1

Introduction

1.1 Basic properties of the neutron

With the advent of nuclear reactors, thermal neutrons have become a valuable tool for investigating many important features of matter – particularly condensed matter. The usefulness of thermal neutrons arises from the basic properties of the neutron. These are listed in Table 1.1.

The value of the mass of the neutron results in the de Broglie wavelength of thermal neutrons being of the order of interatomic distances in solids and liquids. Thus, interference effects occur which yield information on the structure of the scattering system.

Secondly, the fact that the neutron is uncharged means, not only that it can penetrate deeply into the target, but also that it comes close to the nuclei – there is no Coulomb barrier to be overcome. Neutrons are thus scattered by nuclear forces, and for certain nuclides the scattering is large. An important example is light hydrogen which is virtually transparent to X-rays but which scatters neutrons strongly.

Thirdly, the energy of thermal neutrons is of the same order as that of many excitations in condensed matter. So when the neutron is inelastically scattered by the creation or annihilation of an excitation, the change in the energy of the neutron is a large fraction of its initial energy. Measurement of the neutron energies thus provides accurate information on the energies of the excitations, and hence on the interatomic forces.

Fourthly, the neutron has a magnetic moment, which means that neutrons interact with the unpaired electrons in magnetic atoms. Elastic scattering from this interaction gives information on the arrangement of electron spins and the density distribution of unpaired electrons. Inelastic magnetic scattering gives the energies of

Table 1.1 Basic properties of the neutron and values of physical constants

Basic properties of neutron	
mass	$m = 1.675 \times 10^{-27}$ kg
charge	0
spin	$\frac{1}{2}$
magnetic dipole moment	$\mu_n = -1.913\ \mu_N$
Values of physical constants	
elementary charge	$e = 1.602 \times 10^{-19}$ C
mass of electron	$m_e = 9.109 \times 10^{-31}$ kg
mass of proton	$m_p = 1.673 \times 10^{-27}$ kg
Planck constant	$h = 6.626 \times 10^{-34}$ J s
Boltzmann constant	$k_B = 1.381 \times 10^{-23}$ J K^{-1}
Avogadro constant	$N_A = 6.022 \times 10^{23}$ mol^{-1}
Bohr magneton	$\mu_B = 9.274 \times 10^{-24}$ J T^{-1}
nuclear magneton	$\mu_N = 5.051 \times 10^{-27}$ J T^{-1}

magnetic excitations, and in general permits a study of time-dependent spin correlations in the scattering system.

It is convenient to develop the theories of nuclear and magnetic scattering separately. Thus Chapters 1 to 6 of the book are concerned mainly with nuclear scattering, though the definitions in Chapter 1 and the theoretical development in Chapter 2 give basic results that apply to both types of scattering. Chapters 7 and 8 are devoted to magnetic scattering. Chapter 9 deals with polarisation effects and includes both nuclear and magnetic scattering.

1.2 Numerical values for velocity, energy, wavelength

At present the source of thermal neutrons in most scattering experiments is a nuclear reactor. In the thermal region, the velocity spectrum of the neutrons emerging from the reactor is close to Maxwellian, with the temperature T that of the moderator.

The Maxwellian distribution for flux is

$$\phi(v) \propto v^3 \exp(-\tfrac{1}{2}mv^2/k_B T), \tag{1.1}$$

where $\phi(v)\,dv$ is the number of neutrons through unit area per second with velocities between v and $v+\mathrm{d}v$, m is the mass of the neutron, and k_B is the Boltzmann constant. The maximum of the function $\phi(v)$ occurs at

$$v=\left(\frac{3k_BT}{m}\right)^{1/2}, \tag{1.2}$$

which corresponds to a kinetic energy

$$E=\tfrac{1}{2}mv^2=\tfrac{3}{2}k_BT. \tag{1.3}$$

It is conventional to say that a neutron with energy E corresponds to a temperature T, given by

$$E=k_BT. \tag{1.4}$$

The de Broglie wavelength of a neutron with velocity v is

$$\lambda=\frac{h}{mv}, \tag{1.5}$$

where h is the Planck constant. The wavevector $\boldsymbol{k}$ is defined to have magnitude

$$k=\frac{2\pi}{\lambda}, \tag{1.6}$$

its direction being that of $\boldsymbol{v}$. The momentum of the neutron is

$$\boldsymbol{p}=\hbar\boldsymbol{k}. \tag{1.7}$$

We thus have

$$E=k_BT=\tfrac{1}{2}mv^2=\frac{h^2}{2m\lambda^2}=\frac{\hbar^2k^2}{2m}. \tag{1.8}$$

