Beyond Hauser-Feshbach in the compound nucleus

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The program

"The purpose of the program is to bring together physicists from the low-energy nuclear structure and reaction communities to identify avenues for achieving reliable and predictive descriptions of reactions involving nuclei across the isotopic chart."

A goal

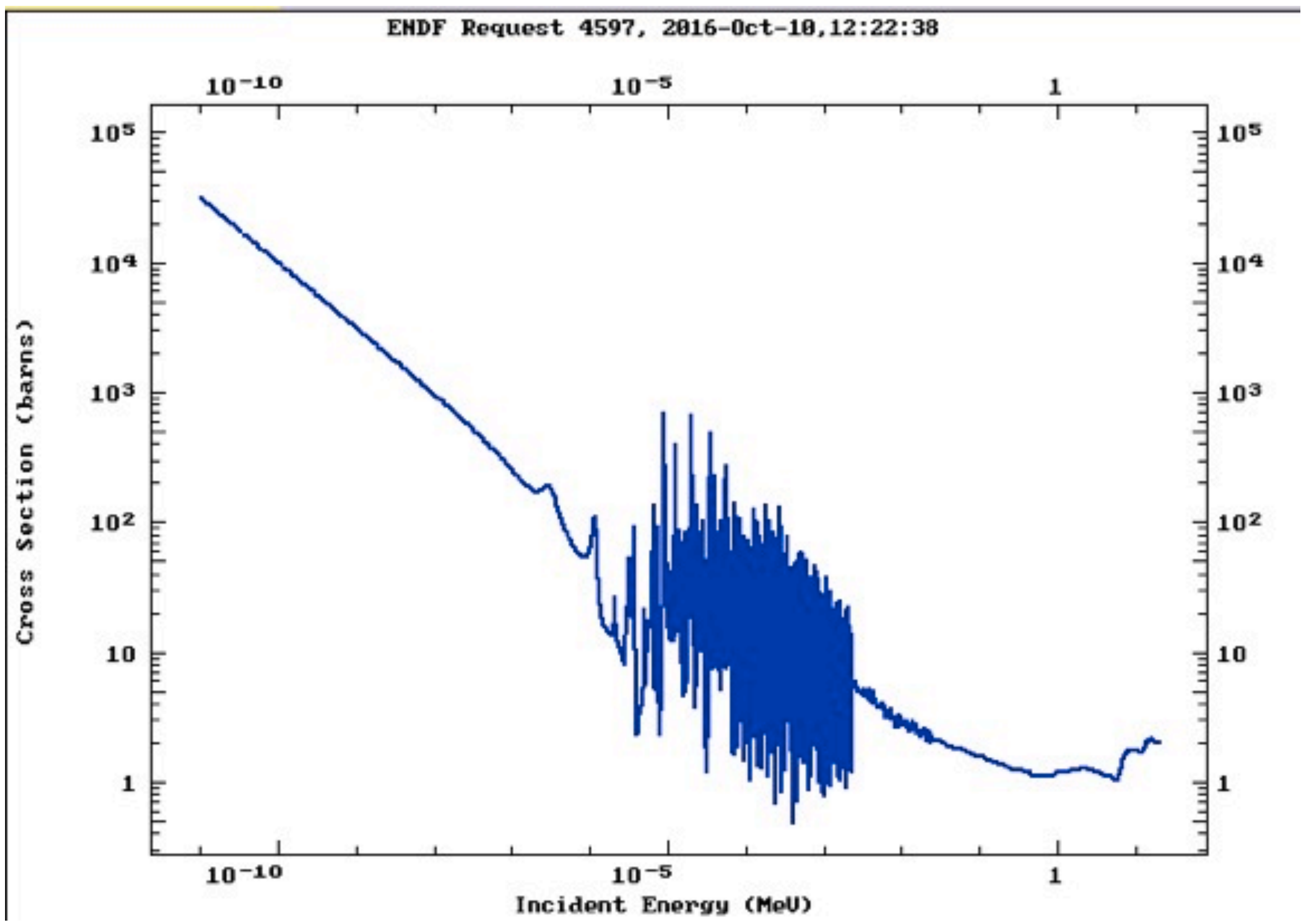
"Determine strategies for moving towards microscopic theories of heavy nuclei to achieve increasingly more predictive descriptions of the structure and reactions of heavy nuclei."

Outline of my talk

1. Motivation: theory of induced fission
2. A new approach: CI
3. Mazama: a flexible code to implement CI methods
4. First results

Motivation

I would like an understanding of fission dynamics, based on a nucleonic Hamiltonian.



