Part I

Basics of neutron scattering

Chapter 1

Introduction to neutron scattering

Neutron scattering is one of the most powerful and versatile experimental methods to study the structure and dynamics of materials on the atomic and nanometer scale. Quoting the Nobel committee, when awarding the prize to C. Shull and B. Brockhouse in 1994, these pioneers have "helped answer the question of where atoms are and ... the question of what atoms do" [4].

Neutron scattering is presently used by more than 5000 researchers worldwide, and the scope of the method is continuously broadening. In the 1950'ies and 1960'ies, neutron scattering was an exotic tool in Solid State Physics and Chemical Crystallography, but today it serves communities as diverse as Biology, Earth Sciences, Planetary Science, Engineering, Polymer Chemistry, and Cultural Heritage. In brief, neutrons are used in all scientific fields that deal with hard, soft, or biological materials.

It is, however, appropriate to issue a warning already here. Although neutron scattering is a great technique, it is also time-consuming and expensive. Neutron scattering experiments last from hours to days and are performed at large international facilities. Here, the running costs correspond to several thousand Euros per instrument day. Hence, neutron scattering should be used only where other methods are inadequate.

For the study of atomic and nanometer-scale structure in materials, X-ray scattering is the technique of choice. X-ray sources are by far more abundant and are, especially for synchrotron X-ray sources, much stronger than neutron sources. Hence, the rule of thumb goes: "If an experiment can be performed with X-rays, use X-rays". For an introduction to X-ray scattering, see, *e.g.*, the excellent recent textbook by D. F. McMorrow and J. Als-Nielsen [5].

However, neutrons have a number of properties that make them extremely useful for purposes where X-rays are not sufficient. This chapter is devoted to presenting the properties of the neutron and describing the essential differences between neutron and X-ray scattering.

1.1 Basic properties of the neutron

The neutron is a nuclear particle with a mass rather close to that of the proton [6]

$$m_\mathrm{n} = 1.675 \cdot 10^{-27}\,\mathrm{kg}. \tag{1.1}$$

The neutron does not exist naturally in free form, but decays into a proton, an electron, and an anti-neutrino. The neutron lifetime, $\tau = 886$ s [7], is much longer than the time a neutron spends within a scattering experiment, which is merely a fraction of a second. Hence, neutron decay can typically be neglected in experiments.

The neutron is electrically neutral but still possesses a magnetic moment

$$\mu = \gamma \mu_\mathrm{N}, \tag{1.2}$$

where $\gamma = -1.913$ is the neutron magnetogyric ratio and the nuclear magneton is given by $\mu_\mathrm{N} = e\hbar/m_\mathrm{p} = 5.051 \cdot 10^{-27}$ J/T. The neutron magnetic moment is coupled antiparallel to its spin, which has the value $s = 1/2$.

The neutron interacts with nuclei via the strong nuclear force and with magnetic moments via the electromagnetic force. Most of this text deals with the consequences of these interactions; *i.e.* the scattering and absorption of neutrons by atoms and nuclei inside materials, as well as reflection from surfaces and interfaces.

1.2 Particle-wave duality

One of the remarkable consequences of quantum mechanics is that matter has both particle- and wave-like nature [8]. The neutron is no exception from this. In neutron scattering experiments, neutrons behave predominantly as particles when they are created in a nuclear process, as interfering waves when they are scattered, and again as particles when they are detected by another nuclear process.

To be more specific on the wave nature of matter, a particle moving with constant velocity, v, can be ascribed a corresponding (de-Broglie) wavelength, given by

$$\lambda = \frac{2\pi\hbar}{mv}. \tag{1.3}$$

In neutron scattering, the wave nature is often referred to in terms of the neutron *wave number*,

$$\boxed{k = 2\pi/\lambda}, \tag{1.4}$$

or the *wave vector* of length k and with same direction as the velocity:

$$\mathbf{k} = \frac{m_\mathrm{n}\mathbf{v}}{\hbar}. \tag{1.5}$$

By tradition, wavelengths are measured in Å (10^{-10} m), and wave numbers in Å^{-1}, while the neutron velocity is measured in SI units: m/s. For our purpose

	v [ms^{-1}]	λ^{-1} [Å^{-1}]	k [Å^{-1}]	$\sqrt{E}$ [meV$^{1/2}$]
v [ms^{-1}]	1	2.528×10^{-4}	1.588×10^{-3}	2.286×10^{-3}
λ^{-1} [Å^{-1}]	3956	1	6.283	9.045
k [Å^{-1}]	629.6	0.1592	1	1.440
$\sqrt{E}$ [meV$^{1/2}$]	437.4	0.1106	0.6947	1

Table 1.1: Conversion table between different neutron parameters in the most commonly used units. Examples of use: $v\,[\mathrm{ms}^{-1}] = 629.6\,k\,[\text{Å}^{-1}]$ and $(\lambda[\text{Å}])^{-1} = 0.1106\sqrt{E[\mathrm{meV}]}$. Adapted from Ref. [3].

Energy interval	λ interval	Common name	Usual origin
less than 0.05 meV	> 40 Å	ultra cold	special sources below 4 K
0.05 meV - 14 meV	2.4 - 40 Å	cold	H_2 moderators at 25 K
14 meV - 200 meV	0.6 - 2.4 Å	thermal	H_2O moderators at 300 K
200 meV - 1 eV	0.3 - 0.6 Å	hot	graphite moderators at 2000 K
1 eV - 10 keV	< 0.3 Å	epithermal	background from moderators

Table 1.2: Common names for neutron energy ranges, and typical origin of neutrons with these energies. The "standard" thermal energy is 25 meV, corresponding to $\lambda_{\rm th} = 1.798$ Å, or $v_{\rm th} = 2200$ m/s.

we consider the neutrons as non-relativistic, and the neutron kinetic energy is given by

$$\boxed{E = \frac{\hbar^2 k^2}{2m_{\rm n}}}, \tag{1.6}$$

which is measured in eV or meV, where 1 eV$= 1.602 \cdot 10^{-19}$ J. A useful conversion table between velocity, wave number, wavelength, and energy, is shown in Table 1.1.

1.3 Neutron scattering facilities

Neutron sources with flux densities adequate for neutron scattering investigations of materials are based on one of two principles, also illustrated in Fig. 1.1:

- **Fission.** A high continuous flux of neutrons is produced in the core of a conventional fission reactor.
- **Spallation.** A pulsed production of neutrons is obtained by bombarding a target of heavy elements with high-energy particles, typically accelerated protons.

Common to both types of sources is that neutrons are moderated to "thermal" or "cold" velocities close to the source and then transported to the neutron scattering instruments in neutron guide systems. For the naming of neutron energy intervals, see Table 1.2.

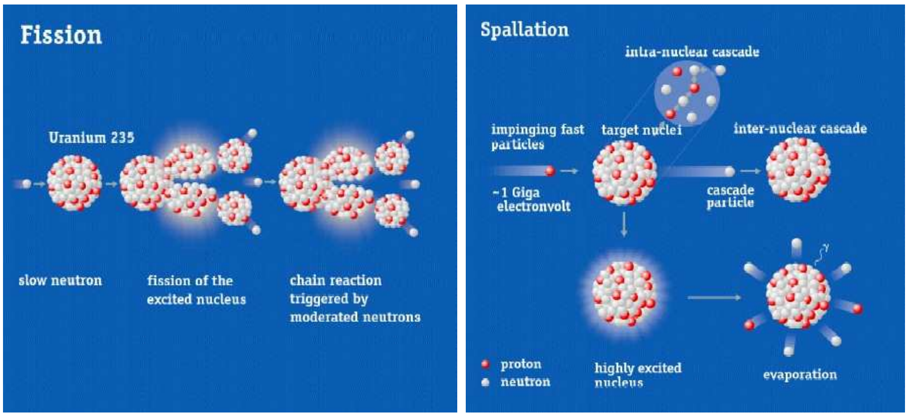

Figure 1.1: The two main methods of neutron production. Left: Traditional nuclear reactors make use of production of neutrons for maintaining the chain reaction; surplus of neutrons can be used for neutron scattering. Right: Protons accelerated into the GeV regime can split heavy nuclei with a large neutron surplus, creating free neutrons among the reaction products.

