

Statistical Nuclear Reactions: The secret confessions of a closet Hauser-Feshbach maniac

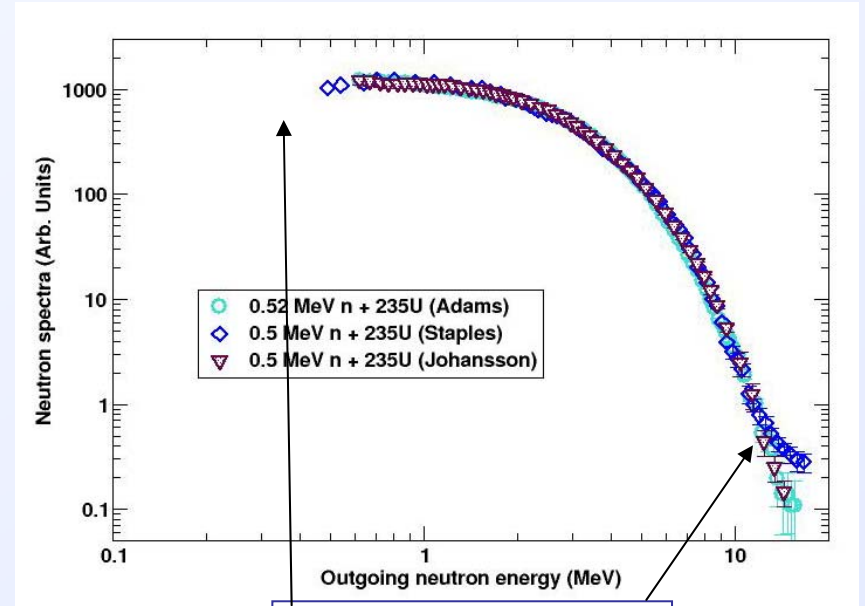


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Accurate simulation of statistical processes: Compound reactions & fission fragments

- Neutron-induced reactions are important for:
 - Astrophysics
 - National security
 - Nuclear power
- Need to predict a wide range of processes
 - From eV to 30 MeV neutrons
 - (n,2n), (n,f), etc.
- Decay of excited nuclei
 - Neutron evaporation from fission fragments - decay of ~ 100 pairs of fission fragments
- Experiment is not always possible - Theory needed to fill in



Larger uncertainties

Quick survey showed that there were significant issues with available codes, such as TALYS & EMPIRE. So, I had to write my own!

By the way, this is a really interesting and difficult DFT problem!