$^{235}U(n,f)$

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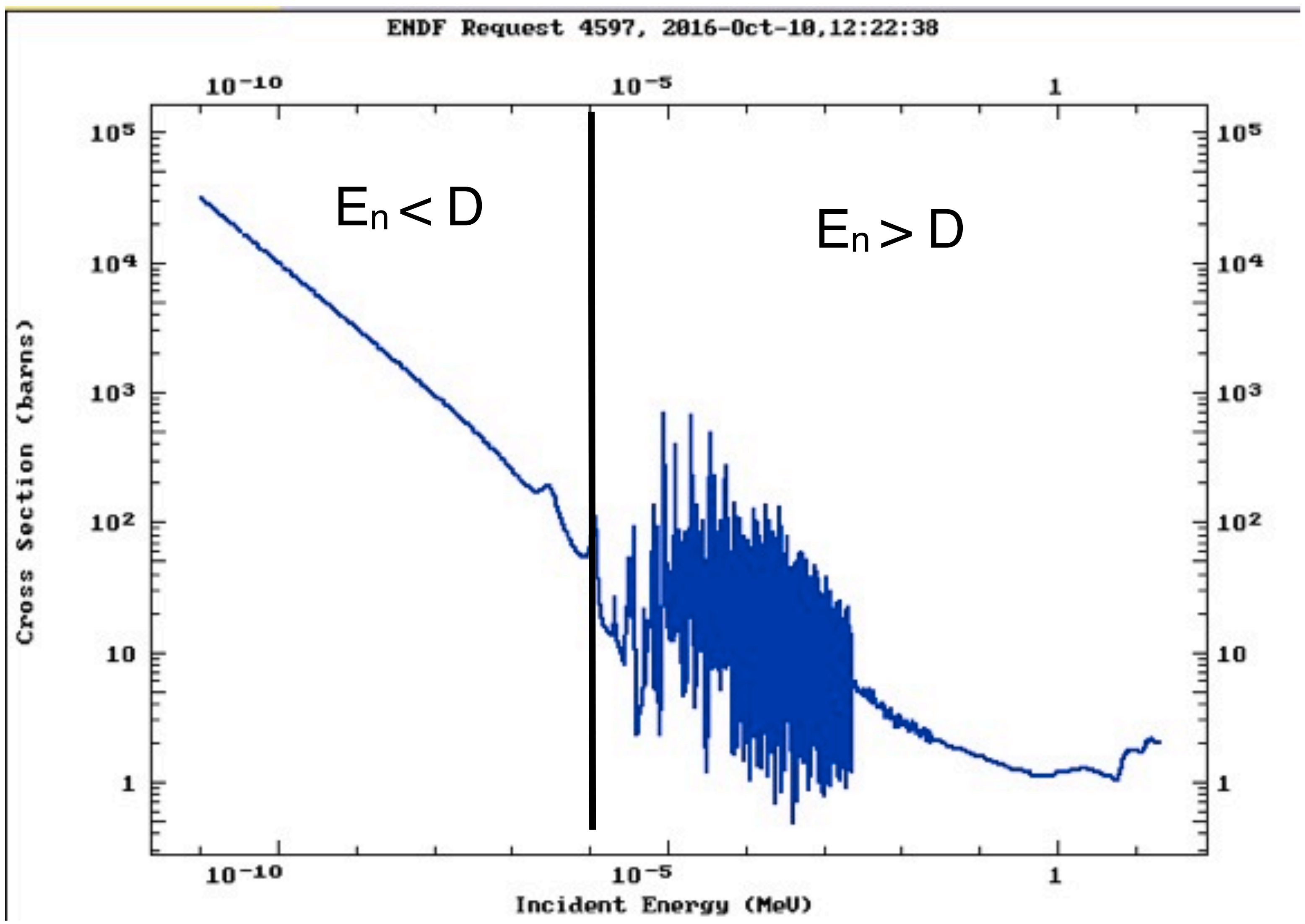
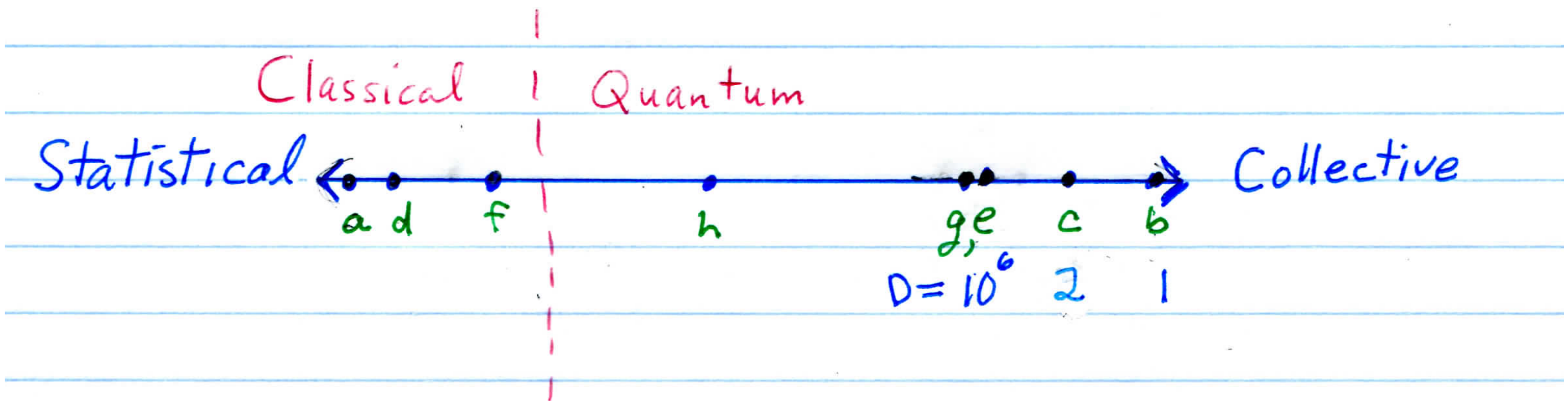


$^{235}U(n,f)$ Text

Spectrum of models



a) Fong, PR 102 434 (1956)
d) Lemaitre, PRC 92 034617 (2015)
f) Randrup & Moller, PRL 106 132503 (2011)

b) Bjornholm & Lynn, RMP 52 725 (1980)
c) Goutte, PRC 71 024316 (2005)
e) Bernard, PRC 84 044308 (2011)
g) Bulgac, PRL
h) Bouland, PRC 88 054612 (2013)

Only Guet et al. and Bulgac et al. dynamics relate to the nucleonic Hamiltonian.

