22.05 Lecture 9

Thermal Scattering

Benoit Forget

March 6, 2023

Massachusetts Institute of Technology

Outline

Massachusetts Institute of Technology

Outline

Massachusetts Institute of Technology

Objectives

- Review of resonance self-shielding
- Temperature effects on Elastic Scattering
- Resonance upscattering near resonances
- Scattering the the thermal energy region

Massachusetts Institute of Technology

Outline

Massachusetts Institute of Technology

Probability Table Approach

If we look at the IR flux model in lethargy space

$$\phi_{IR}(u) = \frac{\sigma_b + \lambda\sigma_p^*}{\sigma_b + \sigma_a^*(u) + \lambda\sigma_s^*(u)}.$$

we notice that the flux is a function only of the cross-sections. All lethargy dependence is in the cross-sections themselves. Thus, we can integrate the reaction rate in a group by its cross-sections rather than lethargy.

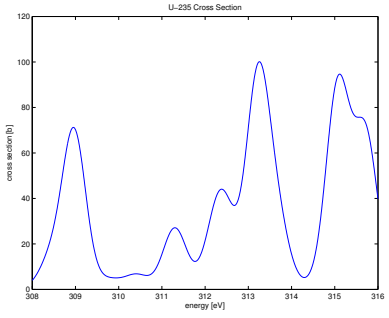
$$\sigma_g = \frac{\int_0^\infty \sigma\phi(\sigma)p(\sigma)\,\mathrm{d}\sigma}{\int_0^\infty \phi(\sigma)p(\sigma)\,\mathrm{d}\sigma},$$

where $p(\sigma)$ is the probability the cross section takes the value σ in the multigroup. This transforms the usual Riemann integral in a Lebesque integral.

Massachusetts Institute of Technology

Basic Idea

The flux is much smoother in the Lebesgue form that we can use a low order quadrature to perform the integral. For a given cross-section



Massachusetts Institute of Technology

Flux Shape

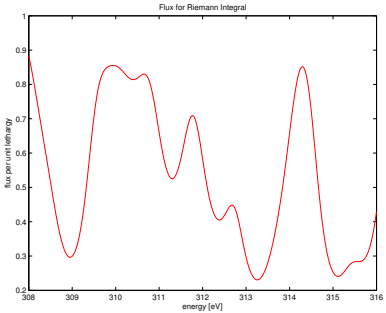


Figure: NR Flux - Riemann

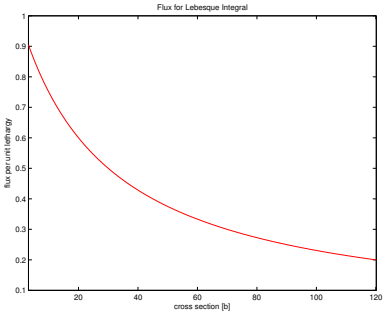


Figure: NR Flux - Lebesque

Massachusetts Institute of Technology

Conceptually

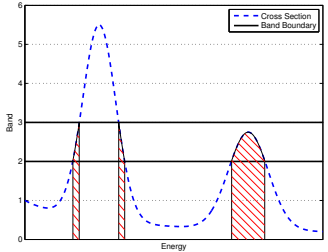


Figure: Direct Subgroup Integration

Massachusetts Institute of Technology

Quadrature

- Quadrature is generated by a minimization problem that tries to match as accurately as possible a set of reference problems (homogeneous or heterogeneous)
- Separate set of parameters is needed for each isotope and each energy group
- Cross section becomes

$$\sigma_{a0} = \frac{\sum_n w_n \phi_n \sigma_{a0,n}}{\sum_n w_n \phi_n}$$

Massachusetts Institute of Technology

Quadrature generation - Fitting

- Generate a reference set of resonance integrals (or effective cross-sections) $\{\langle RI \rangle_k\}$
  - Commonly, an infinite homogeneous resonance model is used at various background levels.
  - Recently, some have generated references using pin cell models with varying densities, enrichments, pin radius, pitch, ...
- For each reference k we write down the subgroup approximation

$$\tilde{RI}_k = \sum_n w_n \sigma_{a0,n} \phi_k(\sigma_n)$$

Massachusetts Institute of Technology

Objective Function

Minimize the square relative error between the estimates and references to obtain a quadrature set

$$\{w_n, \sigma_n\} = argmin \sum_k \left(\frac{\langle RI \rangle_k - \tilde{RI}_k(\{w_n, \sigma_n\})}{\langle RI \rangle_k} \right)^2$$