Both types of neutron sources are built as dedicated facilities, each hosting tens of instruments. All major sources are user facilities, meaning that they serve a research community much larger than the staff affiliated with the facilities. Typically, user experiments are selected through a competitive proposal system.

At the time of writing, more than twenty neutron facilities are in operation worldwide, the most important being the reactor source ILL, Grenoble, France, and the spallation source ISIS, Oxfordshire, UK. However, the European dominance is challenged by the powerful, newly commissioned spallation sources: Spallation Neutron Source (SNS), Oak Ridge, USA, and Japan Proton Accelerator Research Complex (J-PARC), Tokai, Japan [9]. For this and other reasons, it was has long been proposed to build a European Spallation Source (ESS). In 2009, it was decided to initiate the construction of this source, by deciding upon a location close to Lund, Sweden[10].

A list of the most significant neutron sources is given in Chapter 3.

1.4 Five reasons for using neutrons

At last in this introductory chapter, we will present some of the assets of neutron scattering. We will focus on cases where neutrons can be preferred to X-rays or where neutrons are needed to complement X-rays. It is commonly agreed in the neutron scattering community that this can be formulated in five general points:

1. **Energy and wavelength.** Thermal neutrons have a wavelength (around 1.8 Å) similar to inter-atomic distances, and an energy (around 25 meV)

similar to elementary excitations in solids. One can thus obtain simultaneous information on the structure and dynamics of materials and *e.g.* measure dispersion relations (energy-wavelength dependence) of excitations in crystalline solids.

2. **Isotopes and light elements.** The neutron scattering cross section varies in an almost random fashion between elements and even between different isotopes of the same element. One can thus use neutrons to study light isotopes. In particular, this is important for hydrogen, which is almost invisible to X-rays. With neutrons, the large difference in scattering between usual hydrogen (^{1}H) and deuterium, (^{2}D) can be used in biological and soft matter sciences to change the contrast in the scattering and also "highlight" selected groups within large molecules or aggregates.

3. **Quantitative experiments.** The interaction between neutrons and (most) matter is rather weak, implying that neutrons can probe the bulk of the sample, and not only its surface. The weak interaction also diminishes higher order effects. Hence, quantitative comparisons between neutron scattering data and theoretical models can be performed to a high precision.

4. **Transparency.** Since neutrons penetrate matter easily, neutron scattering can be performed with samples stored in all sorts of sample environment: Cryostats, magnets, furnaces, pressure cells, *etc.* Furthermore, very bulky samples can be studied, up to tens of cm thickness, depending on their elemental composition, and the sample is left relatively unharmed by the neutron experiment, although beam experiments should still not be performed on living organisms.

5. **Magnetism.** The neutron magnetic moment makes neutrons scatter from magnetic structures or magnetic field gradients. Unpolarized neutrons are used to learn about the periodicity and magnitude of the magnetic order, while scattering of spin-polarized neutrons can reveal the direction of the atomic magnetic moments.

In most cases, neutron scattering is performed in combination with other experimental techniques; often with neutron scattering as one of the final techniques to be applied before conclusions can be drawn.

1.5 On these notes

After this brief introduction, we will continue the introductory part by presenting the formalism of the neutron scattering process (chapter 2). In part II, we go into details with neutron sources, moderators, and guide systems (chapter 3), components for neutron optics and instruments (chapter 4), and with Monte Carlo ray-tracing techniques for simulating the effect of the combined geometry of neutron scattering instruments (chapter 5).

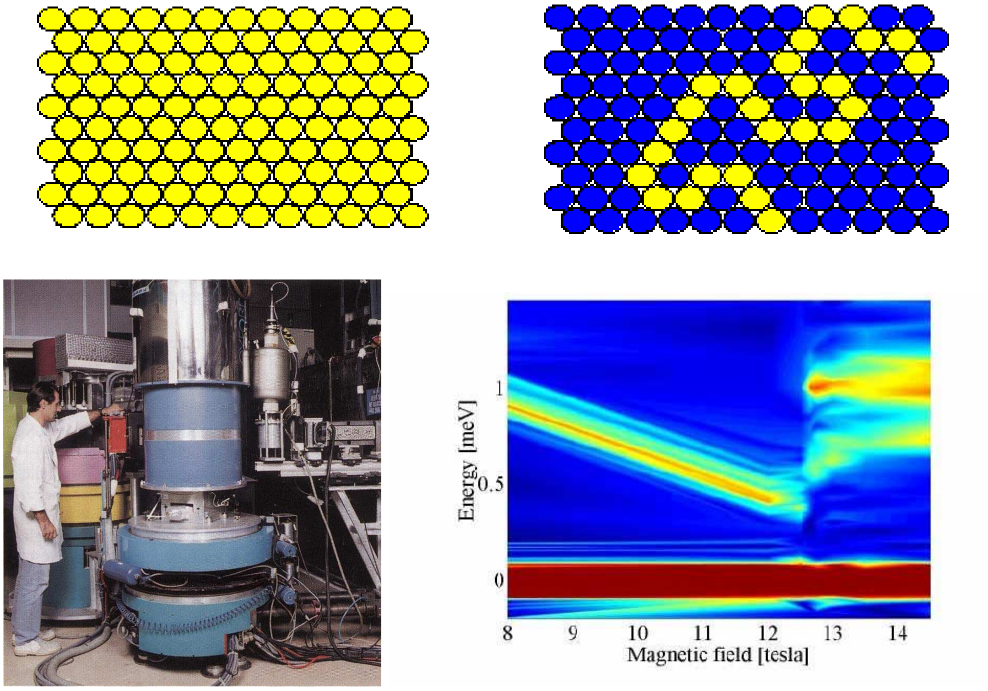

Figure 1.2: Illustration of two of the "five reasons" for neutron scattering. Top row shows schematically the neutron visibility of one polymer chain in two different solutions (left) hydrogenous solvent, (right) deuterated solvent. The enhanced contrast from the deuterated solvent gives a significant effect in a small-angle scattering experiment. Bottom row shows the measurement of magnetic excitations in an applied magnetic field. To perform the measurements, the neutron beam must penetrate the Al walls of a large cryomagnet (left). The data from the $CuGeO_3$ sample is shown with neutron counts presented as a colour scale as a function of neutron energy transfer and magnetic field value (right). Adapted from [11].

In the later parts, we will describe the actual applications of neutron scattering. For each case, we give the necessary theoretical background, a description of the experimental set-up, and a number of corresponding problems, Part III describes the study of material structure by elastic neutron scattering and imaging. Small angle neutron scattering (SANS) is presented in chapter 6, reflectometry in chapter 7, diffraction from crystals in chapter 8. Part IV deals with the study of dynamics in materials by inelastic neutron scattering. We start with the study of coherent lattice vibrations (phonons) in chapter 9. Part V describes elastic and inelastic scattering from magnetic materials in chapters 10 and 11.