The transmission coefficient, a key concept.

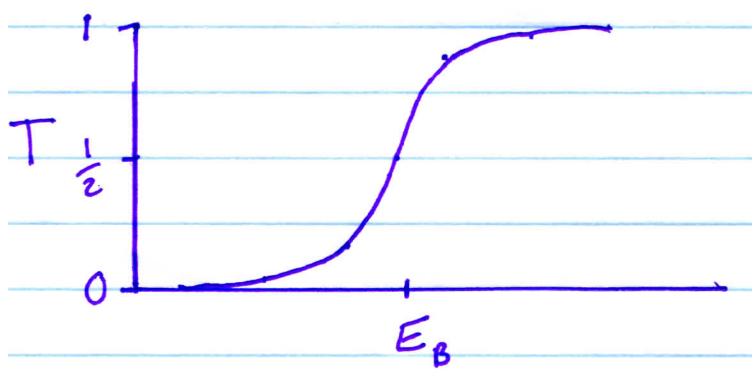
Wigner, Eyring, Weisskopf (1930-1937)

Bohr-Wheeler (1939)

$$\Gamma_F(E) = \frac{1}{2\pi\rho}\sum_c T_c(E)$$

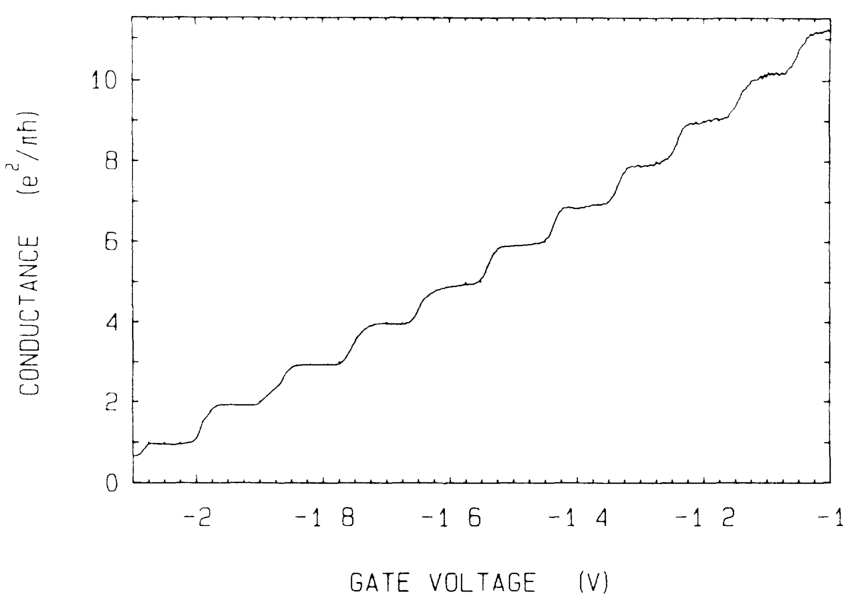
Hill-Wheeler (1953)

$$T(E) = \frac{1}{1+\exp(2\pi(E_B - E)/\hbar\omega)}$$



Well-known in mesoscopic physics as the Landauer formula for quantized conductance.
(See Bertsch, J. Phys. Condens. Matter 3 373 (1991).

$$G = 1/R = \frac{e^2}{2\pi\hbar}\sum_c T_c$$

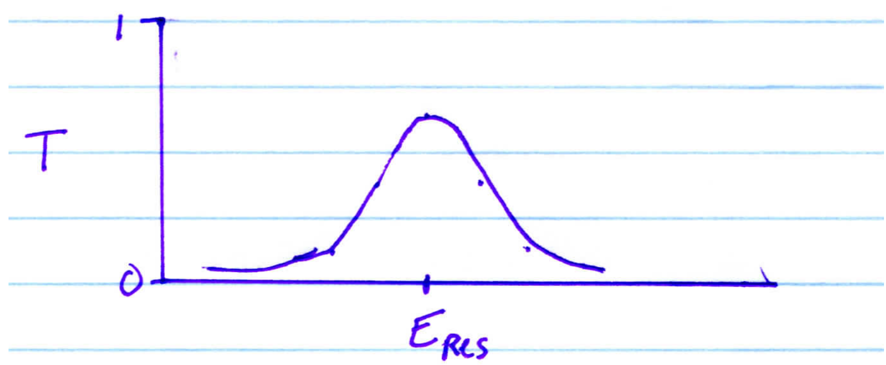


B.J. van Wees, et al. Phys. Rev. Lett. 60 848 (1988).

Transport through quantum dots (resonances)

