Summary of what we did last time:

1. So far, focused on how neutrons are produced
2. How neutrons are slowed down

Today:

• We will finish off our discussion on the slowing down of neutrons
• Maxwellian distribution of neutrons
• How to monochromate a neutron beam
In terms of neutron's lab. energy:

\[ E_\ell = \frac{1}{2} m v_\ell^2, \quad E'_\ell = \frac{1}{2} m v'_\ell^2 \]

thus,

\[ E'_\ell = E_\ell \left[ \frac{A^2 + 2A \cos \theta + 1}{(A+1)^2} \right] \]

Call \[ \alpha = \left( \frac{A-1}{A+1} \right)^2 \]

then,

\[ E'_\ell = \frac{1}{2} E_\ell \left[ (1+\alpha) + (1-\alpha) \cos \theta \right] \]

\[ (E'_\ell)_{\text{max}} = E_\ell, \quad \theta = 0 \]

\[ (E'_\ell)_{\text{min}} = \frac{1}{2} E_\ell, \quad \theta = \pi \]
\[ P(E \rightarrow E') dE' = \text{probability that a neutron with lab energy } E \text{ will emerge with energy } E' \text{ in } dE' \]

\[ \int_{\alpha E}^{E} P(E \rightarrow E') dE' \]

Cross-section for scattering:

\[ N = \text{no of target nuclei} / \text{cm}^3 \]

\[ \delta V = A \delta x \]

Prob. for scattering in \( \delta x \) = \( \frac{\sigma_s N \delta V}{A} = \sigma_s N \delta x \)

\[ \Sigma_s = \sigma_s N \text{ [cm}^{-1}\text{]} = \text{probability for scattering} \]
Probability that a nuclide is scattered into \(d\theta\) at \(\theta\) per unit of path length is,

\[
\mathcal{Z}_s(\theta) = N \sigma_s(\theta)
\]

Total cross section

\[
\text{Total cross section} = \int \sigma_s(\theta) \, d\theta = \sigma_s
\]

Probability that a nuclide, if scattered, is scattered into \(d\theta\) at \(\theta\) is

\[
\frac{\sigma_s(\theta) \, d\theta}{\sigma_s} = \frac{\sigma_s(\theta) \, 2\pi \sin \theta \, d\theta}{\sigma_s}
\]

Thus, since each scattering angle \(\theta\) in c.m. corresponds to a given energy loss:

\[
P(E \to E') \, |dE'| = \frac{\sigma_s(\theta) \, 2\pi \sin \theta \, |d\theta|}{\sigma_s}
\]

But

\[
dE' = -\frac{1}{2} E (1-\alpha) \sin \theta \, d\theta
\]

Therefore,

\[
P(E \to E') = \frac{4\pi \, \sigma_s(\theta)}{E (1-\alpha) \, \sigma_s} \quad \text{for } dE < E' < E
\]
Now assume, that scattering is isotropic in c.m.:

\[ \sigma_s(\theta) = \frac{\sigma_s}{4\pi}, \quad (kR \ll 1) \]

Therefore,

\[ P(E \rightarrow E') = \begin{cases} \frac{1}{E(1-\alpha)}, & dE < E' < E \\ 0, & \text{otherwise} \end{cases} \]

Now define the scattering rate / volume for neutrons of energy \( E \) in \( dE \):

\[ F(E) = \Sigma_s(E) \phi(E). \]

\[ F(E)dE = \text{no. of neutrons in } dE \text{ per cm}^3 \text{ that are scattered per second}. \]
Slowing down in H:

Suppose we have a source $S$ of neutrons/cm$^3$/sec of energy $E_0$. Exactly this number must be scattered per cm$^3$ per second at steady state.

$$P(E_0 \rightarrow E) \, dE = \frac{dE}{E_0}$$
$$P(E' \rightarrow E) \, dE = \frac{dE}{E'}$$

$$F(E') \, dE' \frac{dE}{E'} = \text{no. of neutrons/cm}^3/\text{sec scattered down from } dE' \text{ to } dE.$$
Thus,

\[ F(E) = \frac{S}{E_0} + \int_{E}^{E_0} \frac{F(E')dE'}{E'} \]  

or,

\[ \frac{dF(E)}{dE} = -\frac{F(E)}{E} \]

\[ \text{Solution: } F(E) = \frac{C}{E} \]

\[ u = \ln \frac{E_0}{E} \]

\[ du = \frac{dE}{E} \]

\[ F(u) = \frac{S}{E_0} - \int_{0}^{u} F(u') \]

at \( E = E_0 \), eq. (A) requires \( F(E_0) = \frac{S}{E_0} \).