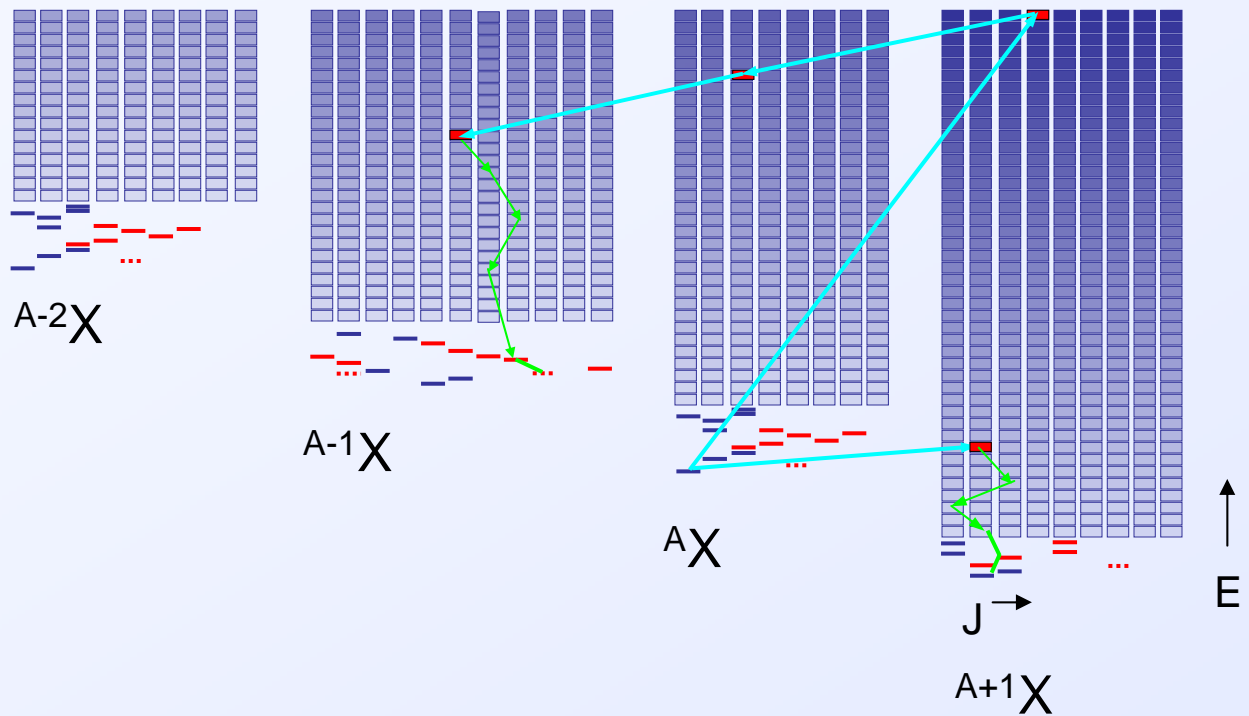


- For most nuclei of interest here, i.e., intermediate to heavy near the valley of stability, we capture at $E_x > 6$ MeV into a region of high density with overlapping states
- Capture into fairly simple “particle-hole” excited states that are not eigenstates of the $A+1$ system
 - If the decay width of these states is smaller than their damping width, they will spread out into the large density of states in to form the so-called “compound nucleus”
 - Niels Bohr - The compound nucleus loses memory of how it was formed
 - Statistical decay: Hauser-Feshbach
 - Otherwise, they will decay via pre-equilibrium emission
 - Usually this starts to be important for $E_n \sim 10$ MeV
 - With a lower density, and for some low-lying states, we can have direct transitions, where structure actually matters