The final chapter contains a number of working problems shaped as "virtual experiments", where the student investigate a problem in neutron science or instrumentation by means of simulations [12].

1.5.1 Reading the text

The text is intended so that after the introduction in part I, each part can in principle be studied independently. However, parts IV and V relies to some extent on basic results from part III.

The reader is assumed to have a general knowledge of classical physics and complex numbers for the description of waves. The first three parts of the text assumes very little knowledge of quantum mechanics. At places where a deeper quantum mechanical presentation could be elucidating for some students, there will be alternative sections containing the formal derivation of the results. These sections can be omitted without loss of context; they are marked by an asterisk (*).

1.5.2 Future extensions

In later versions of this note, we aim to include a number of advanced utilizations of neutron scattering, like scattering with polarized neutrons, radiography/tomography, single crystal diffraction, quasielastic scattering from diffusion, scattering from liquids, and ultracold neutrons.

It is also likely that material on analytical calculations of instrumental resolution will be added.

Chapter 2

Basics of neutron scattering theory

This chapter contains the basics of scattering formalism. The present description is specialised to neutron scattering, but is in general valid also for other scattering processes, like electrons or X-rays.

In this chapter, neutrons are scattered by the nuclei by the strong nuclear forces. The range of these forces are femtometers (fm), much smaller than the neutron wavelength (measured in Å). Thus, the neutron cannot probe the internal structure of the nucleus, and the scattering from a single nucleus is isotropic [13].

The process of neutron scattering is unavoidably of quantum mechanical nature. However, most of this chapter is kept less rigorous, since for many applications a full formal treatment is unnecessary. In particular, this is the case for section 2.2, for which an alternative quantum-based section is given as 2.3*. Although vastly different, these two approaches lead to identical results.

The contents if this chapter form the basis for the understanding of the later parts of these notes, in particular elastic and inelastic neutron scattering from systems like particles, surfaces, powders, and crystals.

2.1 The neutron cross sections

In this section, we introduce the terms by which we describe the scattering of a neutron beam. In particular, we describe the interaction of a neutron beam with materials by introducing the central concept of cross sections.

2.1.1 Neutron flux

We define the flux of a neutron beam as the neutron rate per area

$$\boxed{\Psi = \frac{\text{number of neutrons impinging on a surface per second}}{\text{surface area perpendicular to the neutron beam direction}}}, \tag{2.1}$$

usually given in the unit n/(cm^{2}s).

2.1.2 The scattering cross section

The *neutron scattering cross section*, σ, of a system is defined by its ability to scatter neutrons:

$$\boxed{\sigma = \frac{1}{\Psi} \text{ number of neutrons scattered per second}}, \tag{2.2}$$

which has units of area. The scattering intensity is divided by the neutron flux to ensure that σ is an intrinsic property, independent on the neutron flux at the particular experimental set-up.

For a single nucleus, σ can now be seen as the effective area of the nucleus perpendicular to the neutron beam, as will be elaborated in problem 2.6.1. The scattering cross section used here is the total cross section, which depends on the system (sample) volume, V. For thin samples, σ can be described by the volume specific cross section, Σ, through

$$\sigma = V\Sigma. \tag{2.3}$$

For thicker samples, beam attenuation must be taken into account; see section 2.1.5.

2.1.3 The differential scattering cross section

The angular dependence of the scattered neutrons is a most important aspect of all neutron scattering. To describe this dependence, we define the *differential scattering cross section*:

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{1}{\Psi} \frac{\text{number of neutrons scattered per second into solid angle } d\Omega}{d\Omega}}. \tag{2.4}$$

The total number of scattered neutrons is of course the sum of neutrons in all of the 4π solid angle, whence

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega. \tag{2.5}$$

2.1.4 The partial differential scattering cross section

In some scattering processes, the neutron delivers energy to or absorbs energy from the scattering system. This type of scattering we denote *inelastic scattering*. We define the neutron energy transfer by

$$\boxed{\hbar\omega = E_{\mathrm{i}} - E_{\mathrm{f}} = \frac{\hbar^2(k_{\mathrm{i}}^2 - k_{\mathrm{f}}^2)}{2m_{\mathrm{n}}}}, \tag{2.6}$$

where the indices "i" and "j" denote *initial* and *final*, respectively. Note that the energy change is defined with opposite sign of most definitions of changing properties, so that neutron energy loss gives a positive value of $\hbar\omega$.

In inelastic scattering processes, energy is transfered to - or taken from - the sample. Energy conservation gives that the energy change of the sample is

$$\Delta E = \hbar\omega. \tag{2.7}$$

For describing inelastic scattering, one needs to take into account the energy dependence of the scattered neutrons. This is described by the *partial differential scattering cross section*:

$$\boxed{\frac{d^2\sigma}{d\Omega dE_{\mathrm{f}}} = \frac{1}{\Psi}\frac{\begin{array}{c}\text{no. of neutrons scattered per sec. into } d\Omega \\ \text{with energies } [E_{\mathrm{f}}; E_{\mathrm{f}} + dE_{\mathrm{f}}]\end{array}}{d\Omega dE_{\mathrm{f}}}}. \tag{2.8}$$

Integrating over all final energies, E_{f}, we reach the differential cross section described earlier:

$$\frac{d\sigma}{d\Omega} = \int \frac{d^2\sigma}{d\Omega dE_{\mathrm{f}}} dE_{\mathrm{f}}. \tag{2.9}$$

Following (2.5), the total cross section is found by a double integration:

$$\sigma = \iint \frac{d^2\sigma}{d\Omega dE_{\mathrm{f}}} d\Omega dE_{\mathrm{f}}. \tag{2.10}$$

For a closer description of inelastic scattering, a quantum mechanical treatment of the scattering process is required, as initiated in section 2.3 and described in detail in part IV.

2.1.5 Beam attenuation due to scattering

Since the number of neutrons scattered is necessarily limited by the number of incoming neutrons, the total cross section cannot be truly proportional to volume, at least not for large, strongly scattering systems. Hence, (2.3) should be understood only as what is called the *thin sample approximation*. This equation is valid only when the total scattering cross section of a given sample is much smaller than its area perpendicular to the beam.

For a thick sample, we must consider successive thin slices of thickness dz, each attenuating the incident beam (which we take to travel in the positive z direction):

$$\text{no. of neutrons scattered per sec. from } dz = \Psi(z)\Sigma A dz, \tag{2.11}$$

where A is the area of a sample slice perpendicular to the beam. We assume that A and Σ are constants and that the scattering cross section is uniform within the sample. The flux of the incident beam in the neutron flight direction is then attenuated inside the sample according to

$$\boxed{\Psi(z) = \Psi(0)\exp(-\mu z)}, \tag{2.12}$$

where we have defined the attenuation coefficient

$$\mu = \mu_{\rm s} = \Sigma. \tag{2.13}$$

The derivation is simple and is left as an exercise to the reader, see problem 2.6.2.

When the attenuation coefficient varies along the neutron path, (2.12) is generalized to

$$\boxed{\Psi(z) = \Psi(0)\exp\left(-\int_0^z \mu(z')dz'\right)}. \tag{2.14}$$

This equation is essential in the use of neutrons transmission for real-space *imaging* of samples, in analogy to medical X-ray images. This application of neutrons will be elaborated more in later versions of these notes.