Inserting the values of the constants m, e, h, k_B in Table 1.1 in (1.8) gives the following relations between the wavelength, wavevector, velocity, energy, and temperature for thermal neutrons:

$$\begin{aligned}\lambda&=6.283\frac{1}{k}=3.956\frac{1}{v}=9.045\frac{1}{\sqrt{E}}=30.81\frac{1}{\sqrt{T}},\\ E&=0.08617T=5.227v^2=81.81\frac{1}{\lambda^2}=2.072k^2.\end{aligned} \tag{1.9}$$

In these equations, λ is in Å, k in $10^{10}\,\mathrm{m}^{-1}$, v in $\mathrm{km\,s^{-1}}$, E in meV, and T in kelvin.

The value $v=2.20\,\mathrm{km\,s^{-1}}$ is conventionally taken as a standard velocity for thermal neutrons. For example, the absorption cross-section is usually proportional to $1/v$, and its value is then quoted

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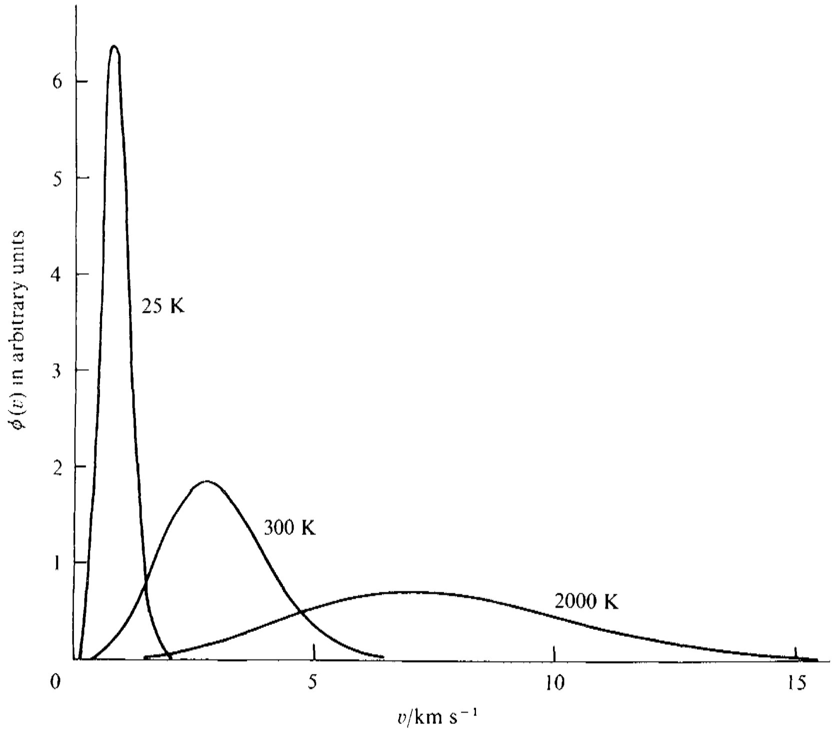
for this value of v. For the standard velocity

$$v = 2.20\ \text{km s}^{-1}, \qquad \frac{1}{v} = 455\ \mu\text{s m}^{-1},$$
$$E = 25.3\ \text{meV}, \qquad T = 293\ \text{K}, \qquad (1.10)$$
$$\lambda = 1.798\ \text{Å}, \qquad k = 3.49 \times 10^{10}\ \text{m}^{-1}.$$

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

Fig. 1.1 Maxwellian flux distribution $\phi(v) \propto v^3 \exp(-mv^2/2k_{\mathrm{B}}T)$ for $T = 25$, 300, 2000 K. The curves are normalised to have the same area.



