22.106 Neutron Interactions and Applications (Spring 2005)
Lecture 15 (4/26/05)

Thermal Neutron Scattering Basics

References --

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M. M. R. Williams, *The Slowing Down and Thermalization of Neutrons* (North Holland, Amsterdam, 1966).
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Neutron thermalization is the study of the distribution of thermal neutrons in energy, space, and time in moderating materials. It is clearly an essential topic in the analysis of nuclear systems where thermal neutrons play an important role. The part of neutron thermalization which concerns us in the present context is the scattering kernel that appears in the scattering gain term in the neutron transport equation (see Eq.(8.3)),

$$\int dE' d\Omega \Sigma_s(E')\phi(\underline{r},E',\underline{\Omega}')F(E'\underline{\Omega}' \rightarrow E,\underline{\Omega})$$

In our discussion of neutron slowing down (Lec9) we were justified in using a rather simple expression for the scattering kernel F, because in the energy range above thermal energy (~0.025 eV), neutrons lose energy upon elastic scattering and the effects of chemical binding and thermal motion of the scattering nuclei can be ignored. In the thermal energy region, neutrons can be up-scattered in elastic scattering, and chemical binding and thermal motion effects now need to be taken into account (see also Lecs2-4). Notice that it is conventional to call the neutron scattering processes in the thermal energy region *inelastic* (as in the title of this lecture). In this usage inelastic refers to neutron exchanging energy with the scattering nucleus, which is chemically bound and in thermal motion (therefore the nucleus is capable of giving or receiving energy). The process of energy exchange involves the interaction between the neutron and the molecular degrees of freedom, or excitation of molecular energy levels. It is also still correct to call the neutron scattering process in the thermal region elastic, provided that elastic here means nuclear interaction, that is, the neutron does not leave the scattering nucleus in an excited nuclear state. Any possible confusion would be eliminated if we just use instead the terms 'nuclear elastic' and 'molecular inelastic'. In both neutron slowing down and thermalization, the scattering process is 'nuclear elastic', whereas in neutron slowing the scattering process is 'molecular elastic' and in neutron thermalization it is 'molecular inelastic'.

The purpose of this and the following lecture is to present the theory of neutron 'molecular inelastic' scattering. We will see that we will need to extend the previous method of cross section calculation based on the phase shift analysis. While the former method is sufficient to give the angular differential cross section $\sigma(\theta)$, it is not suitable for treating the new effects of thermal motion and chemical binding which dominate the behavior of thermal neutrons. Our strategy is to develop the theory of thermal neutron scattering in several stages. In this lecture we will introduce a different method of cross section calculation, that is based on the so-called Born approximation, also a very well known approach in the general theory of scattering. Then we will show that in order to apply the Born approximation we will need to develop a new potential for the neutron-nucleus interaction, a result that will be called the Fermi pseudopotential. In the following lecture we will combine the Born approximation and the Fermi pseudopotential to obtain an expression for the double differential scattering cross section, the kernel that appears in the neutron transport equation. As an application we examine the cross section to arrive at an expression for the scattering law $S(\alpha,\beta)$; as we have seen in our discussions of MCNP, the scattering law is part of the ENDF-B database. In this way, Lecs 15 and 16 serve to connect our theoretical studies of neutron interactions and transport with inelastic scattering experiments.

The Integral Equation Approach to Potential Scattering

In Chap4 we have studied the method of cross section calculation based on an expansion in partial waves, lead to the determination of a phase shift for each partial wave. The phase-shift method is well suited to nuclear reactions, as demonstrated in various applications such as the optical model of nuclear reactions. For thermal neutron scattering, another method of calculating the scattering amplitude $f(\theta)$ turns out to be much more appropriate; this is the Born approximation where $f(\theta)$ is given by the Fourier transform of the interaction potential. Since this is a basic and well-known approach in scattering theory, we will first derive the approximation in general and then apply it to neutron scattering.