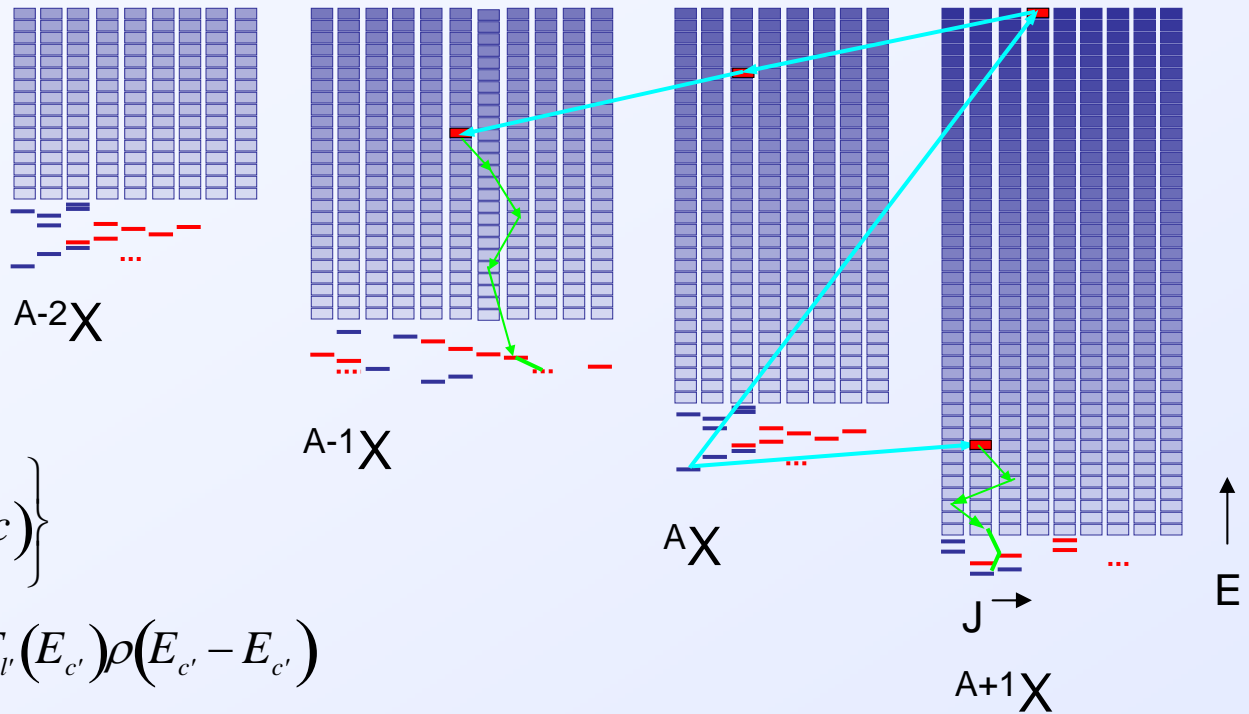
Example reaction networks

- Neg. parity
- Pos. parity
- ... Isomer



Hauser-Feshbach

- Neg. parity
- Pos. parity
- ... Isomer



$$\sigma_c^{comp} = \frac{\pi}{k_c^2} \left\{ \sum_{s,l} g_J T_l(c) \right\}$$

$$P_{Decay}(E_{c'}) = \frac{\sum_{l'} T_{l'}(E_{c'}) \rho(E_{c'} - E_{c'})}{\sum_{c''l''} T_{l''}(E_{c''}) \int_0^{E_{c'}} \rho(E_{c''} - E_{c''}) dE_{c''}}$$

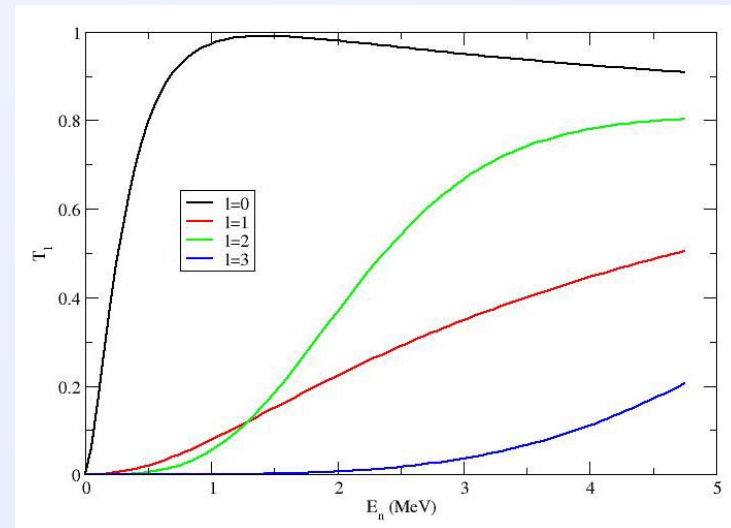
- Transmission coefficient for each Channel
 - Gamma, neutron, proton, ..., fission
- Density of states
- Need estimates of uncertainties



Input #1 - Optical Potential

- Reaction cross section
 - And the population of J^π states in the compound
- Optical potentials are determined empirically
 - Total cross section fairly well known
 - But usually not the reaction cross section
 - There are MANY optical potentials
 - Not as many as there are Skyrme potentials - but almost - **UGH!**
 - This is an art - energy dependent
 - What do we do for nuclei where we don't have data?
 - r-process and FRIB nuclei

$$U(r) = V(r) + iW(r)$$



– **UGH!!!** We need a fundamental and microscopic theory

$$\langle \chi_k | U_{HF} | \chi_k \rangle + \sum_{RPA} \langle \chi_{k'} \psi_f^A | V | RPA_{A+1}^{2p-1h} \rangle \frac{1}{E - E_{RPA} + i\varepsilon} \langle RPA_{A+1}^{2p-1h} | V | \psi_i^A \chi_k \rangle$$



Input #2 - Gamma-strength function

- Essential for (n,γ)
- Γ_γ known for stable targets
 - $T_{XL} \propto \sigma_{XL}$
- E1 dominants
 - Brink hypothesis
 - Generally Lorentzian is very poor
 - Virtually no data below S_n
 - Kopecky & Uhl



- M1 is usually normalized to E1

$$T_{M1} = T_{E1} / 0.0588 A^{0.878}$$

- Explicit structure can still matter
- We can use our sophisticated theories to compute this