2.1.6 The absorption cross section

Neutron absorption takes place as a result of neutron-induced nuclear processes, which destroy the neutrons, emitting secondary radiation (α, β, or γ) as a result. In most cases, the absorption cross section, $\sigma_{\rm a}$, of thermal neutrons is inversely proportional to the neutron velocity. In other words, the absorption is proportional to the neutron wavelength: $\sigma_{\rm a} \propto \lambda$.

The neutron absorption cross sections are measured and tabelized for all but the rarest isotopes, see *e.g.* the Neutron Data Booklet [14], or the NIST home page [15]. Traditionally, the absorption cross sections are given as $\sigma_{\rm a,\,th}$ per nucleus in units of "barns" (1 barn = 10^{-28} m^2) and is listed at the standard "thermal" velocity $v_{\rm th}$ = 2200 ms^{-1} ($\lambda_{\rm th}$ = 1.798 Å, see also table 1.1). The actual absorption cross section is then given by

$$\sigma_{\rm a} = \sigma_{\rm a,\,th}\frac{v_{\rm th}}{v} = \sigma_{\rm a,\,th}\frac{\lambda}{\lambda_{\rm th}}. \tag{2.15}$$

As in (2.12), the resulting attenuation coefficient is

$$\mu_{\rm a} = \sum_i \frac{N_i \sigma_{{\rm a},i}}{V} = \sum_i n_i \sigma_{{\rm a},i}. \tag{2.16}$$

In this sum, N_i represents the number of nuclei of isotope i in the sample volume V, and $n_i = N_i/V$ is the corresponding atomic density. The attenuation coefficients for scattering and absorption are additive due to the rule of addition of probabilities (see problem 2.6.2):

$$\mu_{\rm t} = \mu_{\rm s} + \mu_{\rm a}. \tag{2.17}$$

An abbreviated list of absorption and scattering cross sections for selected isotopes/elements is given in table 2.1.

Experimental consideration. For a single neutron, the probabilty of scattering or absorption will typically be much smaller than unity. However, real experiments deal with thousands to billions of neutrons onto the sample per second, so here the many small probabilities will give rise to an average counting number, N, which can often be considerable. The actual counting number is a stocastic variable, which follows a Poisson distribution with mean N and standard deviation $\sqrt{N}$. For $N > 10$, it can be approximated with a normal distribution with the same average and standard deviation, meaning that 68% of the times the count value will lie in the interval $N \pm \sqrt{N}$ - and 95% in the interval $N \pm 2\sqrt{N}$. Although this approximation does not hold for small count numbers, is in practice often used down to $N = 1$ or even to $N = 0$.

2.2 Wave description of nuclear scattering

In this section, we discuss the basics of scattering of waves from a semi-classical point of view. For an equivalent, fully quantum mechanical treatment of this topic, see section 2.3*.

2.2.1 The neutron wave

The incoming (or initial) neutron can be described as a (complex) plane wave

$$\boxed{\psi_{\rm i}(\mathbf{r}) = \frac{1}{\sqrt{Y}} \exp(i\mathbf{k}_{\rm i} \cdot \mathbf{r})}\,, \tag{2.18}$$

where Y is a normalization constant, implying that the density of the incoming neutron wave is $|\psi_{\rm i}|^2 = 1/Y$. This has no implication on the final results, since Y will eventually cancel in the final equations, but we keep the normalization for completeness. We have in (2.18) omitted an explicit time dependence, $\exp(-i\omega t)$, which plays no role until we discuss inelastic scattering.

From (1.5), the velocity of a neutron described by a plane wave is

$$v = \frac{\hbar k_{\rm i}}{m_{\rm n}}. \tag{2.19}$$

Similarly, the corresponding incoming neutron flux is

$$\Psi_{\rm i} = |\psi_{\rm i}|^2 v = \frac{1}{Y}\frac{\hbar k_{\rm i}}{m_{\rm n}}. \tag{2.20}$$

Z	Nucleus	b (10^{-15} m)	σ_{inc} (10^{-28} m^2)	$\sigma_{\mathrm{a,th}}$ (10^{-28} m^2)
1	H	-3.741	80.26 *	0.3326
1	^{1}H	-3.742	80.27 *	0.3326
1	^{2}D	6.674	2.05	0.000519
2	^{3}He	5.74	1.532	5333
2	^{4}He	3.26	0	0
3	Li	-1.90	0.92	70.5
3	^{6}Li	2.0	0.46	940
3	^{7}Li	-2.22	0.78	0.0454
4	Be	7.79	0.0018	0.0076
5	B	5.30	1.70	767
5	^{10}B	-0.2	3.0	3835
5	^{11}B	6.65	0.21	0.0055
6	C	6.6484	0.001	0.00350
7	N	9.36	0.50	1.90
8	O	5.805	0	0.00019
9	F	5.654	0.0008	0.0096
10	Ne	4.566	0.008	0.039
11	Na	3.63	1.62	0.530
12	Mg	5.375	0.08	0.063
13	Al	3.449	0.0082	0.231
14	Si	4.1507	0.004	0.171
15	P	5.13	0.005	0.172
16	S	2.847	0.007	0.53
17	Cl	9.5792	5.3	33.5
18	Ar	1.909	0.225	0.675
19	K	3.67	0.27	2.1
20	Ca	4.70	0.05	0.43
21	Sc	12.1	4.5	27.5
22	Ti	-3.37	2.87	6.09
23	V	-0.443	5.08	5.08
24	Cr	3.635	1.83	3.05
25	Mn	-3.750	0.40	13.3
26	Fe	9.45	0.40	2.56
27	Co	2.49	4.8	37.18
28	Ni	10.3	5.2	4.49
29	Cu	7.718	0.55	3.78
30	Zn	5.68	0.077	1.11
31	Ga	7.288	0.16	2.75
32	Ge	8.185	0.18	2.20
48	Cd	4.83	3.46	2520
51	Sb	5.57	0	4.91
58	Ce	4.84	0	0.63
60	Nd	7.69	9.2	50.5
64	Gd	9.5	151	49700
65	Tb	7.34	0.004	23.4
82	Pb	9.401	0.0030	0.171

Table 2.1: Neutron cross sections and scattering lengths for the first 32 elements (isotopic average using the natural abundancies). In addition, data from selected isotopes and some heavier elements are presented. Data taken from [14].
* It should be noted that the important incoherent cross section for H varies with wavelength. The value listed is valid for $\lambda >$1.798 Å [16, 17].

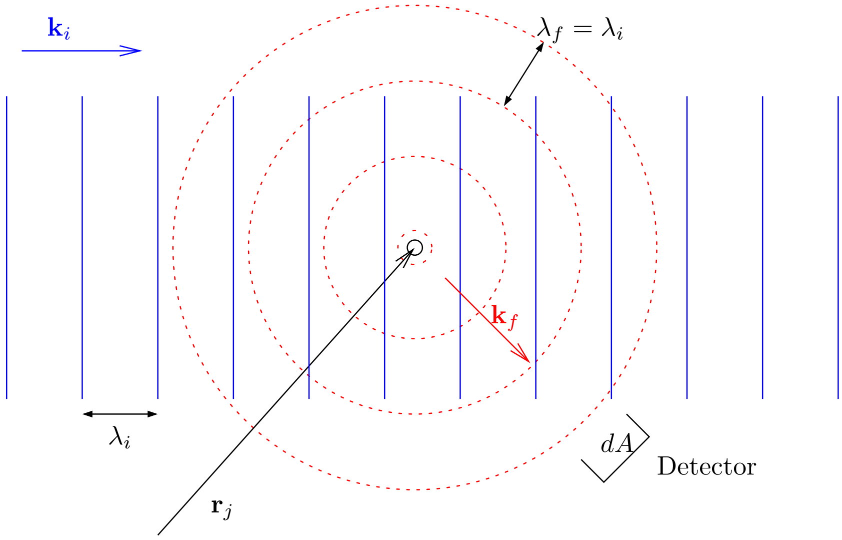

Figure 2.1: An illustration of the initial wave, ψ_i, of wavelength λ_i, and the final wave, ψ_f, of wavelength λ_f, describing a neutron scattering off a single nucleus with positive scattering length (meaning a phase shift of π). The area, dA, for measuring the flux of the outgoing neutrons is the detector area as sketched.

