# 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 $\lambda$. Denote the wavefunction of the neutron by $\psi_{\boldsymbol{k}}$ and of the scattering system by $\chi_\lambda$. 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 $\lambda'$.

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 $j$th 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 $\lambda$ to $\lambda'$, 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 $\theta$, $\phi$, the values of $\boldsymbol{k}$, $\lambda$, and $\lambda'$ remaining constant (Fig. 2.2). From the definition of $d\sigma/d\Omega$ given in





(1.12) we have

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} = \frac{1}{\Phi}\frac{1}{d\Omega}\sum_{\substack{\boldsymbol{k}' \\ \text{in } d\Omega}} W_{\boldsymbol{k},\lambda\to\boldsymbol{k}',\lambda'}, \tag{2.1}$$

where $W_{\boldsymbol{k},\lambda\to\boldsymbol{k}'\lambda'}$ is the number of transitions per second from the state $\boldsymbol{k}$, $\lambda$ to the state $\boldsymbol{k}'$, $\lambda'$, and $\Phi$ is the flux of incident neutrons.

To evaluate the expression on the right-hand side of (2.1) we use a fundamental result in quantum mechanics, known as *Fermi's golden*

Fig. 2.1 Coordinates of nucleus and neutron.

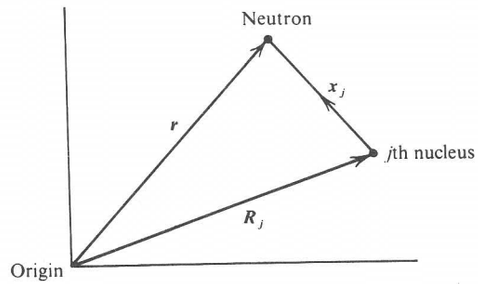
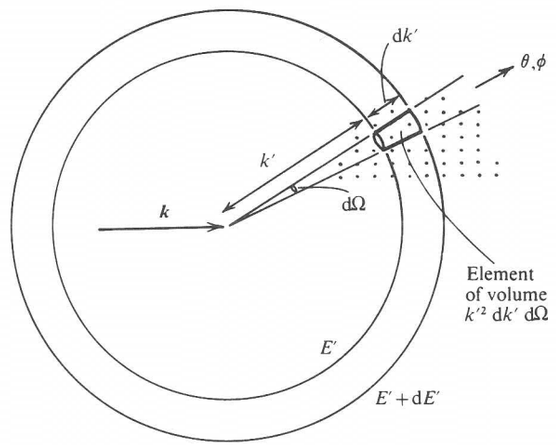



Fig. 2.2 Calculation of $\rho_{\boldsymbol{k}'}$. The points represent $\boldsymbol{k}'$ values permitted by box normalisation. The spheres corresponding to neutron energies $E'$ and $E' + dE'$ are shown.



*rule.*† This is

$$\sum_{\substack{k' \\ \text{in } d\Omega}} W_{k,\lambda\to k',\lambda'} = \frac{2\pi}{\hbar}\rho_{k'}|\langle k'\lambda'|V|k\lambda\rangle|^2. \tag{2.2}$$

In this expression $\rho_{k'}$ is the number of momentum states in $d\Omega$ per unit energy range for neutrons in the state $k'$. The matrix element is given explicitly by

$$\langle k'\lambda'|V|k\lambda\rangle = \int \psi^*_{k'}\chi^*_{\lambda'} V \psi_k \chi_\lambda \, d\boldsymbol{R}\, d\boldsymbol{r}, \tag{2.3}$$

where

$$d\boldsymbol{R} = d\boldsymbol{R}_1\, d\boldsymbol{R}_2 \ldots d\boldsymbol{R}_N. \tag{2.4}$$

$d\boldsymbol{R}_j$ is an element of volume for the $j$th nucleus, and $d\boldsymbol{r}$ is an element of volume for the neutron. The integral is taken over all space for each of the $N+1$ variables.

It may be noted that although the sum on the left-hand side of (2.2) is over a range of neutron states, the expression on the right-hand side is evaluated at a *particular* state $k'$. In the quantum mechanical derivation of the golden rule, a summation is made over all values of $|k'|$. The derivation shows that, for fixed $k$, $\lambda$, and $\lambda'$, the probability of a transition $k$, $\lambda$ to $k'$, $\lambda'$ is negligible except for a narrow range of $|k'|$ values. The centre of this range is the value of $|k'|$ corresponding to conservation of energy for the overall system of neutron plus scattering system, and it is this particular $k'$ which must be inserted on the right-hand side of (2.2).

