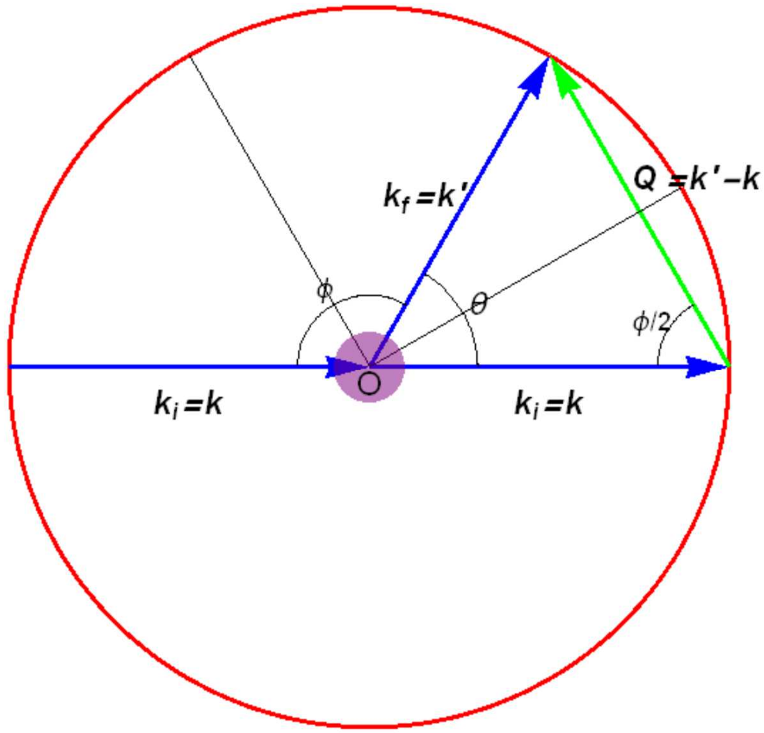


Fig. Ewald sphere for the present system (elastic scattering). $\boldsymbol{k}_{\rm i} = \boldsymbol{k}$. $\boldsymbol{k}_{\rm f} = \boldsymbol{k}'$. $\boldsymbol{Q} = \boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}'$ (scattering wave vector). $|\boldsymbol{Q}| = 2k\sin\dfrac{\theta}{2}$.

((**Ewald sphere**)) **x-ray and neutron scattering**

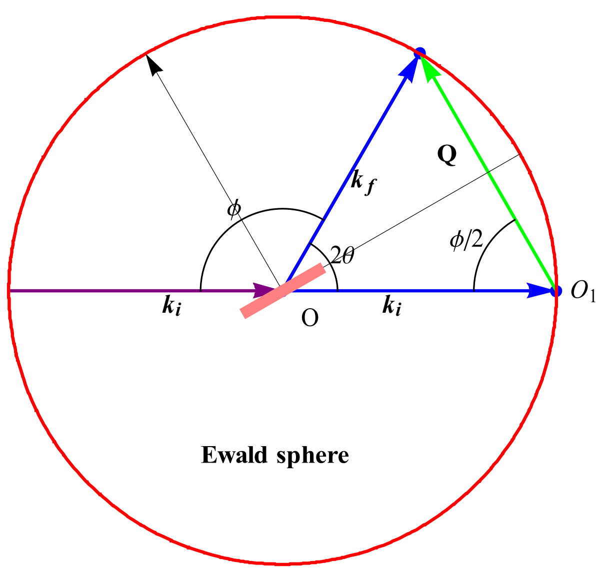


Fig. Ewald sphere used for the x-ray and neutron scattering experiments. $\boldsymbol{k}_i = \boldsymbol{k}$. $\boldsymbol{k}_f = \boldsymbol{k}'$. $\boldsymbol{Q} = \boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}'$ (scattering wave vector). Note that in the conventional x-ray and neutron scattering experiments, we use the angle 2θ, instead of θ for both the x-ray and neutron scattering,

4. Spherical symmetric potential

When the potential energy $V(\boldsymbol{r})$ is dependent only on r, it has a spherical symmetry. For simplicity we assume that θ' is an angle between $\boldsymbol{Q}$ and $\boldsymbol{r}'$.

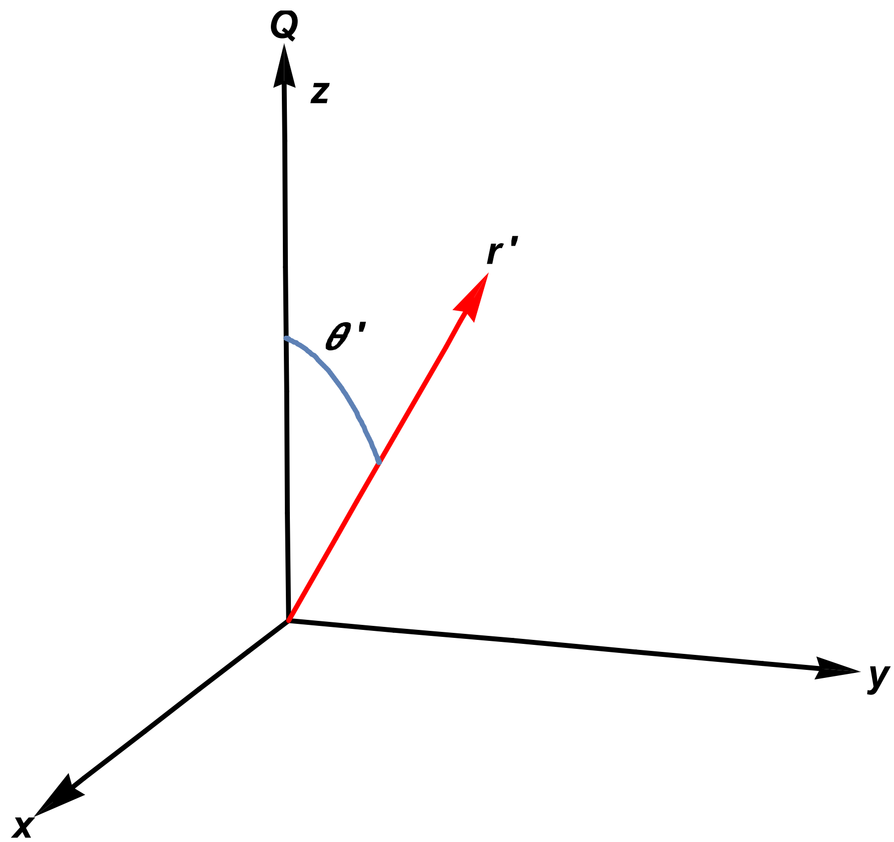
$$\boldsymbol{Q}\cdot\boldsymbol{r}' = Qr'\cos\theta' .$$

We can perform the angular integration over θ'.

$$\begin{aligned}
f^{(1)}(\theta) &= -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' e^{-i\boldsymbol{Q}\cdot\boldsymbol{r}} V(\boldsymbol{r}') \\
&= -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int_0^\infty dr' \int_0^\pi d\theta' e^{-iQr'\cos\theta'} 2\pi r'^2 \sin\theta' V(r') \\
&= -\frac{\mu}{\hbar^2}\int_0^\infty dr' \int_0^\pi d\theta' e^{-iQr'\cos\theta'} r'^2 \sin\theta' V(r')
\end{aligned}$$

Note that

$$\int_0^\pi d\theta' e^{-iQr'\cos\theta'} \sin\theta' = \frac{2}{Qr'}\sin(Qr')$$



Then

$$f^{(1)}(\theta) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int_0^\infty dr' 2\pi r'^2 V(r')\frac{2}{Qr'}\sin(Qr')$$
$$= -\frac{1}{Q}\frac{2\mu}{\hbar^2}\int_0^\infty dr' r' V(r')\sin(Qr')$$

(spherical symmetry)

Then the differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \left|f^{(1)}(\theta)\right|^2 = \frac{1}{Q^2}\left(\frac{2\mu}{\hbar^2}\right)^2\left|\int_0^\infty dr' r' V(r')\sin(Qr')\right|^2$$

We find that $f^{(1)}(\theta)$ is a function of Q.

$$Q = 2k\sin(\frac{\theta}{2}),$$

where θ is an angle between ***k***' and ***k*** (Ewald's sphere).