This objective function is not unique and many others are found in the literature. This process can be simplified by using pre-determined subgroup levels which transforms the optimization problem into a least square fit. Additionally, many constraints can be set

- Preserve infinitely dilute cross-sections
- Ensure that weights are all positive

Massachusetts Institute of Technology

How to use the subgroups?

The starting point will be the IR model:

$$r_{0,IR}\left[\varphi(u)\right] = \lambda_g \sigma_{p0} + (1-\lambda_g)\sigma_{s0}(u)\varphi(u)$$

The λ_g parameter is group dependent and will also depend on dilution. The transport equation is then solved within a group for each subgroup. For the homogeneous case,

$$(\sigma_d + \sigma_{t0}(u))\varphi(u) = r_0\left[\varphi(u)\right] + \sigma_d$$

with

$$\sigma_d = \frac{\sum_{i=1}^{N} \lambda_i N_i \sigma_{pi}}{N_0}$$

Massachusetts Institute of Technology

Homogeneous Solution

Since the lethargy dependence is entirely captured by the cross-sections, we can solve the slowing down flux for each subgroup.

$$\varphi_{IR,n}(u) = \frac{\lambda_g \sigma_{p0} + \sigma_d}{\sigma_{a0,n}(u) + \lambda_g \sigma_{s0}(u) + \sigma_d}$$

$$\sigma_d = \frac{\sum_{i=1}^{N} \lambda_i N_i \sigma_{pi}}{N_0}$$

and compute the group cross-section

$$\sigma_{a0} = \frac{\sum_n w_n \phi_n \sigma_{a0,n}}{\sum_n w_n \phi_n}$$

Massachusetts Institute of Technology

Heterogeneous System

The real advantage of subgroup is that it allows to avoid the need to compute Dancoff factors, since we can solve explicitly for the subgroup flux using the same transport solver.

$$\Omega \cdot \nabla \phi_n(\vec{r},\Omega) + (N_0(\vec{r})\sigma_n + \Sigma_s(\vec{r}))\phi_n(\vec{r},\Omega) = \frac{1}{4\pi}\lambda\Sigma_s(\vec{r}) + (1-\lambda)\Sigma_s(\vec{r})\phi_n(\vec{r},\Omega)$$

which we can re-arrange to

$$\Omega \cdot \nabla \phi_n(\vec{r},\Omega) + (N_0(\vec{r})\sigma_n + \lambda\Sigma_s(\vec{r}))\phi_n(\vec{r},\Omega) = \frac{1}{4\pi}\lambda\Sigma_s(\vec{r})$$

Solutions are needed for each subgroup level of each group and for every resonant isotope. All spatial regions can be solved simultaneously if we approximate $\Sigma_s = \Sigma_p$. The major inconvenience is that the scattering source is represented by the IR model.

Massachusetts Institute of Technology

Self-shielded Cross-section

Since the subgroup levels are defined only for absorption, we must now find a way to obtain self-shielded cross-sections for scattering, fission, ... There are in general two ways to do so

- Relate the self-shielded absorption cross-section to an equivalent homogeneous dilution cross-section. Use this equivalent dilution cross-section to read the other partial cross-sections from a table.
- Fit all partial cross-sections using the fitting method but keeping the weights constant (i.e. find corresponding levels for scattering and fission).