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temperature. In the high-flux reactor at the Laue–Langevin Institute in Grenoble, a vessel containing 25 litres of liquid deuterium acts as a cold moderating source, providing a velocity distribution with $T \sim 25$ K, while a block of hot graphite of about half this volume provides a distribution with $T \sim 2000$ K. Curves of the velocity distribution for $T = 25$, 300, and 2000 K are shown in Fig. 1.1. The approximate ranges for energy, temperature, and wavelength of the neutrons for the three types of source are given in Table 1.2.

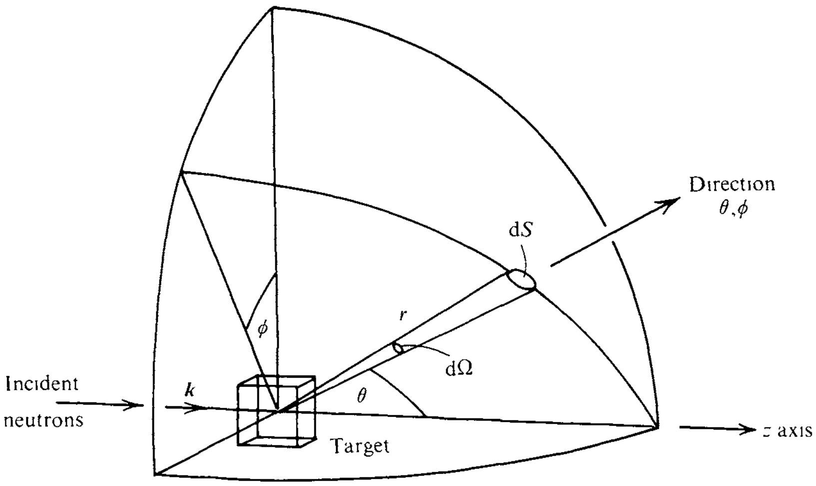
Table 1.2 Approximate values for the range of energy, temperature, and wavelength for three types of source in a reactor

Source	Energy E/meV	Temperature T/K	Wavelength $\lambda/10^{-10}$ m
cold	0.1– 10	1– 120	30–3
thermal	5–100	60–1000	4–1
hot	100–500	1000–6000	1–0.4

1.3 Definitions of scattering cross-sections

Consider a beam of thermal neutrons, all with the same energy E, incident on a target (Fig. 1.2). The target is a general collection of

Fig. 1.2 Geometry for scattering experiment.



atoms – it may be a crystal, an amorphous solid, a liquid, or a gas. We shall call it the *scattering system*. Various types of measurement can be made on the neutrons after they have interacted with the scattering system. The results in each case can be expressed in terms of a quantity known as a *cross-section*.

Suppose we set up a neutron counter and measure the number of neutrons scattered in a given direction as a function of their energy E'. The distance of the counter from the target is assumed to be large compared to the dimensions of the counter and the target, so the small angle $d\Omega$ subtended by the counter at the target is well defined. To specify the geometry of the scattering process we use polar coordinates, taking the direction of the incident neutrons as the polar axis. Let the direction of the scattered neutrons be θ, ϕ. The *partial differential cross-section* is defined by the equation

$$\frac{d^2\sigma}{d\Omega\, dE'} = \text{(number of neutrons scattered per second into a small solid angle } d\Omega \text{ in the direction } \theta, \phi \text{ with final energy between } E' \text{ and } E'+dE')/\Phi\, d\Omega\, dE', \qquad (1.11)$$

where Φ is the flux of the incident neutrons, i.e. the number through unit area per second, the area being perpendicular to the direction of the neutron beam. Note that the dimensions of the numerator on the right-hand side of the equation are [time^{-1} energy]. The dimensions of flux are [area^{-1} time^{-1}]. Thus the dimensions of the cross-section are [area], as we would expect from the name.

Suppose we do not analyse the energy of the scattered neutrons, but simply count all the neutrons scattered into the solid angle $d\Omega$ in the direction θ, ϕ. The cross-section corresponding to these measurements, known as the *differential cross-section*, is defined by

$$\frac{d\sigma}{d\Omega} = \text{(number of neutrons scattered per second into } d\Omega \text{ in the direction } \theta, \phi)/\ \Phi\, d\Omega. \qquad (1.12)$$

The *total scattering cross-section* is defined by the equation

$$\sigma_{\text{tot}} = \text{(total number of neutrons scattered per second)}/\ \Phi. \qquad (1.13)$$

By 'total number' we mean the number scattered in all directions.