5 Lippmann-Schwinger equation

The Lippmann–Schwinger equation is equivalent to the Schrödinger equation plus the typical boundary conditions for scattering problems. In order to embed the boundary conditions, the Lippmann–Schwinger equation must be written as an integral equation. For scattering problems, the Lippmann–Schwinger equation is often more convenient than the original Schrödinger equation (http://en.wikipedia.org/wiki/Lippmann%E2%80%93Schwinger_equation)

The Hamiltonian H of the system is given by

$$\hat{H} = \hat{H}_0 + \hat{V},$$

where H_0 is the Hamiltonian of free particle. Let $|\phi\rangle$ be the eigenket of H_0 with the energy eigenvalue E,

$$\hat{H}_0|\phi\rangle = E|\phi\rangle.$$

The basic Schrödinger equation is

$$(\hat{H}_0 + \hat{V})|\psi\rangle = E|\psi\rangle. \qquad (1)$$

Both $\hat{H}_0$ and $\hat{H}_0 + \hat{V}$ exhibit continuous energy spectra. We look for a solution to Eq.(1) such that as $V \to 0$, $|\psi\rangle \to |\phi\rangle$, where $|\phi\rangle$ is the solution to the free particle Schrödinger equation with the same energy eigenvalue E.

$$\hat{V}|\psi\rangle = (E - \hat{H}_0)|\psi\rangle.$$

Since $\hat{H}_0|\phi\rangle = E|\phi\rangle$ or $(E - \hat{H}_0)|\phi\rangle$ = 0, this can be rewritten as

$$\hat{V}|\psi\rangle = (E - \hat{H}_0)|\psi\rangle - (E - \hat{H}_0)|\phi\rangle,$$

which leads to

$$(E-\hat{H}_0)(|\psi\rangle - |\phi\rangle) = \hat{V}|\psi\rangle,$$

or

$$|\psi\rangle = |\phi\rangle + (E-\hat{H}_0)^{-1}\hat{V}|\psi\rangle.$$

The presence of $|\phi\rangle$ is reasonable because $|\psi\rangle$ must reduce to $|\phi\rangle$ as $\hat{V}$ vanishes.

<u>Lippmann-Schwinger equation:</u>

$$|\psi^{(\pm)}\rangle = |\boldsymbol{k}\rangle + (E_k - \hat{H}_0 \pm i\varepsilon)^{-1}\hat{V}|\psi^{(\pm)}\rangle$$

by making E_k (= $\hbar^2\boldsymbol{k}^2/2\mu$) slightly complex number (ε>0, $\varepsilon \approx 0$). This can be rewritten as

$$\langle \boldsymbol{r}|\psi^{(\pm)}\rangle = \langle \boldsymbol{r}|\boldsymbol{k}\rangle + \int d\boldsymbol{r}'\langle \boldsymbol{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}|\boldsymbol{r}'\rangle\langle \boldsymbol{r}'|\hat{V}|\psi^{(\pm)}\rangle$$

where

$$\langle \boldsymbol{r}|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}},$$

and

$$\hat{H}_0|\boldsymbol{k}'\rangle = E_{k'}|\boldsymbol{k}'\rangle,$$

with

$$E_{k'} = \frac{\hbar^2}{2\mu}k'^2.$$

$$-\frac{2\mu}{\hbar^2}G_0^{(\pm)}(\boldsymbol{r},\boldsymbol{r}') = \langle \boldsymbol{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}|\boldsymbol{r}'\rangle$$

Note that

$$\langle \boldsymbol{r}|\psi^{(+)}\rangle = \langle \boldsymbol{r}|\boldsymbol{k}\rangle + \int dr' \langle \boldsymbol{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}|\boldsymbol{r}'\rangle V(\boldsymbol{r}')\langle \boldsymbol{r}'|\psi^{(+)}\rangle$$
$$= \langle \boldsymbol{r}|\boldsymbol{k}\rangle - \frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' G_0^{(\pm)}(\boldsymbol{r},\boldsymbol{r}')V(\boldsymbol{r}')\langle \boldsymbol{r}'|\psi^{(+)}\rangle$$
$$= \langle \boldsymbol{r}|\boldsymbol{k}\rangle - \frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}V(\boldsymbol{r}')\langle \boldsymbol{r}'|\psi^{(+)}\rangle$$

The Green's function is defined by

$$G_0^{(\pm)}(\boldsymbol{r},\boldsymbol{r}') = -\frac{\hbar^2}{2\mu}\langle \boldsymbol{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}|\boldsymbol{r}'\rangle = \frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}e^{\pm ik|\boldsymbol{r}-\boldsymbol{r}'|}$$

((**Proof**))

$$I = -\frac{\hbar^2}{2\mu}\langle \boldsymbol{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}|\boldsymbol{r}'\rangle$$
$$= -\frac{\hbar^2}{2\mu}\int\int d\boldsymbol{k}' d\boldsymbol{k}''\langle \boldsymbol{r}|\boldsymbol{k}'\rangle(E_k - \frac{\hbar^2}{2\mu}\boldsymbol{k}'^2 \pm i\varepsilon)^{-1}\langle \boldsymbol{k}'|\boldsymbol{k}''\rangle\langle \boldsymbol{k}''|\boldsymbol{r}'\rangle$$

or

$$I = -\frac{\hbar^2}{2\mu}\int\int d\boldsymbol{k}' d\boldsymbol{k}''\langle \boldsymbol{r}|\boldsymbol{k}'\rangle(E_k - \frac{\hbar^2}{2\mu}\boldsymbol{k}'^2 \pm i\varepsilon)^{-1}\delta(\boldsymbol{k}'-\boldsymbol{k}'')\langle \boldsymbol{k}''|\boldsymbol{r}'\rangle$$
$$= -\frac{\hbar^2}{2\mu}\int d\boldsymbol{k}'\langle \boldsymbol{r}|\boldsymbol{k}'\rangle(E_k - \frac{\hbar^2}{2\mu}\boldsymbol{k}'^2 \pm i\varepsilon)^{-1}\langle \boldsymbol{k}'|\boldsymbol{r}'\rangle$$
$$= -\frac{\hbar^2}{2\mu}\int \frac{d\boldsymbol{k}'}{(2\pi)^3}\frac{e^{i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{E_k - \frac{\hbar^2}{2\mu}\boldsymbol{k}'^2 \pm i\varepsilon}$$

where

$$E_k = \frac{\hbar^2}{2\mu}\boldsymbol{k}^2.$$

Then we have

$$I = -\frac{\hbar^2}{2\mu}\int \frac{d\boldsymbol{k}'}{(2\pi)^3}\frac{e^{i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{\frac{\hbar^2}{2\mu}(\boldsymbol{k}^2-\boldsymbol{k}'^2)\pm i\varepsilon}$$
$$= \int \frac{d\boldsymbol{k}'}{(2\pi)^3}\frac{e^{i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{k'^2-(k^2\pm i\varepsilon)}$$