We will use this result as a stepping stone in the following calculations.

2.2.2 Elastic neutron scattering from a single nucleus

We consider the idealized situation where a neutron with a well defined velocity is scattered by a single nucleus, labeled j, which is (somehow) fixed in position. The scattered neutron can be described as a spherical wave leaving the nucleus, which is centered at $\mathbf{r}_j$, as shown in Fig. 2.1. The scattered, or final, wave function reads:

$$\boxed{\psi_\mathrm{f}(\mathbf{r}) = \psi_\mathrm{i}(\mathbf{r}_j)\frac{-b_j}{|\mathbf{r}-\mathbf{r}_j|}\exp(ik_\mathrm{f}|\mathbf{r}-\mathbf{r}_j|)}\,, \tag{2.21}$$

where b_j is a quantity characteristic for the particular isotope. Since b_j has the unit of length, it is usually denoted *scattering length* and is of the order fm. This above equation is valid only "far" from the nucleus, *i.e.* for $|\mathbf{r}-\mathbf{r}_j| \gg b$, The minus sign in (2.21) is a convention chosen so that most nuclei will have a positive value of b_j.

In experiments, r is typically of the order 1 m. In addition, we choose to place origo close to the centre of the "relevant" part of the sample. Hence, the nuclear coordinate, r_j, is typically of the order 1 mm or less, and the density of outgoing neutrons can be approximated by $|\psi_\mathrm{f}|^2 \approx b_j^2/(Yr^2)$, omitting $\mathbf{r}_j$ in the denominator of (2.21) The number of neutrons per second intersecting a small surface, dA, is $v|\psi_\mathrm{f}|^2 dA = vb_j^2/(Yr^2)dA$. Using (2.19) and the expression for solid angle $d\Omega = dA/r^2$, we reach

$$\text{number of neutrons per second in } d\Omega = \frac{1}{Y}\frac{b_j^2 \hbar k_\mathrm{f}}{m_\mathrm{n}} d\Omega. \tag{2.22}$$

Since the scattering nucleus is fixed, energy conservation requires that the energy of the neutron is unchanged. In this so-called *elastic scattering*, we therefore have $k_\mathrm{i} = k_\mathrm{f}$. Using (2.4) and (2.20), this leads to the simple expression for the differential cross section for one nucleus:

$$\boxed{\frac{d\sigma}{d\Omega} = b_j^2}, \tag{2.23}$$

giving the total scattering cross section of

$$\sigma = 4\pi b_j^2. \tag{2.24}$$

2.2.3 Scattering from two nuclei – interference

In the field of neutron scattering from materials, we are concerned with the effect of scattering from a system of particles. We begin by considering the scattering from two nuclei, labeled j and j', again placed at fixed positions. This simple system will reveal some very important features, which we will utilize later.

The neutron wave that is scattered from the two nuclei is in fact describing just one single neutron. Nevertheless, this neutron "senses" the presence of both nuclei, meaning that the wave scattered from one nucleus will add to the wave scattered from another nucleus. This *interference* is a central aspect in most scattering techniques.

Let us describe this in more precise terms. We assume elastic scattering, $k_\mathrm{i} = k_\mathrm{f} \equiv k$ and identical nuclei, $b_j = b_{j'} \equiv b$. Generalizing (2.21), the outgoing (final) wave can be described as

$$\psi_\mathrm{f}(\mathbf{r}) = -b\left(\frac{\psi_\mathrm{i}(\mathbf{r}_j)}{|\mathbf{r}-\mathbf{r}_j|}\exp(ik_f|\mathbf{r}-\mathbf{r}_j|) + \frac{\psi_\mathrm{i}(\mathbf{r}_{j'})}{|\mathbf{r}-\mathbf{r}_{j'}|}\exp(ik_f|\mathbf{r}-\mathbf{r}_{j'}|)\right), \tag{2.25}$$

where $\psi_\mathrm{i}(\mathbf{r})$ is the plane wave given by (2.18). The two nuclei are assumed to be closely spaced compared with the distance to the observer: $|\mathbf{r}_j - \mathbf{r}_{j'}| \ll r$. Choosing the origin to lie close to the two particles, the denominators can be considered equal, giving

$$\begin{aligned}\psi_\mathrm{f}(\mathbf{r}) = \frac{1}{\sqrt{Y}}\frac{-b}{r}\big[&\exp(i\mathbf{k}_\mathrm{i}\cdot\mathbf{r}_j)\exp(ik_f|\mathbf{r}-\mathbf{r}_j|) \\ &+ \exp(i\mathbf{k}_\mathrm{i}\cdot\mathbf{r}_{j'})\exp(ik_f|\mathbf{r}-\mathbf{r}_{j'}|)\big]\end{aligned} \tag{2.26}$$

We now want to calculate the length $|\mathbf{r} - \mathbf{r}_j|$, since it enters the phase of the complex wave function. It is convenient to write the nuclear coordinate, $\mathbf{r}_j$, as a component parallel to and perpendicular to $\mathbf{r}$:

$$|\mathbf{r}-\mathbf{r}_j| = |\mathbf{r}-\mathbf{r}_{j,||}-\mathbf{r}_{j,\perp}| = \sqrt{\left|\mathbf{r}-\mathbf{r}_{j,||}\right|^2 + |\mathbf{r}_{j,\perp}|^2}, \tag{2.27}$$

where the last step is due to Pythagoras. The last term in the square root is by far the smallest and vanishes to first order. To check the order of magnitude, we take a "large" distance between nuclei of $|r_j| \approx 2\,\mu$m and $|\mathbf{r} - \mathbf{r}_{j,||}| \approx 1$ m. This gives an error in the approximation of ≈ 0.02 Å; much smaller than the typical neutron wavelength we consider. This means that effectively only one nuclear coordinate, $\mathbf{r}_{j,||}$, contributes and that the square root can be lifted to give $|\mathbf{r} - \mathbf{r}_j| = |\mathbf{r} - \mathbf{r}_{j,||}|$. Now, we can write

$$k_f|\mathbf{r} - \mathbf{r}_{j,||}| = \mathbf{k}_\mathrm{f} \cdot (\mathbf{r} - \mathbf{r}_{j,||}), \tag{2.28}$$

where $\mathbf{k}_\mathrm{f}$ is a wave vector with length k_f (which here equals k), oriented parallel to $\mathbf{r}$. Since $\mathbf{k}_\mathrm{f} \cdot \mathbf{r}_{j,\perp} = 0$, we reach

$$\exp(ik_f|\mathbf{r} - \mathbf{r}_j|) = \exp(i\mathbf{k}_\mathrm{f} \cdot (\mathbf{r} - \mathbf{r}_j)). \tag{2.29}$$

Rearranging terms, the final wave can be written as

$$\psi_\mathrm{f}(\mathbf{r}) = -\frac{1}{\sqrt{Y}}\frac{b}{r}\exp(i\mathbf{k}_\mathrm{f} \cdot \mathbf{r})\left[\exp(i(\mathbf{k}_\mathrm{i} - \mathbf{k}_\mathrm{f}) \cdot \mathbf{r}_j) + \exp(i(\mathbf{k}_\mathrm{i} - \mathbf{k}_\mathrm{f}) \cdot \mathbf{r}_{j'})\right] \tag{2.30}$$

This shows that the observer at position $\mathbf{r}$ will experience a scattered neutron wave that locally seems like a plane wave with wavevector $\mathbf{k}_\mathrm{f}||\mathbf{r}$.

