Luiz Leal
Oak Ridge National Laboratory

Lectures Presented at the Nuclear Engineering Department of the Massachusetts Institute of Technology (MIT)

Thermal Neutron Scattering Kernel Development

The procedure consists of finding the amplitude of the scattering wave function that leads to the differential scattering cross section. In doing so, a few things will be assumed:

(1) First Born approximation;

(2) Fermi Pseudo-potential;

(3) Time-dependent Schrödinger equation (TDSE)

The first two assumptions have already been discussed. Why assume the TDSE is explained as follows: the energy dependency (explicitly) in the Schrödinger equation implies that the eigenstates of the scattering system are known, i.e., initials and final states. Usually they are not known and even if they are known there will a large number. It is desired to “eliminate” the explicit appearance of the eigenstates.

In so doing one uses

$$E \rightarrow i\hbar \frac{\partial \psi}{\partial t}$$

$$or$$

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \psi = i\hbar \frac{\partial \psi}{\partial t}$$

Leo Van Hove championed this idea. The time dependence is subsequently used in a Fourier transformation.

Assuming that the interaction occurred at $t = t_0$. The wave function at the detector at the position $\vec{r}$ for $t > t_0$ is a solution of the equation

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r},t) \right] \psi(\vec{r},t) = i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t}$$

For $t < t_0$ before the collision has occurred the incident-neutron wave function is

$$\psi_{inc}(\vec{r},t) = e^{i(\vec{k}.\vec{r}-w_0 t)}$$

$$where$$

$$\hbar\vec{k} \rightarrow neutron\ momentum$$

$$\hbar w_0 \rightarrow neutron\ energy$$

The solution at the detector at $(\vec{r},t)$ is

$$\psi(\vec{r},t) = \psi_{inc}(\vec{r},t) + \psi_{scat}(\vec{r},t)$$

Given that for the incident wave ψ_{inc} away from the potential region

$$\left[\frac{\hbar^2}{2m}\nabla^2 + i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}\right]\psi_{inc}(\vec{r},t) = 0$$

then

$$\left[\frac{\hbar^2}{2m}\nabla^2 + i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}\right]\psi_{scat}(\vec{r},t) = V(\vec{r},t)\psi(\vec{r},t)$$

Approximations:

(a) Born approximation

In the right-hand side of the above equation:

$$\psi(\vec{r},t) \rightarrow \psi_{inc}(\vec{r},t)$$

(b) Fermi Pseudo-potential

$$V_n(\vec{r},t) = \frac{2\pi\hbar^2}{m} a_n \delta[\vec{r} - \vec{R}_n(t)]$$

where

$\vec{R}_n \rightarrow$ *position of nucleus n at time t*

$a_n \rightarrow$ *bound scattering related to the bound cross* sec*tion as*

$$\sigma_b = 4\pi a_n^2 \qquad (a_n^2 = \frac{\sigma_b}{4\pi})$$

Hence the equation to be solved is

$$\left[\nabla^2 + \frac{2mi}{\hbar}\frac{\partial}{\partial t}\right]\psi_{scat}(\vec{r},t) = 4\pi\left[\sum_n a_n \delta[(\vec{r} - \vec{R}_n(t_0))]\right]\psi_{inc}(\vec{r},t)$$

Note that $R_n(t_0)$ is for reactions that occurred at the $t = t_0$.

Making use of the Green's function method to solve the equation above. Let $G(\vec{r} - \vec{r}',t - t_0)$ be the Green's function, hence:

$$\left[\nabla^2 + \frac{2mi}{\hbar}\frac{\partial}{\partial t}\right]G(\vec{r} - \vec{r}',t - t_0) = 4\pi\delta(\vec{r} - \vec{r}')\delta(t - t_0)$$

The solution for $\psi_{scat}(\vec{r},t)$ is

$$\psi_{scat}(\vec{r},t) = \int_{\tau}\int_{t_0} d\tau\, dt_0 G(\vec{r}-\vec{r}\,',t-t_0)\psi_{inc}(\vec{r}\,',t_0)\sum_n a_n \delta[r-\vec{R}_n(t_0)]$$

where τ is the volume.