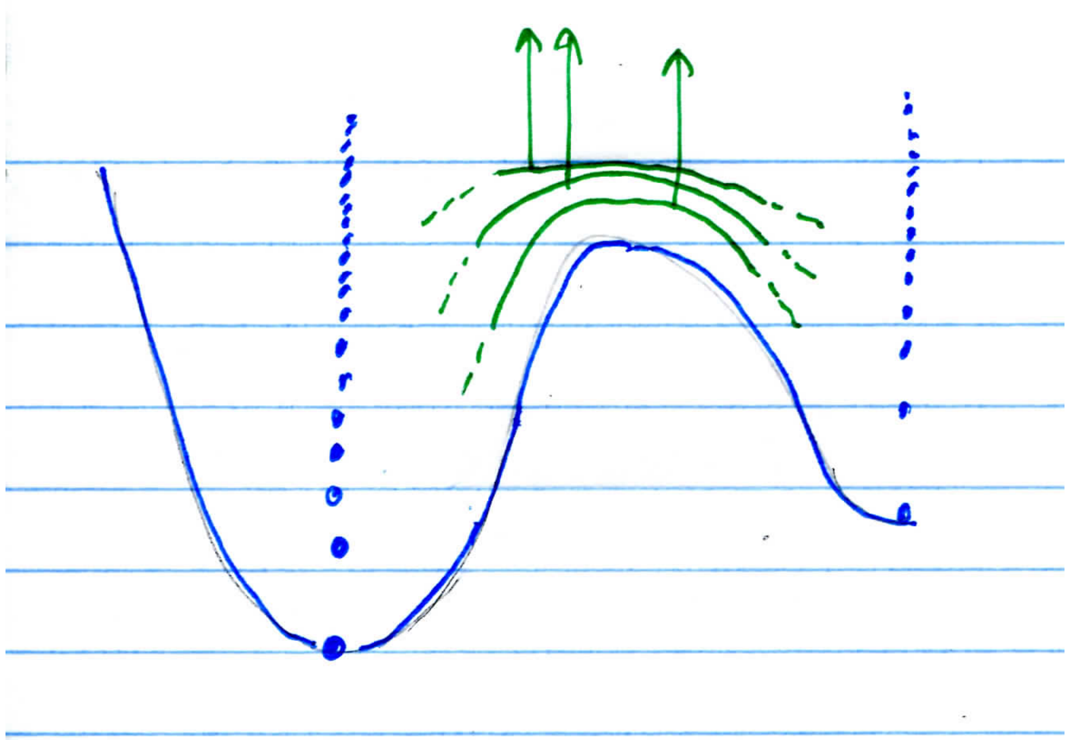
See Alhassid, RMP **72** 895 (2000)

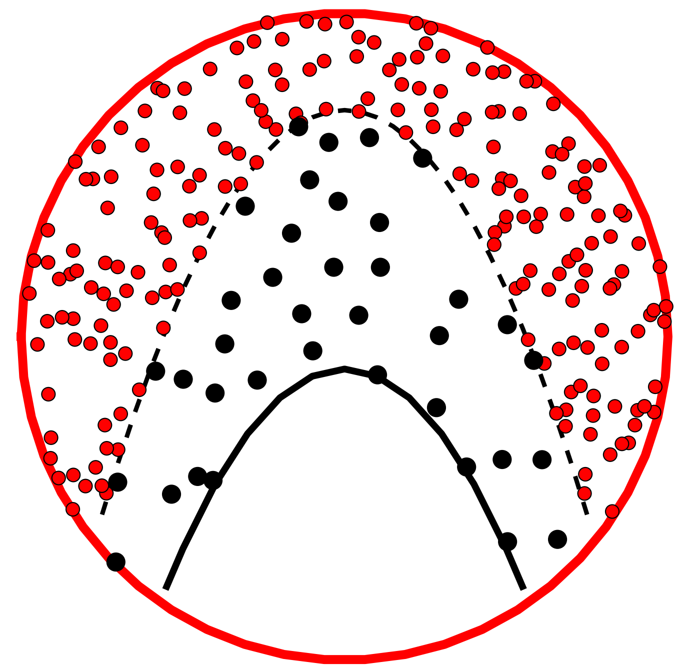
$$T_{res}(E) = \frac{\Gamma_R \Gamma_L}{(E - E_{res})^2 + (\Gamma_R + \Gamma_L)^2/4}$$



Maximum T=1, when left and right widths are equal.

States or Channels?





Remarks:
1)There is (as yet) no way to connect the states to the channels with the nucleonic interaction.

2)Transport through intermediate states is well established in mesoscopic physics.

3) Meager evidence for collectivity in the shape degree of freedom near the ground state.

4) Are there any observable consequences?

Can we make a predictive theory through the CI approach?

$$\hat{H} = \hat{e} + \hat{v} = \sum_i \epsilon_i a_i^\dagger a_i + 1/4 \sum v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$$

Separate configuration space into interacting subspaces q.

$$\hat{H} = \sum_q \hat{V}(q) + \sum_q \hat{e}_q + \sum_q (\hat{v}_q + \hat{v}_{q,q+1})$$

Remarks:
1) How can we systematically define a discrete basis? (see arXiv:1611.09484, PRL 113 262503)
2) DFT gives our best theory of V(q). (Skyrme,.. , hybrid H?)
3) e_q must give a good account of level density (consistent with 2?)
4) v_q can be postponed by invoking the GOE.
5) pairing interaction in v_(q,q+1) is important at low excitation.
6) At high excitation, v_(q,q+1) should have a Porter-Thomas parameterization.