We adopt a standard device in quantum mechanics, known as *box normalisation*, which is to imagine the neutron and scattering system to be in a large box. This enables us to calculate $\rho_{k'}$, and it also fixes the normalisation constant of the neutron wavefunctions. The only allowed neutron states are those whose de Broglie waves are periodic in the box. The wavevectors of such states form a lattice in $k$ space. The volume of the unit cell of the lattice is

$$v_k = \frac{(2\pi)^3}{Y}, \tag{2.5}$$

where $Y$ is the volume of the box.

The final energy of the neutron is

$$E' = \frac{\hbar^2}{2m}k'^2 \tag{2.6}$$

† The rule is derived in most textbooks on quantum mechanics. See for example Merzbacher (1970), Chapter 18.



with

$$dE' = \frac{\hbar^2}{m}k'\, dk'. \tag{2.7}$$

By definition $\rho_{k'}\, dE'$ is the number of states in $d\Omega$ with energy between $E'$ and $E'+dE'$, which is the number of wavevector points in the element of volume $k'^2\, dk'\, d\Omega$ (Fig. 2.2). Thus

$$\rho_{k'}\, dE' = \frac{1}{v_k}k'^2\, dk'\, d\Omega. \tag{2.8}$$

Eqs. (2.5) to (2.8) give

$$\rho_{k'} = \frac{Y}{(2\pi)^3}k'\frac{m}{\hbar^2}d\Omega. \tag{2.9}$$

We now consider the wavefunction $\psi_k$. It is a plane wave and has the form $\exp(i\boldsymbol{k}\,.\,\boldsymbol{r})$. There is one neutron in the box of volume $Y$. So the neutron density is $1/Y$. Thus

$$\psi_k = \frac{1}{\sqrt{Y}}\exp(i\boldsymbol{k}\,.\,\boldsymbol{r}). \tag{2.10}$$

The matrix element in (2.3) is

$$\begin{aligned}\langle k'\lambda'|V|k\lambda\rangle &= \int \psi^*_{k'}\chi^*_{\lambda'} V\psi_k\chi_\lambda \, d\boldsymbol{R}\, d\boldsymbol{r} \\ &= \frac{1}{Y}\int \exp(-i\boldsymbol{k}'\,.\,\boldsymbol{r})\chi^*_{\lambda'} V \exp(i\boldsymbol{k}\,.\,\boldsymbol{r})\chi_\lambda \, d\boldsymbol{R}\, d\boldsymbol{r}.\end{aligned} \tag{2.11}$$

We shall write the last line as $\langle k'\lambda'|V|k\lambda\rangle/Y$, so from now on the neutron wavefunction in the matrix element is $\exp(i\boldsymbol{k}\,.\,\boldsymbol{r})$.

The flux of the incident neutrons is the product of their density and velocity, i.e.

$$\Phi = \frac{1}{Y}\frac{\hbar}{m}k. \tag{2.12}$$

## 2.3 Expression for $d^2\sigma/d\Omega\, dE'$

We now derive a basic expression for the cross-section $d^2\sigma/d\Omega\, dE'$. We start by substituting (2.2), (2.9), (2.11), and (2.12) into (2.1), which gives

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar^2}\right)^2 |\langle k'\lambda'|V|k\lambda\rangle|^2. \tag{2.13}$$

All the $Y$s have cancelled out in (2.13), as they must do since the volume of the normalisation box is arbitrary.

$(\mathrm{d}\sigma/\mathrm{d}\Omega)_{\lambda\to\lambda'}$ is the cross-section for neutrons scattered into $\mathrm{d}\Omega$ in the direction of $\boldsymbol{k}'$. However, as already mentioned, since $\boldsymbol{k}$, $\lambda$, and $\lambda'$ are fixed, the scattered neutrons all have the same energy, determined by conservation of energy. If $E$ and $E'$ are the initial and final energies of the neutron, and $E_\lambda$ and $E_{\lambda'}$ are the initial and final energies of the scattering system, then

$$E+E_\lambda = E'+E_{\lambda'}. \tag{2.14}$$

In mathematical terms the energy distribution of the scattered neutrons is a $\delta$-function (see Appendix A). So the expression for the partial differential cross-section is

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar^2}\right)^2 |\langle \boldsymbol{k}'\lambda'|V|\boldsymbol{k}\lambda\rangle|^2 \delta(E_\lambda - E_{\lambda'} + E - E'). \tag{2.15}$$

