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

# **Neutron Interaction**

Time Independent Transport Equation for  $\Phi(E,\vec{r},\hat{\Omega})$ 

$$\hat{\Omega}.\nabla\Phi + \Sigma_t \Phi = \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE' \Sigma_s(E' \to E, \hat{\Omega}' \to \Omega) \Phi(E', \vec{r}', \hat{\Omega}) + S$$

- $\sum_{t}$  Macroscopic total cross section
- $\Sigma_s$  Macroscopic scattering cross section

### How are these quantities treated?

- (a) Measurement by time-of-flight machine, reactors, etc;
- (b) Evaluated using nuclear physics models;
- (c) Generated using nuclear physics codes

# (Poor Choice!)

How is nuclear physics applied to get the cross sections?

# **Neutron Interaction**

# $n + target \rightarrow ???$



# In all three regions there are always:

#### SCATTERING and REACTION

**Region 1:** High energy neutrons – direct and compound nucleus formation;

**Region 2:** Resonance region (resolved and unresolved) – Definitely compound nucleus formation and some direct interactions;

**Region 3:** Chemical region – neutron energy of incident neutron is comparable to the chemical binding energy of atoms in the molecules;

The neutron reaction cross sections such as (n, fission), (n, gamma) are affected only by the motion of the target atoms (Doppler broadening effects).

In the treatment of the <u>neutron scattering</u> <u>cross section in the chemical region</u> one must consider:

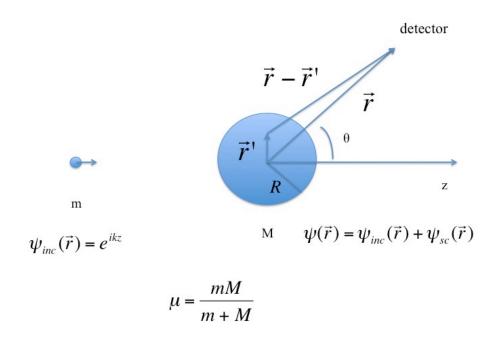
(a) Kinetic energy of the incident neutrons is comparable to the binding energy of the atom in the target (molecule, solid, liquid).

#### ATOMS ARE NOT FREE!!!

- (b) Neutron wavelength is of the order of the interatomic spacing in molecules of crystals;
- (c) Scattering from various nuclei in the same molecule of crystal interfere (coherent, incoherent);
- (d) Neutron may GAIN or lose energy;

# Born approximation And Fermi pseudo potential

Consider the situation: Scattering by a single spinless nucleus



 $\psi(ec{r})$  at the detector satisfy the equation:

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r})$$

Or

$$\left[\nabla^2 + k^2\right]\psi(\vec{r}) = F(\vec{r})$$

Where:

$$k^2 = \frac{2\mu E}{\hbar^2}$$

and

$$F(\vec{r}) = \frac{2\mu}{\hbar^2} V(\vec{r}) \, \psi(\vec{r})$$

The incident wave describes a free particle traveling in the z direction. It is given as

$$\psi_{inc}(\vec{r}) = e^{ikz}$$

We also know that

$$\left[\nabla^2 + k^2\right]e^{ikz} = 0$$

Suggested homework: Demonstrate that

$$\left[\nabla^2 + k^2\right]e^{ikz} = 0$$

Therefore, the equations to be solved is

$$\left[\nabla^2 + k^2\right] \psi_{sc}(\vec{r}) = F(\vec{r})$$

with

$$F(\vec{r}) = \frac{2\mu}{\hbar^2} V(\vec{r}) \, \psi(\vec{r})$$

Recall that  $\psi(\vec{r})$  is included in  $F(\vec{r})$ 

# Green's Function $\psi_0(\vec{r})$

Solution at the detector due to a point source at  $\vec{r} - \vec{r}'$ 

$$\left[ \nabla^2 + k^2 \right] \psi_0(\vec{r}) = \delta(\vec{r} - \vec{r}')$$

$$\psi_0(\vec{r}) \text{ is given as}$$

$$\psi_0(\vec{r}) = -\frac{e^{ik|\vec{r} - \vec{r}'|}}{4\pi |\vec{r} - \vec{r}'|}$$