Massachusetts Institute of Technology

Limitations of Subgroup

- Assumes that subgroup parameters are independent of dilution
- No resonance overlap treatment
- Source is assumed uniform throughout the fixed source problem
- Not clear that it can treat fuel subdivision with more accuracy than other methods
- Difficult to handle varying properties in fuel

Massachusetts Institute of Technology

Square wave example

Using the narrow resonance model and assuming a dilution of 50 barns, compute the absorption group average cross section (group bounds of 1 to 3 keV) for an isotope with a square wave (peak of 4 barns) between 2 and 2.25 keV with a potential scattering component of 1 barn.

$$\sigma_{a,g} = \frac{\int_1^3 \sigma_a(E)\phi(E)dE}{\int_1^3 \phi(E)}$$

from factorization of the flux, we know

$$\phi(E) = \psi(E)\varphi_{NR}(E) = \frac{1}{E}\varphi_{NR}(E)$$

and

$$\varphi_{NR}(E) = \frac{\sigma_p + \sigma_d}{\sigma_t(E) + \sigma_d} = \frac{1 + 50}{\sigma_t(E) + 50}$$

Massachusetts Institute of Technology

Square wave example

Replacing and separating the integrals

$$\sigma_{a,g} = \frac{\int_1^2 \frac{1}{E}\sigma_a \varphi dE + \int_2^{2.25} \frac{1}{E}\sigma_a \varphi dE + \int_{2.25}^3 \frac{1}{E}\sigma_a \varphi dE}{\int_1^2 \frac{1}{E}\varphi dE + \int_2^{2.25} \frac{1}{E}\varphi dE + \int_{2.25}^3 \frac{1}{E}\varphi dE}$$

Replacing the values

$$\sigma_{a,g} = \frac{\int_2^{2.25} \frac{1}{E} 3\frac{51}{54} dE}{\int_1^2 \frac{1}{E} dE + \int_2^{2.25} \frac{1}{E}\frac{51}{54} dE + \int_{2.25}^3 \frac{1}{E} dE}$$

thus

$$\sigma_{a,g} = \frac{2.8333 \ln 1.125}{\ln 2 + 0.95 \ln 1.125 + \ln 1.333} = 0.306b$$

Massachusetts Institute of Technology

Subgroup example

For a simple square resonance, the subgroups can easily be defined

- $w_1 = \ln 2.667 / \ln 3 = 0.893$, $\sigma_{a,1} = 0$ and $\sigma_{s,1} = 1$
- $w_2 = \ln 1.125 / \ln 3 = 0.107$, $\sigma_{a,2} = 3$ and $\sigma_{s,2} = 1$

The subgroup flux using the NR model is equal to

$$\phi_{NR,1} = \frac{\sigma_p + \sigma_d}{\sigma_{t,1} + \sigma_s} = \frac{51}{51} = 1$$

$$\phi_{NR,2} = \frac{\sigma_p + \sigma_d}{\sigma_{t,2} + \sigma_s} = \frac{51}{54}$$

Massachusetts Institute of Technology

Subgroup example

The weights are obtained by computing the lethargy width that subtends each subgroup cross section.

$$w_1 = \frac{(\ln 2 - \ln 1) + (\ln 3 - \ln 2.25)}{\ln 3 - \ln 1} = \frac{\ln 2.6667}{\ln 3} = 0.893$$

$$w_2 = \frac{\ln 2.25 - \ln 2}{\ln 3 - \ln 1} = \frac{\ln 1.125}{\ln 3} = 0.107$$

and we can then compute the group average cross section

$$\sigma_a = \frac{\sum w_n \phi_n \sigma_{a,n}}{\sum w_n \phi_n} = \frac{0.107 \times 0.9444 \times 3}{0.107 \times 0.9444 + 0.893 \times 1} = 0.306b$$

Massachusetts Institute of Technology

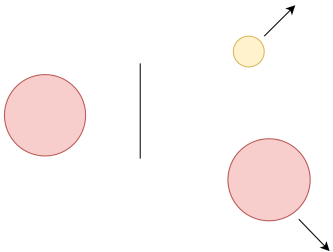
Outline

Massachusetts Institute of Technology

Scattering Review

- Elastic scattering = kinetic energy is conserved
- Target is initially at rest

  $E_n + \cancelto{0}{E_t} = E'_n + E'_t$
- Target atom is "free"



Are these valid assumptions for keV neutrons?