This follows from (1.14) and the result

$$\int \delta(E_\lambda - E_{\lambda'} + E - E')\,\mathrm{d}E' = 1. \tag{2.16}$$

***Fourier transform of the potential function***

The first step in evaluating the matrix element is to integrate with respect to $\boldsymbol{r}$, the neutron coordinate. The potential of the neutron due to the $j$th nucleus has the form $V_j(\boldsymbol{r}-\boldsymbol{R}_j)$. So the potential for the whole scattering system is

$$V = \sum_j V_j(\boldsymbol{r}-\boldsymbol{R}_j). \tag{2.17}$$

Put

$$\boldsymbol{x}_j = \boldsymbol{r}-\boldsymbol{R}_j. \tag{2.18}$$

Now

$$\langle \boldsymbol{k}'\lambda'|V|\boldsymbol{k}\lambda\rangle$$

$$= \sum_j \int \chi^*_{\lambda'} \exp(-\mathrm{i}\boldsymbol{k}'\,.\,\boldsymbol{r}) V_j(\boldsymbol{r}-\boldsymbol{R}_j)\chi_\lambda \exp(\mathrm{i}\boldsymbol{k}\,.\,\boldsymbol{r})\,\mathrm{d}\boldsymbol{R}\,\mathrm{d}\boldsymbol{r} \tag{2.19}$$

$$= \sum_j \int \chi^*_{\lambda'} \exp\{-\mathrm{i}\boldsymbol{k}'\,.\,(\boldsymbol{x}_j+\boldsymbol{R}_j)\} V_j(\boldsymbol{x}_j)\chi_\lambda \exp\{\mathrm{i}\boldsymbol{k}\,.\,(\boldsymbol{x}_j+\boldsymbol{R}_j)\}\,\mathrm{d}\boldsymbol{R}\,\mathrm{d}\boldsymbol{x}_j \tag{2.20}$$

$$= \sum_j V_j(\boldsymbol{\kappa})\langle\lambda'|\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j)|\lambda\rangle, \tag{2.21}$$

where

$$V_j(\boldsymbol{\kappa}) = \int V_j(\boldsymbol{x}_j)\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{x}_j)\,\mathrm{d}\boldsymbol{x}_j, \tag{2.22}$$

$$\langle\lambda'|\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j)|\lambda\rangle = \int \chi^*_{\lambda'}\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j)\chi_\lambda\,\mathrm{d}\boldsymbol{R}, \tag{2.23}$$



and

$$\boldsymbol{\kappa} = \boldsymbol{k}-\boldsymbol{k}'. \tag{2.24}$$

$\boldsymbol{\kappa}$ is known as the *scattering vector*. The logic in going from (2.19) to (2.20) is that, for each $j$ term in the sum, integrating with respect to $\boldsymbol{r}$ and to $\boldsymbol{x}_j$ give the same result, because both integrations are done at fixed $\boldsymbol{R}_j$ over all space. We see from (2.22) that $V_j(\boldsymbol{\kappa})$ is the Fourier transform of the potential function for the $j$th nucleus.

***Fermi pseudopotential***

The next step is to insert a specific function for $V_j(\boldsymbol{x}_j)$. To find a suitable mathematical function we make an apparent digression and calculate $\mathrm{d}\sigma/\mathrm{d}\Omega$ for a single fixed nucleus using the present formalism. Consider (2.19). There is only one term, $j=1$, in the sum over $j$. Since the nucleus is fixed at the origin, $\boldsymbol{R}_1 = 0$, and $\lambda' = \lambda$. Thus

$$\langle \boldsymbol{k}'\lambda'|V|\boldsymbol{k}\lambda\rangle = \int \chi^*_\lambda\chi_\lambda\,\mathrm{d}\boldsymbol{R}_1 \int V(\boldsymbol{r})\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}$$

$$= \int V(\boldsymbol{r})\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}, \tag{2.25}$$

since $\chi_\lambda$ is normalised. Inserting this result in (2.13), together with $k'=k$, gives

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\int V(\boldsymbol{r})\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}\right|^2. \tag{2.26}$$

Now we know that $V(\boldsymbol{r})$ is short range. Let us make it really short range and put

$$V(\boldsymbol{r}) = a\delta(\boldsymbol{r}), \tag{2.27}$$

where $a$ is a real constant. $\delta(\boldsymbol{r})$ is a three-dimensional Dirac delta function, i.e.

$$\int_{\substack{\text{all}\\\text{space}}} \delta(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = 1. \tag{2.28}$$

Then

$$\int V(\boldsymbol{r})\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = a\int \delta(\boldsymbol{r})\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = a. \tag{2.29}$$

Therefore

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 a^2. \tag{2.30}$$

But from Section 1.4

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = b^2, \tag{2.31}$$

where $b$ is the scattering length. Therefore

$$a = \frac{2\pi\hbar^2}{m} b. \tag{2.32}$$

Inserting this value in (2.27) gives

$$V(\boldsymbol{r}) = \frac{2\pi\hbar^2}{m} b\,\delta(\boldsymbol{r}). \tag{2.33}$$

This potential, known as the *Fermi pseudopotential*, is the one we shall adopt. The positive sign in (2.32) comes from the definition of $b$ in (1.18), which implies a positive scattering length for a repulsive potential.

