

## 22.101 Applied Nuclear Physics (Fall 2006)

### Lecture 18 (11/20/06)

#### Neutron Interactions: Energy and Angular Distributions, Thermal Motions

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##### References:

R. D. Evans, *Atomic Nucleus* (McGraw-Hill New York, 1955), Chap. 12.

W. E. Meyerhof, *Elements of Nuclear Physics* (McGraw-Hill, New York, 1967), Sec. 3.3.

John R. Lamarsh, *Nuclear Reactor Theory* (Addison-Wesley, Reading, 1966), Chap 2.

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We will use the expressions relating energy and scattering angles derived in the previous chapter to determine the energy and angular distributions of an elastically scattered neutron. The energy distribution, in particular, is widely used in the analysis of neutron energy moderation in systems where neutrons are produced at high energies (MeV) by nuclear reactions and slow down to thermal energies. This is the problem of neutron slowing down, where the assumption of the target nucleus being initially at rest is justified. When the neutron energy approaches the thermal region ( $\sim 0.025$  eV), the stationary target assumption is no longer valid. One can relax this assumption and derive a more general distribution which holds for neutron elastic scattering at any energy. This then is the result that should be used for the analysis of the spectrum (energy distribution) of thermal neutrons, a problem known as neutron thermalization. As part of this discussion we will have an opportunity to study the energy dependence of the elastic scattering cross section.

We have seen from our study of cross section calculation using the method of phase shift that for low-energy scattering ( $kr_0 \ll 1$ , which is equivalent to neutron energies below about 10-100 keV) only s-wave contribution to the cross section is important, and moreover, the angular distribution of the scattered neutron is spherically symmetric in CMCS. This is the result that we will make use of in deriving the energy distribution of the elastically scattered neutron.

### ***Energy Distribution of Elastically Scattered Neutrons***

We define  $P(\underline{\Omega}_c)$  as the probability that the scattered neutron will be going in the direction of the unit vector  $\underline{\Omega}_c$  (recall this is a unit vector in angular space). We should also understand that a more physical way of defining P is to say that

$$P(\underline{\Omega}_c)d\Omega_c = \text{the probability that the neutron will be scattered into an element of solid angle } d\Omega_c \text{ about } \underline{\Omega}_c$$

For s-wave scattering one has therefore

$$P(\underline{\Omega}_c)d\Omega_c = \frac{d\Omega_c}{4\pi} \quad (16.1)$$

Notice that  $P(\underline{\Omega}_c)$  is a probability distribution in the two angular variables,  $\varphi_c$  and  $\theta_c$ , and is properly normalized,

$$\int_0^{2\pi} d\varphi_c \int_0^\pi \cos\theta_c d\theta_c P(\underline{\Omega}_c) = 1 \quad (16.2)$$

Since there is a one-to-one relation between  $\theta_c$  and  $E_3$  (cf. (15.13)), we can transform (16.1) to obtain a probability distribution in the outgoing energy,  $E_3$ . To do this we first need to reduce (16.1) from a distribution in two variables to a distribution in the variable  $\theta_c$ . Let us define  $G(\theta_c)$  as the probability of the scattering angle being  $\theta_c$ . This quantity can be obtained from (16.1) by simply integrating (16.1) over all values of the azimuthal angle  $\varphi_c$ ,

$$G(\theta_c)d\theta_c = \int_0^{2\pi} d\varphi P(\underline{\Omega}_c) \sin\theta_c d\theta_c \quad (16.3)$$

$$= \frac{1}{2} \sin\theta_c d\theta_c \quad (16.4)$$

Now we can write down the transformation from  $G(\theta_c)$  to the energy distribution in the outgoing energy. For the purpose of general discussion our notation system of labeling particles as 1 through 4 is not a good choice. It is more conventional to label the energy of the neutron before and after the collision as either  $E$  and  $E'$ , or vice versa. We will therefore switch notation at this point and let  $E_1 = E$  and  $E_3 = E'$ , and denote the probability distribution for  $E'$  as  $F(E \rightarrow E')$ . The transformation between  $G(\theta_c)$  and  $F(E \rightarrow E')$  is the same as that for any distribution function,