The *Schrödinger* equation to be solved describes the scattering of an effective particle by a central potential. We will rewrite this second-order differential equation in the form of an integral equation

$$(\nabla^2 + k^2)\psi(\underline{r}) = U(r)\psi(\underline{r}) \tag{15.1}$$

where we have defined

$$U(r) \equiv \frac{2\mu}{\hbar^2} V(r) \tag{15.2}$$

We now regard the right-hand side of (15.1) as a 'source' or inhomogeneous term and write down the formal solution to (15.1) as the sum of the solution to the homogeneous equation and a particular solution due to the source term. The homogeneous equation is

$$(\nabla^2 + k^2)\varphi(\underline{r}) = 0 \tag{15.3}$$

The particular solution is a superposition of the Green's function and the source term (15.2). By the Green's function we mean the solution to the equation

$$(\nabla^2 + k^2)G(\underline{r} - \underline{r}') = -\delta(\underline{r} - \underline{r}') \qquad (15.4)$$

The formal solution to (15.1) is therefore

$$\psi(\underline{r}) = \varphi(\underline{r}) - \int d^3r' G(\underline{r} - \underline{r}')U(r')\psi(\underline{r}') \qquad (15.5)$$

The best way to see that this is indeed a general solution to (15.1) is by direct substitution. The advantage of writing the solution to the *Schrödinger* equation in this form is that we can generate a series solution by assuming the second term in (15.5) as being 'small' in some sense. This assumption then imposes certain condition on the interaction potential V(r), as we will see.

The homogeneous equation (15.3) should be familiar to us. We will work with the solution in the form of a plane wave,

$$\varphi(\underline{r}) = \exp(i\underline{k} \cdot \underline{r}) \equiv e^{ikz} \qquad (15.6)$$

where we have taken incident wave vector to be along the z-axis. Thus (15.6) corresponds to the incident plane wave in our description. The solution to the Green's function equation (15.4) is also quite well-known; it can be written in the form of a spherical outgoing wave, which is how we want to represent the scattered wave,

$$G(\underline{r} - \underline{r}') = \frac{e^{ik|\underline{r} - \underline{r}'|}}{4\pi|\underline{r} - \underline{r}'|} \qquad (15.7)$$

Because (15.7) is a result one is likely to encounter in other problems, given that (15.3) is the Helmholtz equation, we digress a bit to show that (15.7) can be obtained using the method of Fourier transform.

Without loss of generality, we can set $\underline{r}' = 0$ in (15.4). We introduce the Fourier transform of $G(\underline{r})$ as

$$F(\underline{\kappa}) = \int d^3r e^{-i\underline{\kappa}\cdot\underline{r}} G(\underline{r}) \qquad (15.8)$$

Taking the Fourier transform of (15.4) we obtain an algebraic equation in F which gives

$$F(\underline{\kappa}) = -(k^2 - \kappa^2)^{-1} \qquad (15.9)$$

To find $G(\underline{r})$ we invert (15.9),

$$G(\underline{r}) = (2\pi)^{-3}\int d^3\kappa e^{i\underline{\kappa}\cdot\underline{r}}(\kappa^2 - k^2)^{-1} \tag{15.10}$$

The angular integrations can be readily carried out since the only dependence is in the factor $\exp(i\kappa r\cos\theta)$,

$$G(r) = \frac{1}{2\pi^2 r}\int_0^\infty \kappa\sin\kappa r\frac{1}{\kappa^2 - k^2}d\kappa \tag{15.17}$$

Notice that since $F(\underline{\kappa})$ depends only the magnitude of $\underline{\kappa}$, its Fourier transform depends only on the magnitude of $\underline{r}$. The integrand of (15.17) is manifestly an even function of κ, we can extend the integration from $-\infty$ to ∞,

$$G(r) = \frac{1}{4i\pi^2 r}\int_{-\infty}^\infty \kappa\frac{e^{i\kappa r}}{(\kappa + k)(\kappa - k)}d\kappa \tag{15.18}$$