We recall that our entire derivation of the cross-section is based on Fermi's golden rule, which, for scattering processes, is equivalent to the Born approximation; both are based on first-order perturbation theory. Now the conditions for this theory to apply do not hold for the nuclear scattering of thermal neutrons. The justification for the use of the golden rule in these circumstances is that, when combined with the pseudopotential, it gives the required result of isotropic scattering for a single fixed nucleus.†

It may be noted that the pseudopotential does not correspond even approximately to the actual potential. Equation (2.33) shows that a repulsive pseudopotential gives a positive, and an attractive pseudopotential a negative scattering length. However, a positive scattering length does not imply that the actual potential is repulsive. If we simulate the actual potential by a hypothetical 'square-well' (or square-barrier) of range $r_0$ and depth or height $V$, we can solve the Schrödinger equation without approximation. The relation between the scattering length and the parameter $x = (2mV)^{1/2} r_0/\hbar$ is shown in Fig. 2.3. For a repulsive potential $b$ is positive for all values of $x$. For an attractive potential it may be negative or positive. The actual potential is basically attractive. The details of its shape, depth, and range determine the magnitude and sign of the scattering length.

The scattering length defined in (1.18) relates to a fixed nucleus and is sometimes known as the *bound* scattering length. If the nucleus is free, the scattering must be treated in the centre-of-mass system. The result is the same as if the nucleus were fixed, but the mass $m$ of the neutron must be replaced by the reduced mass $\mu$ of the nucleus–neutron system. This is given by

$$\mu = \frac{mM}{m+M}, \tag{2.34}$$

where $M$ is the mass of the nucleus. The scattering length for this process is called the *free* scattering length. Denote it by $b_f$. Since the potential is the same whether the nucleus is fixed or free, the expression for the pseudopotential (2.33) shows that

$$\frac{b_f}{\mu} = \frac{b}{m}, \tag{2.35}$$

i.e.

$$b_f = \frac{M}{m+M} b. \tag{2.36}$$

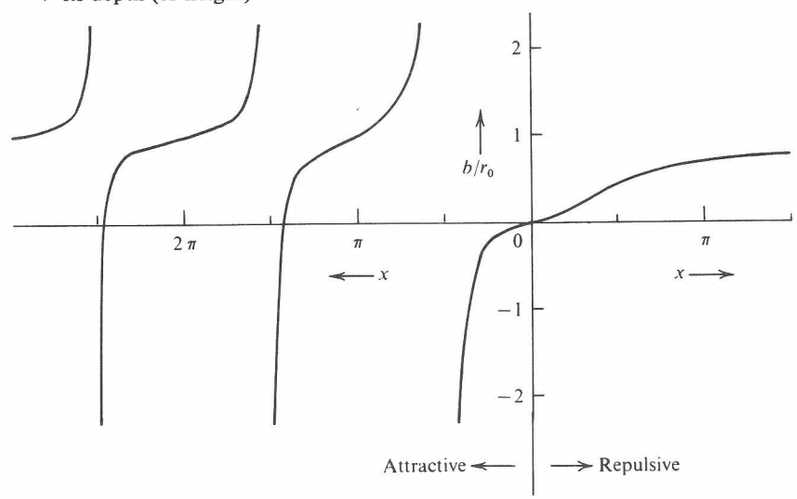
For most nuclei the free scattering length is only slightly less than the bound one. But in the extreme case of light hydrogen

$$b_f = \tfrac{1}{2} b. \tag{2.37}$$

We return to the expression for the cross-section for a general scattering system. If the $j$th nucleus has scattering length $b_j$, its potential is

$$V_j(\boldsymbol{x}_j) = \frac{2\pi\hbar^2}{m} b_j \delta(\boldsymbol{x}_j). \tag{2.38}$$

Fig. 2.3 Relation between scattering length $b$ and the parameter $x = (2mV)^{1/2} r_0/\hbar$ for a square-well potential. $r_0$ is the range of the potential and $V$ its depth (or height).




† For further discussion of this point see Fermi (1936) and Breit (1947).

Inserting this in (2.22) gives

$$V_j(\boldsymbol{\kappa}) = \frac{2\pi\hbar^2}{m} b_j. \tag{2.39}$$

From (2.15), (2.21), and (2.39)

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\lambda'\to\lambda} = \frac{k'}{k}\left|\sum_j b_j\langle\lambda'|\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j)|\lambda\rangle\right|^2 \delta(E_\lambda - E_{\lambda'} + E - E'). \tag{2.40}$$

***Integral representation of the δ-function for energy***

We now express the $\delta$-function for energy as an integral with respect to time. The reason for doing this will become apparent later in the section.

$$\delta(E_\lambda - E_{\lambda'} + E - E') = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp\{\mathrm{i}(E_{\lambda'} - E_\lambda)t/\hbar\}\exp(-\mathrm{i}\omega t)\,\mathrm{d}t, \tag{2.41}$$

where $\omega$ is defined by

$$\hbar\omega = E - E'. \tag{2.42}$$

Eq. (2.41) is derived in Appendix A.2.