$$F(E \rightarrow E')dE' = G(\theta_c)d\theta_c \quad (16.5)$$

With  $G(\theta_c)$  given by (16.4) we obtain

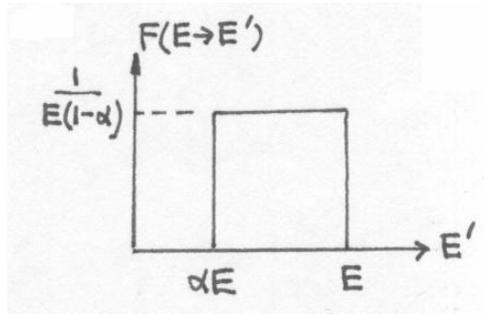
$$F(E \rightarrow E') = G(\theta_c) \left| \frac{d\theta_c}{dE'} \right| \quad (16.6)$$

The Jacobian of transformation can be readily evaluated from (15.13) after relabeling  $E_1$  and  $E_3$  as  $E$  and  $E'$ . Thus,

$$F(E \rightarrow E') = \frac{1}{E(1-\alpha)} \quad \alpha E \leq E' \leq E$$

$$= 0 \quad \text{otherwise} \quad (16.7)$$

The distribution, which is sketched in Fig. 16.1, is so simple that one can understand completely all its features. The distribution is uniform in the interval  $(\alpha E, E)$  because the scattering is spherically symmetric (independence of scattering angle translates into independence of outgoing energy because of the one-to-one correspondence). The fact that the outgoing energy can only lie in a particular interval follows from the range of scattering angle  $(0, \pi)$ . Since  $\alpha$  depends on the mass of the target, being zero for hydrogen and approaching unity as  $M \gg m$ , the interval can vary from  $(0, E)$  for hydrogen to a vanishing value as  $A \gg 1$ . In other words, the neutron can lose all its energy in one collision with hydrogen, and loses practically no energy if it collides with a



**Fig. 16.1.** Scattering frequency giving the probability that a neutron elastic scattered at energy  $E$  will have an energy in  $dE'$  about  $E'$ .

very heavy target nucleus. Although simple, the distribution is quite useful for the analysis of neutron energy moderation in the slowing down regime. It also represents a reference behavior for discussing conditions when it is no longer valid to assume the scattering is spherically symmetric in CMCS, or to assume the target nucleus is at rest. We will come back to these two situations later.

Notice that  $F$  is a distribution, so its dimension is the reciprocal of its argument, an energy.  $F$  is also properly normalized, its integral over the range of the outgoing energy is necessarily unity as required by particle conservation. Knowing the probability distribution  $F$  one can construct the energy differential cross section

$$\frac{d\sigma_s}{dE'} = \sigma_s(E)F(E \rightarrow E') \quad (16.7)$$

such that

$$\int dE' \frac{d\sigma_s}{dE'} = \sigma_s(E) \quad (16.8)$$

which is the ‘total’ (in the sense that it is the integral of a differential) scattering cross section. It is important to keep in mind that  $\sigma_s(E)$  is a function of the initial (incoming)

neutron energy, whereas the integration in (16.8) is over the final (outgoing) neutron energy. The quantity  $F(E \rightarrow E')$  is a distribution in the variable  $E'$  and also a function of  $E$ . We can multiply (16.7) by the number density of the target nuclei  $N$  to obtain

$$N\sigma_s(E)F(E \rightarrow E') \equiv \Sigma_s(E \rightarrow E') \quad (16.9)$$

which is sometimes known as the scattering kernel. As its name suggests, this is the quantity that appears in the neutron balance equation for neutron slowing down in an absorbing medium,

$$[\Sigma_s(E) + \Sigma_a(E)]\phi(E) = \int_E^{E/\alpha} dE' \Sigma_s(E' \rightarrow E)\phi(E') \quad (16.10)$$

where  $\phi(E) = vn(E)$  is the neutron flux and  $n(E)$  is the neutron number density.

