Chapter 7 - **NEUTRON SCATTERING THEORY**

Elements of neutron scattering theory are described here. The scattering amplitude, scattering lengths and cross sections are introduced and discussed.

1. SOLUTION OF THE SCHRODINGER EQUATION

Neutron scattering theory involves quantum mechanics tools such as the solution of the Schrodinger equation even though the scattering problem is not a quantum mechanical problem (no bound states are involved). A simple solution of the Schrodinger equation involving perturbation theory is presented here. This is to so-called Born Approximation method.

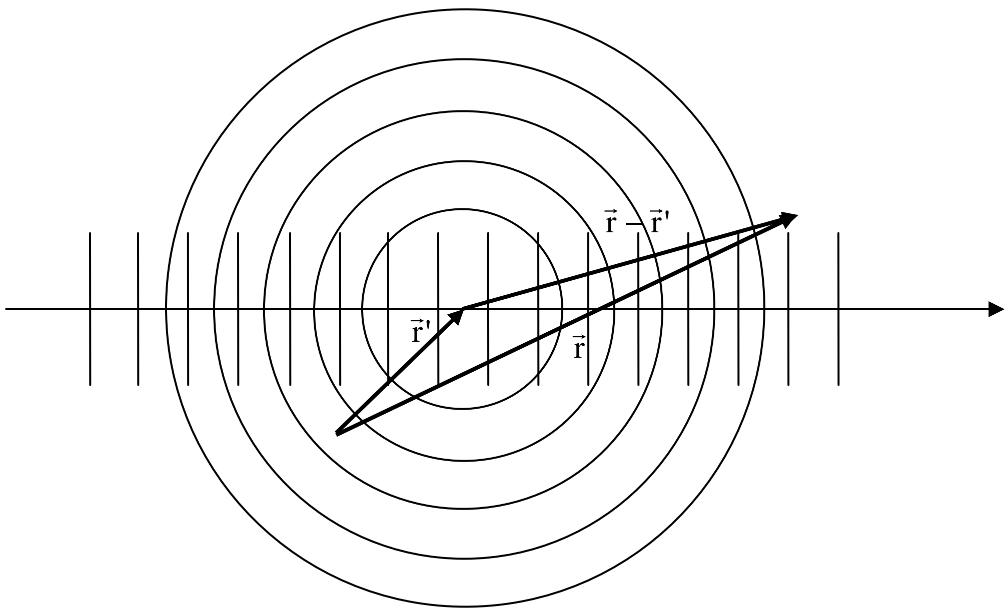

Figure 1: Incident plane wave and scattered spherical wave.

The Schrodinger equation is expressed as follows:

$$H_i \psi_i = E_i \psi_i \qquad (1)$$
$$H\psi = E_s \psi$$
$$H = H_i + V.$$

H is the full Hamiltonian operator, H_i is the incident neutron kinetic energy operator and V is the neutron-nucleus interaction potential. E_i and E_s are the eigenvalue energies for the incident neutron and for the scattered neutron. Ψ_i and Ψ are the eigenfunctions for the incident (non-interacting) neutron and for the interacting neutron-nucleus pair.

$$H_i = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2 \qquad (2)$$

$\vec{p} = i\hbar\vec{\nabla}$ is the momentum operator.

$$E_i = \frac{\hbar^2 k_i^{\,2}}{2m}.$$

E_i is the incident neutron kinetic energy and k_i is its incident wavenumber. Ψ_i is the solution of the homogeneous differential equation:

$$(H_i - E_i)\Psi_i(\vec{r}) = -\frac{\hbar^2}{2m}(\nabla^2 + k_i^{\,2})\Psi_i(\vec{r}) = 0. \qquad (3)$$

The solution is an incident plane wave $\Psi_i(r) = \exp(i\vec{k}_i.\vec{r})$ using vector notation. The full differential equation is written as:

$$-\frac{\hbar^2}{2m}(\nabla^2 + k_s^{\,2})\Psi(\vec{r}) = -V(\vec{r})\Psi(\vec{r}). \qquad (4)$$