■ **UGH!!!!**

$$T_{XL} = K \varepsilon_\gamma^{2L+1} \sigma_r \Gamma_r \left[\frac{\varepsilon_\gamma \Gamma(\varepsilon_\gamma, T_f)}{(\varepsilon_\gamma^2 - E_r^2)^2 + (\varepsilon_\gamma \Gamma(\varepsilon_\gamma, T_f))^2} + 0.7 \frac{\Gamma(\varepsilon_\gamma = 0, T_f)}{E_r^3} \right]$$

$$\Gamma(\varepsilon_\gamma, T_f) = \frac{\Gamma_r}{E_r^2} \left[\varepsilon_\gamma^2 + (2\pi T_f)^2 \right]$$

$$T = \sqrt{(E_x - \varepsilon_\gamma) / a}$$

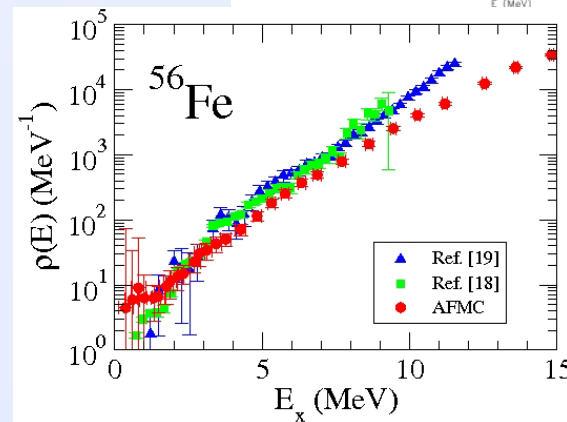
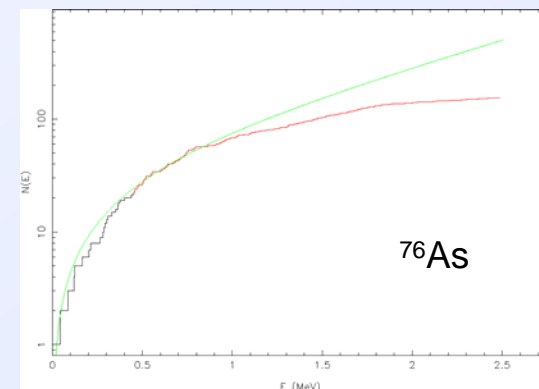


Input #3 - Level densities

- Important because it is exponentially growing, thus phase space rules
- Tends to help determine threshold behaviors, as in (n,2n), also (n, γ)
- How accurately do we know it?
 - Discrete levels
 - D_0 Models
 - Gilbert-Cameron - Back-shifted Fermi gas
 - Level-density parameter a
 - Spin cutoff parameter
 - Better microscopic theories are needed
- **UGH!**

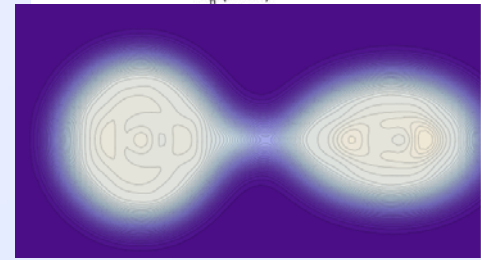
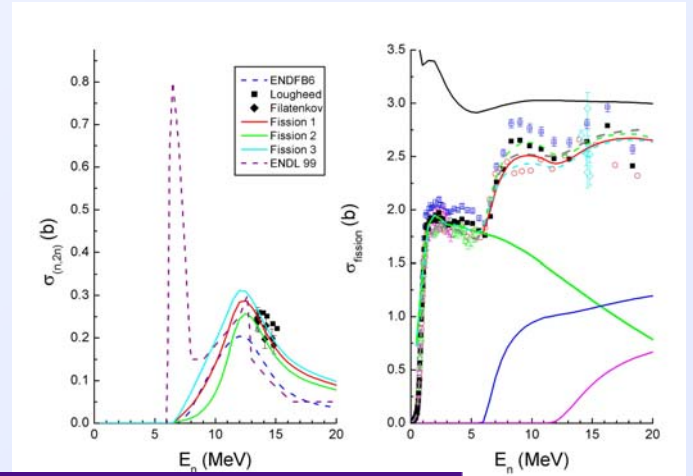
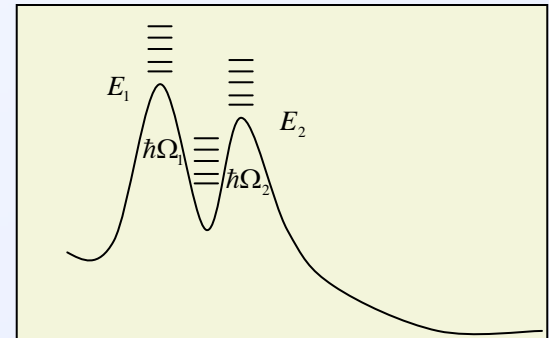
$$\rho(E) = \frac{\sqrt{\pi}}{12a^{1/4}(E-\Delta)^{5/4}} e^{2\sqrt{a(E-\Delta)}}$$