Substituting the values for $G(\vec{r}-\vec{r}\,',t-t_0)$ and ψ_{inc} we have

$$\psi_{scat}(\vec{r},t) = i\sqrt{\frac{m}{2\pi\hbar}}\int_{-\infty}^{t} dt_0 (t-t_0)^{3/2}\sum_n a_n \int d\tau\, \delta[r-\vec{R}_n(t_0)] \times$$
$$\exp\left[\frac{im}{2\hbar}\frac{\left|\vec{r}-\vec{r}\,'\right|^2}{(t-t_0)}\right] \times \exp[i(\vec{k}_0.\vec{r}-w_0 t)]$$

The above expression is the solution for the scattered wave ψ_{scat} at the detector at the position $\vec{r}$ for the time $t > t_0$ for an incident neutron of energy $\hbar w_0$ and momentum $\hbar \vec{k}_0$. It is not clear how to obtain the scattered amplitude from the above equation. Leon Van Hove came up with a cleaver idea of using a Fourier transform of the type

$$\psi_{scat}(\vec{r},t) = \sum_{w'} f(\vec{r},w')\, e^{iw't}$$

and

$$f(\vec{r},w') = \frac{1}{T}\int_0^T dt\, e^{iw't}\psi_{scat}(\vec{r},t)$$

$f(\vec{r},w)$ relates to the scattered wave amplitude.

After LOTS OF ALGEBRA

$$f(\vec{r},w') = \frac{1}{Tr'}\int_0^T dt_0\, e^{iw't_0} \sum_n a_n \int d\tau\delta[\vec{r} - \vec{R}_n(t_0)]e^{i\vec{\kappa}\cdot}$$

For derivation of the above equation see: Thermal Neutron Scattering by Engelstaff pages 49-52

The scattered neutron has

$$\vec{\kappa} = \vec{k}_0 - \vec{k} \rightarrow momentum\ change$$
$$w' = w_0 - w \rightarrow energy\ change$$

The scattering differential cross section is defined as

$$\frac{d^2\sigma}{dEd\Omega} = r'^2 \frac{T}{h} \frac{\upsilon}{\upsilon_0} \left| f(\vec{r}, w) \right|^2$$

$$\upsilon_0\ and\ \upsilon\ initial\ and\ final\ neutron\ velocity$$

Read: The Elements of Neutron Interaction Theory Anthony Foderaro page 555

$$\left| f(\vec{r}, w) \right|^2 = \frac{1}{T^2 r'^2} \int_{-\infty}^{+\infty} d\tau\, e^{-iw\tau} \sum_{m,n} a_m^* a_n \int d\vec{r}\,'' \int d\vec{r}\, e^{i\vec{\kappa}.(\vec{r}-\vec{r}\,'')} \times \overline{\delta[\vec{r}\,'' - \vec{R}_n(0)]\delta[\vec{r} - \vec{R}_n(\tau)]}$$

The bar indicates time averaging.

The double differential cross section is finally obtained as

$$\frac{d^2\sigma}{dEd\Omega} = \frac{1}{h}\frac{\upsilon}{\upsilon_0}\int_{-\infty}^{+\infty} d\tau\, e^{-iw\tau} \sum_{m,n} a_m^* a_n \int d\vec{r}\,' \int d\vec{r}\, e^{i\vec{\kappa}.\vec{r}} \times$$

$$\delta[\vec{r}\,'' - \vec{R}_n(0) - \vec{r}\,]\delta[\vec{r} - \vec{R}_n(\tau)]$$

The Space-Time Correlation Function (Van Hove)

$$G(\vec{r},\tau) = \frac{1}{N}\sum_{m,n}\int dr'\,\delta[\vec{r}\,' - \vec{R}_n(0) - \vec{r}\,]\delta[\vec{r} - \vec{R}_n(\tau)]$$

$G(\vec{r},\tau)$ *is not the Green's function!!*

Interpretation of the $G(\vec{r},\tau)$

Two parts:

for $m = n$ (diagonal terms) $G_s(\vec{r},\tau)$
for $m \neq n$ (off-diagonal terms) $G_d(\vec{r},\tau)$

Interpretation:

$G_s(\vec{r},\tau) \rightarrow self-correlation\ \ function$: a second IDENTICAL nucleus is present