Eq.(16.10) is an example of the usefulness of the energy differential scattering cross section (16.7).

The scattering distribution  $F(E \rightarrow E')$  can be used to calculate various energy-averaged quantities pertaining to elastic scattering. For example, the average loss for a collision at energy  $E$  is

$$\int_{\alpha E}^E dE' (E - E')F(E \rightarrow E') = \frac{E}{2}(1 - \alpha) \quad (16.11)$$

For hydrogen the energy loss in a collision is one-half its energy before the collision, whereas for a heavy nucleus it is  $\sim 2E/A$ .

### ***Angular Distribution of Elastically Scattered Neutrons***

We have already made use of the fact that for s-wave scattering the angular distribution is spherically symmetric in CMCS. This means that the angular differential scattering cross section in CMCS is of the form

$$\frac{d\sigma_s}{d\Omega_c} = \sigma_s(\theta_c) \equiv \sigma_s(E) \frac{1}{4\pi} \quad (16.12)$$

One can ask what is the angular differential scattering cross section in LCS? The answer can be obtained by transforming the results (16.12) from a distribution in the unit vector  $\underline{\Omega}_c$  to a distribution in  $\underline{\Omega}$ . As before (cf. (16.5)) we write

$$\sigma_s(\theta)d\Omega = \sigma_s(\theta_c)d\Omega_c \quad (16.13)$$

or

$$\sigma_s(\theta) = \sigma_s(\theta_c) \frac{\sin \theta_c}{\sin \theta} \frac{d\theta_c}{d\theta} \quad (16.14)$$

From the relation between  $\cos \theta$  and  $\cos \theta_c$ , (15.15), we can calculate

$$\frac{d(\cos \theta)}{d(\cos \theta_c)} = \frac{\sin \theta_c d\theta_c}{\sin \theta d\theta}$$

Thus

$$\sigma_s(\theta) = \frac{\sigma_s(E)}{4\pi} \frac{(\gamma^2 + 2\gamma \cos \theta_c + 1)^{3/2}}{1 + \gamma \cos \theta_c} \quad (16.15)$$

with  $\gamma = 1/A$ . Since (16.15) is a function of  $\theta$ , the factor  $\cos \theta_c$  on the right hand side should be expressed in terms of  $\cos \theta$  in accordance with (15.15). The angular distribution in LCS, as given by (16.15), is somewhat too complicated to sketch simply. From the relation between LCS and CMCS indicated in Fig. 15.2, we can expect that if the distribution is isotropic in LCS, then the distribution in CMCS should be peaked in the forward direction (simply because the scattering angle in LCS is always less than the angle in CMCS). One way to demonstrate that this is indeed the case is to calculate the average value of  $\mu = \cos \theta$ ,

$$\bar{\mu} = \frac{\int d\Omega \cos \theta \sigma_s(\theta)}{\int d\Omega \sigma_s(\theta)} = \frac{\int_{-1}^1 d\mu \mu \sigma_s(\mu)}{\int_{-1}^1 d\mu \sigma_s(\mu)} = \frac{\int_{-1}^1 d\mu_c \mu(\mu_c) \sigma_s(\mu_c)}{\int_{-1}^1 d\mu_c \sigma_s(\mu_c)} = \frac{2}{3A} \quad (16.16)$$

The fact that  $\bar{\mu} > 0$  means that the angular distribution is peaked in the forward direction. This bias becomes less pronounced the heavier the target mass; for  $A \gg 1$  the distinction between LCS and CMCS vanishes.