Its solution is an integral equation of the form:

$$\Psi(\vec{r}) = \Psi_i(\vec{r}) + \left(\frac{m}{2\pi\hbar^2}\right)\int d\vec{r}\,'G(\vec{r}-\vec{r}\,')V(\vec{r}\,')\Psi(\vec{r}\,') \qquad (5)$$

Here $G(\vec{r}-\vec{r}\,')$ is a Green's function satisfying the following differential equation:

$$(H - E_s)G(\vec{r}) = -\frac{\hbar^2}{2m}(\nabla^2 + k_s^{\,2})G(\vec{r}) = \delta(\vec{r}) \qquad (6)$$

k_s is the scattered neutron wavenumber. Its solution is a spherical outgoing wave of the form:

$$G(\vec{r}) = \frac{\exp(ik_s r)}{r}. \qquad (7)$$

In order to verify this result, the following relations valid in spherical coordinates are used:

$$\nabla\left(\frac{1}{r}\right) = \frac{\partial}{\partial r}\left(r^2\frac{1}{r}\right) = \frac{1}{r^2} \qquad (8)$$

$$\nabla^2\left(\frac{1}{r}\right)=\frac{1}{r^2}\left[\frac{\partial}{\partial r}r^2\left(\frac{\partial}{\partial r}\right)\right]\left(\frac{1}{r}\right)=\delta(r)\,.$$

Therefore:

$$\Psi(\vec{r})=\Psi_i(\vec{r})+\left(\frac{m}{2\pi\hbar^2}\right)\int d\vec{r}\,'\frac{\exp(ik_s\,|\vec{r}-\vec{r}\,'|)}{|\vec{r}-\vec{r}\,'|}V(\vec{r}\,')\Psi(\vec{r}\,') \qquad (9)$$

Vector $\vec{r}\,'$ is within the sample and $\vec{r}$ is far from the sample so that r >> r' and therefore one can approximate $|\vec{r}-\vec{r}\,'|\cong r-\frac{\vec{r}.\vec{r}\,'}{r}$.

$$G(|\vec{r}-\vec{r}\,'|)=\frac{\exp(ik_s r)}{r}\exp\left(\frac{-ik_s\vec{r}.\vec{r}\,'}{r}\right)=\frac{\exp(ik_s r)}{r}\exp(-i\vec{k}_s.\vec{r}\,')\,. \qquad (10)$$

Here, the scattered neutron wavevector $\vec{k}_s$ has been defined as $\vec{k}_s=k_s\vec{r}/r$.

The general solution of the Schrodinger equation is an integral equation that can be solved iteratively through the expansion:

$$\Psi(\vec{r})=\Psi_i(\vec{r})+\left(\frac{m}{2\pi\hbar^2}\right)\int d\vec{r}\,'G(\vec{r}-\vec{r}\,')V(\vec{r}\,')\Psi_i(\vec{r}\,')+$$
$$\left(\frac{m}{2\pi\hbar^2}\right)^2\int d\vec{r}\,'G(\vec{r}-\vec{r}\,')V(\vec{r}\,')\int d\vec{r}\,''G(\vec{r}-\vec{r}\,'')\Psi_i(\vec{r}\,'')+\ldots \qquad (11)$$

Keeping only the first integral term corresponds to the first Born approximation which can be presented in the form:

$$\Psi(\vec{r})=\Psi_i(\vec{r})+\left(\frac{m}{2\pi\hbar^2}\right)\int d\vec{r}\,'G(\vec{r}-\vec{r}\,')V(\vec{r}\,')\Psi_i(\vec{r}\,') \qquad (12)$$
$$\Psi(\vec{r})=\exp(i\vec{k}_i.\vec{r})+\frac{\exp(ik_s r)}{r}\left(\frac{m}{2\pi\hbar^2}\right)\int d\vec{r}\,'\exp(-i\vec{k}_s.\vec{r}\,')V(\vec{r}\,')\exp(i\vec{k}_i.\vec{r}\,')$$
$$\Psi(\vec{r})=\exp(i\vec{k}_i.\vec{r})+\frac{\exp(ik_s r)}{r}f(\theta)\,.$$