Thus, \( C = S \), and

\[ F(E) = \frac{S}{E} \]

But \( F(E) = \sum_s(E) \phi(E) \)

so that

\[ \phi(E) = \frac{S}{E \sum_s(E)} \]

If \( \sum_s(E) \) is independent of \( E \), we get the \( \frac{S}{E} \) slowing

\[ \phi(E) = \frac{S}{E \sum_s} \]
When a chemical system achieves equilibrium, it is through a process of energy transfer between the components, with
energetic parts constantly giving energy away. This means that the probability distribution should favor situations where the energy is spread throughout the system and disfavor situations where any system component has a great deal of energy. The exact form of the probability distribution is an exponential function:

\[ P(i) = C e^{-E_i/k_B T} \]

or

\[ P(x) = C' e^{-E(x)/k_B T} \]

This equation means that the probability of finding a particle in state \( i \) or \( x \) (use \( i \) for discrete distributions and \( x \) for continuous ones) is proportional to the exponential of \(-E\) (minus the energy of the state) divided by the product of \( k_B \) (Boltzmann's constant) and \( T \) (the temperature in Kelvins). What is meant by a state? Each state corresponds to a set of possible measured values. For an atom in an ideal gas, each state has particular values of the three velocity components \( u_x, u_y, \) and \( u_z \). States of a molecule can be indexed by the same three velocity components, plus vibrational and rotational energy levels. Since we know that any probability distribution must be normalized, we can determine the constants \( C \) and \( C' \) explicitly:

\[ P(i) = \frac{e^{-E_i/k_B T}}{\sum_{j=1}^{N} e^{-E_j/k_B T}} \]

or

\[ P(x) = \frac{e^{-E(x)/k_B T}}{\int_{E_{\text{min}}}^{E_{\text{max}}} dx \, e^{-E(x)/k_B T}} \]

(The denominator in each case is called the "partition function".) This probability distribution describes how energy is distributed at equilibrium for an amazingly wide variety of chemical and physical systems. This probability distribution (in discrete and continuous forms) is the Maxwell-Boltzmann distribution.

Maxwell-Boltzmann distribution
Maxwell-Boltzmann Flux Spectrum

Number of neutrons / m^3 in d^3V = \( n(\vec{v}) \, d^3\vec{v} \).

\[ n(\vec{v}) = \frac{d^3N}{dV^3} = C \, e^{-E/kt} \quad \text{no. of neutrons / m}^3 \quad \text{per unit volume in } \vec{v} \text{-sp.} \]

where the K.E. is

\[ E = \frac{1}{2} m v^2. \]

\[ d^3\vec{v} = \sin \theta d\theta d\phi \, v^2 \, dv \Rightarrow 4\pi v^2 \, dv \]

box integrate shell.
Maxwellian distribution
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The normalization constant, \( c \):

\[
N_0 = \text{no. of neutrons} / \text{cm}^3.
\]

\[
= \int n(u) d^3\mathbf{u} = c \int_0^\infty e^{-\frac{m v^2}{2 K T}} d v
\]

Gaussian integrals:

**normalized gaussian**:

\[
g(x) = \frac{1}{\sqrt{2 \pi} \, \sigma} \, e^{-x^2/2 \sigma^2}
\]

\[
\int_{-\infty}^{\infty} g(x) \, dx = 1
\]

Half-width = \( x_{1/2} \)

\[
\frac{1}{2} = e^{-x_{1/2}^2 / 2 \sigma^2}
\]

\[
\sqrt{2 \ln 2} = 2.507
\]

\[
\ln 2 = x_{1/2}^2 / 2 \sigma^2
\]

\[
x_{1/2} = \sqrt{2 \ln 2} \, \sigma
\]
Half-line integral:

\[ \int_0^\infty g(x) \, dx = \frac{1}{2} \]

Let \( \alpha = \frac{1}{2n^2} \), \( n = \frac{1}{\sqrt{2\alpha}} \)

Then, \( g(x) = \sqrt{\frac{\alpha}{\pi}} \, e^{-\alpha x^2} \).