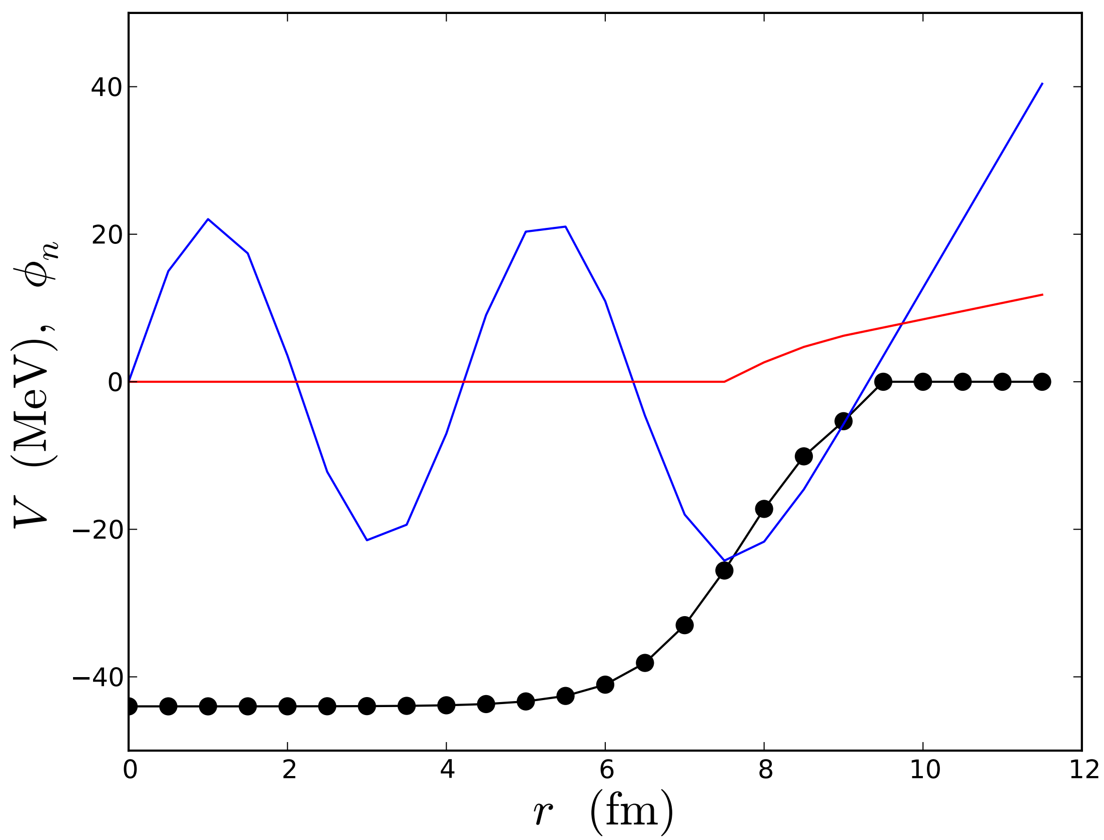
The Mazama code: implementing the H_q framework for neutron-induced reactions.

The Hamiltonian is set up in stages, each one connects only with its neighbors.
-Entrance channel
-Internal stage I
-internal stage 2
-...

Entrance channel: continuum neutron wave function represented on an r-space mesh.
Woods-Saxon potential:

$$V(r_i) = \frac{V_0}{1 + \exp((r_i - R)/a)}$$

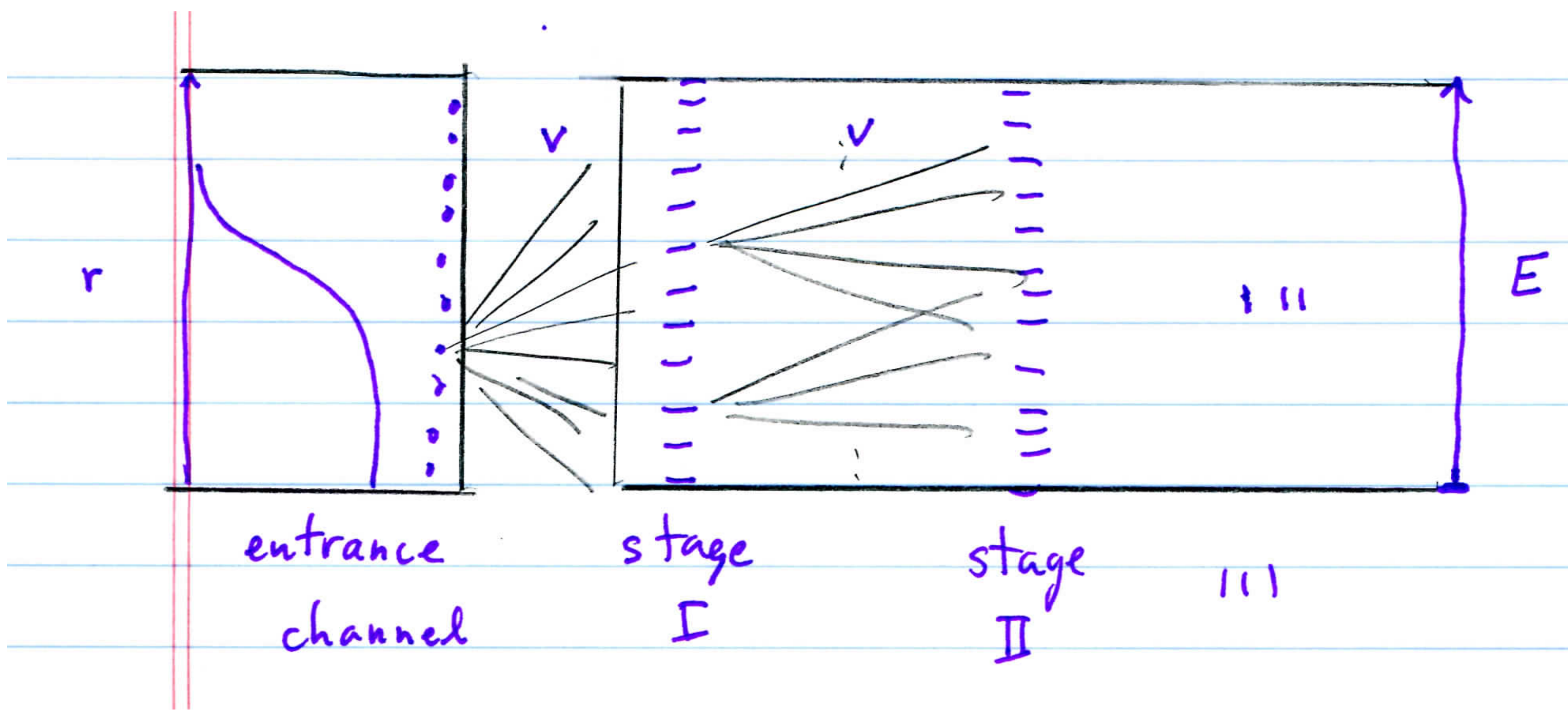
No imaginary W!