So (15.18) amounts to a contour integration. The integrand is seen to have two simple poles on the real axis, at $\kappa = \pm k$. We will choose the path for the contour integral to close on itself in the upper half plane while enclosing the pole at $+k$ (see Fig. 15.1). For

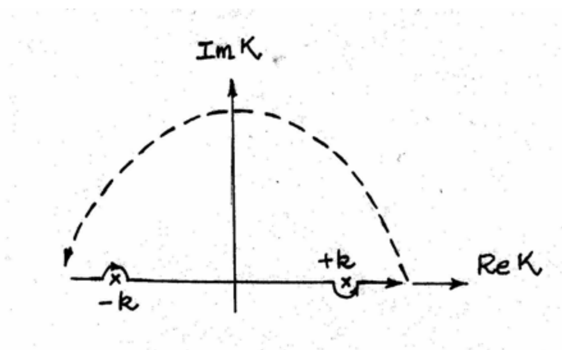

Fig. 15.1. Contour for the inverse Fourier transform.

this particular choice gives a contribution from the enclosed pole and nothing else. Thus,

$$G(r) = \frac{1}{4i\pi^2 r}\cdot 2\pi i\cdot k\frac{e^{ikr}}{2k} = \frac{e^{ikr}}{4\pi r} \tag{15.19}$$

which is the desired result, (15.7). Our choice of the contour is motivated by the physical consideration of having G(r) to be in the form of a spherical outgoing wave for G(r), since then (15.5) would coincide with the boundary condition for the scattering problem. If we had chosen the contour to enclose the other pole, $\kappa = -k$, we would have obtained a spherical incoming wave for the Green's function. What if one encloses both poles? This would give a standing spherical wave sin(kr)/r. This ends our digression.

Returning to our formal solution to the *Schrödinger* equation, we combine (15.5) and (15.7) to give

$$\psi(\underline{r}) = e^{ikz} - \int d^3r' \frac{e^{ik|\underline{r}-\underline{r}'|}}{4\pi|\underline{r}-\underline{r}'|} U(r')\psi(\underline{r}') \qquad (15.20)$$

We will refer to (15.20) as the integral equation of scattering; it is entirely equivalent to the *Schrödinger* equation since no approximation has been made. The advantage of this form is that the boundary condition where one introduces the scattering amplitude has been explicitly incorporated. However, it is not yet in a form from which one can directly extract $f(\theta)$. Because we are only interested in the solution in the asymptotic region of large r compared to the range of interaction r_o, we can simplify (17.20) by noting that the presence of U(r') means the integral over r' will be restricted to $r' \le r_o$. Thus, the that fact that r'/r << 1 means we can write

$$|\underline{r}-\underline{r}'| \sim r - \underline{\hat{r}} \cdot \underline{\hat{r}}' \qquad (15.21)$$

in the exponent in (15.20), and just simply take r for $|\underline{r}-\underline{r}'|$ in the denominator. Then (15.20) becomes

$$\psi(\underline{r}) \sim e^{ikz} - \frac{e^{ikr}}{4\pi r} \int d^3r' e^{-ik\underline{\hat{r}}\cdot\underline{r}'} U(r')\psi(\underline{r}'), \quad r >> r_o \qquad (15.22)$$

We compare this with the boundary condition for the scattering problem,

$$\psi(\underline{r}) \sim e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \qquad (15.23)$$

to obtain a formal expression for the scattering amplitude. But such a result is not useful since it still contains the unknown wave function ψ. To turn (15.22) into a useful result we need to introduce an approximation for ψ.