$G_d(\vec{r},\tau) \rightarrow distinct-correlation\ \ function$: a second DISTINCT nucleus is present

$$G(\vec{r},\tau) = G_s(\vec{r},\tau) + G_d(\vec{r},\tau)$$

where

$$G_s(\vec{r},\tau) = \frac{1}{N}\sum_{n=1}^{N}\int dr'\,\delta[\vec{r}\,'-\vec{R}_n(0)-\vec{r}\,]\delta[\vec{r}-\vec{R}_n(\tau)]$$

and

$$G_d(\vec{r},\tau) = \frac{1}{N}\sum_{m\neq n=1}^{N}\int dr'\,\delta[\vec{r}\,'-\vec{R}_n(0)-\vec{r}\,]\delta[\vec{r}-\vec{R}_n(\tau)]$$

Defining

$$< a^2 >= \frac{1}{N}\sum_{m,n} a_m^* a_n \delta_{mn}$$

$$< a >^2 = \frac{1}{N^2} \sum_{m \neq n} a_m^* a_n$$

$$\frac{d^2\sigma}{dEd\Omega} = \frac{d^2\sigma_{coh}}{dEd\Omega} + \frac{d^2\sigma_{incoh}}{dEd\Omega}$$

Assuming only coherent inelastic scattering present, i.e., $< a^2 > = < a >^2 = a$

$$\frac{d^2\sigma}{dEd\Omega} = \frac{d^2\sigma_{coh}}{dEd\Omega}$$

$$\frac{d^2\sigma}{dEd\Omega} = \frac{a^2}{h} \frac{\upsilon}{\upsilon_0} \int \int d\vec{r} d\tau \, e^{i(\vec{\kappa} . \vec{r} - w' \tau)} G(\vec{r}, \tau)$$

Recall that

$$a^2 = \frac{\sigma_b}{4\pi}$$

$$and$$

$$\frac{\upsilon}{\upsilon_0} = \sqrt{\frac{E}{E_0}}$$

$$\frac{d^2\sigma}{dEd\Omega} = \frac{\sigma_b}{4\pi}\sqrt{\frac{E}{E_0}}\tilde{S}(\vec{\kappa},w')$$

where

$$\tilde{S}(\vec{\kappa},w') = \frac{1}{h}\int\int d\vec{r}\,d\tau\, e^{i(\vec{\kappa}.\vec{r}-w'\tau)}G(\vec{r},\tau)$$

$$\tilde{S}(\vec{\kappa},w') \rightarrow Scattering\ Law$$

$\tilde{S}(\vec{\kappa},w')$ can be obtained directly from measurements of $\frac{d^2\sigma}{dEd\Omega}$

Properties of $\tilde{S}(\vec{\kappa}, w')$

(a) Depends only on the dynamics of the scatter center

(b) Sum ruler

$$\int w \, \tilde{S}(\vec{\kappa}, w) \, dw = \frac{\kappa^2}{2M}$$

(c) Condition derived from the detailed balance

$$\tilde{S}(-\vec{\kappa}, w-) = e^{-\frac{\hbar w}{KT}} \tilde{S}(\vec{\kappa}, w)$$

Definitions:

$$\tilde{S}(\vec{\kappa}, w) = e^{-\frac{\beta}{2}} S(\alpha, \beta)$$

Where

$$\alpha = \frac{\hbar^2 \kappa^2}{2mAKT} \qquad and \qquad \beta = \frac{E - E_0}{KT}$$

Since

$$\vec{\kappa} = \vec{k}_0 - \vec{k} \longrightarrow \quad \kappa^2 = k_0^2 + k^2 - 2\vec{k}_0 . \vec{k} \cos\theta$$

$$\alpha = \frac{\hbar^2 \kappa^2}{2mAKT} = \frac{\hbar^2 (k_0^2 + k^2 - 2\vec{k}_0 . \vec{k} \cos\theta)}{2mAKT}$$

$$\alpha = \frac{E_0 + E - 2\sqrt{EE_0} \cos\theta)}{AKT}$$

Hence the double differential cross section becomes

$$\frac{d^2\sigma}{dEd\Omega} = \frac{\sigma_b}{4\pi KT}\sqrt{\frac{E}{E_0}}e^{-\frac{\beta}{2}}S(\alpha,\beta)$$