Thus,

\[ I_0(\alpha) = \int_0^\infty e^{-\alpha x^2} \, dx = \frac{1}{2} \sqrt{\frac{\pi}{\alpha}} \]

\[ I_2(\alpha) = \int_0^\infty x^2 e^{-\alpha x^2} \, dx = -\frac{d}{d\alpha} I_0(\alpha) = \frac{\sqrt{\pi}}{4} \, \alpha^{-3/2} \]

For our normalization integral:

\( \alpha = \frac{m}{2kT} \), \( N_0 = C \cdot 4\pi \cdot I_2(\alpha) \)

Thus,

\[ N_0 = C \cdot \frac{\sqrt{\pi}}{4} \left( \frac{2kT}{m} \right)^{3/2} \cdot 4\pi \]

and,

\[ c = \frac{N_0 (\frac{m}{2})^{3/2}}{L} \]
And therefore,

\[ n(v^2) = N_0 \left( \frac{m}{2\pi kT} \right)^{3/2} e^{-mv^2/2kT} \]

= no. of neutrinos/cm^3/unit volume in v space

Distribution in energy:

\[ \tilde{n}(E) \, dE = n(v^2) \, 4\pi v^2 \, dv \]

\[ \tilde{n}(E) = \frac{n(v^2) \, 4\pi v^2 \, dv}{dE} \]

where, \( E = \frac{1}{2} mv^2 \), \( dE = mv \, dv \)

so that

\[ \frac{dv}{dE} = \frac{1}{mv} = \frac{1}{\sqrt{2mE}} \]

Thus,

\[ \tilde{n}(E) = C_0 \sqrt{E} \, e^{-E/kT} \]

where \( C_0 = \frac{2}{\sqrt{\pi}} \frac{N_0}{(kT)^{3/2}} \),

independent of mass m.
At $E = E_{\text{max}}$:

$$\frac{d \tilde{n}}{d E} = 0$$

$$= C_0 \left\{ \frac{1}{a} E^{-\frac{1}{2}} e^{-E/kT} - \frac{1}{kT} E^{\frac{1}{2}} e^{-E/kT} \right\}$$

$$\Rightarrow E_{\text{max}} = \frac{1}{a} kT$$
Flux

\[ \phi(E) \equiv \nu \tilde{\rho}(E) \quad \text{neutrons/cm}^2/\text{sec/} \text{unit} \]

where \( \nu = \sqrt{2E/m} \)

Thus,

\[ \phi(E) = \left( \frac{2}{\sqrt{\pi}m} \right) \frac{N_0}{(kT)^{3/2}} E e^{-E/kT} \]

at \( E = E_p \):

\[ \frac{d\phi}{dE} = 0 = \sqrt{\frac{2}{\pi m}} C_0 \left\{ E \left( -\frac{1}{kT} \right) e^{-E/kT} + e^{-E/kT} \right\} \]

\[ \therefore \quad E_p = kT \]
Total thermal flux

\[
\phi_0 = \int_0^\infty \phi(E) \, dE = \sqrt{\frac{2}{m}} \frac{2}{\sqrt{\pi}} \frac{N_0}{(kT)^{3/2}} \int_0^\infty E e^{-E/kT} \, dE = (kT)^2
\]

\[
= 2N_0 \left( \frac{2kT}{m\pi} \right)^{1/2}
\]

Define thermal velocity as \( \frac{1}{2} m v_T^2 = kT \)

\[
v_T = \sqrt{\frac{2kT}{m}}
\]

Thus,

\[
\phi_0 = \left( \frac{2}{\sqrt{\pi}} \right) v_T N_0
\]

\[
= 1.128 \text{ neutrons/cm}^2/\text{s}
\]

We can rewrite \( \phi(E) \) in terms of \( \phi_0 \)

\[
\phi(E) = \phi_0 \frac{E \, e^{-E/kT}}{(kT)^2}
\]
de Broglie wave length $\lambda$.

$$E = \frac{1}{2} mv^2 = \frac{p^2}{2m} = \frac{h^2 k^2}{2m} = \frac{h^2}{2m \lambda^2}$$

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

wave packet.