The solution for  $\psi_{sc}(\vec{r})$  is obtained by integrating in volume  $oldsymbol{\mathcal{T}}$ 

$$\psi_{sc}(\vec{r}) = -\int_{\tau} \frac{e^{ik|\vec{r} - \vec{r}'|}}{4\pi |\vec{r} - \vec{r}'|} F(\vec{r}') d\tau$$

or

$$\psi_{sc}(\vec{r}) = -\frac{\mu}{2\pi\hbar^2} \int_{\tau} \frac{e^{ik|\vec{r} - \vec{r}'|}}{4\pi |\vec{r} - \vec{r}'|} V(\vec{r}') \psi(\vec{r}') d\tau$$

Nice solution of little value since neither  $V(\vec{r})$  nor  $\psi(\vec{r})$  are known quantities. Before proceeding further note that for

$$|\vec{r}| >> |\vec{r}'|$$

$$|\vec{r} - \vec{r}'| \approx r \left[ 1 - 2 \frac{\vec{r}' \cdot \hat{u}}{r} \right]^{1/2}$$

or

$$|\vec{r} - \vec{r}'| \approx r - \vec{r}' \cdot \hat{u}$$

where

$$\hat{u} = \frac{\vec{r}}{r}$$

Suggested homework: Show that

$$|\vec{r} - \vec{r}'| \approx r - \vec{r}' \cdot \hat{u}$$

The function  $\psi_{sc}(\vec{r})$  becomes,

$$\psi_{sc}(\vec{r}) = \left[ -\frac{\mu}{2\pi\hbar^2} \int_{\tau} e^{-ik\vec{r}'\cdot\hat{u}} V(\vec{r}') \psi(\vec{r}') d\tau \right] \frac{e^{ikr}}{r}$$

Defining

$$f(\theta) = -\frac{\mu}{2\pi\hbar^2} \int_{\tau} e^{-ik\vec{r}'\cdot\hat{u}} V(\vec{r}') \psi(\vec{r}') d\tau$$

Hence

$$\psi_{sc}(\vec{r}) = f(\theta) \frac{e^{ikr}}{r}$$

We know that the differential scattering cross section is given as

$$\sigma(\theta) = \frac{d^2\sigma}{dEd\Omega} = |f(\theta)|^2$$

$$\sigma(\theta) = \left| -\frac{\mu}{2\pi\hbar^2} \int_{\tau} e^{-ik\vec{r}'\cdot\hat{u}} V(\vec{r}') \psi(\vec{r}') d\tau \right|^2$$

The functions  $\psi(\vec{r})$  and  $V(\vec{r})$  are still not Known!!!

# **Born Approximation**

# **Assumption:**

The complete wave function  $\psi(\vec{r})$  in the potential region is replaced by the incident wave function, that is,

$$\psi(\vec{r}) = e^{ikz} = e^{ik\vec{r} \cdot \hat{u}_z}$$

#### Rationale:

Incident particle is weakly scattered in the potential region,

$$\sigma(\theta) = \left| -\frac{\mu}{2\pi\hbar^2} \int_{\tau} e^{-ik\vec{r}'\cdot(\hat{u}_z - \hat{u})} V(\vec{r}') d\tau \right|^2$$

 $V(\vec{r})$  is still not known!!

# Fermi Pseudopotencial

Fermi came up with a clever idea for an expression for  $V(\vec{r})$  when the neutron energy is very low.

### **Assumptions:**

- (a) The potential is applied to s-wave, angular momentum l=0, that is, the potential is spherically symmetric;
- (b) Short range potential The potential suggested by Fermi is

$$V(\vec{r}) = \frac{2\pi\hbar^2}{\mu} a\delta(\vec{r})$$

Where a is the scattering length

To understand the concept introduced by Fermi let's continue examining the scattering of neutrons by a single nucleus with no spin effect considered.

