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

Erich Ormand

Physical Sciences

Lawrence Livermore National Laboratory

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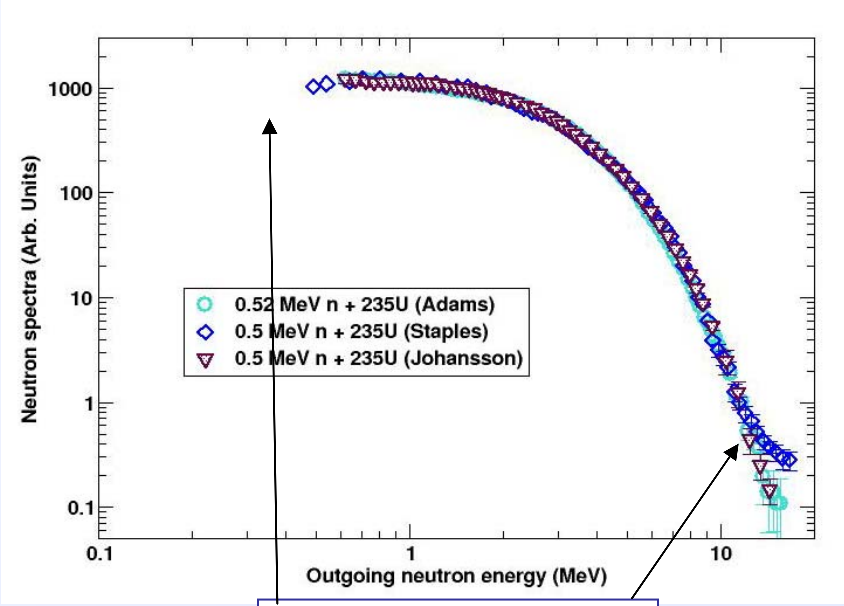
Accurate simulation of statistical processes: Compound reactions & fission fragments

- 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!

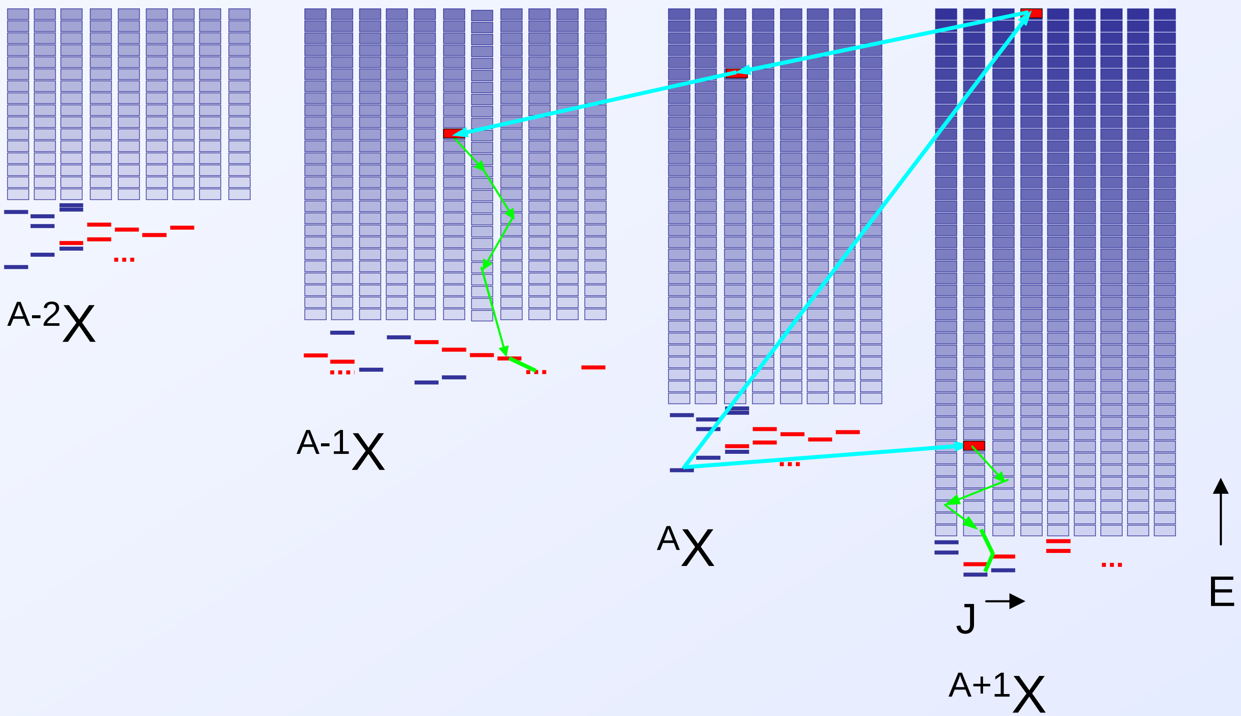
By the way, this is a really interesting and difficult DFT problem!