So we have

$$G_0^{(\pm)}(\boldsymbol{r}-\boldsymbol{r}') = \frac{1}{(2\pi)^3}\int d\boldsymbol{k}'\frac{e^{i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{k'^2-(k^2\pm i\varepsilon)} = \frac{e^{\pm ik|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}$$

where $\varepsilon>0$ is infinitesimally small value (see the **Appendix III** for the derivation)

In summary, we get

$$\langle \boldsymbol{r}|\psi^{(\pm)}\rangle = \langle \boldsymbol{r}|\boldsymbol{k}\rangle + \int dr'\langle \boldsymbol{r}|(E_k-\hat{H}_0\pm i\varepsilon)^{-1}|\boldsymbol{r}'\rangle\langle \boldsymbol{r}'|\hat{V}|\psi^{(\pm)}\rangle$$

$$\langle \boldsymbol{r}|\psi^{(\pm)}\rangle = \langle \boldsymbol{r}|\boldsymbol{k}\rangle - \frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' G_0^{(\pm)}(\boldsymbol{r},\boldsymbol{r}')\langle \boldsymbol{r}'|\hat{V}|\psi^{(\pm)}\rangle$$

or

$$\langle \boldsymbol{r}|\psi^{(\pm)}\rangle = \langle \boldsymbol{r}|\boldsymbol{k}\rangle - \frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' G_0^{(\pm)}(\boldsymbol{r},\boldsymbol{r}')V(\boldsymbol{r}')\langle \boldsymbol{r}'|\psi^{(\pm)}\rangle .$$

More conveniently the Lippmann-Schwinger equation can be rewritten as

$$|\psi^{(\pm)}\rangle = |\boldsymbol{k}\rangle + (E_k-\hat{H}_0\pm i\varepsilon)^{-1}\hat{V}|\psi^{(\pm)}\rangle$$

with

$$\hat{G}_0^{(\pm)} = -\frac{\hbar^2}{2\mu}(E_k-\hat{H}_0\pm i\varepsilon)^{-1},$$

and

$$-\frac{2\mu}{\hbar^2}\hat{G}_0^{(\pm)}\hat{V} = (E_k-\hat{H}_0\pm i\varepsilon)^{-1}\hat{V}$$

When two operators $\hat{A}$ and $\hat{B}$ are not commutable, we have very useful formula as follows,

$$\frac{1}{\hat{A}} - \frac{1}{\hat{B}} = \frac{1}{\hat{A}}(\hat{B} - \hat{A})\frac{1}{\hat{B}} = \frac{1}{\hat{B}}(\hat{B} - \hat{A})\frac{1}{\hat{A}},$$

We assume that

$$\hat{A} = (E_k - \hat{H}_0 \pm i\varepsilon), \quad \hat{B} = (E_k - \hat{H} \pm i\varepsilon)$$

$$\hat{B} - \hat{A} = -\hat{H} + \hat{H}_0 = -\hat{V}$$

Then

$$(E_k - \hat{H}_0 \pm i\varepsilon)^{-1} = (E_k - \hat{H} \pm i\varepsilon)^{-1} - (E_k - \hat{H} \pm i\varepsilon)^{-1}\hat{V}(E_k - \hat{H}_0 \pm i\varepsilon)^{-1},$$

or

$$(E_k - \hat{H} \pm i\varepsilon)^{-1} = (E_k - \hat{H}_0 \pm i\varepsilon)^{-1} + (E_k - \hat{H}_0 \pm i\varepsilon)^{-1}\hat{V}(E_k - \hat{H} \pm i\varepsilon)^{-1}.$$

Here we newly define the two operators by

$$(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}, \qquad (E_k - \hat{H} \pm i\varepsilon)^{-1}$$

Note that $(E_k - \hat{H}_0 + i\varepsilon)^{-1}$ denotes an outgoing spherical wave and $(E_k - \hat{H}_0 - i\varepsilon)^{-1}$ denotes an incoming spherical wave. Then we have

$$\begin{aligned}(E_k - \hat{H}_0 \pm i\varepsilon)^{-1} &= (E_k - \hat{H} \pm i\varepsilon)^{-1} - (E_k - \hat{H} \pm i\varepsilon)^{-1}\hat{V}(E_k - \hat{H}_0 \pm i\varepsilon)^{-1} \\ &= (E_k - \hat{H} \pm i\varepsilon)^{-1}[\hat{1} - \hat{V}(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}]\end{aligned}$$

$$\begin{aligned}(E_k - \hat{H} \pm i\varepsilon)^{-1} &= (E_k - \hat{H}_0 \pm i\varepsilon)^{-1} + (E_k - \hat{H}_0 \pm i\varepsilon)^{-1}\hat{V}(E_k - \hat{H} \pm i\varepsilon)^{-1} \\ &= (E_k - \hat{H}_0 \pm i\varepsilon)^{-1}[\hat{1} + \hat{V}(E_k - \hat{H} \pm i\varepsilon)^{-1}]\end{aligned}$$

Then $\left|\psi^{(\pm)}\right\rangle$ can be rewritten as

$$
\begin{aligned}
\left|\psi^{(\pm)}\right\rangle &= \left|\boldsymbol{k}\right\rangle + (E_k - \hat{H}_0 \pm i\varepsilon)^{-1}\hat{V}\left|\psi^{(\pm)}\right\rangle \\
&= \left|\boldsymbol{k}\right\rangle + (E_k - \hat{H} \pm i\varepsilon)^{-1}[\hat{1} - \hat{V}(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}]\hat{V}\left|\psi^{(\pm)}\right\rangle \\
&= \left|\boldsymbol{k}\right\rangle + (E_k - \hat{H} \pm i\varepsilon)^{-1}\hat{V}(\left|\psi^{(\pm)}\right\rangle - (E_k - \hat{H}_0 \pm i\varepsilon)^{-1}]\hat{V}\left|\psi^{(\pm)}\right\rangle \\
&= \left|\boldsymbol{k}\right\rangle + (E_k - \hat{H} \pm i\varepsilon)^{-1}\hat{V}\left|\boldsymbol{k}\right\rangle \\
&= [\hat{1} + (E_k - \hat{H} \pm i\varepsilon)^{-1}\hat{V}]\left|\boldsymbol{k}\right\rangle
\end{aligned}
$$

or

$$
\left|\psi^{(\pm)}\right\rangle = \left|\boldsymbol{k}\right\rangle + \frac{1}{E_k - \hat{H} \pm i\varepsilon}\hat{V}\left|\boldsymbol{k}\right\rangle.
$$

7 The higher order Born Approximation

From the iteration, $\left|\psi^{(+)}\right\rangle$ can be expressed as

$$
\begin{aligned}
\left|\psi^{(+)}\right\rangle &= \left|\boldsymbol{k}\right\rangle + (E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V}\left|\psi^{(+)}\right\rangle \\
&= \left|\boldsymbol{k}\right\rangle + (E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V}(\left|\boldsymbol{k}\right\rangle + (E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V}\left|\psi^{(+)}\right\rangle) \\
&= \left|\boldsymbol{k}\right\rangle + (E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V}\left|\boldsymbol{k}\right\rangle + (E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V}(E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V}\left|\boldsymbol{k}\right\rangle + \ldots
\end{aligned}
$$