#### Recall that:

$$\psi(\vec{r}) = e^{ikz} + f(\theta) \frac{e^{ikr}}{r}$$
for  $r > R$ 

Low energy neutron, since  $k^2 = \frac{2\mu E}{\hbar^2}$ , implies that  $k \to 0$ 

Hence

$$\lim_{k \to 0} r \psi(r) = r + \lim_{k \to 0} f(\theta)$$

$$k \to 0$$

$$r > R$$

$$r > R$$

The scattering length *a* is defined as

$$a = -\lim f(\theta)$$
$$k \to 0$$
$$r > R$$

# Interpretation of the scattering length a

For r=R at the nuclear surface we have

$$R \psi(R) = R - a$$

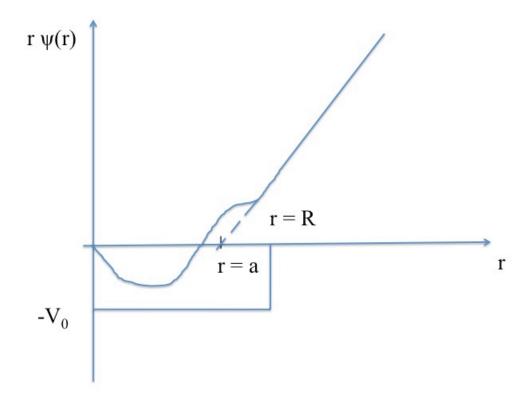
$$a = R[1 - \psi(R)]$$

(a)  $\psi(R) = 0$  impenetrable sphere and a=R

(b) 
$$\psi(R) < 1$$

# a > 0 and a < R

Realistic potential indicating bound states



(c) 
$$\psi(R) > 1$$

No bound states!!

The differential scattering cross section with the Fermi pseudopotential is then

$$\sigma(\theta) = \left| -\frac{\mu}{2\pi\hbar^2} \int_{\tau} e^{-ik\vec{r}.(\hat{u}_z - \hat{u})} \frac{2\pi\hbar^2}{\mu} a\delta(\vec{r}) d\tau \right|^2$$

for  $k \rightarrow 0$  (low energy neutrons)

$$\sigma(\theta) = \left| a \right|^2$$

The total scattering cross section is

$$\sigma_{s} = \int_{4\pi} \sigma_{s}(\theta) d\Omega$$

or

$$\sigma_s = 4\pi |a|^2$$

The derivation so far assumes that the incident neutrons have very low energy. It is also assumed that the nucleus of mass M is not bound; therefore, the scattering length is called  $a_{free}$ . If the neutron interacts with a molecule of mass M' in which the nucleus of mass M is included, i.e., nucleus bound to the molecule, the Schrödinger equation for the system neutron-molecule will include the mass between the neutron (m) and the molecule (M').

The scenarios are:

(a) System m and M

$$\left[ -\frac{\hbar^2}{2\mu} \nabla^2 + V(\vec{r}) \right] \psi(\vec{r}) = E\psi(\vec{r})$$

where

$$\mu = \frac{mM}{m+M}$$

# (b) System m and M'

$$\left[-\frac{\hbar^2}{2\mu'}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r})$$

where

$$\mu' = \frac{mM'}{m+M'}$$

The Schrödinger equation for the system m and M' can be written as

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\vec{r}) + \frac{\mu'}{\mu}V(\vec{r})\psi(\vec{r}) = \frac{\mu'}{\mu}E\psi(\vec{r})$$

We see an effective potential for the system m-M' as

$$V_{eff}(\vec{r}) = \frac{\mu'}{\mu} V(\vec{r})$$

As we have seen, in the Born approximation together with the Fermi pseudopotential the scattering length with the effective potential is

$$a_{bound} = \frac{\mu}{2\pi\hbar^2} \int_{\tau} V_{eff}(\vec{r}) d\tau$$

or

$$a_{bound} = \frac{m + M}{M} \frac{\mu}{2\pi\hbar^2} \int_{\tau} V(\vec{r}) d\tau$$

The relation between  $a_{bound}$  and  $a_{free}$  is

$$a_{bound} = \frac{m + M}{M} a_{free}$$

Defining A as the ratio between the nucleus mass M and the neutron mass m, A=M/m we have

$$a_{bound} = \frac{A+1}{A} a_{free}$$

Since the low-energy bound-scattering crosssection is

$$\sigma_s^{bound} = 4\pi a_{bound}^2$$

The relation between the bound and unbound scattering cross section is

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

As an example, for A=1 (hydrogen)

$$\sigma_s^{bound} = 4 \, \sigma_{free}$$

Suggested homework:

- (a) Which one is measured  $\sigma_s^{bound}$  or  $\sigma_s^{free}$ ?
- (b) If both, how?

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