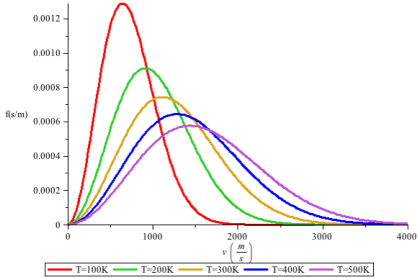
- Molecular bonds are $<\sim 1$ eV
  (so atoms can be considered "free")
- Target atoms move much slower than neutrons (up-scattering rare)

Massachusetts Institute of Technology

Maxwell-Boltzmann

$$P(E) = \frac{2\pi N_0}{(\pi kT)^{3/2}} \sqrt{E} e^{-E/kT}$$

$$P(v) = \frac{4\pi v^2 N_0}{(2\pi kT/m)^{3/2}} e^{-mv^2/2kT}$$



Massachusetts Institute of Technology

Most probable velocity

$$\frac{dP}{dv} = \frac{d}{dv}\left[\frac{4\pi v^2 N_0}{(2\pi kT/m)^{3/2}} e^{-mv^2/2kT}\right] = 0$$

$$\frac{dP}{dv} = \frac{4\pi N_0}{(2\pi kT/m)^{3/2}}\left[2ve^{-mv^2/2kT} + v^2\left(\frac{-mv}{kT}\right)e^{-mv^2/2kT}\right]$$

$$0 = 2v - \frac{mv^3}{kT}$$

$$v_p = \sqrt{\frac{2kT}{m}}$$

Massachusetts Institute of Technology

Average Energy and Velocity

$$E_{avg} = \frac{\int_0^\infty P(E)EdE}{\int_0^\infty P(E)dE}$$

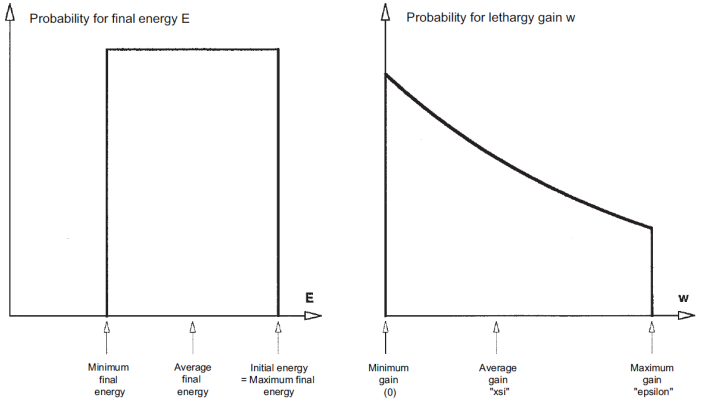
$$v_{avg} = \frac{\int_0^\infty P(v)vdv}{\int_0^\infty P(v)dv}$$

	Energy	Velocity
Average	$E_{avg} = \frac{3}{2}kT$	$v_{avg} = \frac{2}{\sqrt{\pi}}v_p$
Most probable	$E_p = \frac{1}{2}kT$	$v_p = \sqrt{\frac{2kT}{m}}$

The energy of the most probable velocity v_p is equal to kT.

Massachusetts Institute of Technology

Review of slowing down



$$v_n \overline{\sigma_x(E' \to E, \mu)} = \int d^3 v_T P(v_T) |\vec{v_n} - \vec{v_T}| \sigma_s(E_R \to E, \mu)$$

Massachusetts Institute of Technology

Temperature effect

The scattering kernel of unbound isotopes is impacted by temperature (i.e. it will impact outgoing angle and energy). We must perform the convolution integral on the scattering kernel and not just the cross-section. If we assume that the scattering cross-section is constant (or slowly varying), we can obtain an analytical solution.