$$\tilde{\phi}(\lambda) d\lambda = \phi(E) dE$$

$$\tilde{\phi}(\lambda) = \phi(E) \left| \frac{dE}{d\lambda} \right|$$

$$\frac{dE}{d\lambda} = - \frac{h^2}{m \lambda^3} = -\frac{2E}{\lambda}$$

Thus,

$$\phi(\lambda) = \phi_0 \frac{2E^2}{(kT)^2} \frac{1}{\lambda} \ e^{-\frac{E}{kT}}$$

or

$$\phi(\lambda) = \phi_0 \frac{2 \left( \frac{h^4}{4m^2} \right)}{(kT)^2} \frac{1}{\lambda^5} \ e^{-\frac{h^2}{2m kT \lambda^2}}$$
at $\lambda = \lambda_p$:

$$\frac{d\Phi}{d\lambda} = 0$$

$\phi(\lambda)$ is

$$\phi(\lambda) = c \lambda^{-5} e^{-a/\lambda^2}, \quad a = \frac{h^2}{2m}$$

$$\frac{d\phi}{d\lambda} = c \left[ -5\lambda^{-6} e^{-a/\lambda^2} + 2a \lambda^{-8} e^{-a/\lambda^2} \right]_{\lambda_p}$$

$$\Rightarrow \lambda_p^2 = \frac{2}{5} a = \frac{h^2}{5mkT}$$

The energy corresponding to this wavelength is

$$E(\lambda_p) = \frac{5}{2} kT$$
Diffraction pattern from Mg$_3$V$_2$O$_8$

Neutron diffraction
Bragg's Law (crystals):

\[ n\lambda = 2d \sin \theta \]

Scattered intensity:

\[ I \propto |F_N|^2 \]

where \( F_N = \sum b_n \exp(iQ.r_n) \) \textit{Structure Factor}
Electron diffraction

Mono1
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2-axis spectrometer

- 12 ft biological shield
- Monochromator crystal
- Monochromator shield
- Detector
- Sample
- "Antiparallel side"
- "Parallel side"

Reactor Core
- 4" to 6" diameter beam tube
- Primary collimator
- Secondary collimator
- Soller collimators
- 2θ_4 and 2θ_5

Bragg Law: \[ 2d \sin \theta_B = \lambda \]

Scattering triangle:
- \( \vec{Q} = \vec{G}_{hk0} \)
- \( \vec{k} \)
- \( \vec{k}' \)
- \( 2\theta_B \)

Miller indices:
- \( d_{hk0} = \frac{2\pi}{G_{hk0}} \)

\( \vec{k} - \vec{k}' = \vec{Q} = \vec{G} \)
\[ \phi(E) = \phi_0 \frac{E}{(RT)^2} e^{-E/kT} \]

- Neutrons reflected by monochromators:
  - Energy: \( E = E_1 \) for first-order neutrons.
  - Energy: \( E = E_2 \) for second-order neutrons.

\[ E_1 = \frac{81.78}{\lambda_1^2 (\text{Å})} \]
\[ E_2 = \frac{81.78}{\lambda_2^2 (\text{Å})} = \frac{4 \times 81.78}{\lambda_1^2 (\text{Å})} = 4E_1 \]
\[ \phi(E) = \frac{\phi_0 E}{(kT)^2} e^{-E/kT} \]

\[ E_a = 4E_1 \quad E_3 = 9E_1 \]

\[ \int_0^\infty \phi(E) dE = \phi_0 = 2 \times 10^{14} \text{ m}^2/\text{sr} \]

Bragg's Law

\[ 2d \sin \theta = \lambda \]

\[ \vec{G} = \frac{2\pi}{\lambda} \]

\[ \vec{G}_{hkl} = \text{reciprocal lattice vector} \]
What is the flux at the monochromator?

At the source end of the primary collimator, let

\[ \phi_0 = 2 \times 10^{14} \text{ m}^2/\text{m}^2/\text{sec} \]

\[ L_1 = 16 \text{ ft} \]

\[ H_0 = 6^\circ \]

\[ H_0 = 15^\circ \]

\[ L = 1/30 \]

\[ w = \infty \]

\[ W_0 = \infty \]

\[ \alpha_H = 1/2 \text{ deg} = 0.0087 \text{ rad} \]

\[ \Delta \Omega = \alpha_H \alpha_V = (3.1)(8.7) \times 10^{-5} = 23 \times 10^{-5} \]

\[ = \frac{1}{4} \text{ mrad} \]

Flux at monochromator = \[ \phi_0 \frac{\Delta \Omega}{4\pi} \text{ all energy} \]

\[ = 2 \times 10^{14} \frac{1/4 \times 10^{-3}}{4\pi} = 0.034 \times 10^{-6} \approx 4 \times 10^{-9} \]
What is the flux at the Sample?