<u>The Born Approximation</u>

A simple way to solve an inhomogeneous integral equation is to iterate with the inhomogeneous term assuming the integral kernel is in some sense 'small' (since the kernel contains the interaction potential, we may think of the potential as being 'weak'). This leads to a perturbation approach that generates a solution in the form of a series expansion. Under proper conditions one may be justified in truncating this series and thereby obtain a useful approximate solution directly. The zeroth-order solution, which denote by a superscript, is obtained by ignoring completely the integral term in (15.22),

$$\psi^{(o)}(\underline{r}) = e^{ikz} \qquad (15.24)$$

The next approximation is to replace the wave function ψ in (15.22) by (15.24), thus giving the first-order solution. In the asymptotic region, this would read

$$\psi^{(1)}(\underline{r}) \sim e^{ikz} - \frac{e^{ikr}}{4\pi r}\int d^3r' e^{-i\underline{k}\cdot\underline{r}'} U(r') e^{i\underline{k}'\cdot\underline{r}'} \tag{15.25}$$

where we have set $\underline{k}' \equiv k\hat{\underline{z}}$. Eq.(15.25) is known as the first Born approximation. Comparing it with (15.23) one obtains an expression for the scattering amplitude,

$$f(\theta) = -\frac{2\mu}{4\pi\hbar^2}\int d^3r e^{i\underline{\kappa}\cdot\underline{r}} V(r) \tag{15.26}$$

with

$$\underline{\kappa} \equiv \underline{k}' - \underline{k} \tag{15.27}$$

Eq.(15.26) shows that in the Born approximation the scattering amplitude is given by the Fourier transform of the interaction potential. The Fourier transform variable $\underline{\kappa}$ is a wave vector, the difference between the wave vectors of the scattered and incident waves respectively, $\underline{k}'$ and $\underline{k}$. We will refer to $\underline{\kappa}$ as the wave vector transfer (see Fig. 15.2),

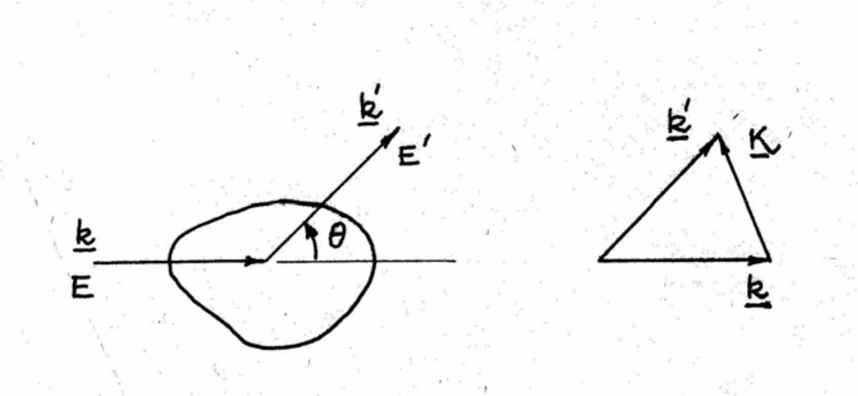

Fig. 15.2. Schematic of scattering of a particle with incoming energy E, wave-vector k at an angle θ and outgoing energy E', wave-vector k'. The momentum triangle shows the relation between the momentum transfer $\hbar\underline{\kappa}$ and the scattering angle, the angle between k and k'.

and note that $\hbar\underline{\kappa}$ is the momentum gained by the particle in scattering through an angle θ. Since in potential scattering there is no energy transfer, the incident and scattered wave vectors have the same magnitude. This means the magnitude of $\underline{\kappa}$ is

$$\kappa = 2k\sin(\theta/2) \tag{15.28}$$

In the Born approximation the dependence on the scattering angle enters therefore through the wave vector transfer.