The Lippmann-Schwinger equation is given by

$$
\left|\psi^{(+)}\right\rangle = \left|\boldsymbol{k}\right\rangle + (E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V}\left|\psi^{(+)}\right\rangle = \left|\boldsymbol{k}\right\rangle + (E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{T}\left|\boldsymbol{k}\right\rangle,
$$

where the transition operator $\hat{T}$ is defined as

$$
\hat{V}\left|\psi^{(+)}\right\rangle = \hat{T}\left|\boldsymbol{k}\right\rangle
$$

or

$$
\hat{T}\left|\boldsymbol{k}\right\rangle = \hat{V}\left|\psi^{(+)}\right\rangle = \hat{V}\left|\boldsymbol{k}\right\rangle + \hat{V}(E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{T}\left|\boldsymbol{k}\right\rangle
$$

This is supposed to hold for any $\left|\boldsymbol{k}\right\rangle$ taken to be any plane-wave state.

$$
\hat{T} = \hat{V} + \hat{V}(E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{T}.
$$

The scattering amplitude $f(\boldsymbol{k}',\boldsymbol{k})$ can now be written as

$$f(\boldsymbol{k}',\boldsymbol{k}) = -\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\left\langle \boldsymbol{k}'\middle|\hat{V}\middle|\psi^{(+)}\right\rangle = -\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\left\langle \boldsymbol{k}'\middle|\hat{T}\middle|\boldsymbol{k}\right\rangle.$$

Using the iteration, we have

$$\begin{aligned}\hat{T} &= \hat{V} + \hat{V}(E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{T} \\ &= \hat{V} + \hat{V}(E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V} + \hat{V}(E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V}(E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V} + \ldots\end{aligned}$$

Correspondingly we can expand $f(\boldsymbol{k}',\boldsymbol{k})$ as follows:

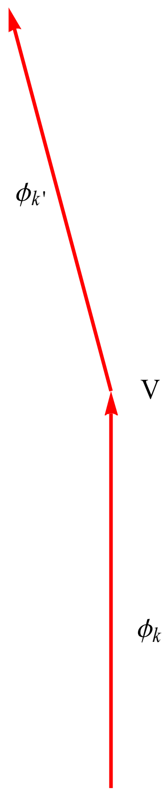
$$f(\mathbf{k}',\mathbf{k}) = f^{(1)}(\mathbf{k}',\mathbf{k}) + f^{(2)}(\mathbf{k}',\mathbf{k}) + f^{(3)}(\mathbf{k}',\mathbf{k}) + ...$$

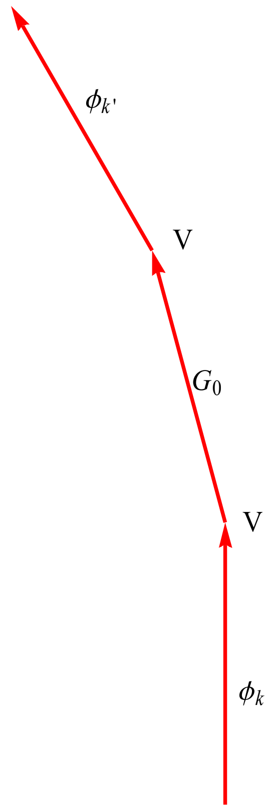
with

$$f^{(1)}(\boldsymbol{k}',\boldsymbol{k}) = -\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\left\langle \boldsymbol{k}'\middle|\hat{V}\middle|\boldsymbol{k}\right\rangle,$$

$$f^{(2)}(\boldsymbol{k}',\boldsymbol{k}) = -\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\left\langle \boldsymbol{k}'\middle|\hat{V}(E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V}\middle|\boldsymbol{k}\right\rangle,$$

$$f^{(3)}(\boldsymbol{k}',\boldsymbol{k}) = -\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\left\langle \boldsymbol{k}'\middle|\hat{V}(E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V}(E_k - \hat{H}_0 + i\varepsilon)^{-1}\hat{V}\middle|\boldsymbol{k}\right\rangle.$$


$\phi_{k'}$
V
ϕ_k


$\phi_{k'}$
V
G_0
V
ϕ_k

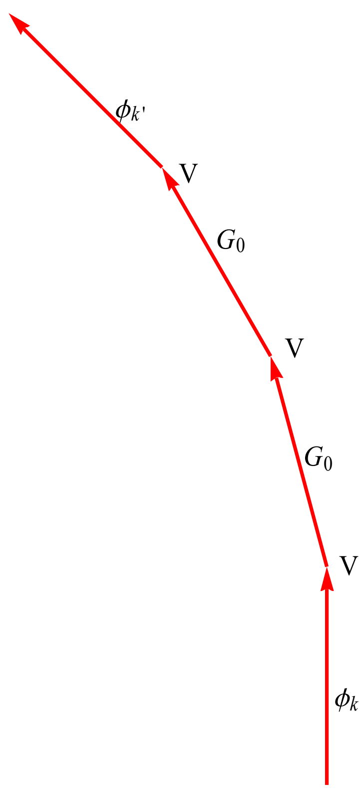

$\phi_{k'}$
V
G_0
V
G_0
V
ϕ_k

Fig. Feynman diagram. First order, 2nd order, and 3rd order Born approximations. $\phi_k = |\boldsymbol{k}\rangle$ is the initial state of the incoming particle and $\phi_{k'} = |\boldsymbol{k}'\rangle$ is the final state of the incoming particle. $\hat{V}$ is the interaction.

8 Optical Theorem

The scattering amplitude and the total cross section are related by the identity

$$\mathrm{Im}[f(\theta = 0)] = \frac{k}{4\pi}\sigma_{tot},$$

where

$f(\theta = 0) = f(\boldsymbol{k}, \boldsymbol{k})$: scattering in the forward direction.

$$\sigma_{tot} = \int \frac{d\sigma}{d\Omega} d\Omega.$$

This formula is known as the optical theorem, and holds for collisions in general.