From their definitions the three cross-sections are related by the following equations

$$\frac{d\sigma}{d\Omega} = \int_0^\infty \left(\frac{d^2\sigma}{d\Omega\, dE'}\right) dE', \qquad (1.14)$$

$$\sigma_{\text{tot}} = \int_{\text{all directions}} \left(\frac{d\sigma}{d\Omega}\right) d\Omega. \tag{1.15}$$

If the scattering is axially symmetric, i.e. if $d\sigma/d\Omega$ depends only on θ and not on ϕ, the last equation becomes

$$\sigma_{\text{tot}} = \int_0^\pi \frac{d\sigma}{d\Omega} 2\pi \sin\theta \, d\theta. \tag{1.16}$$

The cross-sections are the quantities actually measured in a scattering experiment. The basic problem, with which this whole book is concerned, is to derive theoretical expressions for these quantities. Experimental cross-sections are quoted per atom or per molecule, i.e. the cross-sections defined above are divided by the number of atoms or molecules in the scattering system.

The present cross-sections do not take account of the initial and final spin states of the neutron. The definitions are extended to do this in Chapter 9 when we consider polarisation experiments.

1.4 Scattering of neutrons by a single fixed nucleus

The definitions of cross-sections apply to any kind of scattering. We now consider a simple case – nuclear scattering by a single nucleus fixed in position. The nuclear forces which cause the scattering have a range of about 10^{-14} to 10^{-15} m. The wavelength of thermal neutrons is of the order of 10^{-10} m, and is thus much larger than the range of the forces. In these circumstances the scattering, analysed in terms of partial waves, comes entirely from the S waves ($l = 0$). The angular distribution for S-wave scattering is spherically symmetric. We do not need the theory of partial waves to see that the angular distribution has this form. It is a basic result from diffraction theory that if waves of any kind are scattered by an object small compared to the wavelength of the waves, then the scattered wave is spherically symmetric.

We take the origin to be at the position of the nucleus, and the z axis to be along the direction of $\boldsymbol{k}$, the wavevector of the incident neutrons (Fig. 1.2). Then the incident neutrons can be represented by the wavefunction

$$\psi_{\text{inc}} = \exp(ikz). \tag{1.17}$$

As the scattering is spherically symmetric, the wavefunction of the scattered neutrons at the point $\boldsymbol{r}$ can be written in the form

$$\psi_{sc} = -\frac{b}{r}\exp(ikr), \tag{1.18}$$

where b is a constant, independent of the angles θ, ϕ. The minus sign in the equation is arbitrary and corresponds to a positive value of b for a repulsive potential (see Section 2.3).

Note that the magnitude of the wavevector is the same for the scattered and incident neutrons. The energy of thermal neutrons is too small to change the internal energy of the nucleus. And since we are taking the position of the nucleus to be fixed, the neutron cannot give the nucleus kinetic energy. Thus the scattering is elastic. The energy of the neutron, and hence the magnitude of $\boldsymbol{k}$, is unchanged.

The quantity b in ψ_{sc} is known as the *scattering length*. We may distinguish two types of nucleus. In the first type the scattering length is complex and varies rapidly with the energy of the neutron. The scattering for such nuclei is a resonance phenomenon and is associated with the formation of a compound nucleus (original nucleus plus neutron) with energy close to an excited state. Examples of nuclei which show this behaviour are ^{103}Rh, ^{113}Cd, ^{157}Gd, and ^{176}Lu. Since the imaginary part of the scattering length corresponds to absorption, such nuclei strongly absorb neutrons. The majority of nuclei are of the second type, in which the compound nucleus is not formed near an excited state. The imaginary part of the scattering length is small, and the scattering length is independent of the energy of the neutron. We shall confine the discussion to such nuclei and take the scattering length to be a real quantity.