The intensity of neutrons impinging on a small area is again given as $v|\psi_\mathrm{f}(\mathbf{r})|^2 dA$. Hereby we can write the scattering cross section as

$$\text{no. of neutrons per sec. in } d\Omega$$
$$= \frac{1}{Y}\frac{b^2\hbar k_\mathrm{f}}{m_\mathrm{n}} d\Omega \left|\exp(i\mathbf{q} \cdot \mathbf{r}_j) + \exp(i\mathbf{q} \cdot \mathbf{r}_{j'})\right|^2, \tag{2.31}$$

where we have defined the very central concept of neutron scattering, the *scattering vector*, as

$$\boxed{\mathbf{q} = \mathbf{k}_\mathrm{i} - \mathbf{k}_\mathrm{f}}\,. \tag{2.32}$$

The final expression for the differential scattering cross section for elastic scattering from nuclei now becomes:

$$\frac{d\sigma}{d\Omega} = b^2\big|\exp(i\mathbf{q} \cdot \mathbf{r}_j) + \exp(i\mathbf{q} \cdot \mathbf{r}_{j'})\big|^2 = 2b^2\big(1 + \cos[\mathbf{q} \cdot (\mathbf{r}_j - \mathbf{r}_{j'})]\big). \tag{2.33}$$

At some values of $\mathbf{q}$, this cross section vanishes, while at others the value is up to 4 times that of a single nucleus. This is the essence of interference.

2.3 * Quantum mechanics of scattering

We will now go through the principles of neutron scattering from nuclei in a way, which is more strictly quantum mechanical than section 2.2.

This section does not contain new results, but may be more satisfactory for readers with a physics background. Further, the formalism developed here carries on to the detailed treatment of inelastic scattering of phonons and magnetic scattering in subsequent chapters.

This section is strongly inspired by the treatments in the textbooks by Marshall and Lovesey [2] and Squires [3].

2.3.1 * The initial and final states

We define the state of the incoming wave as

$$\boxed{|\psi_\mathrm{i}\rangle = \frac{1}{\sqrt{Y}}\exp(i\mathbf{k}_\mathrm{i}\cdot\mathbf{r})}\,, \tag{2.34}$$

where $Y = L^3$ can be identified as the (large) normalization volume for the state which is assumed enclosed in a cubic box with a side length L. The incoming neutron flux is given as (2.20)

$$\Psi_\mathrm{i} = |\psi_\mathrm{i}|^2 v = \frac{1}{Y}\frac{\hbar k_\mathrm{i}}{m_\mathrm{n}}. \tag{2.35}$$

In contrast to the spherical outgoing wave from section 2.2, we express the final state as a (superposition of) plane wave(s)

$$\boxed{|\psi_\mathrm{f}\rangle = \frac{1}{\sqrt{Y}}\exp(i\mathbf{k}_\mathrm{f}\cdot\mathbf{r})}\,. \tag{2.36}$$

We here ignore the spin state of the neutron, which will be discussed in the chapter on neutron polarization.

2.3.2 * Density of states

For the spinless states, we calculate the number density in $\mathbf{k}$-space:

$$\frac{dn}{dV_k} = \left(\frac{2\pi}{L}\right)^{-3} = \frac{Y}{(2\pi)^3}. \tag{2.37}$$

We now consider a spherical shell in $\mathbf{k}$-space to calculate the (energy) density of states,

$$\frac{dn}{dE_\mathrm{f}} = \frac{dn}{dV_k}\frac{dV_k}{dk_\mathrm{f}}\left(\frac{dE_\mathrm{f}}{dk_\mathrm{f}}\right)^{-1} = \frac{Y}{(2\pi)^3}4\pi k_\mathrm{f}^2\frac{m_\mathrm{n}}{k_\mathrm{f}\hbar^2} = \frac{Yk_\mathrm{f}m_\mathrm{n}}{2\pi^2\hbar^2}. \tag{2.38}$$

In order to describe the differential scattering cross sections, we would like to describe the fraction of the wavefunction which is emitted into directions of $\mathbf{k}_\mathrm{f}$, corresponding to a solid angle $d\Omega$. Here, the densities are given by

$$\left.\frac{dn}{dV_k}\right|_{d\Omega} = \frac{dn}{dV_k}\frac{d\Omega}{4\pi} = \frac{Y}{(2\pi)^3}\frac{d\Omega}{4\pi}. \tag{2.39}$$

Following the calculations leading to (2.38), we can now calculate the density of states within the scattering direction $d\Omega$:

$$\left.\frac{dn}{dE}\right|_{d\Omega} = \frac{Y k_{\mathrm{f}} m_{\mathrm{n}}}{(2\pi)^3 \hbar^2} d\Omega. \tag{2.40}$$

We will need this expression in the further calculations.

2.3.3 * The master equation for scattering

We describe the interaction responsible for the scattering by an operator denoted $\hat{V}$. The scattering process itself is described by the *Fermi Golden Rule* [18]. This gives the rate of change between the neutron in the single incoming state, $|\psi_{\mathrm{i}}\rangle$ and a final state, $|\psi_{\mathrm{f}}\rangle$, where $|\psi_{\mathrm{f}}\rangle$ resides in a continuum of possible states.

$$W_{\mathrm{i}\to\mathrm{f}} = \frac{2\pi}{\hbar} \frac{dn}{dE_{\mathrm{f}}} \left|\langle\psi_{\mathrm{i}}|\hat{V}|\psi_{\mathrm{f}}\rangle\right|^2, \tag{2.41}$$

We wish to consider only neutrons scattered into the solid angle $d\Omega$. Using (2.40) and (2.41), we reach

$$W_{\mathrm{i}\to\mathrm{f},d\Omega} = \frac{Y k_{\mathrm{f}} m_{\mathrm{n}}}{(2\pi)^2 \hbar^3} d\Omega \left|\langle\psi_{\mathrm{i}}|\hat{V}|\psi_{\mathrm{f}}\rangle\right|^2. \tag{2.42}$$

$W_{\mathrm{i}\to\mathrm{f},d\Omega}$ is the number of neutrons scattered into $d\Omega$ per second. We now only need the expression for the incoming flux (2.20) to reach the result for the differential scattering cross section (2.4)

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{1}{\Psi} \frac{W_{\mathrm{i}\to\mathrm{f},d\Omega}}{d\Omega} \\ &= Y^2 \frac{k_{\mathrm{f}}}{k_{\mathrm{i}}} \left(\frac{m_{\mathrm{n}}}{2\pi\hbar^2}\right)^2 \left|\langle\psi_{\mathrm{i}}|\hat{V}|\psi_{\mathrm{f}}\rangle\right|^2. \end{aligned} \tag{2.43}$$

In this expression, the normalization volume, Y, will eventually vanish due to the factor $1/\sqrt{Y}$ in the states $|k_{\mathrm{i}}\rangle$ and $|k_{\mathrm{f}}\rangle$, since the interaction, $\hat{V}$, is independent of Y. We will thus from now on neglect the Y dependence in the states and in the cross sections.