We also need the following results. Let $H$ be the Hamiltonian of the scattering system. The states $\lambda$ and $\lambda'$ are eigenfunctions of $H$ with eigenvalues $E_\lambda$ and $E_{\lambda'}$, i.e.

$$H|\lambda\rangle = E_\lambda|\lambda\rangle, \quad \text{and} \quad H|\lambda'\rangle = E_{\lambda'}|\lambda'\rangle. \tag{2.43}$$

Then

$$H^n|\lambda\rangle = E_\lambda^n|\lambda\rangle, \tag{2.44}$$

a result obtained from (2.43) by operating $n$ times on $|\lambda\rangle$ with $H$. Further

$$\exp(-\mathrm{i}Ht/\hbar)|\lambda\rangle = \exp(-\mathrm{i}E_\lambda t/\hbar)|\lambda\rangle. \tag{2.45}$$

This result is obtained by expanding the exponential

$$\exp(-\mathrm{i}Ht/\hbar) = 1 - \mathrm{i}Ht/\hbar + \frac{1}{2!}(-\mathrm{i}Ht/\hbar)^2 + \ldots \tag{2.46}$$

and using (2.44).

The matrix element in (2.40) is the sum of $N$ terms ($j = 1, \ldots N$). So the square of the matrix element is the sum of $N^2$ terms, of which a typical member is

$$b_{j'}^* b_j\langle\lambda'|\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_{j'})|\lambda\rangle^*\langle\lambda'|\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j)|\lambda\rangle$$
$$= b_{j'}b_j\langle\lambda|\exp(-\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_{j'})|\lambda'\rangle\langle\lambda'|\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j)|\lambda\rangle. \tag{2.47}$$



In this equation we have used the fact that the scattering length is real, and also the relation (C.3). From (2.40), (2.41), and (2.47)

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\lambda\to\lambda'}$$
$$= \frac{k'}{k}\sum_{jj'} b_{j'}b_j\langle\lambda|\exp(-\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_{j'})|\lambda'\rangle\langle\lambda'|\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j)|\lambda\rangle$$
$$\times\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\exp\{\mathrm{i}(E_{\lambda'} - E_\lambda)t/\hbar\}\exp(-\mathrm{i}\omega t)\,\mathrm{d}t \tag{2.48}$$
$$= \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{jj'} b_{j'}b_j\int_{-\infty}^{\infty}\langle\lambda|\exp(-\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_{j'})|\lambda'\rangle$$
$$\times\langle\lambda'|\exp(\mathrm{i}Ht/\hbar)\exp(\mathrm{i}\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j)\exp(-\mathrm{i}Ht/\hbar)|\lambda\rangle\exp(-\mathrm{i}\omega t)\,\mathrm{d}t. \tag{2.49}$$

The last step follows from (2.45).

***Sum over λ′, average over λ***

In an actual experiment we do not measure the cross-section for a process in which the scattering system goes from a specific state $\lambda$ to another state $\lambda'$. Instead we measure $\mathrm{d}^2\sigma/\mathrm{d}\Omega\,\mathrm{d}E'$, the cross-section defined in (1.11). To obtain this quantity we must first sum $(\mathrm{d}^2\sigma/\mathrm{d}\Omega\,\mathrm{d}E')_{\lambda\to\lambda'}$ over all final states $\lambda'$, keeping the initial state $\lambda$ fixed, and then average over all $\lambda$.

To carry out the first step we use the closure relation proved in Appendix C. For a pair of operators $A$ and $B$

$$\sum_{\lambda'}\langle\lambda|A|\lambda'\rangle\langle\lambda'|B|\lambda\rangle = \langle\lambda|AB|\lambda\rangle. \tag{2.50}$$

To average the last quantity over $\lambda$, we multiply by $p_\lambda$, the probability that the scattering system is in the state $\lambda$, and then sum over $\lambda$. $p_\lambda$ is given by the Boltzmann distribution. If the temperature of the scattering system is $T$

$$p_\lambda = \frac{1}{Z}\exp(-E_\lambda\beta), \tag{2.51}$$

where

$$Z = \sum_\lambda \exp(-E_\lambda\beta), \tag{2.52}$$

and

$$\beta = \frac{1}{k_\mathrm{B}T}. \tag{2.53}$$

$Z$ is known as the *partition function* and is inserted to ensure that $\sum_\lambda p_\lambda = 1$.