The scattering amplitude $f(\theta)$ has been defined as:

$$f(\theta)=\left(\frac{m}{2\pi\hbar^2}\right)\int d\vec{r}\,'\exp(-i\vec{Q}.\vec{r}\,')V(\vec{r}\,') \qquad (13)$$

$\vec{Q} = \vec{k}_s - \vec{k}_i$ is the scattering vector. f(θ) is the Fourier transform of the interaction potential V(r'). f(θ) has been assumed to be independent of the azimuthal angle.

The first Born approximation applies to thermal/cold neutrons neutron scattering corresponding to "s wave" scattering (i.e., corresponding to a zero orbital angular quantum number). This includes all of neutron scattering except for neutron reflectivity whereby higher order terms in the Born expansion have to be included. Neutron reflectometry involves refraction (not diffraction).

$\vec{Q}$ characterizes the probed length scale and its magnitude is given for elastic scattering in terms of the neutron wavelength λ and scattering angle θ as $Q = (4\pi/\lambda)\sin(\theta/2)$. For small angles (SANS), it is simply approximated by $Q = 2\pi\theta/\lambda$. Since Q is the Fourier variable (in reciprocal space) conjugate to scatterer positions (in direct space), investigating low-Q probes large length scales in direct space and vice versa.

In summary, the solution of the Schrodinger equation is an incident plane wave plus a scattered spherical wave multiplied by the scattering amplitude.

2. SCATTERING CROSS SECTIONS

The microscopic differential scattering cross section is defined here. It represents the fraction of neutrons scattered into solid angle dΩ with a scattering angle θ.

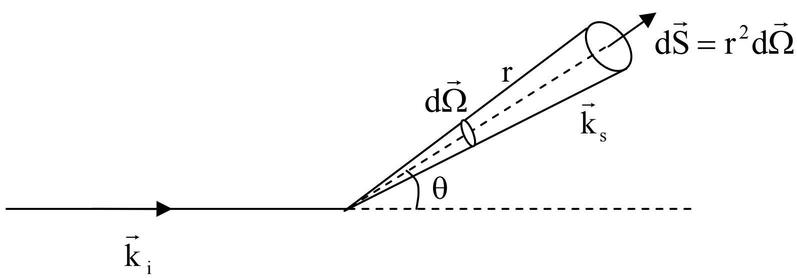

Figure 2: Representation of neutrons scattered with angle θ inside a solid angle dΩ.

Consider incident neutrons of wavenumber k_i and scattered neutrons of wavenumber k_s. The incident neutron flux also called current density (neutrons/cm^2.s) is given by:

$$\vec{J}_i = \frac{i\hbar}{2m}\left(\Psi_i \vec{\nabla}\Psi_i^* - \Psi_i^* \vec{\nabla}\Psi_i\right). \tag{14}$$

Here * represents the complex conjugate and $\Psi_i = \exp(i\vec{k}_i.\vec{r})$ is the incident plane wave. Performing the simple operation $\vec{\nabla}\Psi = i\vec{k}_i\Psi$, one obtains $\vec{J}_i = \hbar\vec{k}_i / m$. Similarly for the scattered neutron flux:

$$\vec{J}_s = \frac{i\hbar}{2m}\left(\chi\vec{\nabla}\chi^* - \chi^*\vec{\nabla}\chi\right). \qquad (15)$$

Where $\chi = \Psi - \Psi_i = \frac{\exp(ik_s r)}{r} f(\theta)$. Here also, performing the differentiations, one obtains: $\vec{J}_s = \frac{\hbar\vec{k}_s}{m}\frac{|f(\theta)|^2}{r^2}$. Note that the current densities $\vec{J}_i$ and $\vec{J}_s$ have units of velocity (speed). In order to obtain the standard units for a current density (neutrons/cm^2.s), one has to divide by the volume formed by a unit area and the distance travelled by the neutrons per second.