The factor $k_{\mathrm{f}}/k_{\mathrm{i}}$ in (2.43) is of importance only for inelastic neutron scattering, where it always appears in the final expressions. For elastic scattering, $k_{\mathrm{f}} = k_{\mathrm{i}}$.

2.3.4 * Elastic scattering from one and two nuclei

The interaction between the neutron and the nuclei is expressed by the *Fermi pseudopotential*

$$\boxed{\hat{V}_j(\mathbf{r}) = \frac{2\pi\hbar^2}{m_{\mathrm{n}}} b_j \delta(\mathbf{r} - \mathbf{r}_j)}\,. \tag{2.44}$$

Here, b_j has the unit of length and is of the order fm. It is usually denoted the *scattering length*. The spatial delta function represents the short range of the strong nuclear forces and is a sufficient description for the scattering of thermal neutrons.

It should here be noted that a strongly absorbing nucleus will have an significant imaginary contribution to the scattering length. We will, however, not deal with this complication here.

For a single nucleus, we can now calculate the scattering cross section. We start by calculating the matrix element

$$\begin{aligned} \langle \psi_\mathrm{f} | \hat{V}_j | \psi_\mathrm{i} \rangle &= \frac{2\pi\hbar^2}{m_\mathrm{n}} b_j \int \exp(-i\mathbf{k}_\mathrm{f} \cdot \mathbf{r}) \delta(\mathbf{r} - \mathbf{r}_j) \exp(i\mathbf{k}_\mathrm{i} \cdot \mathbf{r}) d^3\mathbf{r} \\ &= \frac{2\pi\hbar^2}{m_\mathrm{n}} b_j \exp(i\mathbf{q} \cdot \mathbf{r}_j), \end{aligned} \tag{2.45}$$

where we have defined the very central concept of neutron scattering, the *scattering vector*, as

$$\boxed{\mathbf{q} = \mathbf{k}_\mathrm{i} - \mathbf{k}_\mathrm{f}}\,. \tag{2.46}$$

Inserting (2.45) into (2.43), we reassuringly reach the same result as found from the semi-classical calculation (2.23):

$$\boxed{\frac{d\sigma}{d\Omega} = b_j^2}\,. \tag{2.47}$$

For a system of two nuclei, we obtain interference between the scattered waves. We can write the scattering potential as a sum $\hat{V} = \hat{V}_j + \hat{V}_{j'}$. In this case, the matrix element becomes

$$\langle \psi_\mathrm{f} | \hat{V} | \psi_\mathrm{i} \rangle = \frac{1}{Y} \frac{2\pi\hbar^2}{m_\mathrm{n}} \big(b_j \exp(i\mathbf{q} \cdot \mathbf{r}_j) + b_{j'} \exp(i\mathbf{q} \cdot \mathbf{r}_{j'}) \big). \tag{2.48}$$

Inserting into (2.43), we reach the same result (2.33) as found by the simpler approach in section 2.2.

2.3.5 * Formalism for inelastic scattering

When describing the quantum mechanics of the inelastic scattering process, it is important to keep track of the quantum state of the scattering system (the sample), since it changes during the scattering process (for $\hbar\omega \neq 0$). The initial and final sample states are denoted $|\lambda_\mathrm{i}\rangle$ and $|\lambda_\mathrm{f}\rangle$, respectively. The partial differential cross section for scattering from $|\lambda_\mathrm{i}, \mathbf{k}_\mathrm{i}\rangle$ to $|\lambda_\mathrm{f}, \mathbf{k}_\mathrm{f}\rangle$ is given in analogy with (2.43) by

$$\boxed{\left.\frac{d^2\sigma}{d\Omega dE_\mathrm{f}}\right|_{\lambda_\mathrm{i} \to \lambda_\mathrm{f}} = \frac{k_\mathrm{f}}{k_\mathrm{i}} \left(\frac{m_\mathrm{n}}{2\pi\hbar^2} \right)^2 \left| \langle \lambda_\mathrm{i} \psi_\mathrm{i} | \hat{V} | \psi_\mathrm{f} \lambda_\mathrm{f} \rangle \right|^2 \delta(E_{\lambda_\mathrm{i}} - E_{\lambda_\mathrm{f}} + \hbar\omega)}\,, \tag{2.49}$$

where the δ-function expresses explicit energy conservation and the normalization factor Y^2 is omitted.

This expression will be our starting point in the chapters on inelastic scattering from lattice vibrations and magnetic excitations.

2.4 Coherent and incoherent scattering

Very often, the neutron scattering length varies randomly from nucleus to nucleus in a sample. This can be caused by the variation of the nuclear spin direction with time, or by variations between isotopes of the same element - or between different elements. We here describe how this affects the scattering cross sections.

2.4.1 The coherent and incoherent cross sections

Variation in scattering length due to element or isotope disorder is a static effect, while nuclear spin variations are dynamic. However, for a macroscopic sample the calculations can be treated in the same way, since we can assume that 1) the sample is large enough to essentially represent an ensemble average and 2) we observe the system over times much longer than nuclear fluctuation times, meaning that the time average equals an ensemble average.

Let us for simplicity assume that the scattering length at site j has the stochastic value

$$b_j = \langle b_j \rangle + \delta b_j , \tag{2.50}$$

where $\langle b_j \rangle$ is shorthand for the average of b_j and δb_j is the local deviation from the average, $\langle \delta b_j \rangle = 0$. The deviations are assumed to be independent between sites, $\langle \delta b_j \, \delta b_{j'} \rangle = 0$. The mean scattering cross section is found from interference terms of the type seen in the two-atom problem.

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle = \left\langle |b_j \exp(i\mathbf{q}\cdot\mathbf{r}_j) + b_{j'} \exp(i\mathbf{q}\cdot\mathbf{r}_{j'})|^2 \right\rangle , \tag{2.51}$$

where the average here means both time and ensemble average. Using (2.50), we now see that the "square terms" in (2.51) give $\langle b_j^2 \rangle = \langle b_j \rangle^2 + \langle \delta b_j^2 \rangle$, while the "interference terms" give $\langle b_j b_{j'} \rangle = \langle b_j \rangle \langle b_{j'} \rangle$. Identifying $\sigma_{\mathrm{inc},j}$ with $4\pi\langle (\delta b_j)^2 \rangle$, we rewrite (2.51) to give

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle = \frac{\sigma_{\mathrm{inc},j} + \sigma_{\mathrm{inc},j'}}{4\pi} + \left| \langle b_j \rangle \exp(i\mathbf{q}\cdot\mathbf{r}_j) + \langle b_{j'} \rangle \exp(i\mathbf{q}\cdot\mathbf{r}_{j'}) \right|^2 . \tag{2.52}$$

Here we notice that σ_{inc} represents a constant scattering of neutrons, *i.e.* in all directions, without interference. Hence, σ_{inc} is called the *incoherent scattering cross section*. The average value $\langle b_j \rangle$ represents the strength of the interferent scattering and is denoted the *coherent scattering length*. In general, the coherent scattering depends on the scattering vector $\mathbf{q}$, and hence on the scattering angle.

One defines *coherent scattering cross section* for a single nucleus j as $\sigma_{\text{coh,j}} = 4\pi\langle b_j\rangle^2$.

Usually, the explicit average notation $\langle b\rangle$ is dropped, and the symbol b almost exclusively means the average scattering length of a certain isotope or element. This is also the notation used in Table 2.1.