black: V
blue: phi_n.real
red: phi_n.imag

Other stages are described by a spectrum of levels with space either uniform or following the GOE ensemble. An imaginary contribution Gamma/2 may be added to the energies to represent decay modes other than coupling to neighboring stages.

Interactions between levels in neighboring stages are taken from a Porter-Thomas distribution (i.e. Gaussian-distributed).



Computational issues

Space dimension

Matrix is already partially diagonalized. Dimensionality of each stage is limited by computer resources, eg. N~1000's for python on a Mac. Number of stages is limited only by round-off errors.

Truncation

Only a limited energy band can be treated exactly. Presents problems when the spacing of levels in the stage is large than the bandwidth.

Example: D = 1 eV in ^{236}U. Thus, bandwidth is ~1 keV.

The Hauser-Feshbach formula

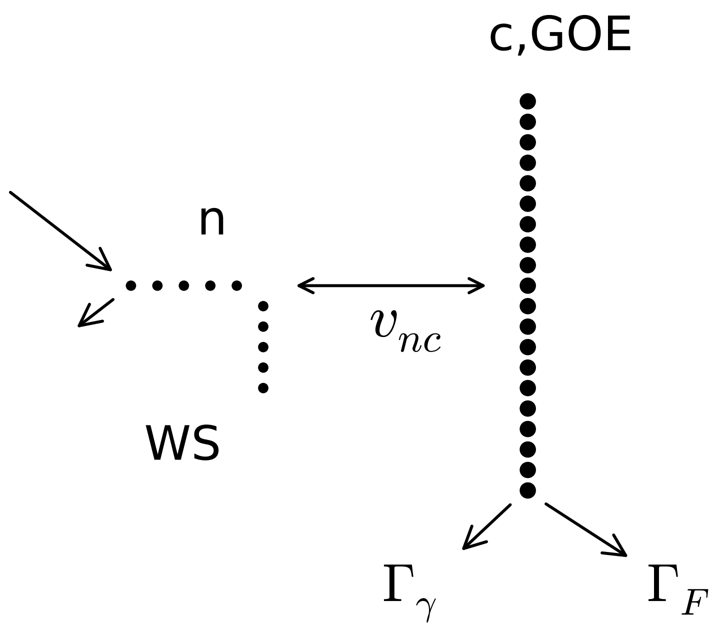
$$\sigma_{\alpha,\beta} = \frac{(2l+1)\pi}{k^2} \frac{\Gamma_\alpha \Gamma_\beta}{\Gamma^2}$$ (prefactor modified by symmetries)

Definition of compound nucleus

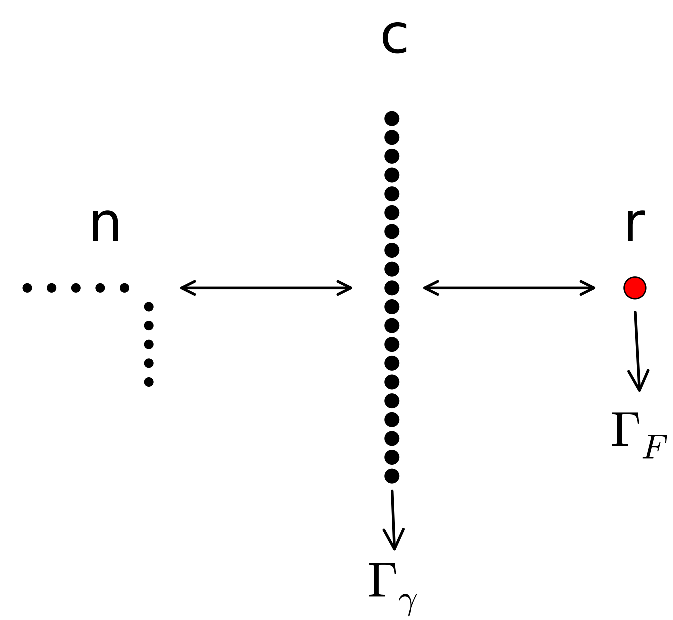
1) level spacing follows GOE spectrum
2) matrix elements $\langle \alpha | v | x \rangle$ follow Porter-Thomas distribution