The differential neutron scattering cross section is defined as:

$$d\sigma_s(\theta) = \frac{J_s r^2 d\Omega}{J_i} = \frac{k_s}{k_i}|f(\theta)|^2 \, d\Omega \qquad (16)$$

This is the ratio of the neutron flux scattered in $d\Omega$ over the incident neutron flux. Within the first Born approximation (also called the Fermi Golden Rule):

$$\frac{d\sigma_s(\theta)}{d\Omega} = \frac{k_s}{k_i}|f(\theta)|^2 \qquad (17)$$

$$\frac{d\sigma_s(\theta)}{d\Omega} = \frac{k_s}{k_i}\left|\left(\frac{m}{2\pi\hbar^2}\right)\int dr' \exp(-i\vec{Q}.\vec{r}')V(\vec{r}')\right|^2.$$

This cross section contains information about what inhomogeneities are scattering and how they are distributed in the sample. The microscopic scattering cross section is its integral over solid angles: $\sigma_s = \int\left(\frac{d\sigma_s}{d\Omega}\right)d\Omega$. Cross sections are given in barn units (1 barn = 10^{-24} cm^2).

Given the (atomic) number density N/V (number of scattering nuclei/cm^3) in a material, a macroscopic cross section is also defined as: $\Sigma_s = (N/V)\,\sigma_s$ (units of cm^{-1}). SANS data are often presented on an "absolute" macroscopic cross section scale independent of instrumental conditions and of sample volume. It is given by $d\Sigma_s/d\Omega = (N/V)\, d\sigma_s/d\Omega$.

3. THE BRA-KET NOTATION

The <bra|ket> approach is useful for simplifying notation. Consider the following definitions:

$$< \vec{r} \,|\, \vec{k}_i >= \exp(i\vec{k}_i.\vec{r}) \qquad (18)$$
$$< \vec{r} \,|\, \Psi >= \Psi(\vec{r})$$
$$< r \,|\, V = V(r)$$
$$< \vec{r} \,|\, G \,|\, \vec{r}') = G(\vec{r} - \vec{r}')$$
$$< \vec{r} \,|\, \vec{r}') = \delta(\vec{r} - \vec{r}')\,.$$

Define the following closure relations:

$$\int |\, \vec{r}'> d\vec{r}' < \vec{r}'| = 1$$

$$\int |\, \vec{k} > d\vec{k} < \vec{k}\,| = 1\,. \qquad (19)$$

The integrations are over all direct $\vec{r}$ or reciprocal $\vec{k}$ space. The scattering amplitude is expressed as:

$$f(\theta) = \left(\frac{m}{2\pi\hbar^2}\right)\int d\vec{r}' \exp(-i\vec{Q}.\vec{r}')V(\vec{r}') \qquad (20)$$

$$= \left(\frac{m}{2\pi\hbar^2}\right)\int d\vec{r}' \exp(-i\vec{k}_s.\vec{r}')\exp(i\vec{k}_i.\vec{r}')V(\vec{r}')\,.$$

Using the <bra|ket> notation, $f(\theta)$ can be also manipulated to the form:

$$f(\theta) = \left(\frac{m}{2\pi\hbar^2}\right) < \vec{k}_s \,|\, V \,|\, \vec{k}_i >. \qquad (21)$$

The scattering cross section is therefore given in terms of the transition probability $< \vec{k}_s \,|\, V \,|\, \vec{k}_i >$ as:

$$\frac{d\sigma_s(\theta)}{d\Omega} = \frac{k_s}{k_i}\left| < \vec{k}_s \,|\left(\frac{m}{2\pi\hbar^2}\right) V \,|\, \vec{k}_i > \right|^2. \qquad (22)$$

This result ignores the effect of spin interactions and therefore does not apply to scattering from magnetic systems.