The Theory

- 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 looses 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 ~ 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
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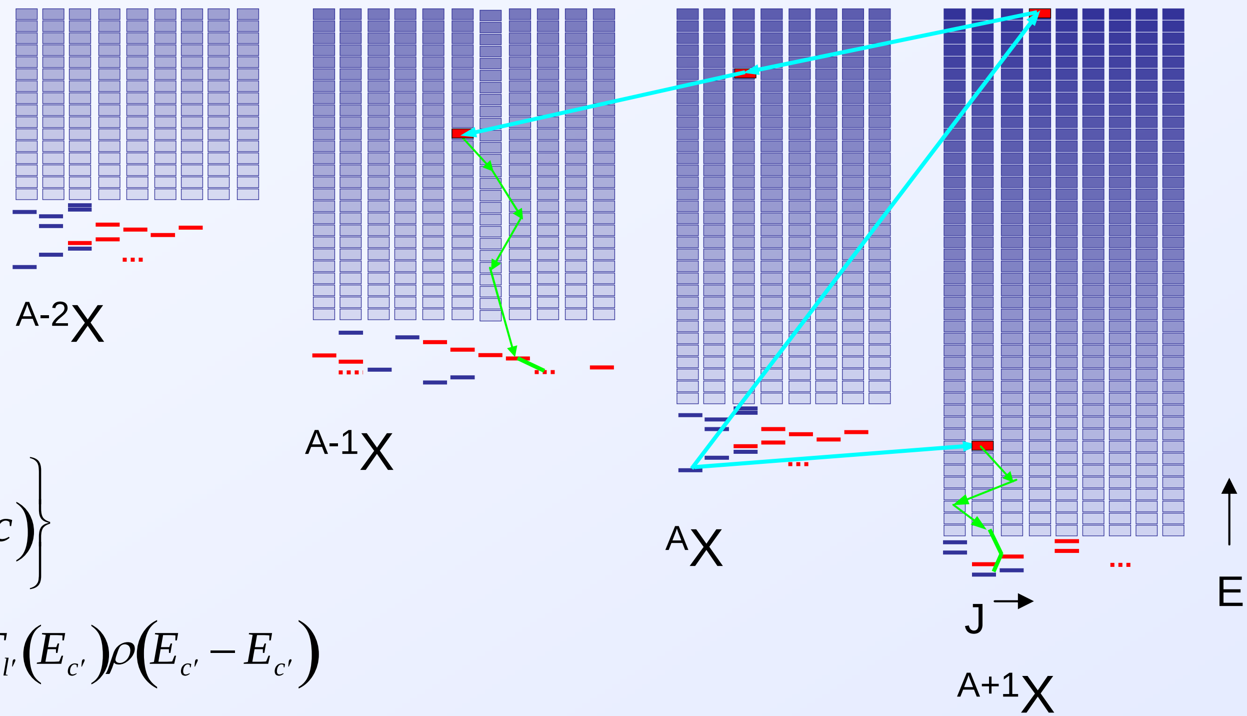