### ***Assumptions in Deriving $F(E \rightarrow E')$***

In arriving at the scattering distribution (also sometimes called the scattering frequency), (16.7), we have made use of three assumptions, namely,

- (i) elastic scattering
- (ii) target nucleus at rest
- (iii) scattering is isotropic in CMCS (s-wave)

These assumptions imply certain restrictions pertaining to the energy of incoming neutron  $E$  and the temperature of the scattering medium. Assumption (i) is valid provided the neutron energy is not high enough to excite the nuclear levels of the compound nucleus formed by the target nucleus plus the incoming neutron. On the other hand, if the neutron energy is high enough to excite the first nuclear energy level above the ground state, then inelastic scattering becomes energetically possible. Inelastic scattering is a threshold reaction ( $Q < 0$ ), it can occur in heavy nuclei at  $E \sim 0.05 - 0.1$  Mev, or in medium nuclei at  $\sim 0.1 - 0.2$  Mev. Typically the cross section for inelastic scattering,  $\sigma(n, n')$ , is of the order of 1 barn or less. In comparison with elastic scattering, which is always present no matter what other reactions can take place and is of order 5 – 10 barns except in the case of hydrogen where it is 20 barns as we have previously discussed.

Assumption (ii) is valid when the neutron energy is large compared to the kinetic energy of the target nucleus, typically taken to be  $k_B T$  assuming the medium is in equilibrium at temperature  $T$ . This would be the case for neutron energies  $\sim 0.1$  ev and above. When the incident neutron energy is comparable to the energy of the target

nucleus, the assumption of stationary target is clearly invalid. To take into account the thermal motions of the target, one should know what is the state of the target since the nuclear (atomic) motions in solids are different from those in liquids, vibrations in the former and diffusion in the latter. If we assume the scattering medium can be treated as a gas at temperature  $T$ , then the target nucleus moves in a straight line with a speed that is given by the Maxwellian distribution. In this case one can derive the scattering distribution which is an extension of (16.7) [see, for example, G. I. Bell and S. Glasstone, *Nuclear Reactor Theory* (Van Nostrand reinhold, New York 1970), p. 336]. We do not go into the details here except to show the qualitative behavior in Fig. 16.2. From the way the scattering distribution changes with incoming energy  $E$  one can get a good intuitive feeling for how the more general  $F(E \rightarrow E')$  evolves from a spread-out distribution (the curves for  $E = k_B T$ ) to the more restricted form given by (16.7).

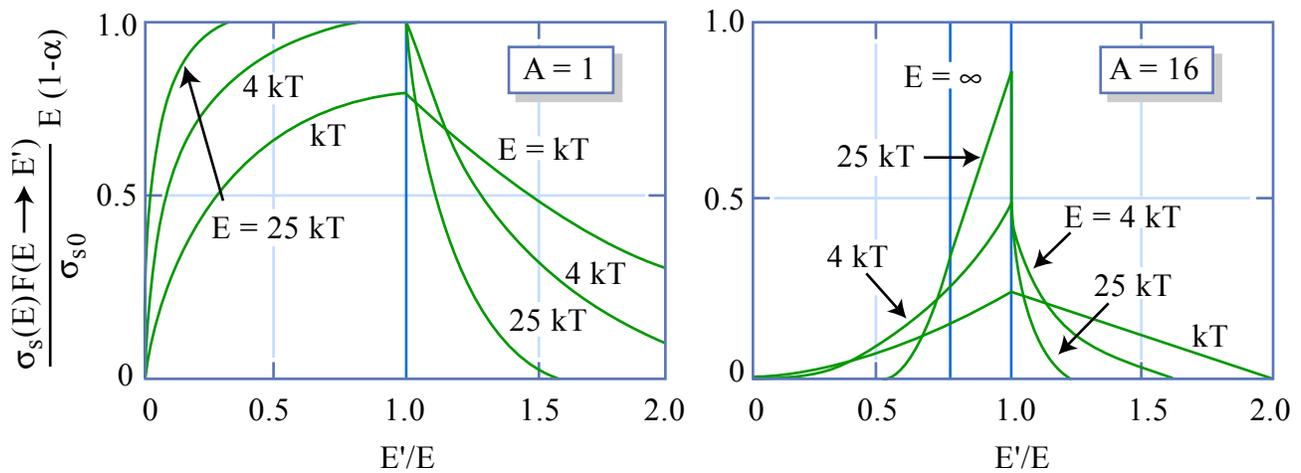


Figure by MIT OCW. Adapted from Bell and Glasstone.