$$\sigma_s(E')f(E' \rightarrow E) = \frac{\sigma_{s0}\eta^2}{2E'}\left(erf\left(\eta\sqrt{\frac{E}{kT}} - \rho\sqrt{\frac{E'}{kT}}\right) \mp erf\left(\eta\sqrt{\frac{E}{kT}} + \rho\sqrt{\frac{E'}{kT}}\right) \right.$$
$$\left. + e^{(E'-E)/kT}\left(erf\left(\eta\sqrt{\frac{E'}{kT}} - \rho\sqrt{\frac{E}{kT}}\right) \pm erf\left(\eta\sqrt{\frac{E'}{kT}} + \rho\sqrt{\frac{E}{kT}}\right)\right)\right)$$

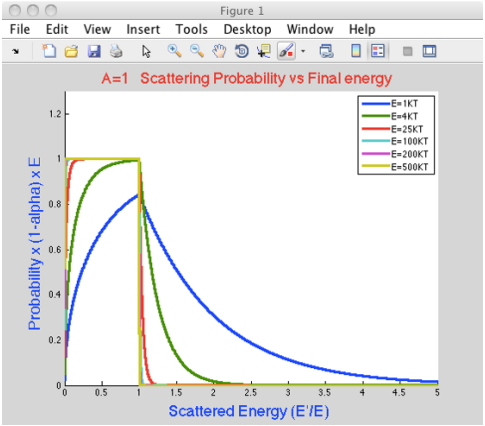
with

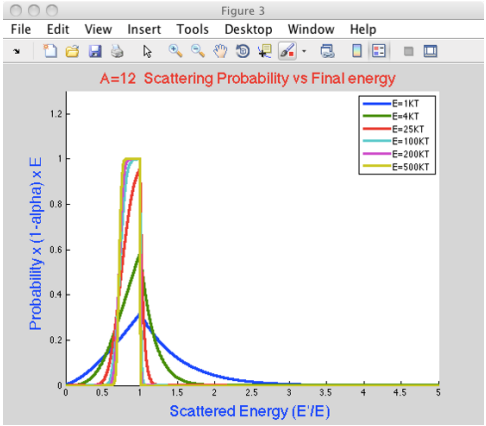
$$\eta = \frac{A+1}{2\sqrt{A}} \qquad \rho = \frac{A-1}{2\sqrt{A}}$$

use top sign if $E' < E$, and bottom sign if $E' > E$

Massachusetts Institute of Technology

Scattering kernel

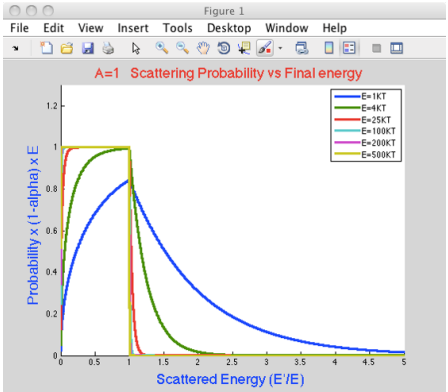




Massachusetts Institute of Technology

Interpreting these curves

kT = 0.025 eV at room temperature, so at T = 586K (coolant temperature), kT = 0.05 eV, 4kT = 0.2 eV, and 25kT = 1.25eV



- If we have a 0.05 eV neutron, use curve kT = 1.
- If we have a 0.2 eV neutron, use curve kT = 4.
- If we have a 1.25 eV neutron, use curve kT = 25.
- If we have a 5 eV neutron, use curve kT = 100.