$$P(\langle \alpha | v | x \rangle) = \exp(-v^2/2v_0^2)$$

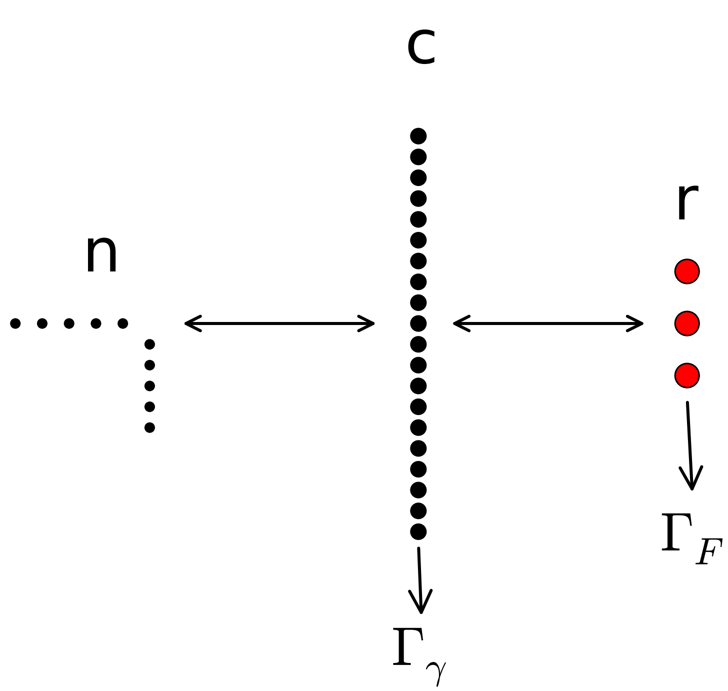
Examples of models that can be analyzed with Mazama.