**Fig. 16.2.** Energy distribution of elastically scattered neutrons in a gas of nuclei with mass  $A = M/m$  at temperature  $T$ . (from Bell and Glasstone)

Notice that for  $E \sim k_B T$  there can be appreciable upscattering which is not possible when assumption (ii) is invoked. As  $E$  becomes larger compared to  $k_B T$ , upscattering becomes less important. The condition of stationary nucleus also means that  $E \gg k_B T$ .

When thermal motions have to be taken into account, the scattering cross section  $\sigma_s(E)$  is also changed; it is no longer a constant,  $4\pi a^2$ , where  $a$  is the scattering length. This occurs in the energy region of neutron thermalization; it covers the range  $(0, 0.1 -$

0.5 eV). We will now discuss the energy dependence of  $\sigma_s(E)$ . For the case of the scattering medium being a gas of atoms with mass A and at temperature T, it is still relatively straightforward to work out the expression for  $\sigma_s(E)$ . We will give the essential steps to give the student some feeling for the kind of analysis that one can carry out even for more complicated situations such as neutron elastically in solids and liquids.

### ***Energy Dependence of Scattering Cross Section $\sigma_s(E)$***

When the target nucleus is not at rest, one can write down the expression for the elastic scattering cross section measured in the laboratory (we will call it the measured cross section),

$$v\sigma_{meas}(v) = \int d^3V |\underline{v} - \underline{V}| \sigma_{theo}(|\underline{v} - \underline{V}|) P(\underline{V}, T) \quad (16.17)$$

where  $v$  is the neutron speed in LCS,  $\underline{V}$  is the target nucleus velocity in LCS,  $\sigma_{theo}$  is the scattering cross section we calculate theoretically, such as what we had previously studied using the phase-shift method and solving the wave equation for an effective one-body problem (notice that the result is a function of the relative speed between neutron and target nucleus), and P is the thermal distribution of the target nucleus velocity which depends on the temperature of the medium. Eq.(16.17) is a general relation between what is calculated theoretically, in solving the effective one-body problem, and what is measured in the laboratory where one necessarily has only an average over all possible target nucleus velocities. What we call the scattering cross section  $\sigma_s(E)$  we mean  $\sigma_{meas}$ . It turns out that we can reduce (16.17) further by using for P the Maxwellian distribution and obtain the result

$$\sigma_s(v) = \frac{\sigma_{so}}{\beta^2} \left[ \left( \beta^2 + \frac{1}{2} \right) \text{erf}(\beta) + \frac{1}{\sqrt{\pi}} \beta e^{-\beta^2} \right] \quad (16.18)$$

where  $\text{erf}(x)$  is the error function integral

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x dt e^{-t^2} \quad (16.19)$$

and  $\beta^2 = AE/k_B T$ , and  $E = mv^2/2$ . Given that the error function has the limiting behavior for small and large arguments,

$$\operatorname{erf}(x) \sim \frac{2}{\sqrt{\pi}} \left( x - \frac{x^3}{3} + \dots \right) \quad x \ll 1 \quad (16.20)$$

$$1 - \frac{e^{-x^2}}{x\sqrt{\pi}} \left( 1 - \frac{1}{2x^2} + \dots \right) \quad x \gg 1$$

we have the two limiting behavior,

$$\sigma_s(v) \sim \sigma_{so} / v \quad \beta \ll 1 \quad (16.21)$$

$$\sigma_s(v) \sim \sigma_{so} \quad \beta \gg 1 \quad (16.22)$$

The physical significance of this calculation is that one sees the elastic scattering cross section has a  $1/v$  behavior at low energy (or high temperature) and a constant behavior at high energy. The expression (16.18) is therefore a useful expression giving the energy variation of the scattering cross section over the entire energy range from thermal to Mev, so far as elastic scattering is concerned. Note that this result has been obtained by assuming the target nuclei move as in a gas of noninteracting atoms. This assumption is not realistic when the scattering medium is a solid or a liquid. For these situations one can also work out the expressions for the cross section, but the results are more complicated (and beyond the scope of this course). We will therefore settle for a brief, qualitative look at what new features can be seen in the energy dependence of the elastic scattering cross sections of typical solids (crystals) and liquids.