Massachusetts Institute of Technology

Free Gas - 50 eV

Hydrogen

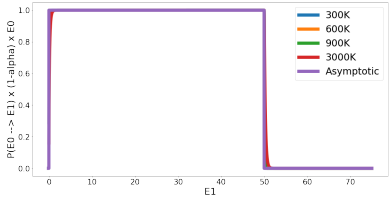


Figure: 50eV - H-1

Carbon

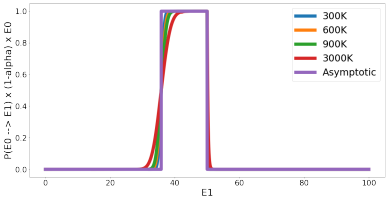


Figure: 50eV - C-12

Free Gas - 5 eV

Hydrogen

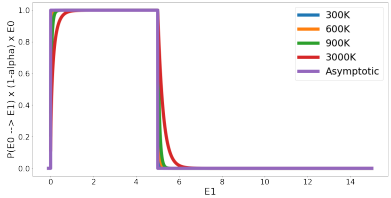


Figure: 5eV - H-1

Carbon

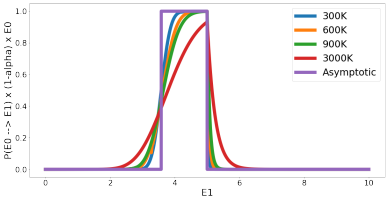


Figure: 5eV - C-12

Free Gas - 0.5 eV

Hydrogen

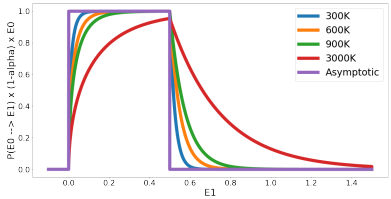


Figure: 0.5eV - H-1

Carbon

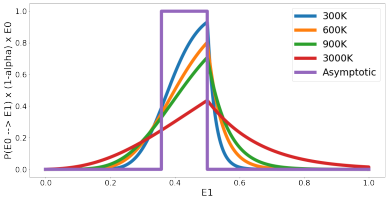


Figure: 0.5eV - C-12

Free Gas - 0.05 eV

Hydrogen

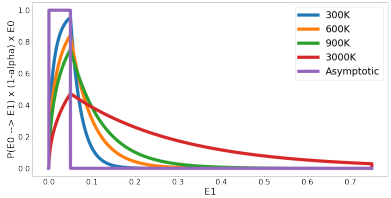


Figure: 0.05eV - H-1

Carbon

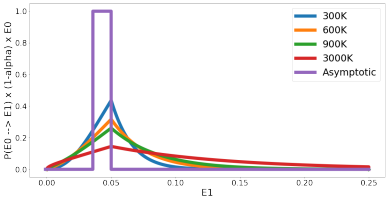


Figure: 0.05eV - C-12

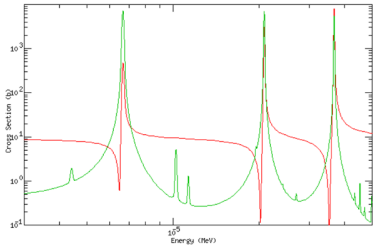
Massachusetts Institute of Technology

Outline

Massachusetts Institute of Technology

Scattering Resonance

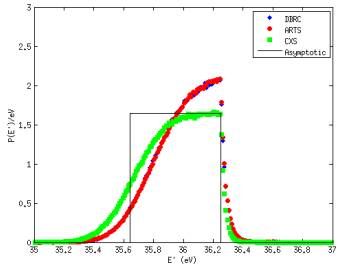
If we can no longer assume that the cross section is slowly varying, the derivation becomes much more complicated (see Ouisloumen and Sanchez, 1991 for details).



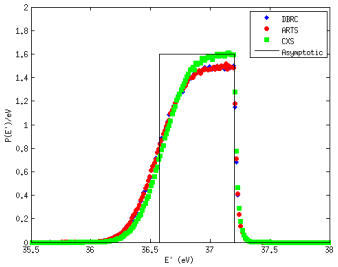
$$\overline{\sigma(E \to E')} = \frac{\beta^{5/2}}{4E} e^{E/kT} \int_{\infty} t\sigma^{tab}(kTt^2/A) e^{-t^2/A} \psi_n(t) dt$$