$$\sigma_c^{comp} = \frac{\pi}{k_c^2}\left\{\sum_{s,l} g_J T_l(c)\right\}$$

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

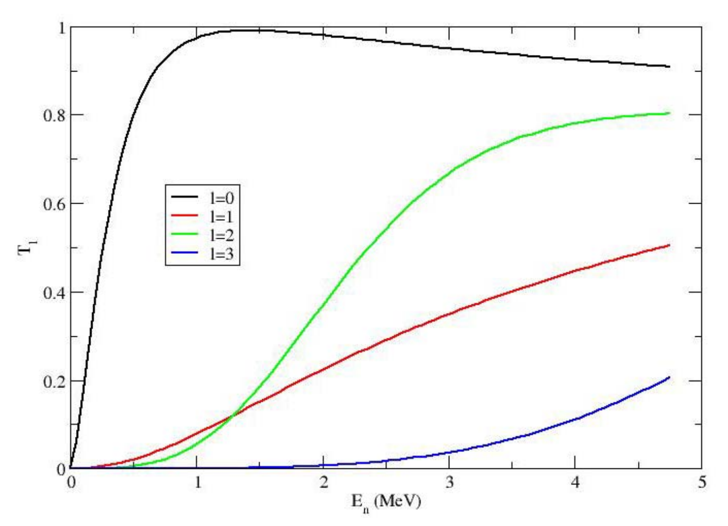
- Transmission coefficient for each Channel
  - Gamma, neutron, proton, …, fission
- Density of states
- Need estimates of uncertainties

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

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

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



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

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!!!!

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

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

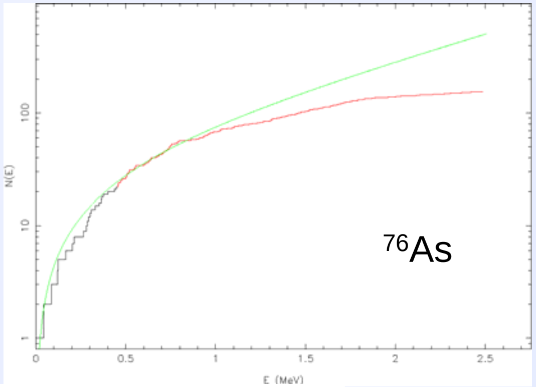
$$T=\sqrt{(E_x-\varepsilon_\gamma)/a}$$

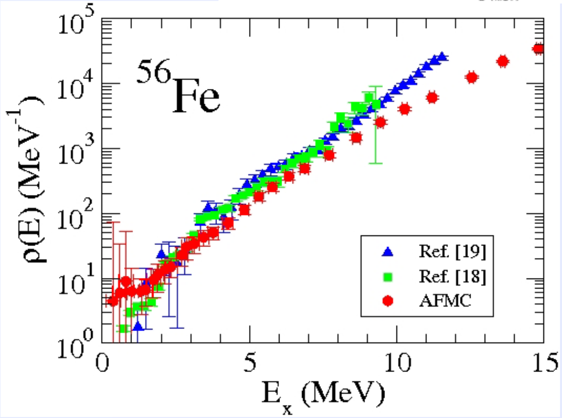
Input #3 - Level densities

- 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!