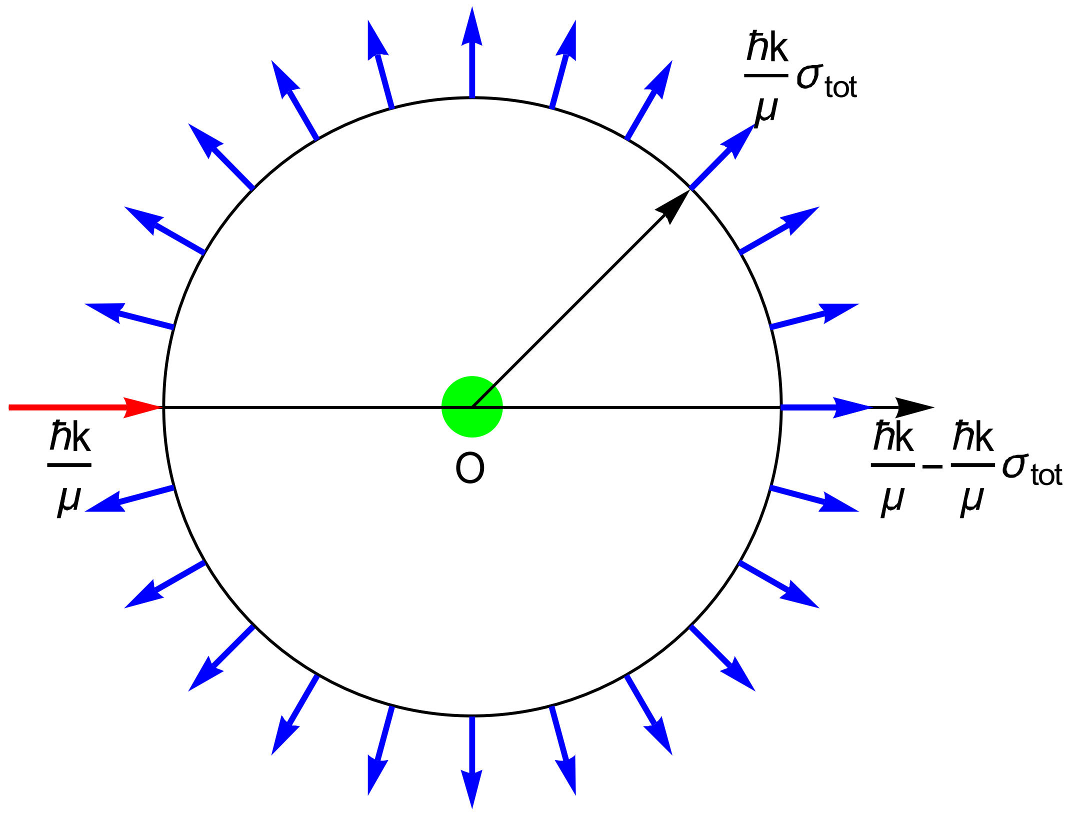


Fig. Optical theorem. The intensity of the incident wave is $\hbar k/\mu$. The intensity of the forward wave is $(\hbar k/\mu)-(4\pi\hbar/\mu)\,\mathrm{Im}[f(0)]$. The waves with the total intensity $(4\pi\hbar/\mu)\,\mathrm{Im}[f(0)]=(\hbar k/\mu)\sigma_{tot}$ is scattered for all the directions, as the scattering spherical waves.

((**Proof**))

$$\mathrm{Im}[f(\boldsymbol{k},\boldsymbol{k})]=-\frac{1}{4\pi}(2\pi)^3\frac{2\mu}{\hbar^2}\mathrm{Im}[\langle\boldsymbol{k}|\hat{T}|\boldsymbol{k}\rangle]$$
$$=-\frac{1}{4\pi}(2\pi)^3\frac{2\mu}{\hbar^2}\mathrm{Im}[\langle\boldsymbol{k}|\hat{V}|\psi^{(+)}\rangle]$$

$$|\psi^{(+)}\rangle=|\boldsymbol{k}\rangle+(E_k-\hat{H}_0+i\varepsilon)^{-1}\hat{V}|\psi^{(+)}\rangle,$$

or

$$|\boldsymbol{k}\rangle=|\psi^{(+)}\rangle-(E_k-\hat{H}_0+i\varepsilon)^{-1}\hat{V}|\psi^{(+)}\rangle,$$

or

$$\langle \boldsymbol{k}| = \langle \psi^{(+)}| - \langle \psi^{(+)}|\hat{V}(E_k - \hat{H}_0 - i\varepsilon)^{-1}.$$

Then

$$\mathrm{Im}[\langle \boldsymbol{k}|\hat{V}|\psi^{(+)}\rangle = \mathrm{Im}[(\langle \psi^{(+)}| - \langle \psi^{(+)}|\hat{V}(E_k - \hat{H}_0 - i\varepsilon)^{-1}|\psi^{(+)}\rangle.$$

Now we use the well-known relation ($i\varepsilon$ representation, see the **Appendix IV**)

$$\begin{aligned}\hat{G}_0(E_k - i\varepsilon) &= \left(\frac{1}{E_k - \hat{H}_0 - i\varepsilon}\right) \\ &= [P\left(\frac{1}{E_k - \hat{H}_0}\right) + i\pi\delta(E_k - \hat{H}_0)]\end{aligned}$$

Then

$$\begin{aligned}\mathrm{Im}[\langle \boldsymbol{k}|\hat{V}|\psi^{(+)}\rangle &= \mathrm{Im}[(\langle \psi^{(+)}|\psi^{(+)}\rangle - [\mathrm{Im}\langle \psi^{(+)}|\hat{V}P\left(\frac{1}{E - \hat{H}_0}\right)\hat{V}|\psi^{(+)}\rangle \\ &\quad + \mathrm{Im}\langle \psi^{(+)}|\hat{V}i\pi\delta(E - \hat{H}_0)\hat{V}|\psi^{(+)}\rangle]\end{aligned}$$

The first two terms of this equation vanish because of the Hermitian operators of $\hat{V}$ and

$$\hat{V}P\left(\frac{1}{E - \hat{H}_0}\right)\hat{V}.$$

Therefore,

$$\mathrm{Im}[\langle \boldsymbol{k}|\hat{V}|\psi^{(+)}\rangle = -\pi\langle \psi^{(+)}|\hat{V}\delta(E_k - \hat{H}_0)\hat{V}|\psi^{(+)}\rangle = -\pi\langle \boldsymbol{k}|\hat{T}^{+}\delta(E - \hat{H}_0)\hat{T}|\boldsymbol{k}\rangle$$

or

$$\mathrm{Im}[\langle \boldsymbol{k}|\hat{V}|\psi^{(+)}\rangle = -\pi\int d\boldsymbol{k}'\langle \boldsymbol{k}|\hat{T}^{+}|\boldsymbol{k}'\rangle\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\delta(E_k - \frac{\hbar^2 k'^2}{2\mu})$$
$$= -\pi\int d\boldsymbol{k}'\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2\delta(E_k - \frac{\hbar^2 k'^2}{2\mu})$$

$$\delta(E - \frac{\hbar^2 k'^2}{2\mu}) = \delta(\frac{\hbar^2 k^2}{2\mu} - \frac{\hbar^2 k'^2}{2\mu})$$
$$= \delta[\frac{\hbar^2}{2\mu}(k^2 - k'^2)] = \delta[\frac{\hbar^2}{2\mu}(k+k')(k-k'))] = \delta[\frac{k\hbar^2}{\mu}(k-k')]$$

or

$$\delta(E - \frac{\hbar^2 k'^2}{2\mu}) = \frac{\mu}{k\hbar^2}\delta(k-k')$$

$$\mathrm{Im}[\langle \boldsymbol{k}|\hat{V}|\psi^{(+)}\rangle = -\pi\frac{\mu}{k\hbar^2}\iint dk' k'^2\, d\Omega'\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2\delta(k-k')$$
$$= -\pi\frac{\mu k}{\hbar^2}\int d\Omega'\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2$$

Thus

$$\mathrm{Im}[f(\theta=0)] = -\frac{1}{4\pi}(2\pi)^3\frac{2\mu}{\hbar^2}\mathrm{Im}[\langle \boldsymbol{k}|\hat{V}|\psi^{(+)}\rangle]$$
$$= -\frac{1}{4\pi}(2\pi)^3\frac{2\mu}{\hbar^2}(-\frac{\pi\mu k}{\hbar^2})\int d\Omega'\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2$$
$$= \frac{k}{4\pi}\frac{16\pi^4\mu^2}{\hbar^4}\int d\Omega'\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2]$$

Since

$$\frac{d\sigma}{d\Omega'} = \left|f(\boldsymbol{k}',\boldsymbol{k})\right|^2$$
$$= \frac{1}{16\pi^2}(2\pi)^6\frac{4\mu^2}{\hbar^4}\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2,$$
$$= \frac{16\pi^4\mu^2}{\hbar^4}\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2$$

$$\sigma_{tot} = \int d\Omega' \frac{d\sigma}{d\Omega'} = \frac{16\pi^4\mu^2}{\hbar^4}\int d\Omega' \left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2$$

Then we obtain

$$\mathrm{Im}[f(\theta = 0)] = \frac{k}{4\pi}\sigma_{tot}. \qquad \text{(optical theorem)}$$

9. Summary

Comparison between the partial wave approximation (low-energy scattering) and high-energy scattering (Born approximation).