The monochromator picks out a band, \( \Delta E \), of neutrons from the incident M-B spectrum. The bandwidth \( \Delta E \) is determined by the primary and secondary collimations and the monochromator "mosaic spread".

Darwin's Mosaic Crystal Model:

\[
W(\Delta) = \frac{1}{\sqrt{2\pi} \eta} e^{-\Delta^2/2\eta^2}
\]

\( \eta \) = mosaic spread parameter
Reflectivity \( R(\lambda) = R_0 \, e^{-\lambda^2 / 2 \sigma^2} \)

\( R_0 = \text{"peak reflectivity"} \)

\text{typically} \approx 30 \text{ to } 70 \% 

Collimation: typically 0.2 degrees to 1.0 degree

All this implies

\( \Delta E / E \approx 10^{-2} \)

for \( E = 81 \, \text{meV} \), \( \lambda = 1 \, \text{Å} \).

\( \Rightarrow \Delta E = 1 \, \text{meV} \).

Since \( E = \frac{81.78}{\lambda^2} \),

\( \Delta E = -2 \frac{81.78}{\lambda^3} \Delta \lambda \)

Thus \( \left| \frac{\Delta \lambda}{\lambda} \right| = \frac{1}{2} \left| \frac{\Delta E}{E} \right| \)
Monochromatic Crystal

Perfect crystal:

\[ R = \frac{I}{I_n(a\theta)} \]

\( \Delta \theta \)

Density width = 1 arcsec.

\( K \)-space

Mosaic crystal.
Flex leaving Monochromator

The vector flux = current density

$$\vec{\phi}(\vec{v}) \cdot \vec{n}(\vec{v}) = \nu N_0 \left( \frac{m}{2\pi kT} \right)^{3/2} e^{-E/kT} \hat{\nu}$$

$$\nu_T = \sqrt{\frac{2kT}{m}}$$

$$\phi(v) = \frac{\nu N_0}{\pi^{3/2}} \frac{1}{\nu_T^3} e^{-E/kT}$$

$$\Delta^3\nu = \nu^{-3} \phi' \nu' \cdot \Delta n \sin \Theta_B$$

$$N_0 = \frac{\sqrt{\pi}}{2} \phi_0 / \nu_T$$

$$\phi(v) = \frac{1}{2\pi} \phi_0 \frac{\nu}{\nu_T^4} e^{-E/kT}$$
Take \( E = E_T = kT = \frac{1}{2} m v_i^2 \),

FWHM \( \eta = \frac{1}{2} \text{ deg} = 9 \times 10^{-3} \), \( \Theta_B = 30^\circ \)

Then,

\[
\phi(\theta) \Delta^3 \nu = \frac{2 \times 10^{14}}{2\pi} \left( \frac{1}{4 \times 10^{-3}} \right) \left( 9 \times 10^{-3} \right) (1.7) \cdot 1 = 1.2 \times 10^8
\]

**Flex at Sample**

Height Flat

\[ h = 4'' \]

\[ \phi_V = 0.066 \text{ rad} = \text{ large.} \]

\[ \text{Take } \phi_m' = \frac{1}{2} \text{ deg } \approx = 8.7 \times 10^{-3} \]
**Vertical Focusing**

\[ d_V = \frac{H_1}{L_2} \]

\[ d_V = \frac{H_0}{L_1 + L_2} \text{ flat} \]

Gain due to focusing

\[
G = \frac{H_1}{H_0} \left( 1 + \frac{L_1}{L_2} \right)
\]

\[
= \frac{4}{6} \left( 1 + \frac{16}{5} \right) = 2.8
\]

\[
\beta(y) = \frac{1}{2 \sin \theta_M} \left( \frac{1}{L_1} + \frac{1}{L_2} \right)
\]
Vertical Plane.

\[ \frac{H_1}{L_2} = \frac{H_0}{L_1 + L_2} \]

\[ H_1 = \frac{L_2 H_0}{L_1 + L_2} = \frac{5}{16 + 5} \cdot \frac{1}{2} = 0.11 \text{ ft} = (1.4 \text{ in.}) \]