Fig. 16.3 shows the total and elastic scattering cross sections of graphite ( $C^{12}$ ) over the entire energy range of interest to this class. At the very low-energy end we see a number of features we have not discussed previously. These all have to do with the fact that the target nucleus (atom) is bound to a crystal lattice and therefore the positions of the nuclei are fixed to well-defined lattice sites and the atomic motions are small-amplitude vibrations about these sites. There is a sharp drop of the cross section below an energy marked Bragg cutoff. Cutoff here refers to Bragg reflection which occurs when the condition for constructive interference (reflection) is satisfied, a condition that depends on the wavelength of the neutron (hence its energy) and the spacing between the lattice planes in the crystal. When the wavelength is too long (energies below the cutoff) for the Bragg condition to be satisfied, the cross section drops sharply. What is then left is the interaction between the neutron and the vibrational motions of the nuclei, this process involves the transfer of energy from the vibrations to the neutron which has much lower energy. Since there is more excitation of the vibrational modes at higher temperatures, this is reason why the cross section below the Bragg cutoff is very sensitive to temperature, increasing with increasing  $T$ .

Above the Bragg cutoff the cross section shows some oscillations. These correspond to the onset of additional reflections by planes which have smaller lattice spacings. At energies around  $k_{BT}$  the cross section approaches a constant value up to  $\sim 0.3$  Mev. This is the region where our previous calculation of cross section would apply. Between 0.3 and 1 Mev the scattering cross section decreases gradually, a behavior which we can still understand using simple theory (beyond what we had discussed). Above 1 Mev one sees scattering resonances, which we have not yet discussed; also there is now a difference between total and scattering cross sections (which should be attributed to absorption).