4. SIMPLE MODEL FOR NEUTRON SCATTERING LENGTHS

A simple argument is used here in order to appreciate the origin of the scattering length (Squires, 1978). Consider a neutron of thermal/cold incident energy E_i being elastically scattered from a nucleus displaying an attractive square well potential $-V_o$ (note that $V_o >> E_i$). Recall the Schrodinger equation for this simplest potential.

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r) = E_s\psi(r). \qquad (23)$$

The Schrodinger equation can be solved in 2 regions (inside and outside of the well region).

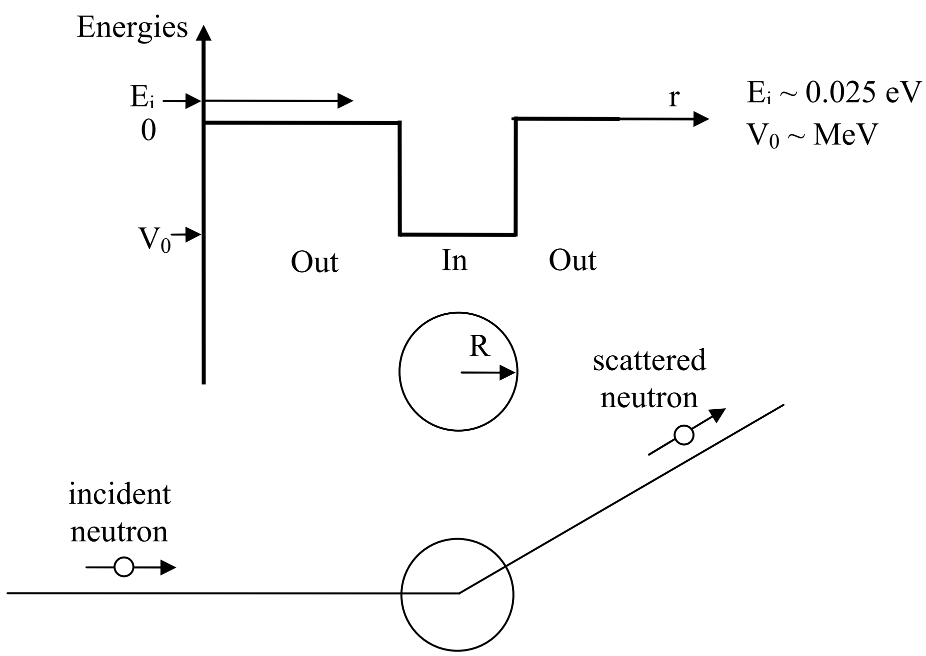

Figure 2: Neutron scattering from the quantum well of a nucleus.

Outside of the well region (i.e., for r > R) where V(r) = 0, the solution has the form:

$$\psi^{Out}(r) = \frac{\sin(k_i r)}{k_i r} - b\frac{\exp(ik_s r)}{r} \text{ (s-wave scattering).} \qquad (24)$$

Here b is the scattering length and for elastic scattering $k_s = k_i = \sqrt{2mE_i}/\hbar$. Note that in this case, the scattering amplitude is simply $f(\theta) = -b$. Note also that the incident plane wave has been averaged over orientation: $\frac{1}{2}\int_{-1}^{1} d\mu \exp(ik_i r\mu) = \frac{\sin(k_i r)}{k_i r}$.