From (2.49) and (2.50) we have

$$\frac{d^2\sigma}{d\Omega\, dE'} = \sum_{\lambda\lambda'} p_\lambda \left(\frac{d^2\sigma}{d\Omega\, dE'}\right)_{\lambda\to\lambda'}$$

$$= \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{jj'} b_j b_{j'} \int_{-\infty}^{\infty} \exp(-i\omega t)\, dt \sum_\lambda p_\lambda \times \langle\lambda|\exp(-i\boldsymbol{\kappa}\,.\,\boldsymbol{R}_{j'})\exp(iHt/\hbar)\exp(i\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j)\exp(-iHt/\hbar)|\lambda\rangle. \tag{2.54}$$

The last expression may be written in terms of the time-dependent Heisenberg operator $\boldsymbol{R}_j(t)$, defined by

$$\boldsymbol{R}_j(t) = \exp(iHt/\hbar)\boldsymbol{R}_j \exp(-iHt/\hbar). \tag{2.55}$$

It follows from the definition that

$$\exp\{i\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j(t)\} = \exp(iHt/\hbar)\exp(i\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j)\exp(-iHt/\hbar). \tag{2.56}$$

Heisenberg operators are discussed in Appendix D, and (2.56) is justified there. Note that

$$\boldsymbol{R}_j(0) = \boldsymbol{R}_j. \tag{2.57}$$

We denote the thermal average of the operator $A$ at temperature $T$ by $\langle A\rangle$, i.e.

$$\langle A\rangle = \sum_\lambda p_\lambda \langle\lambda|A|\lambda\rangle. \tag{2.58}$$

From (2.54), (2.56), and (2.58) we have

$$\frac{d^2\sigma}{d\Omega\, dE'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{jj'} b_j b_{j'} \int_{-\infty}^{\infty} \langle\exp\{-i\boldsymbol{\kappa}\,.\,\boldsymbol{R}_{j'}(0)\}\exp\{i\,\boldsymbol{\kappa}.\,\boldsymbol{R}_j(t)\}\rangle \times\exp(-i\omega t)\, dt. \tag{2.59}$$

This is our basic expression for the partial differential cross-section for nuclear scattering. It is a compact expression and may appear simple, but its evaluation, except for the most elementary scattering systems, is not a simple matter. The properties of the scattering system are contained in the Hamiltonian $H$. They are therefore contained in the Heisenberg operators, and the eigenstates $|\lambda\rangle$. In the next three chapters we shall be concerned with evaluating the cross-section for specific physical systems.

We can see at this stage the purpose of expressing the $\delta$-function for conservation of energy as an integral with respect to time in (2.41). The $E_{\lambda'}$ term in the argument of the $\delta$-function prevents us from using (2.50) to sum over $\lambda'$. By means of (2.41) we are able to bring the $E_{\lambda'}$ term inside one of the matrix elements, where it reappears as an operator depending on the Hamiltonian. There is now no term in $\lambda'$ outside the two matrix elements, and the sum over $\lambda'$ can be carried out immediately.



## 2.4 Coherent and incoherent scattering

Consider a scattering system consisting of a single element where the scattering length $b$ varies from one nucleus to another owing to nuclear spin or the presence of isotopes or both. Let the value $b_i$ occur with relative frequency $f_i$, i.e.

$$\sum_i f_i = 1. \tag{2.60}$$

Then the average value of $b$ for the system is

$$\bar{b} = \sum_i f_i b_i, \tag{2.61}$$

and the average value of $b^2$ is

$$\overline{b^2} = \sum_i f_i b_i^2. \tag{2.62}$$

We assume there is no correlation between the values of $b$ for any two nuclei, that is to say, whatever the value of $b$ for one nucleus, the probability that another nucleus has the value $b_i$ is simply $f_i$.

Imagine that we have a large number of scattering systems. They are identical in every way as regards the positions and motions of the nuclei. Also the total number of each $b_i$ is the same for all the systems. But each system has a different distribution of the $b$s among the nuclei, every possible distribution being represented once. Now, provided the system contains a large number of nuclei – a condition usually well satisfied – the cross-section we measure is very close to the cross-section averaged over all the systems. This is given by

$$\frac{d^2\sigma}{d\Omega\, dE'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{jj'} \overline{b_{j'} b_j} \int \langle j', j\rangle \exp(-i\omega t)\, dt, \tag{2.63}$$

where

$$\langle j', j\rangle = \langle\exp\{-i\boldsymbol{\kappa}\,.\,\boldsymbol{R}_{j'}(0)\}\exp\{i\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j(t)\}\rangle. \tag{2.64}$$

(We use this notation for the moment, because only the $j'$, $j$ values of the matrix element are relevant to the discussion.)