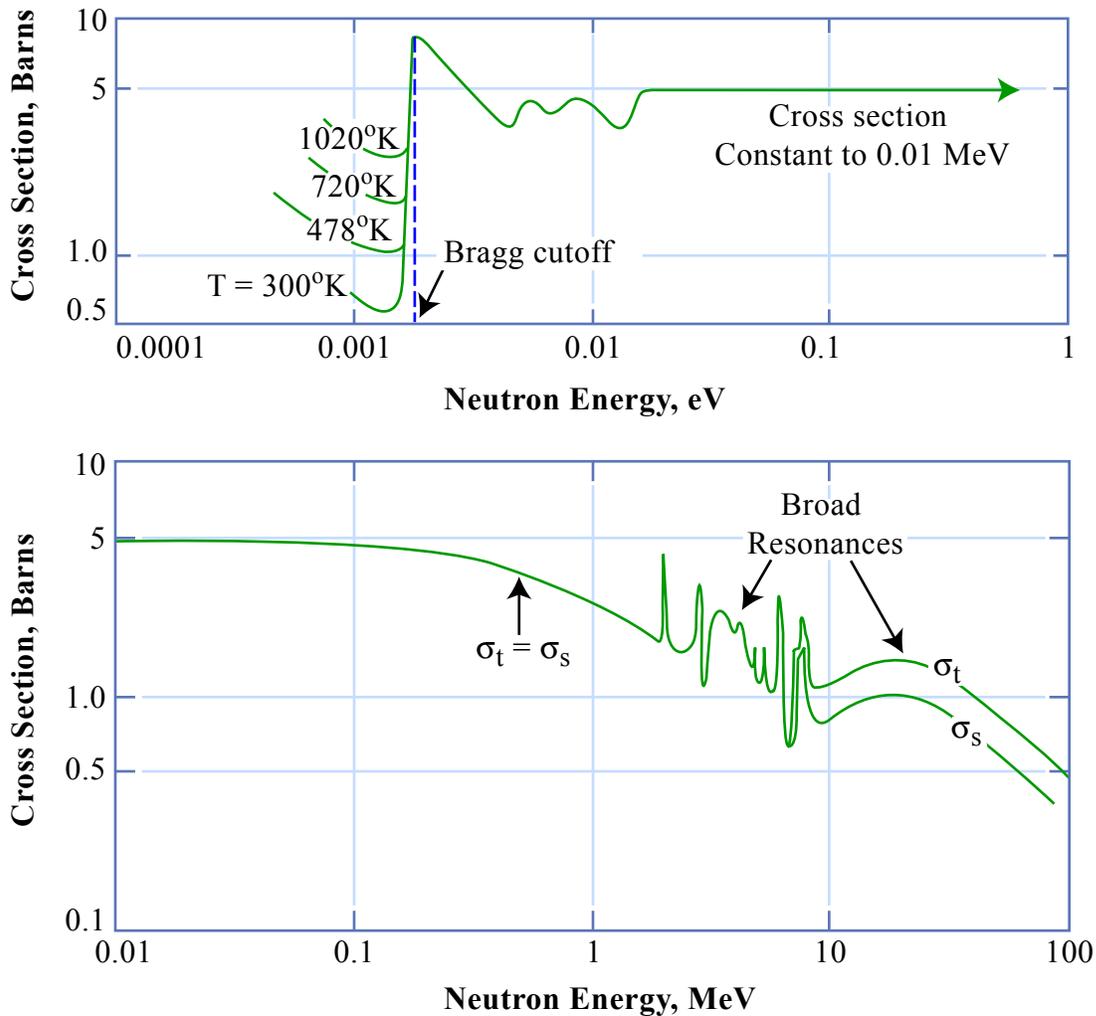


Figure by MIT OCW.

**Fig. 16.3.** Total and elastic scattering cross sections of  $C^{12}$  in the form of graphite. (from Lamarsh).

Fig. 16.4 shows the measured total cross section of  $H_2O$  in the form of water. The cross section is the sum of contributions from two hydrogen and an oxygen. Compared to Fig. 16.3 the low-energy behavior here is quite different. This is not unexpected since a crystal and a liquid are really very different with regard to their atomic structure and atomic motions. In the case of the liquid the cross section rises from a constant value at energies above 1 eV in a manner like the  $1/v$  behavior given by (16.21). Notice that the constant value of about 45 barns is just what we know from the hydrogen cross section  $\sigma_{so}$  of 20 barns per hydrogen and a cross section of about 5 barns for oxygen.

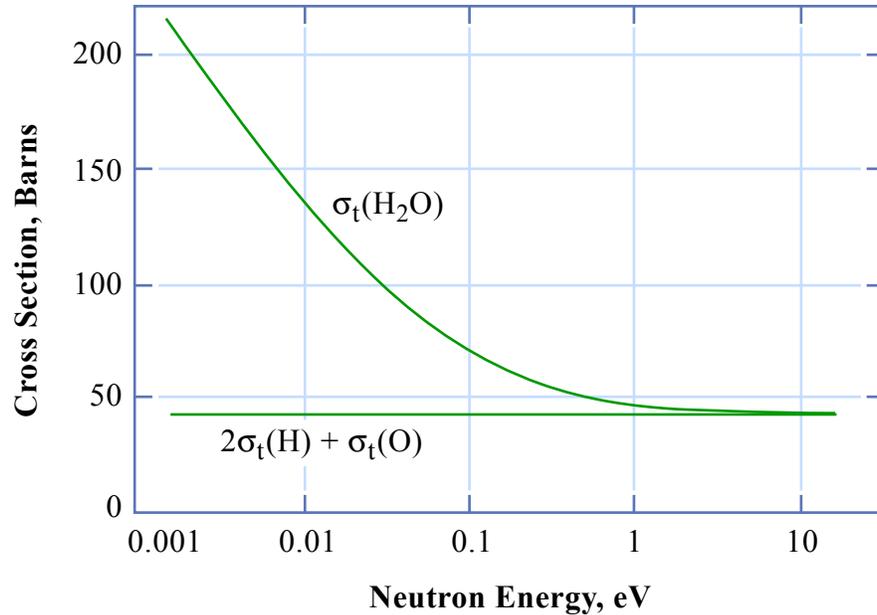


Figure by MIT OCW.