$$\rho(E, J) = \frac{2J+1}{2\sqrt{2}\pi\sigma^3} e^{-(J+1/2)^2/2\sigma^2}$$



Input #4 - Fission

- Fission probabilities affect other processes, e.g., (n,2n)
- No predictive theory of fission
 - Generally, a barrier penetration model is used
 - Bjornholm & Lynn; Nix; Britt
 - Depends on Barriers, curvatures with an inertial parameter, and density of states above the barrier
 - Empirical, and HIGHLY uncertain without data to fit parameters to
- Dynamics affects KE, E_x for fragments, hence the number of neutrons emitted and their spectrum
- DFT can provide better guidance
- UGH!!!

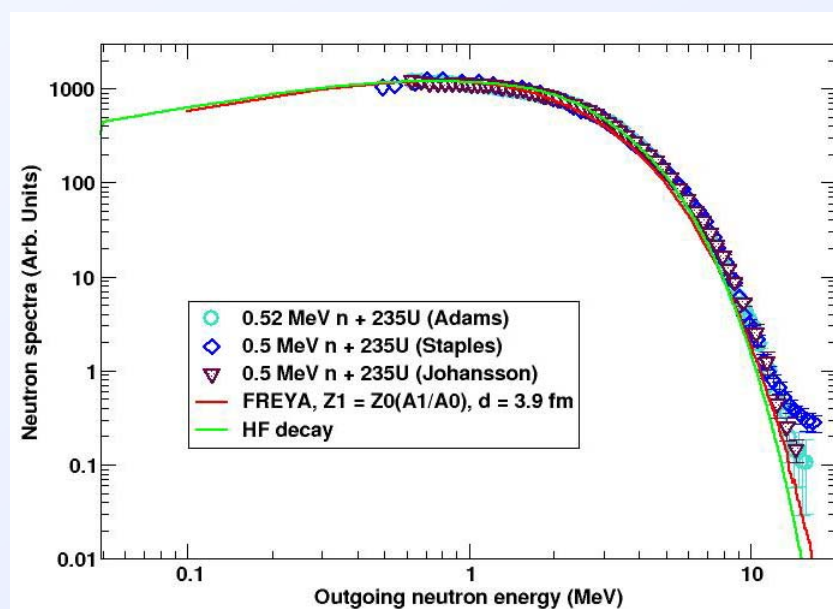


Input #5 Pre-equilibrium processes

- Formation of the compound nucleus is a multi-step process
- Remember the initial states damp into the compound
- If the width for neutron emission is comparable to the damping width, the state can decay prior to formation of the compound nucleus
- Models:
 - Exciton - coupling to particle hole states, and their densities
 - Feshbach-Koonin-Kerman
 - Nishioka, Weidenmüller, Yoshida
 - Tamura, Udagawa, and Lenske
- Suffer from the presence of a rubber matrix
- Computationally demanding
- **UGH!!!**



- Statistical decay is generally not too difficult
 - 50 keV bins, 20 J states for +/- parity ~ 3 mins to decay ^{130}Te with $E_x=20$ MeV
 - CPU ~ N_{bin}^2
- Easy:
 - Cross section for each channel
 - Emission spectrum from each compound
- Difficult:
 - Each input is a complicated structure calculation
 - Spectrum for each exclusive channel
 - e.g., one neutron only when three-neutron channel is open
 - Correlations:
 - e.g., spectrum of 1st and 2nd emitted neutron



1000 fission fragment pairs

$$N(E) = \int \frac{(\sqrt{E} + \sqrt{E_f})^2 \phi(E_{cm}) dE_{cm}}{(\sqrt{E} - \sqrt{E_f})^2 4\sqrt{E_f E_{cm}}} \sim \sqrt{E}$$

- Hauser-Feshbach, or statistical decay, is fairly straight forward and is reasonably grounded in physics
 - Conceptually easy to do
- But, it has many components for the decay channels, each of which are a separate, and computationally demanding challenge
 - Optical potential, pre-equilibrium emission, γ Strength functions, fission probabilities, level densities
 - Each of these inputs is a substantial effort in itself
 - Classic example of GARBAGE IN - GARBAGE OUT