Inside of the well $(r < R)$ where $V(r) = -V_0$ the solution is of the form:

$$\psi^{In}(r) = A\frac{\sin(qr)}{qr} \quad \text{with } q = \sqrt{2m(E_i + V_0)}/\hbar . \tag{25}$$

Note that this wavefunction $\Psi^{In}(r)$ represents a randomly oriented plane wave $\left(\frac{\sin(qr)}{qr} = \frac{1}{2}\int_{-1}^{1} d\mu \exp(iqr\mu)\right)$. The boundary conditions (continuity of the wavefunction and its derivative) are applied at the surface $(r = R)$:

$$\psi^{In}(r = R) = \psi^{Out}(r = R) \tag{26}$$

$$\frac{d}{dr}[\psi^{In}](r = R) = \frac{d}{dr}[\psi^{Out}](r = R).$$

Here $k_i r = k_s r = \sqrt{2mE_i}\, r/\hbar << 1$ (nuclear interactions are short ranged) and therefore $\psi^{Out} \sim 1 - b/r$. Finally:

$$A\frac{\sin(qR)}{qR} = 1 - \frac{b}{R} \tag{27}$$

$$Aq\frac{\cos(qR)}{qR} - A\frac{\sin(qR)}{qR^2} = \frac{b}{R^2}.$$

In another form:

$$A = \frac{1}{\cos(qR)} \tag{28}$$

$$\frac{b}{R} = 1 - \frac{\tan(qR)}{qR}.$$

The solution of this transcendental equation:

$$\frac{b}{R} = 1 - \frac{\tan(qR)}{qR} \tag{29}$$

gives a first order estimate of the scattering length b as a function of the radius of the spherical nucleus R and the depth of the potential well V_0.

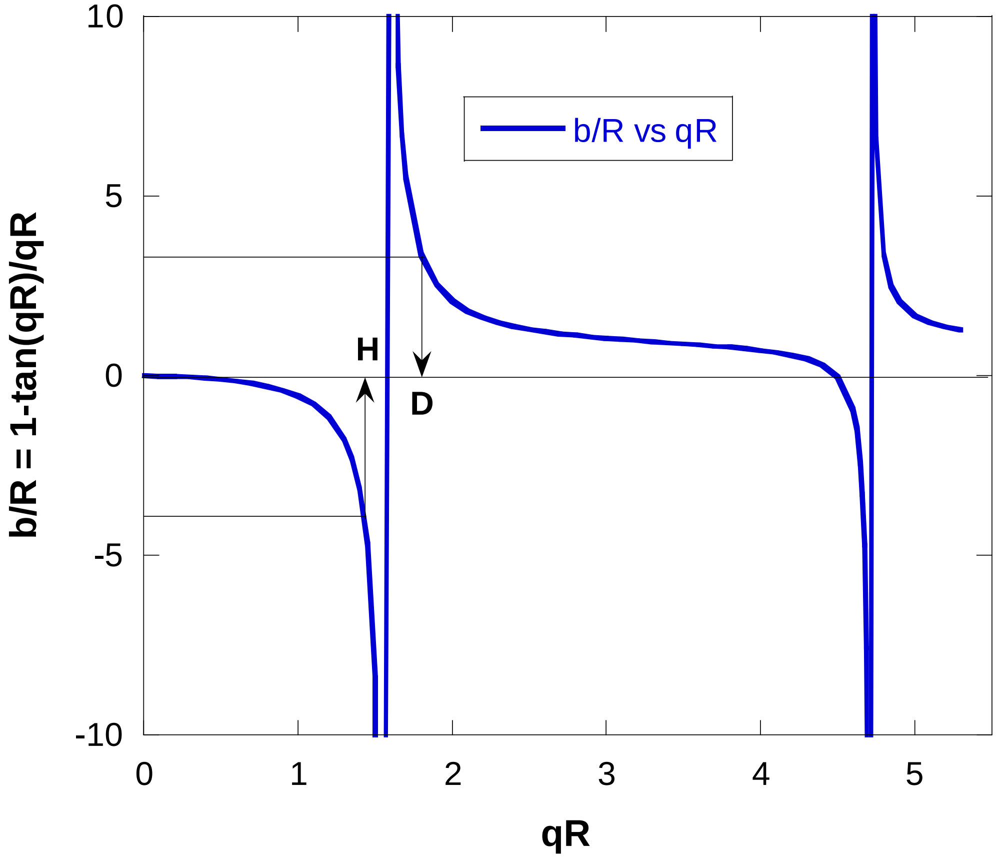

Figure 3: Solution of the Schrodinger equation subject to the boundary conditions.