Notations:

$$\frac{d^2\sigma}{dEd\Omega}$$

or

$$\sigma_s(E_0 \rightarrow E,\theta)$$

or

$$\sigma_s(E_0 \rightarrow E,\mu)$$

where

$$\mu = \cos\theta$$

Simple Example:

(1) Scatterer is a single nucleus of mass M. Only coherent scattering is accounted for;

(2) Scatterer is free and at rest

This corresponds to the situation dealt with in the theory of neutron moderation where the chemical region effects are negligible.

$$\sigma_s(E_0 \rightarrow E, \mu) = \frac{\sigma_b}{4\pi}\sqrt{\frac{E}{E_0}}\tilde{S}(\vec{\kappa}, w)$$

$$\mu = \cos\theta$$

$\tilde{S}(\vec{\kappa}, w')$ is a delta function as

$$\tilde{S}(\vec{\kappa}, w) = \delta(E_0 - E + \frac{E_0 + E - 2(EE_0)^{1/2}\mu}{A})$$

$$\mu = \cos\theta \quad and \quad A = \frac{M}{m}$$

Recall that

$$\hbar w \rightarrow E_0 - E$$

$$\frac{\hbar^2 \kappa^2}{2M} \rightarrow \frac{E_0 + E - 2(EE_0)^{1/2}\mu}{A}$$

Also,

$$d\Omega = 2\pi \sin\theta \, d\theta$$

$$\mu = \cos\theta$$

$$d\mu = -\sin\theta \, d\theta$$

$$d\Omega = 2\pi(-d\mu)$$

and

$$\sigma_s(E_0 \rightarrow E) = \int_{4\pi} \sigma_s(E_0 \rightarrow E, \mu)\, d\Omega$$

$$\sigma_s(E_0 \rightarrow E) = 2\pi \int_{+1}^{-1} \sigma_s(E_0 \rightarrow E, \mu)\, d\mu$$

$$\sigma_s(E_0 \rightarrow E) = 2\pi \frac{\sigma_b}{4\pi} \left(\frac{E}{E_0}\right)^{1/2} \int_{+1}^{-1} \delta(E_0 - E + \frac{E_0 + E - 2(EE_0)^{1/2}\mu}{A})\, d\mu$$

Change of variables

$$x = E_0 - E + \frac{E_0 + E - 2(EE_0)^{1/2}\mu}{A}$$

such that

$$dx = -\frac{2(EE_0)^{1/2}}{A}\, d\mu$$

$$\mu = \pm 1 \rightarrow x_{\mp} = E_0 - E + \frac{(E_0^{1/2} \mp E^{1/2})^2}{A}$$

$$\sigma_s(E_0 \rightarrow E) = 2\pi \frac{\sigma_b}{4\pi} \left(\frac{E}{E_0} \right)^{1/2} \frac{A}{2(E_0 E)^{1/2}} \int_{x_-}^{x_+} \delta(x) dx$$

$$\sigma_s(E_0 \rightarrow E) = \frac{\sigma_b}{4} \frac{A}{E_0}$$

Recall that

$$\sigma_b = \left(\frac{A+1}{A} \right)^2 \sigma_{free}$$

$$\sigma_s(E_0 \to E) = \frac{(A+1)^2}{4A} \frac{1}{E_0} \sigma_{free}$$

$$if \ \alpha = \left(\frac{A-1}{A+1}\right)^2 \quad \to \quad 1-\alpha = \frac{4A}{(A+1)^2}$$

hence

$$\sigma_s(E_0 \to E) = \frac{1}{(1-\alpha)E_0} \ \sigma_{free}$$

$Energy \quad range?$

$$E = \frac{A^2 + 2A\mu + 1}{(A+1)^2} E_0$$

$$\mu = 1 \quad \rightarrow \quad E = E_0$$

$$\mu = -1 \quad \rightarrow \quad E = (1-\alpha) E_0$$

$$\sigma_s(E_0 \rightarrow E) = \begin{cases} \dfrac{1}{(1-\alpha)E_0}\,\sigma_{free} & for \quad (1-\alpha)E_0 < E < E_0 \\ \\ 0 & otherwise \end{cases}$$

(Nuclear Reactor Analysis Duderstadt and Hamilton page 44)