On the assumption of no correlation between the $b$ values of different nuclei

$$\overline{b_{j'}b_j} = (\bar{b})^2, \qquad j' \neq j,$$
$$\overline{b_{j'}b_j} = \overline{b^2}, \qquad j' = j. \tag{2.65}$$

So

$$\frac{d^2\sigma}{d\Omega\, dE'} = \frac{k'}{k}\frac{1}{2\pi\hbar}(\bar{b})^2 \sum_{\substack{jj' \\ j'\neq j}} \int \langle j', j\rangle \exp(-i\omega t)\, dt$$
$$+ \frac{k'}{k}\frac{1}{2\pi\hbar}\overline{b^2}\sum_j \int \langle j, j\rangle \exp(-i\omega t)\, dt \tag{2.66}$$
$$= \frac{k'}{k}\frac{1}{2\pi\hbar}(\bar{b})^2 \sum_{jj'} \int \langle j', j\rangle \exp(-i\omega t)\, dt$$
$$+ \frac{k'}{k}\frac{1}{2\pi\hbar}\{\overline{b^2} - (\bar{b})^2\}\sum_j \int \langle j, j\rangle \exp(-i\omega t)\, dt. \tag{2.67}$$

In going from (2.66) to (2.67) we have added and subtracted $(k'/k)(1/2\pi\hbar)(\bar{b})^2 \int \sum_j \langle j, j\rangle \exp(-i\omega t)\, dt$. The first term in (2.67) is known as the *coherent* and the second term as the *incoherent* scattering cross-section. We write

$$\left(\frac{d^2\sigma}{d\Omega\, dE'}\right)_{coh} = \frac{\sigma_{coh}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{jj'}\int_{-\infty}^{\infty} \langle \exp\{-i\boldsymbol{\kappa}\,.\,\boldsymbol{R}_{j'}(0)\}\exp\{i\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j(t)\}\rangle$$
$$\times \exp(-i\omega t)\, dt, \tag{2.68}$$

$$\left(\frac{d^2\sigma}{d\Omega\, dE'}\right)_{inc} = \frac{\sigma_{inc}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j}\int_{-\infty}^{\infty} \langle \exp\{-i\boldsymbol{\kappa}\,.\,\boldsymbol{R}_{j}(0)\}\exp\{i\boldsymbol{\kappa}\,.\,\boldsymbol{R}_j(t)\}\rangle$$
$$\times \exp(-i\omega t)\, dt, \tag{2.69}$$

where $$\sigma_{coh} = 4\pi(\bar{b})^2, \qquad \sigma_{inc} = 4\pi\{\overline{b^2} - (\bar{b})^2\}. \tag{2.70}$$

We see from the equations that the coherent scattering depends on the correlation between the positions of the *same* nucleus at different times, and on the correlation between the positions of *different* nuclei at different times. It therefore gives *interference* effects. The incoherent scattering depends only on the correlation between the positions of the *same* nucleus at different times. It does not give interference effects.

The physical interpretation of (2.67) is as follows. The actual scattering system has different scattering lengths associated with different nuclei. The coherent scattering is the scattering the same system (same nuclei with the same positions and motions) would give if all the scattering lengths were equal to $\bar{b}$. The incoherent scattering



is the term we must add to this to obtain the scattering due to the actual system. Physically the incoherent scattering arises from the random distribution of the deviations of the scattering lengths from their mean value.

We now derive expressions for the frequencies $f_i$ and for $\bar{b}$ and $\overline{b^2}$. The simplest case is when the scattering system consists of a single isotope with zero nuclear spin. Then all the $b$s are equal, and the scattering is entirely coherent.

Suppose the system consists of a single isotope with nuclear spin $I$. The spin of the nucleus–neutron system has the values $I+\frac{1}{2}$ or $I-\frac{1}{2}$. Denote the scattering lengths for the two spin values by $b^+$ and $b^-$. The number of states associated with spin $I+\frac{1}{2}$ is

$$2(I+\tfrac{1}{2})+1 = 2I+2, \tag{2.71}$$

and the number of states associated with spin $I-\frac{1}{2}$ is

$$2(I-\tfrac{1}{2})+1 = 2I. \tag{2.72}$$

If the neutrons are unpolarised and the nuclear spins are randomly oriented, each spin state has the same *a priori* probability. So the scattering length $b^+$ occurs with frequency

$$f^+ = \frac{2I+2}{4I+2} = \frac{I+1}{2I+1}, \tag{2.73}$$

and the scattering length $b^-$ occurs with frequency

$$f^- = \frac{2I}{4I+2} = \frac{I}{2I+1}. \tag{2.74}$$

Thus $$\bar{b} = \frac{1}{2I+1}\{(I+1)b^+ + Ib^-\}. \tag{2.75}$$

If the neutrons are polarised or the nuclear spins are aligned, the $4I+2$ spin states of the nucleus–neutron system are not equally probable. But unless *both* conditions apply, $f^+$ and $f^-$ have the values shown in (2.73) and (2.74).