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

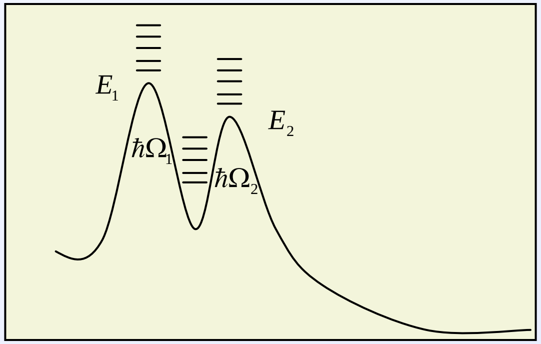
$$\rho(E,J) = \frac{2J+1}{2\sqrt{2\pi}\sigma^3} e^{-(J+1/2)^2/2\sigma^2}$$

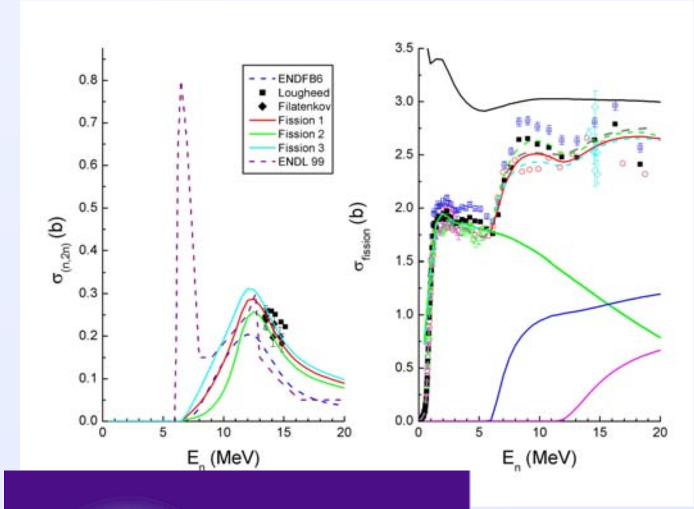


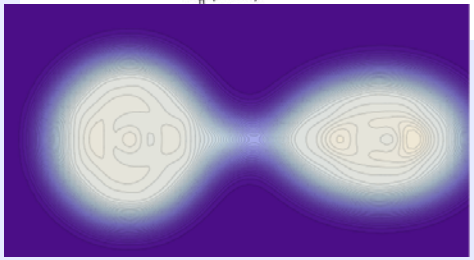


Input #4 - Fission

- 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!!!





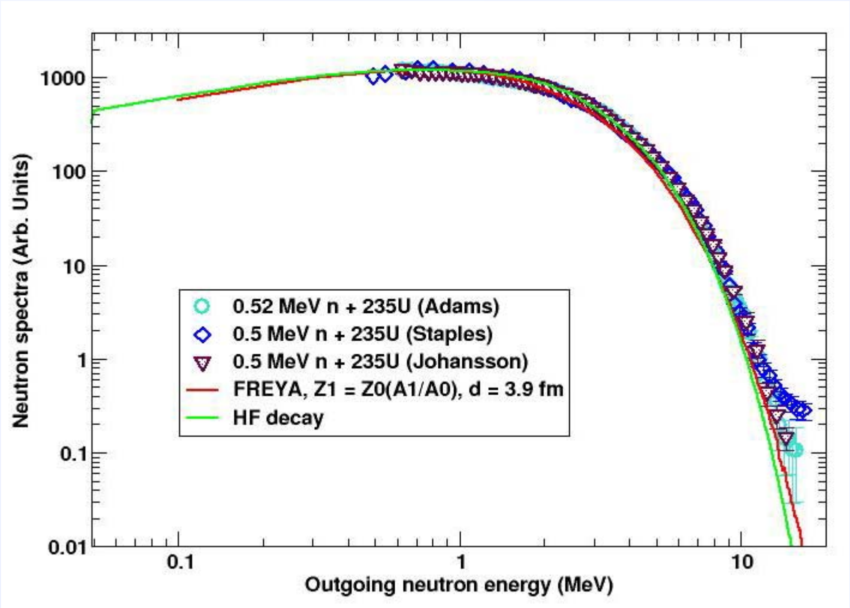


Input #5 Pre-equilibrium processes

- 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!!!

Calculations

- 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^2_{bin}
- 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

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

Summary

- 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