Due to the steep variation of the solution to the above transcendental equation, adding only one nucleon (for example, going from H to D) gives a very large (seemingly random) variation in b. The scattering length can be negative like for H-1, Li-7, Ti-48, Ni-62, etc. The H and D nuclei have been added to the figure knowing their scattering lengths ($b_H = -0.374$ fm and $b_D = 6.671$ fm) and assuming $R_H = 1$ fm and $R_D = 2$ fm. The Fermi (1 fm = 10^{-13} cm) is a convenient unit for scattering lengths. The neutron-nucleus interaction potential can be estimated for the case of H as $V_0 = 30$ MeV. These are huge energies compared to the thermal neutron kinetic energy of 25 meV.

The scattering length itself can be complex if absorption is non negligible: $b = b_R - ib_I$. Neutron absorption is small for most organic materials. It has been neglected completely in the simple model discussed above.

Since no nucleus is completely free, bound scattering lengths should be used instead: $b_{bound} = b_{free} (A + 1)/A$, where A is the atomic number. Free and bound scattering lengths are substantially different only for low mass elements such as hydrogen.

5. MEASUREMENTS OF NEUTRON SCATTERING LENGTHS

Note that the index of refraction n is related to the material atomic density ρ (atoms/cm^3), the neutron scattering length b, and the neutron wavelength λ as:

$$n = 1 - \frac{\rho b}{2\pi}\lambda^2. \qquad (30)$$

The scattering length b can be measured by measuring the index of refraction n using optical methods. Note that most materials have an index of refraction less than one for neutrons and greater than one for light.

Neutron interferometry methods are another way of measuring scattering lengths.

REFERENCES

G.L. Squires, "Introduction to the Theory of Thermal Neutron Scattering" Dover Publications (1978).

QUESTIONS

1. What is the neutron scattering length of an element?
2. What is the scattering cross section of an element? How does it relate to the scattering length?
3. What is the differential scattering cross section?
4. What is the strength of typical neutron-nucleus interaction potentials? What is a typical neutron kinetic energy?
5. Write down the Schrodinger equation.
6. What is the first Born approximation? What type of neutron scattering is not well modeled by the first Born approximation?
7. What is a simple description of the solution of the Schrodinger equation in terms of waves?

ANSWERS

1. The neutron scattering length of an element represents the apparent "size" of this element during scattering.
2. The scattering cross section of an element is the apparent area that it offers during scattering. The scattering cross section σ is related to the scattering length b as $\sigma = 4\pi b^2$.
3. The differential scattering cross section is the cross section per unit solid angle $d\sigma/d\Omega$.
4. Typical neutron-nucleus interaction potentials are of order MeV. Typical neutron kinetic energies are of order meV (thermal neutron energy is 25 meV).

5. The Schrodinger equation is $[\frac{-\hbar^2}{2m}\nabla^2 + V(r)]\ \psi(r) = E\ \psi(r)$ where the first term is the kinetic energy, the second term is the potential energy, V(r) is the neutron-nucleus interaction potential, E is the so-called system energy and $\psi(r)$ is the so-called eigenfunction. This equation can also be written as $H\psi = E\psi$ where H is the system Hamiltonian.

6. The first Born approximation corresponds to keeping only the first term in the expansion solution of the Schrodinger equation. The first Born approximation does not model reflectivity well.

7. The solution of the Schrodinger equation corresponds to an incident plane wave and a scattered spherical wave.