Validity of the Born Approximation

The simplicity of the result of the Born Approximation makes it widely useful. We will find that the theory of thermal neutron scattering depends critically on the use of this approximation. Before going on to discuss this theory, it is just as important to pause and consider the condition under which this approximation can be justified. When we do this, we will see that strictly speaking the condition for the validity of the Born Approximation is not fulfilled in the case of thermal neutron scattering. However, there is a way out of this dilemma; it involves the introduction of a pseudopotential in place of the actual neutron-nucleus interaction which we have studied in the neutron-proton scattering problem. The idea of the pseudopotential that enables the use of the Born Approximation is due to E. Fermi.

The Born Approximation amounts to one iteration of the inhomogeneous integral equation (15.22). (Strictly speaking, we should call it the first Born Approximation since one can iterate further and obtain the second and higher-order Born Approximation results.) The assumption is therefore that the integral term in (15.22) is small compared to the inhomogeneous term. Since the magnitude of the latter is unity, the condition for validity can be expressed as

$$\Delta = \left| \int d^3r' \frac{e^{ikr'}}{4\pi r'} \cdot \frac{2\mu}{\hbar^2} V(r') \cdot e^{i\underline{k}\cdot\underline{r}'} \right| << 1 \qquad (15.29)$$

where we have taken the integral term to be evaluated at r = 0 and require its magnitude to be small compared to unity. Since the potential is spherically symmetric, the angular integrations can be readily performed. For the radial integration we take V(r) to be a spherical well with depth V_o and range r_o,

$$\Delta = \frac{\mu V_o}{\hbar^2 k} \left| \int_o^{r_o} dr (e^{2ikr} - 1) \right|$$

$$= \frac{\mu V_o}{2\hbar^2 k^2} \left| e^{2ikr_o} - 2ikr_o - 1 \right|$$

$$= \frac{\mu V_o}{2\hbar^2 k^2} [y^2 + 2 - 2y \sin y - 2\cos y]^{1/2} << 1 \qquad (15.30)$$

where y = $2kr_o$.

The inequality (15.30) can be satisfied in two ways, the dimensionless parameter y is either small or large. For kr_o >>1, the square root quantity behaves like y. Then (15.30) gives the condition

$$\frac{V_o r_o}{\hbar v} << 1 \tag{15.31}$$

where $v = \hbar k / \mu$ is the incident velocity of the particle. We will call this the high-energy condition since it is derived from $kr_o >>1$. For $kr_o <<1$, the square root in (15.30) becomes $y^2/2$ to lowest order. This then leads to the low-energy condition

$$\frac{\mu V_o r_o^2}{\hbar^2} << 1 \tag{15.32}$$

For thermal neutron scattering the appropriate condition to check is (17.32) since we are in the regime of low-energy scattering, $kr_o <<1$. If one were interested in electron scattering, one would find that the appropriate condition for the use of Born Approximation would be the high-energy condition (15.31).

It is now a simple matter to put in appropriate numerical values for the constants in (15.32) to see whether the condition is satisfied for thermal neutron scattering. For the potential parameters we can take the values for n-p scattering (triplet interaction). The left-hand side of (15.32) becomes

$$\frac{1.6x10^{-24} \cdot 36x10^{6} x1.6x10^{-12} \cdot 4x10^{-26}}{10^{-54}} = 3.7 \tag{15.33}$$

which is manifestly too large for the Born Approximation to be applicable. One would like to see a magnitude typically ~10^{-2}.

<u>The Fermi Pseudopotential</u>

It was pointed out by E. Fermi [Ricerca Scientifica **7**, 13 (1936), reprinted in E. Fermi, *Collected Papers* (Univ. Chicago Press, 1952), vol. I, p. 980.] that there is way to formulate the thermal neutron scattering problem such that the low-energy condition (15.32) can be satisfied. One could see that the difficulty lies in the large value of V_o, which is not all that surprising since nuclear forces are well-known to be strong interactions. It was observed that in addition to the condition for the use of Born Approximation there are two other conditions which need to be preserved, the condition of low-energy scattering, $kr_o << 1$, and the expression for the scattering length,

$$a = -f(\theta)\big|_{kr_o \to 0} = \frac{m}{2\pi\hbar^2} \int d^3 r V(r) \sim V_o r_o^3 \tag{15.34}$$