2.4.2 Incoherent nuclear scattering from randomness

There are several sources of the incoherent scattering, described in general terms above. One source is the spin-dependent term, which is described in detail in [2], and which is the one given by the isotope tables. Below, we will deal with incoherent scattering caused by variations in the scattering length due to isotopic mixture or chemical randomness. From the neutron point of view, all these mechanisms are very similar, as described above. The values of the incoherent scattering cross sections for the elements, found in Table 2.1, deal with the combined effect from spin and isotopic mixture.

For a simple example of site randomness, assume that a material consists of two isotopes with the abundances $a_c = a$, and $a_d = 1-a$, the scattering lengths b_c and b_d, respectively, and no nuclear spin. The average scattering length is

$$\langle b\rangle = ab_c + (1-a)b_d, \tag{2.53}$$

and the average incoherent cross section can be calculated by an average over the isotope abundances:

$$\begin{aligned}\frac{\sigma_{\text{inc}}}{4\pi} &= \langle(\delta b)^2\rangle \\ &= a(b_c - \langle b\rangle)^2 + (1-a)(b_d - \langle b\rangle)^2 \\ &= a(1-a)(b_c - b_d)^2. \end{aligned} \tag{2.54}$$

This means that we see an incoherent scattering due to the isotope mixture, strongest at 50%-50% mixing ratio.

With a little effort, (2.54) can be generalized to more than two isotopes.

2.5 The total cross section for a system of particles

We have seen above that the total cross section can be written as a sum of the coherent and incoherent cross sections. In general, each of these cross sections can have an elastic and an inelastic part, giving rise to four terms:

$$\frac{d^2\sigma}{d\Omega dE_{\text{f}}} = \sum_j \left.\frac{d^2\sigma_j}{d\Omega dE_{\text{f}}}\right|_{\text{inc}} + \left.\frac{d^2\sigma}{d\Omega dE_{\text{f}}}\right|_{\text{coh}} + \sum_j \left.\frac{d\sigma_j}{d\Omega}\right|_{\text{inc}} \delta(\hbar\omega) + \left.\frac{d\sigma}{d\Omega}\right|_{\text{coh}} \delta(\hbar\omega). \tag{2.55}$$

We will in the remainder of these notes concentrate upon the two coherent scattering processes, unless explicitly noticed.

Experimental considerations. The distinction between coherent and incoherent scattering is very important. In most types of experiment you will aim to minimize the incoherent cross section, which creates a uniform background, and maximize the coherent cross section, which generates the features you intend to study. A typical strong source of incoherent scattering is hydrogen, ^{1}H, where the incoherence is due to a strong spin dependence of the interaction between the neutron and the proton.

Inelastic incoherent scattering can, however, be used to study dynamic processes; mostly the motion of hydrogen. This type of scattering is not discussed further in this version of the notes.

2.5.1 Coherent elastic scattering from a system of nuclei

In chapters 6 and 8, we will discuss neutron diffraction from macromolecules and crystals, respectively. These topics essentially deal with interference between waves scattered from a large number of nuclei in the same way as we have seen for two nuclei above. For this purpose, equation (2.33) is easily generalized to several particles

$$\boxed{\left.\frac{d\sigma}{d\Omega}\right|_{\mathrm{coh}} = \left|\sum_j b_j \exp(i\mathbf{q}\cdot\mathbf{r}_j)\right|^2}. \tag{2.56}$$

This is a very important result, which is used in most types of neutron scattering.

2.5.2 The significance of the scattering vector

In a scattering experiment, one will always measure the *scattering angle* with respect to the incoming beam, as illustrated in Fig. 2.2. The scattering angle is known as 2θ. In elastic scattering, $k_{\mathrm{i}} = k_{\mathrm{f}} \equiv k$, and we can see from the figure that

$$\boxed{q = 2k\sin(\theta)}. \tag{2.57}$$

2.6 Problems

2.6.1 The cross section

Imagine a beam of neutrons arriving randomly over a surface of area A perpendicular to the beam, with an arrival rate of N neutrons per second. In a semi-classical approximation, you can consider each neutron to be point shaped. Now, on the surface we place one nucleus with an effective radius of $2b$. Assume that each neutron hitting the nucleus is scattered and all other neutrons are left unscattered.

1. Calculate the neutron flux
2. Calculate the probability for one neutron to hit the nucleus
3. Show that the scattering cross section of the nucleus is $\sigma = 4\pi b^2$

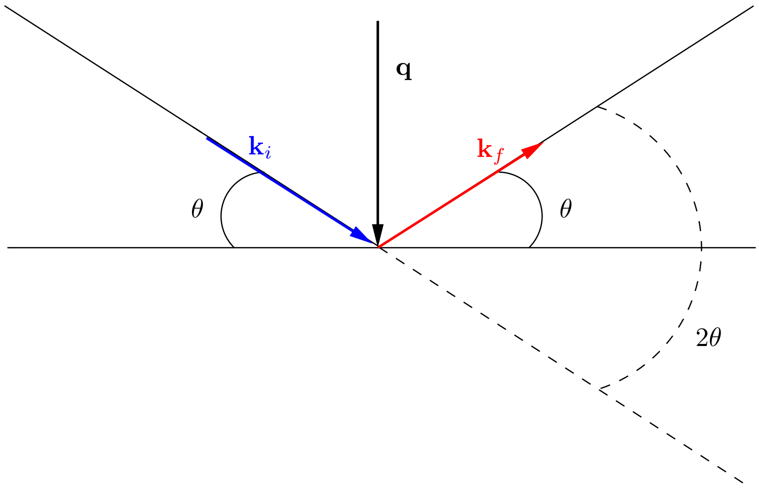

Figure 2.2: An illustration of the scattering process with the incoming and outgoing beam, the wave vectors, $\mathbf{k}_{\mathrm{i}}$ and $\mathbf{k}_{\mathrm{f}}$, and the scattering vector $\mathbf{q}$.

2.6.2 Attenuation of the neutron beam

1. Derive the exponential decay (2.12).

2. Prove that when there is both absorption and scattering, then the total attenuation coefficient is the sum of the individual coefficients.

2.6.3 Selection of materials for neutron scattering experiments

Most nuclei scatter neutrons incoherently, *i.e.* in random directions. Further, some nuclear isotopes are able to absorb neutrons by nuclear processes. We will now take a closer look at these properties for various materials.

1. Consider the incoherent scattering cross section σ_{inc} for the typical elements occuring in organic materials: H, C, N, O and P. How could one reduce the incoherent background from organic samples?

2. Some transition metals (Sc $\rightarrow$ Zn) display a strong incoherent scattering, and one of them is used as a standard incoherent scatterer (for calibration purposes). Try to figure out which one it is.

3. Sometimes other, more easily accessible, materials are used as incoherent scatterers instead. Suggest one.

4. Which metals may be used for neutron shielding? Calculate the penetration depth $1/\mu$ in these materials for neutron energies of 5 meV. Assume that the number density of atoms in the metal is $1/(16\ \text{Å}^3)$.

5. Also boron nitride, BN, (V_0 = 11.81 Å^3) is used for shielding purposes. This material is used *e.g.* to make adjustable diaphragms (*slits*) to control the size of the neutron beam.

   Calculate the thickness of BN needed to reach an attenuation factor of 10^{-6} (that is, only a fraction of 10^{-6} of the neutrons in the beam are left in the beam at this thickness) for 5 meV neutrons. What will the attenuation then be for neutrons of 20 meV and 180 meV?

6. In a neutron scattering experiment, the sample surroundings must be "clean" in the sense of absorption and (incoherent) scattering. Which metal would you suggest for constructing cryostats for neutron experiments?