at 300K

at $E = 36.25$ eV



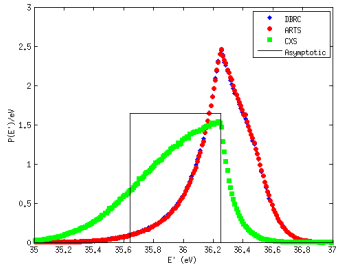
at $E = 37.2$ eV



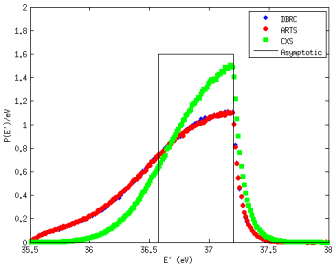
Massachusetts Institute of Technology

at 1000K

at $E = 36.25$ eV



at $E = 37.2$ eV



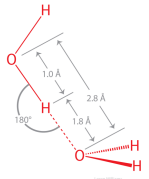
Massachusetts Institute of Technology

Outline

Massachusetts Institute of Technology

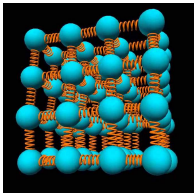
Chemical Region

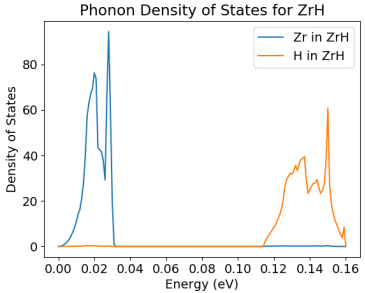
- When neutrons have energy of the same order as the chemical binding energies of atoms in molecules (1eV), we call this the chemical region
- Two phenomena come into play
  - Atoms can no longer be considered to be free. Energy changes can only happen when the vibrational or rotational energy levels of the molecule is excited
  - Waves scattered from multiple nucleus interfere with one another producing diffraction and reflection effects
- Doesn't occur in a monoatomic gas

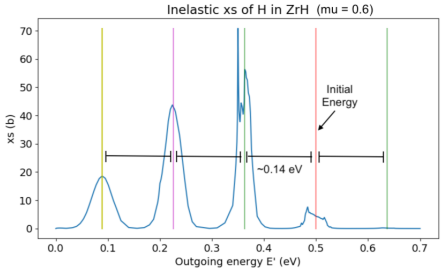


Why is thermal scattering different?

- **Phonon** - An excitation of a normal mode of the material
- **Phonon density of states (DOS)** - # states available each level of energy (represented as PDF)







Massachusetts Institute of Technology

Thermal Cross Section Equation

(Scattering Law, using the incoherent approximation)

$$\sigma_s(E \to E', \mu) = \frac{\sigma_b}{4\pi\hbar}\sqrt{\frac{E'}{E}}\frac{1}{2\pi}\int_{-\infty}^{\infty}\int e^{i(\kappa\cdot\mathbf{r}-\epsilon t/\hbar}\ G_s(\mathbf{r},t)\ d\mathbf{r}\ dt$$

Two Fourier transforms and a change of variables later...

$$\boxed{\sigma(E \to E', \mu) = \frac{\sigma_b}{2k_bT}\sqrt{\frac{E'}{E}}\ S(\alpha,\beta)}$$

$$\text{Momentum Exchange} = \alpha = \frac{E' + E - 2\mu\sqrt{E'E}}{Ak_bT}$$

$$\text{Energy Exchange} = \beta = \frac{E' - E}{k_bT}$$

Massachusetts Institute of Technology

Thermal Cross Section Equation

(Scattering Law, using the incoherent approximation)

$$\sigma(E \to E', \mu) = \frac{\sigma_b}{2k_b T}\sqrt{\frac{E'}{E}}\ S(\alpha, \beta)$$

Obtain $S(\alpha, \beta)$ vis Phonon Expansion

$$S(\alpha, \beta) = \mathrm{e}^{-\alpha\lambda}\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}\ T_n(\beta) \qquad n = 0 \text{ is incoherent elastic}$$

$$T_1(\beta) = \frac{\rho(\beta)\mathrm{e}^{-\beta/2}}{2\beta\sinh(\beta/2)} \qquad \rho(\beta) = \text{phonon distribution}$$

$$T_n(\beta) = \int_{-\infty}^{\infty} T_1(\beta')\ T_{n-1}(\beta - \beta')\ d\beta'$$