**Fig. 16.4.** Total cross section of water. (from Lamarsh)

The importance of hydrogen (water) in neutron scattering has led to another interpretation of the rise of the cross section with decreasing neutron energy, one which focuses on the effect of chemical binding. The idea is that at high energies (relative to thermal) the neutron does not see the water molecule. Instead it sees only the individual nuclei as targets which are free-standing and essentially at rest. In this energy range (1 eV and above) the interaction is the same as that between a neutron and free protons and oxygen nuclei. This is why the cross section is just the sum of the individual contributions.

When the cross section starts to rise as the energy decreases, this is an indication that the chemical binding of the protons and oxygen in a water molecule starts to have an effect. When the neutron energy is at  $k_{BT}$  the neutron now sees the entire water molecule rather than the individual nuclei. In that case the scattering is effectively between a neutron and a water molecule. What this means is that as the neutron energy decreases the target changes from individual nuclei with their individual mass to a water molecule with mass 18. Now one can show the scattering cross section is actually proportional to the square of the reduced mass of the scatterer  $\mu$ ,

$$\sigma_s \propto \mu^2 = \left( \frac{mM}{m+M} \right)^2 = \left( \frac{A}{A+1} \right)^2 \quad (16.23)$$

One can define a *free-atom* cross section appropriate for the energy range where the cross section is a constant, and a *bound-atom* cross section for the energy range where the cross section is rising, with the relation

$$\sigma_{free} = \sigma_{bound} \left( \frac{A}{A+1} \right)^2 \quad (16.24)$$

For hydrogen these two cross sections would have the values of 20 barns and 80 barns respectively.

We close this chapter with a brief consideration of assumption (iii) used in deriving (16.7). When the neutron energy is in the 10 Kev range and higher, the contributions from the higher angular momentum (p-wave and above) scattering may become significant. In that case we know the angular distribution will be more forward peaked. This means one should replace (16.1) by a different form of  $P(\underline{\Omega}_c)$ . Without going through any more details, we show in Fig. 16.5 the general behavior that one can expect in the scattering distribution  $F$  when scattering in CMCS is no longer isotropic.

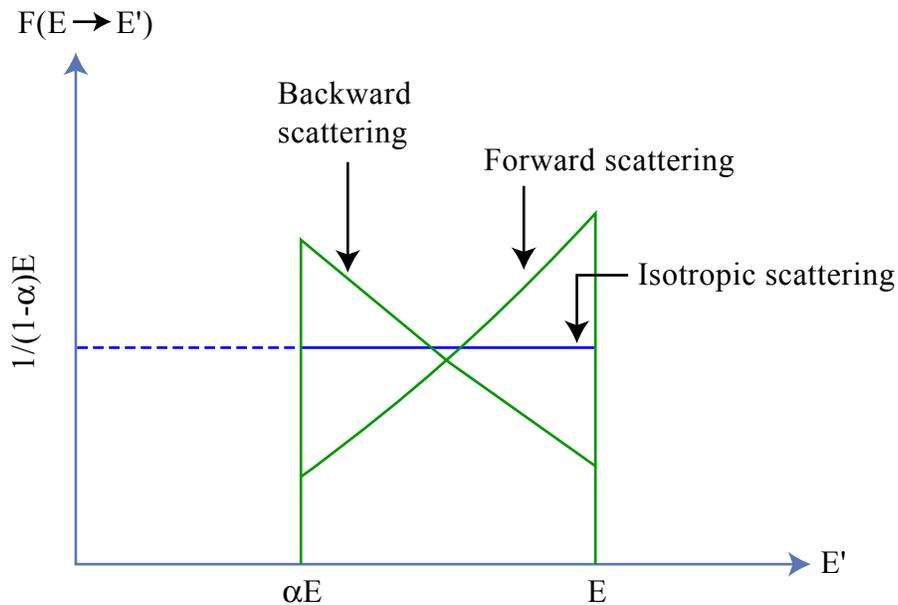


Figure by MIT OCW.

**Fig. 16.5.** Energy distribution of elastically scattered neutrons by a stationary nucleus. (from Lamarsh)