(i) Although the partial wave expansion is "straightforward", when the energy of incident particles is high (or the potential weak), many partial waves contribute. In this case, it is convenient to switch to a different formalism, the Born approximation.

(ii) At low energies, the partial wave expansion is dominated by small orbital angular momentum.

APPENDIX-II
Inelastic neutron scattering data

We use the conversion relation of the units for photon with the dispersion relation

$$E = h\nu = \frac{ch}{\lambda}$$

1 meV = 0.241799 THz
1 THz = 4.13567 meV
100 THz = 0.413567 eV
1 cm^{-1} = 0.123984 meV
1 meV = 8.06556 cm^{-1}
3 THz = 100.069 cm^{-1}.

(a) Rh

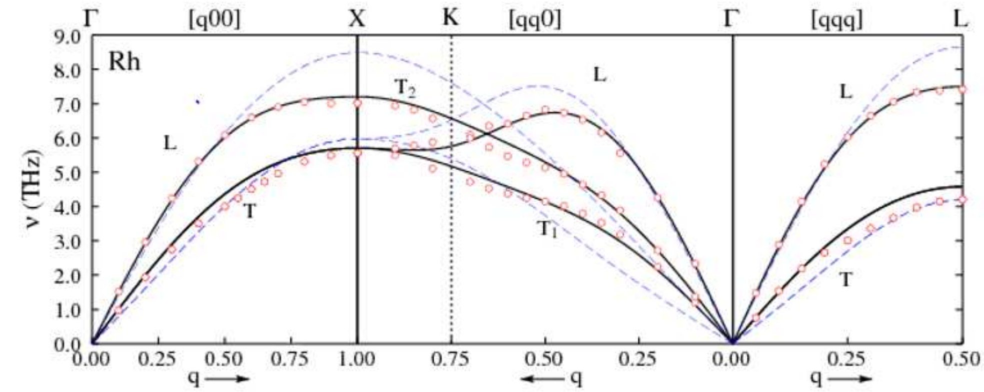


Fig. Phonon dispersion curve of Rh. A. Eichler, K.P. Bohnen, W. Reichardt, and J. Hafner, Phonon dispersion relation in rhodium: Ab initio calculations and neutron-scattering investigations, Phys. Rev. B57, 324 (1998).

(b) Neon

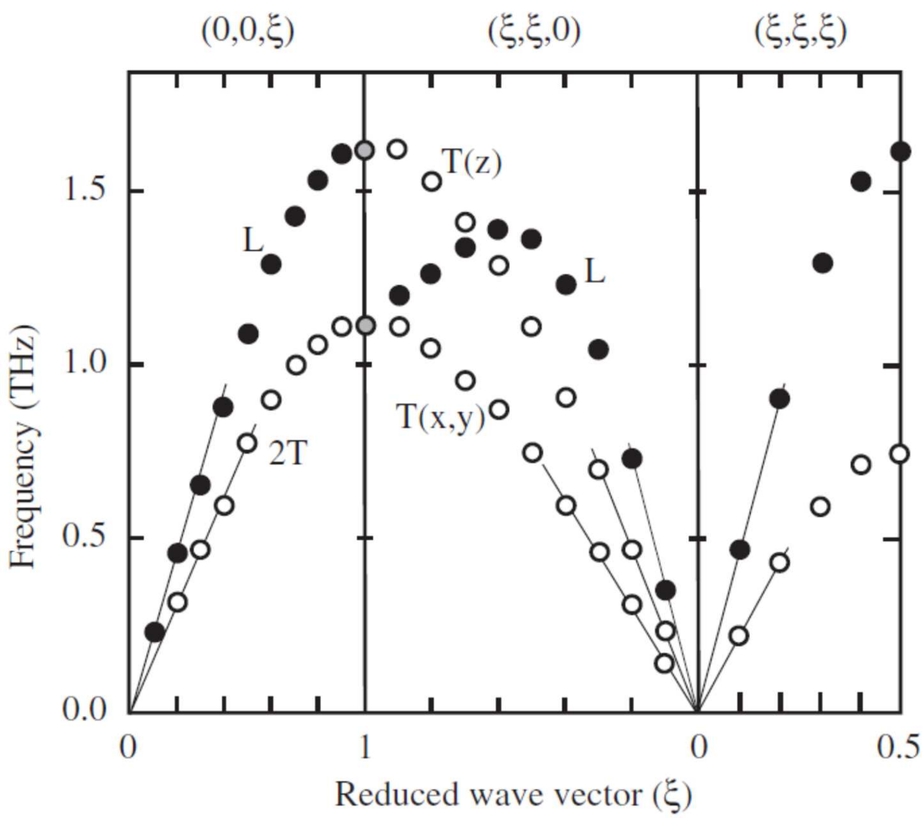


Fig. Acoustic mode dispersion curves for neon (ccp structure) measured by inelastic neutron scattering. (Data taken from Endoh et al. Phys. Rev. B11, 1681, 1975). M.T. Dove, Structure and Dynamics: An Atomic View of Materials (Oxford, 2002).

(c) Lead

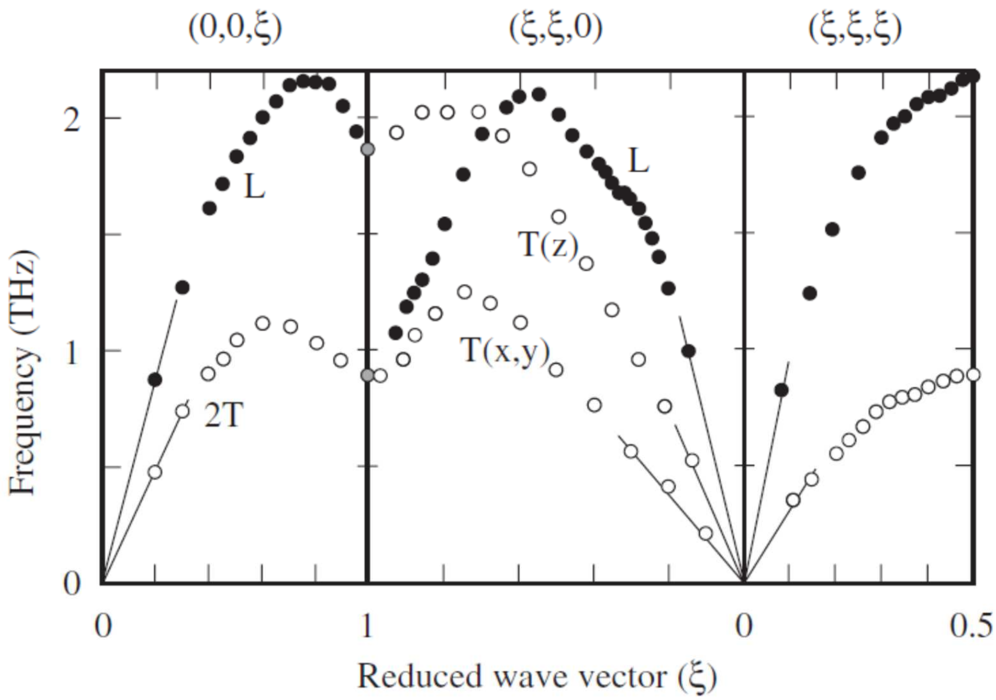


Fig. Acoustic mode dispersion curves for lead (fcc) measured by inelastic scattering (Data taken from Brockhouse et al. Phys. Rev. **128**, 1099, 1962). M.T. Dove, Structure and Dynamics: An Atomic View of Materials (Oxford, 2002).