Massachusetts Institute of Technology

Outline

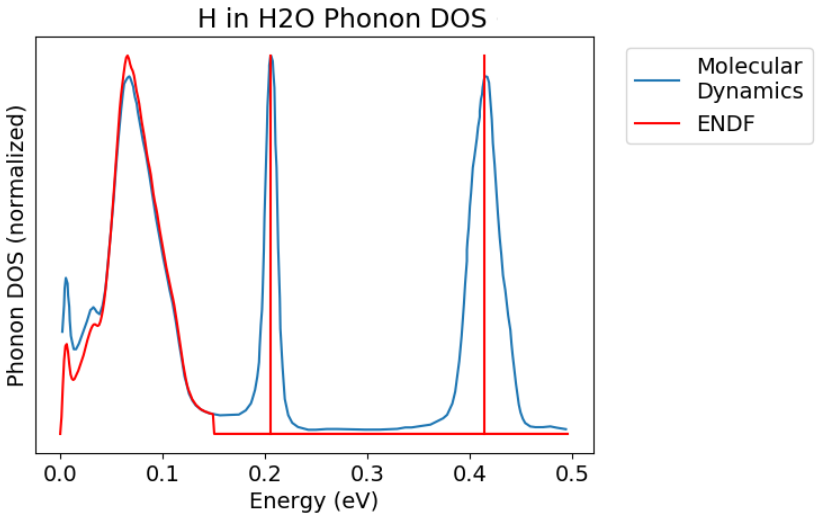
Massachusetts Institute of Technology

Phonon Distributions

- Depend on composition, crystalline structure, and temperature
- Evaluated Nuclear Data Files (ENDF) publishes $\sim$30
- Obtained experimentally, computationally, or approximated analytically and fit to experiments
- Some phonon DOS peaks are approximated as δ functions

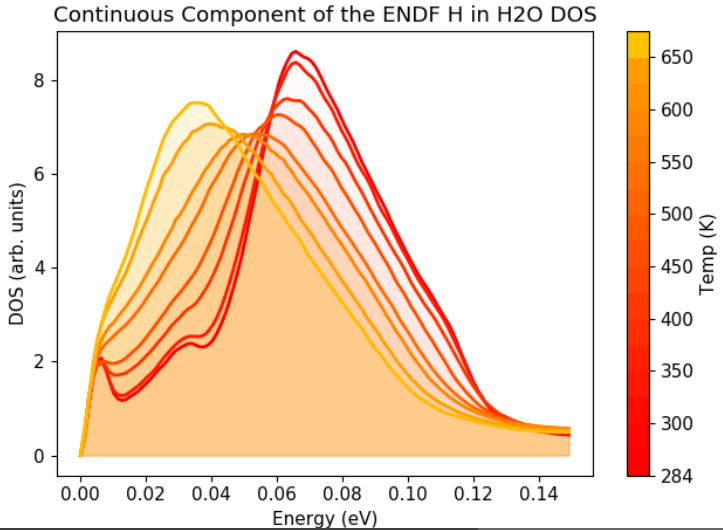
Massachusetts Institute of Technology

Phonon Distributions



Massachusetts Institute of Technology

Phonon Distributions



Massachusetts Institute of Technology

Temperature Effects of Phonon Distributions

- Atoms in a cold material oscillate harmonically
- Higher temperatures induce non-linear restorative forces for the atoms to return home
- High temperature results in anharmonic atom movement
- When atoms get closer and begin to interfere with each others motion in complicated ways, the distinct phonon modes will start to smear
- As atoms become more spaced apart, the vibrations between atoms shifts to a lower energy (downward frequency shift for all phonon modes)

How it is used

- A phonon distribution (determined either experimentally or by simulation) is provided to LEAPR (NJOY module) and a list of α and β values.
- Cross-section sets are then generated as a function of energy and angular distribution
- In Monte Carlo methods, the data is separated in equiprobable bins that must be sampled in multiple dimension.
- In deterministic methods, average scattering kernels (fct of Legendre moments) are generated in multigroup format.

Massachusetts Institute of Technology

Readings

- Lamarsh (p.46-54, 242-245)
- Chapter 3, Section 1

Massachusetts Institute of Technology