If there are several isotopes in the scattering system, then for each isotope the quantities $f^+$ and $f^-$ must be multiplied by the relative abundance of the isotope to obtain the relative frequency of the scattering length. So, in general,

$$\bar{b} = \sum_\xi \frac{c_\xi}{2I_\xi+1}\{(I_\xi+1)b_\xi^+ + I_\xi b_\xi^-\}, \tag{2.76}$$

$$\overline{b^2} = \sum_\xi \frac{c_\xi}{2I_\xi+1}\{(I_\xi+1)(b_\xi^+)^2 + I_\xi(b_\xi^-)^2\}, \tag{2.77}$$

where $c_\xi$ is the relative abundance of the $\xi$th isotope, $I_\xi$ its nuclear spin, and $b_\xi^+$ and $b_\xi^-$ its scattering lengths. The quantity $\bar{b}$ is known as the *coherent* scattering length of the element or nuclide. It is conventional to quote the values of $\bar{b}$ and $\overline{b^2}$ in terms of the two quantities $\sigma_{\text{coh}}$ and $\sigma_{\text{inc}}$ defined in (2.70). A list of the values of $\sigma_{\text{coh}}$ and $\sigma_{\text{inc}}$ for the elements, together with a description of the methods of measuring these quantities, has been given by Koester (1977). A few of the values are given in Table 2.1.

Table 2.1 Values of $\sigma_{\text{coh}}$ and $\sigma_{\text{inc}}$

| Element or nuclide | $Z$ | $\sigma_{\text{coh}}$ | $\sigma_{\text{inc}}$ | Element | $Z$ | $\sigma_{\text{coh}}$ | $\sigma_{\text{inc}}$ |
|---|---|---|---|---|---|---|---|
| $^1$H | 1 | 1.8 | 80.2 | V | 23 | 0.02 | 5.0 |
| $^2$H | 1 | 5.6 | 2.0 | Fe | 26 | 11.5 | 0.4 |
| C | 6 | 5.6 | 0.0 | Co | 27 | 1.0 | 5.2 |
| O | 8 | 4.2 | 0.0 | Ni | 28 | 13.4 | 5.0 |
| Mg | 12 | 3.6 | 0.1 | Cu | 29 | 7.5 | 0.5 |
| Al | 13 | 1.5 | 0.0 | Zn | 30 | 4.1 | 0.1 |

The units of $\sigma_{\text{coh}}$ and $\sigma_{\text{inc}}$ are $10^{-28}$ m$^2$. The values are taken from Koester (1977).

The extension of the theory to scattering systems containing more than one element is readily made. If for example the scattering system is a crystal of NaCl, the coherent scattering is that due to a hypothetical crystal in which all the sodium nuclei have scattering lengths equal to $\bar{b}$ for sodium, and all the chlorine nuclei have scattering lengths equal to $\bar{b}$ for chlorine. The incoherent scattering is the sum of the incoherent scattering from the sodium nuclei and the incoherent scattering from the chlorine nuclei.

# 3

## *Nuclear scattering by crystals*

### 3.1 Introduction

In the present chapter we evaluate the cross-sections when the scattering system is a single crystal. We start by considering a Bravais crystal, i.e. a crystal with one atom per unit cell. Denote the sides of the unit cell by $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ (see Fig. 3.1). Then a lattice vector is given by

$$\boldsymbol{l} = l_1\boldsymbol{a}_1 + l_2\boldsymbol{a}_2 + l_3\boldsymbol{a}_3, \tag{3.1}$$

where $l_1$, $l_2$, $l_3$ are integers. The volume of the unit cell is

$$v_0 = \boldsymbol{a}_1 \,.\, [\boldsymbol{a}_2 \times \boldsymbol{a}_3]. \tag{3.2}$$

We define the reciprocal lattice to be a lattice with unit-cell vectors $\boldsymbol{\tau}_1$, $\boldsymbol{\tau}_2$, $\boldsymbol{\tau}_3$, where

$$\boldsymbol{\tau}_1 = \frac{2\pi}{v_0}[\boldsymbol{a}_2 \times \boldsymbol{a}_3], \qquad \boldsymbol{\tau}_2 = \frac{2\pi}{v_0}[\boldsymbol{a}_3 \times \boldsymbol{a}_1],$$
$$\boldsymbol{\tau}_3 = \frac{2\pi}{v_0}[\boldsymbol{a}_1 \times \boldsymbol{a}_2]. \tag{3.3}$$

The volume of the unit cell in the reciprocal lattice is

$$\boldsymbol{\tau}_1 \,.\, [\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3] = \frac{(2\pi)^3}{v_0}. \tag{3.4}$$

Fig. 3.1 Unit cell of crystal.