(d) Potassium (fcc)

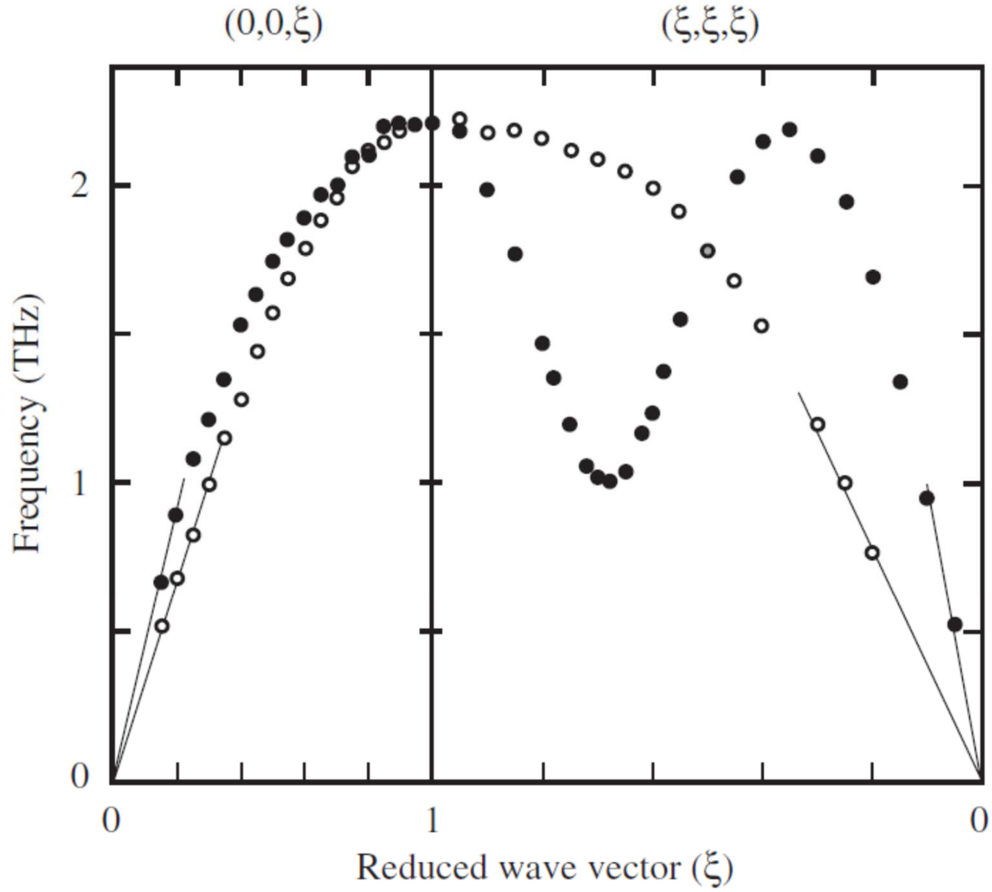


Fig. Acoustic mode dispersion curves for potassium (fcc) measured by inelastic neutron scattering. (Data taken from Cowley et al., Phys. Rev. **150**, 487, 1966). M.T. Dove, Structure and Dynamics: An Atomic View of Materials (Oxford, 2002).

(e) NaCl

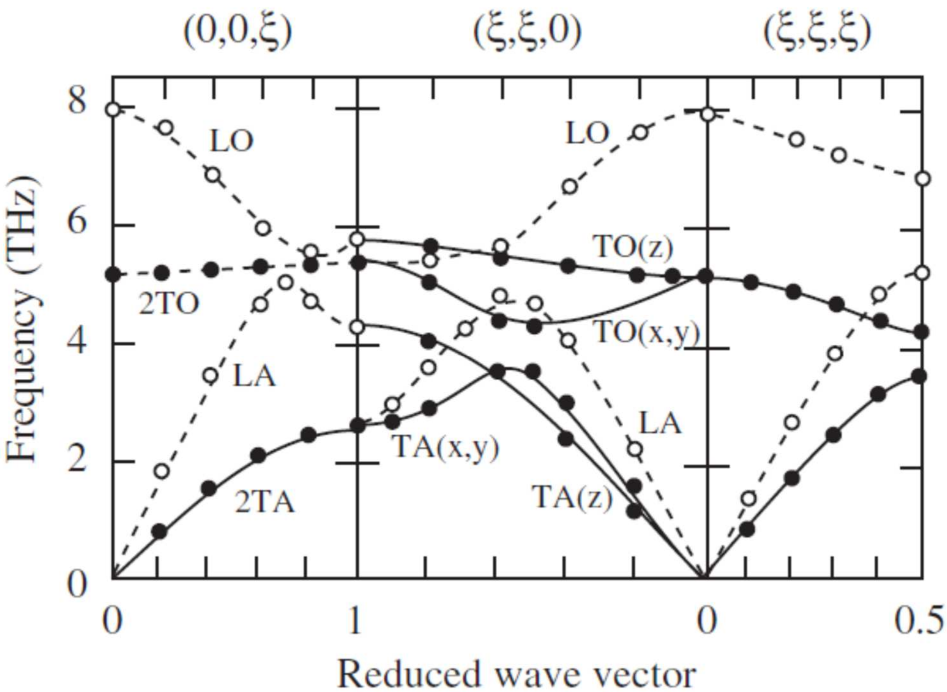


Fig. Dispersion curves for NaCl (inelastic neutron scattering). (Data taken from Raunio et al. Phys. Rev. **178**, 1496, 1969). M.T. Dove, Structure and Dynamics: An Atomic View of Materials (Oxford, 2002).