The value of the scattering length depends on the particular nucleus (i.e. nuclide), and the spin state of the nucleus–neutron system. The neutron has spin $\frac{1}{2}$. Suppose the nucleus has spin I (not zero). Then the spin of the nucleus–neutron system is either $I+\frac{1}{2}$, or $I-\frac{1}{2}$. Each spin state has its own value of b. So every nucleus with non-zero spin has two values of the scattering length. If the spin of the nucleus is zero, the nucleus–neutron system can only have spin $\frac{1}{2}$, and there is only one value of the scattering length.

If we had a proper theory of nuclear forces we would be able to calculate or predict the values of b from other properties of the nucleus. But we do not have such a theory, so we have to treat the scattering lengths as parameters to be determined experimentally. If the nuclides are arranged according to their Z, N values the values of b vary erratically from one nuclide to its neighbour. The actual values have important practical consequences, which we shall see later. A selection of values is given in Table 1.3.

Table 1.3 Values of scattering lengths

Nuclide	Combined spin	b/fm	Nuclide	Combined spin	b/fm
^{1}H	1	10.85	^{23}Na	2	6.3
	0	−47.50		1	−0.9
^{2}H	$\frac{3}{2}$	9.53	^{59}Co	4	−2.78
	$\frac{1}{2}$	0.98		3	9.91

The values for H, Na, and Co are from Koester (1977), Abragam *et al.* (1975), and Koester *et al.* (1974) respectively. The spin values refer to the nucleus–neutron system.

We can readily calculate the cross-section $d\sigma/d\Omega$ for scattering from a single fixed nucleus, using the expressions for ψ_{inc} and ψ_{sc} in (1.17) and (1.18). If v is the velocity of the neutrons (the same before and after scattering), the number of neutrons passing through the area dS per second is

$$v\, dS|\psi_{sc}|^2 = v\, dS\frac{b^2}{r^2} = vb^2\, d\Omega \tag{1.19}$$

(see Fig. 1.2). The flux of incident neutrons is

$$\Phi = v|\psi_{inc}|^2 = v. \tag{1.20}$$

From the definition of the cross-section

$$\frac{d\sigma}{d\Omega} = \frac{vb^2\, d\Omega}{\Phi\, d\Omega} = b^2, \tag{1.21}$$

and in this simple case

$$\sigma_{tot} = 4\pi b^2. \tag{1.22}$$

2

Nuclear scattering – basic theory

2.1 Introduction

We now start on the theory proper and consider the nuclear scattering by a general system of particles. We first derive a general expression for the cross-section $d^2\sigma/d\Omega\, dE'$ for a specific transition of the scattering system from one of its quantum states to another. Although the calculation relates to nuclear scattering there will be no difficulty in applying the basic formula (2.15) to the magnetic case. We start by ignoring the spin of the neutron. This means that the state of the neutron is specified entirely by its momentum, i.e. by its wavevector.

Suppose we have a neutron with wavevector $\boldsymbol{k}$ incident on a scattering system in a state characterised by an index λ. Denote the wavefunction of the neutron by $\psi_{\boldsymbol{k}}$ and of the scattering system by χ_λ. Suppose the neutron interacts with the system via a potential V, and is scattered so that its final wavevector is $\boldsymbol{k}'$. The final state of the scattering system is λ'.

We set up a coordinate system with the origin at some arbitrary point in the scattering system. Denote the number of nuclei in the scattering system by N. Let $\boldsymbol{R}_j$ $(j=1,\ldots N)$ be the position vector of the jth nucleus, and $\boldsymbol{r}$ that of the neutron (Fig. 2.1).

2.2 Fermi's golden rule

Consider the differential scattering cross-section $(d\sigma/d\Omega)_{\lambda\to\lambda'}$, representing the sum of all processes in which the state of the scattering system changes from λ to λ', and the state of the neutron changes from $\boldsymbol{k}$ to $\boldsymbol{k}'$. The sum is taken over all values of $\boldsymbol{k}'$ that lie in the small solid angle $d\Omega$ in the direction θ, ϕ, the values of $\boldsymbol{k}$, λ, and λ' remaining constant (Fig. 2.2). From the definition of $d\sigma/d\Omega$ given in