While (15.34) is not quite a condition in the sense of the low-energy scattering condition and (15.32), it is nevertheless a constraint on the potential parameters. By this we mean that in a theory one may want to vary the potential V(r) for a certain purpose, however this is done one should ensure that the V(r) used still gives the correct scattering length. In other words, one may vary V(r) in the theory, but not the magnitude of the scattering cross section which is a quantity that can be measured (and therefore not something that can be adjusted).

Collecting these three conditions, we see that in thermal neutron scattering the values of V_o and r_o are such that we are in the situation where

$$kr_o \sim 10^{-4} \tag{15.35}$$

$$\frac{\mu V_o r_o^2}{\hbar^2} \sim 3 \tag{15.36}$$

$$V_o r_o^3 = \text{a given constant} \tag{15.37}$$

This situation is unsatisfactory because (15.36) is too large by about two orders of magnitude. What Fermi suggested was to replace the actual neutron-nucleus potential V(r) by a fictitious potential V*(r). Suppose we retain the spherical well shape, but simply scale the well depth and range so that V* is a spherical well with depth V_o* and range r_o*. In particular, suppose we take

$$V_o^* = 10^{-6}\, V_o, \qquad r_o^* = 10^2\, r_o$$

How does this replacement affect the three conditions, (15.35) - (15.37)? With the fictitious potential theses conditions become

$$kr_o^* \sim 10^{-2} \tag{15.38}$$

$$\frac{\mu V_o^* r_o^{*2}}{\hbar^2} \sim 3 \text{ x } 10^{-2} \tag{15.39}$$

$$V_o^* r_o^{*3} = V_o r_o^3 \tag{15.40}$$

which is just what we desire. In other words, replacing (V_o, r_o) by (V_o*, r_o*) one is able to satisfy all the requirements for a theory of thermal neutron scattering based on the Born Approximation.

The suggestion of Fermi was in effect to distort the neutron-nucleus interaction - extending the range and decreasing the depth in such a way that preserves the scattering length. Eqs.(15.38) - (15.40) shows that doing this one can now satisfy the low-energy condition for the Born Approximation. Fermi made one further suggestion. He proposed that the fictitious potential can be expressed in the form

$$V^*(r) = \frac{2\pi\hbar^2}{m} a\delta(r) \tag{15.41}$$

This form has come to be known as the Fermi pseudopotential. We will see in the next lecture that this is a very important result for the calculation of the double differential scattering cross section for thermal neutrons. Physically (15.41) describes the neutron-nucleus collision as an impulse interaction, like the collision between two hard spheres - a sudden interaction only at the moment when the spheres touch. How is this possible, given that we have just gone through an argument where the fictitious potential was introduced to decrease the strength of the interaction V_o in order to satisfy the condition (15.32)? The answer is that indeed for the purpose of justifying the Born Approximation we should be thinking of a potential which is weaker than the n-p interaction by six orders of magnitude with a range that is two orders of magnitude greater. With ro ~ 2 x $10^{-13\ cm}$, this would mean a pseudopotential having a range of 10^{-11} cm. What Fermi means by (15.41) is that on the scale of the wavelength of a thermal neutron, 10^{-8} cm, the interaction range, regardless whether is 10-13 or 10-11 cm, is still so small that the interaction can be described as an impulse interaction, occurring essentially at a point. It is in this sense that (15.41) is physically meaningful. Before closing this discussion we remark that in (15.41) the scattering length a is a parameter that is to be specified externally; it can be calculated by another theory or determined by experiment. A virtue of (15.41) is that the correct scattering cross section is already built into the potential. Recall that in the low-energy limit the scattering cross section is given by the s-wave cross section, $\sigma_s = 4\pi a^2$.