(f) Qaurtz

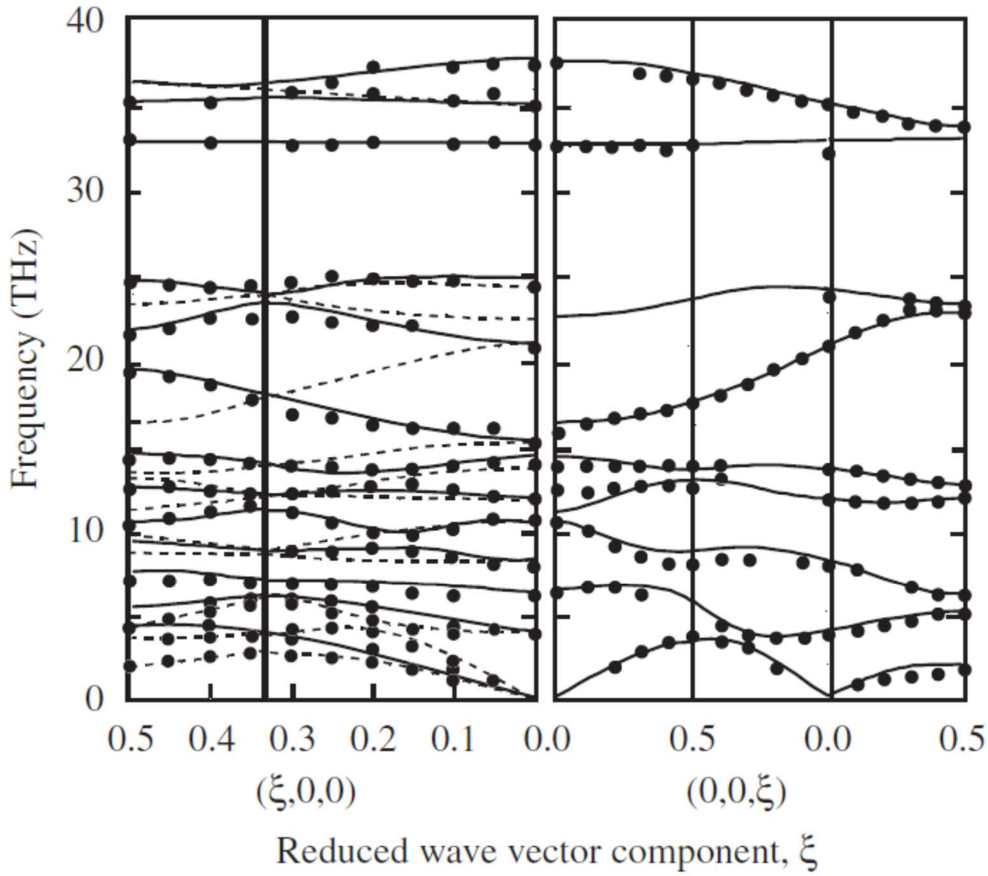


Fig. Dispersion curves for quartz. (Data are taken from Strauch and Dorner, J. Phys. Cond. Matter **5**, 6149, 1993). M.T. Dove, Structure and Dynamics: An Atomic View of Materials (Oxford, 2002).

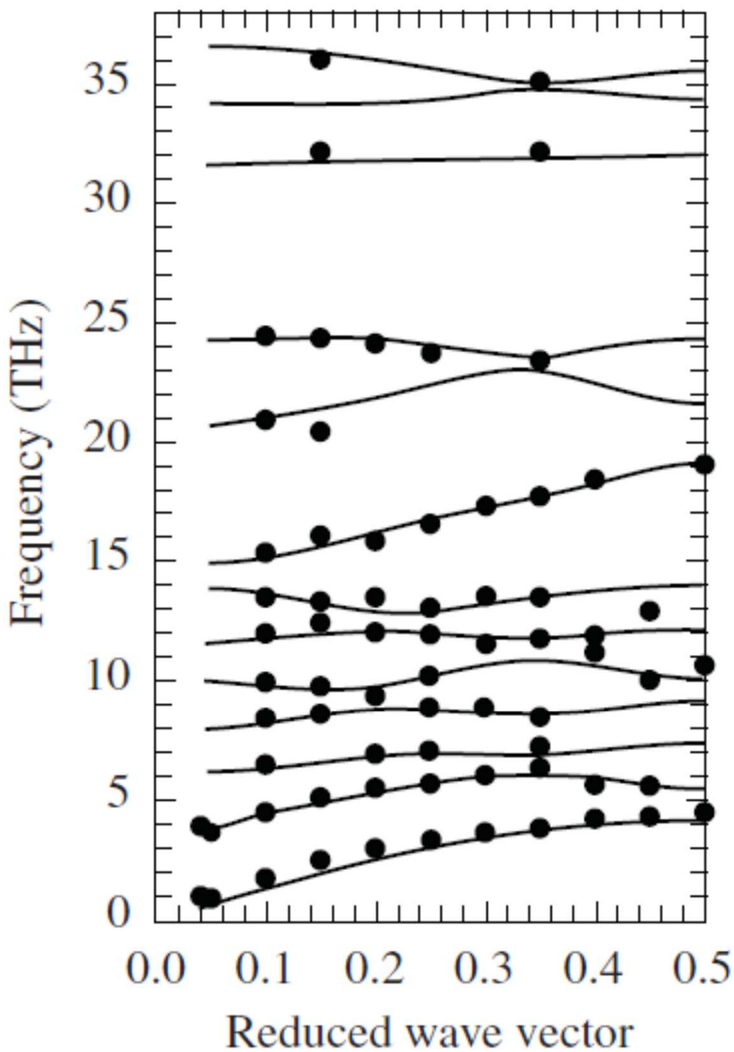


Fig. Phonon dispersion curves of quartz obtained by inelastic x-ray scattering. (Data from Ch. Halcoussis, J. Phys,: Cond. Matter 13, 7627, 2001).

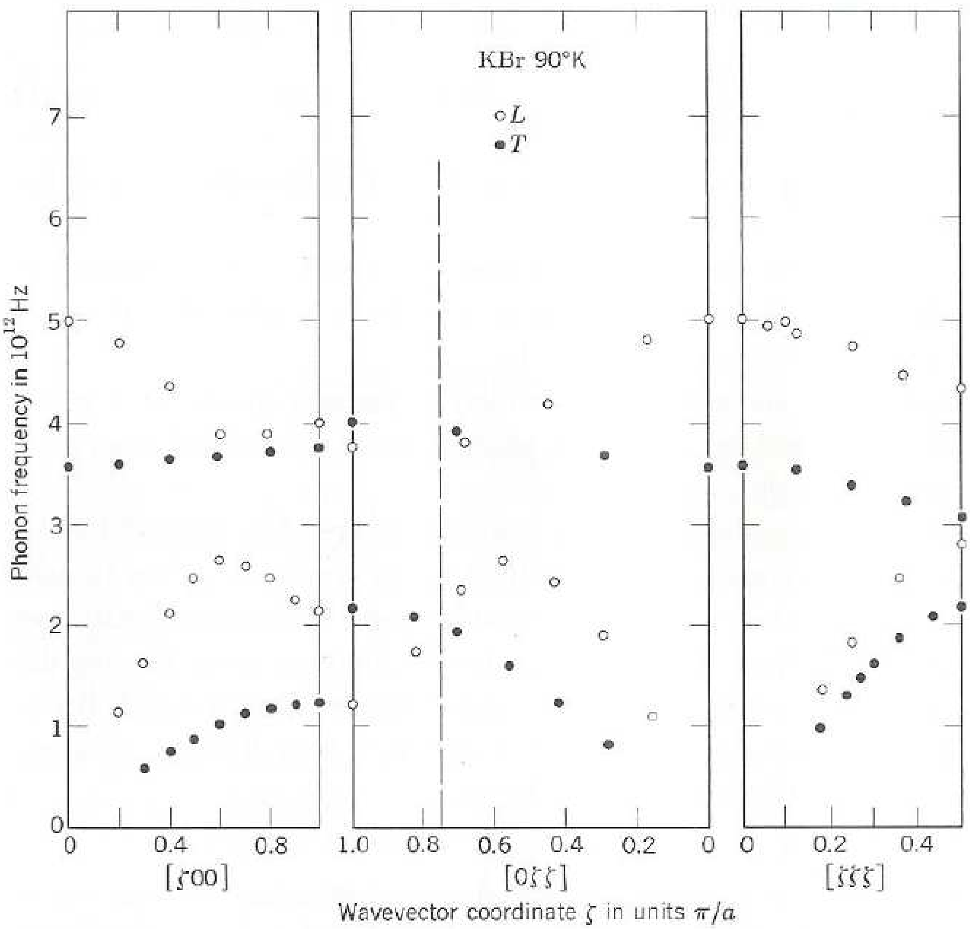


Fig. Dispersion curves for potassium bromide at 90 K. (Woods et al. Phys. Rev. 131, 1025 (1963). C. Kittel, Introduction to Solid State Physics, 4-th edition (John Wiley, 1971).