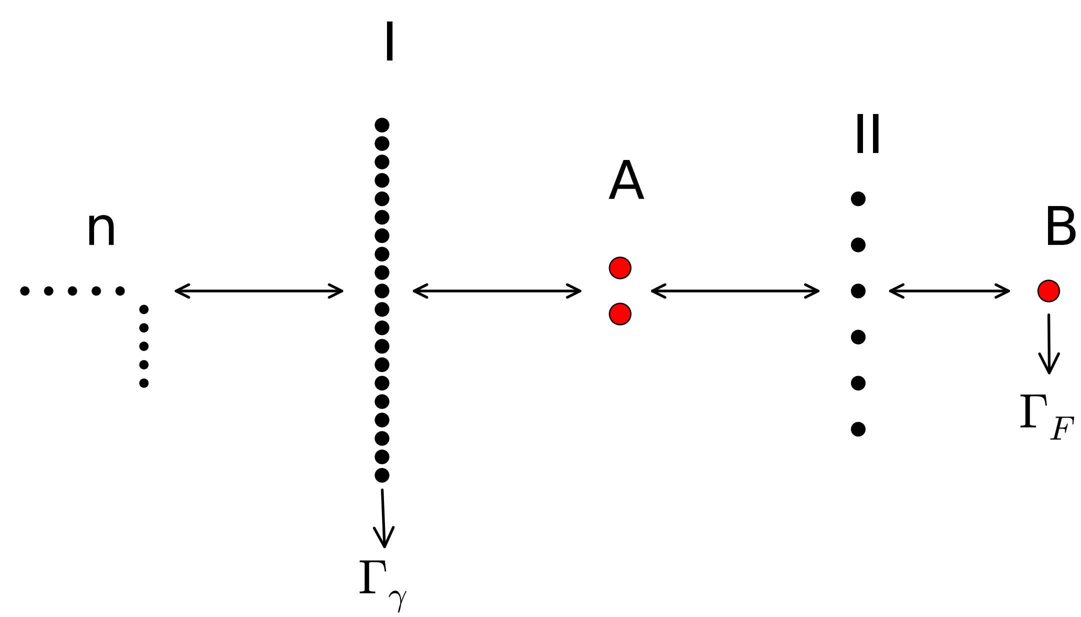
Hauser-Feshbach



Simple barrier model



More transition states

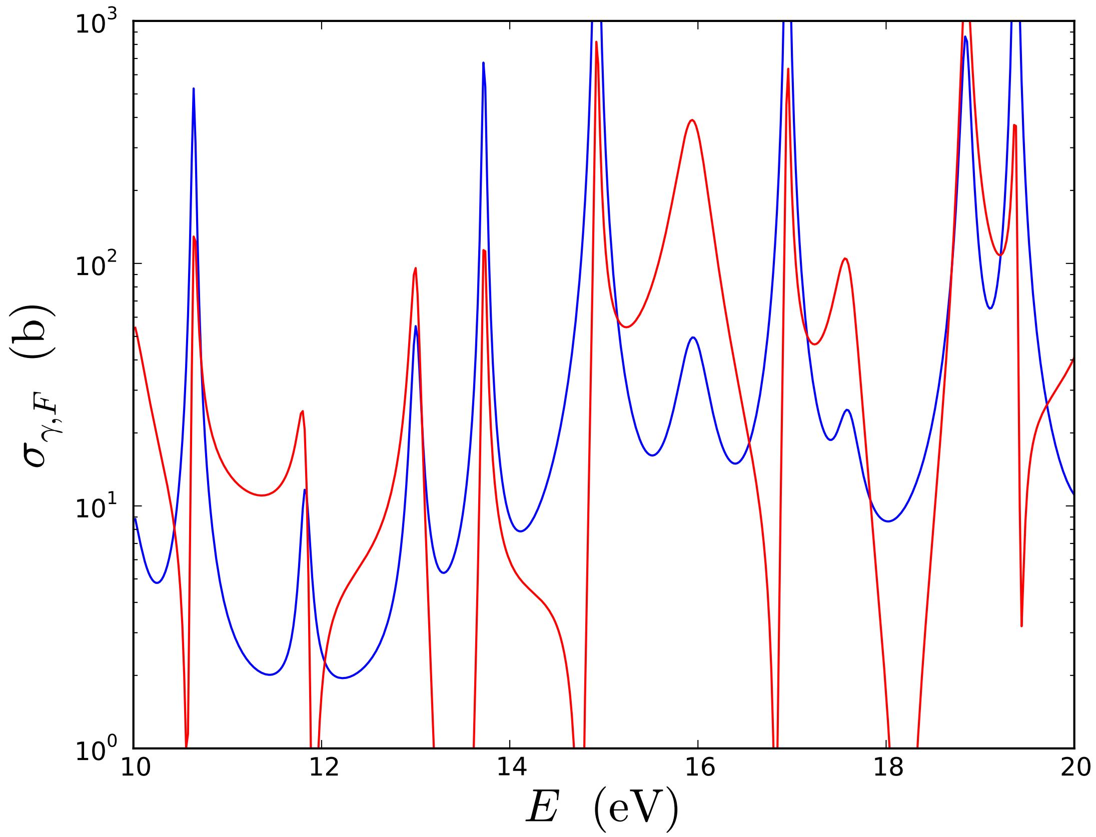


Double-barrier dynamics

How far can we get with the simpler barrier model?

Average low-energy properties of ^{235}U(n,..) :

$$\langle \frac{\Gamma_n}{D} \rangle = 10^{-4} \left(\frac{E_n}{1\mathrm{eV}} \right)^{1/2} \qquad \Gamma_\gamma \approx 35 \text{ meV} \qquad \Gamma_F \approx 100 \text{ meV} \qquad \alpha^{-1} \approx 2.8$$



Blue: capture; red: fission

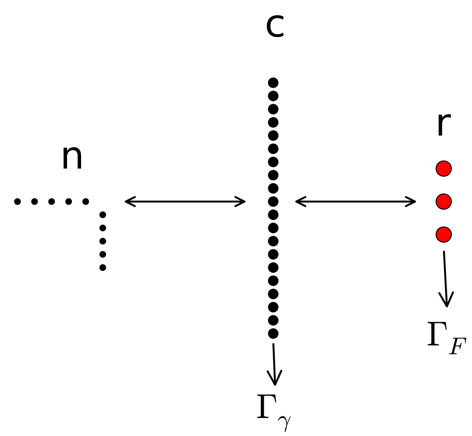
Single transition state

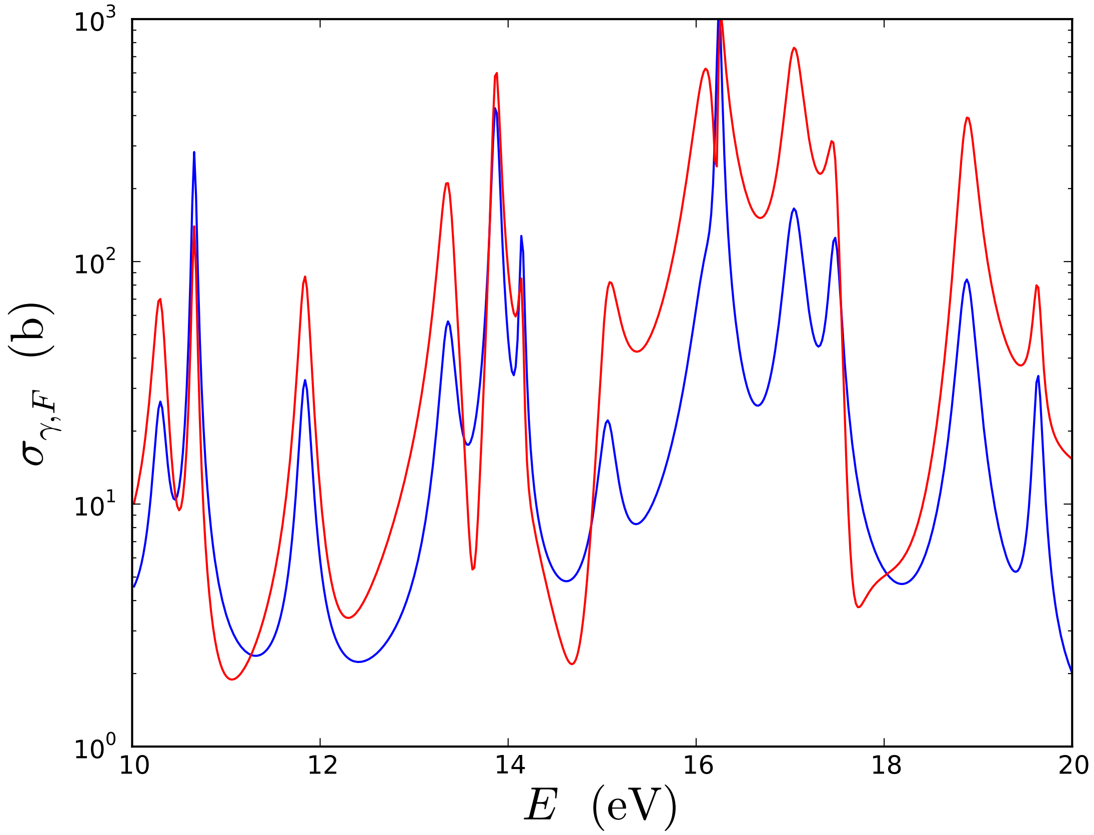
```
0.5  24 15             # delta_r, Nn,  i_vnc
-44.0 0.65 1.25 235. # V_ws a_r r0 A
2  1                   # Nstage seed
200 -50.e-6 1.0e-6 35.0e-9 2.5e-3 w
          #Nc,E0c,dEc,gamma_c,v_nc
1  50.0e-6  0.0 2.0e-5 1.0 u
          # 100.e_9 *200 = 2.e_5
10.0e-6 2.0e-8 1000 sig # E0, delE, NE, S/sigma
```

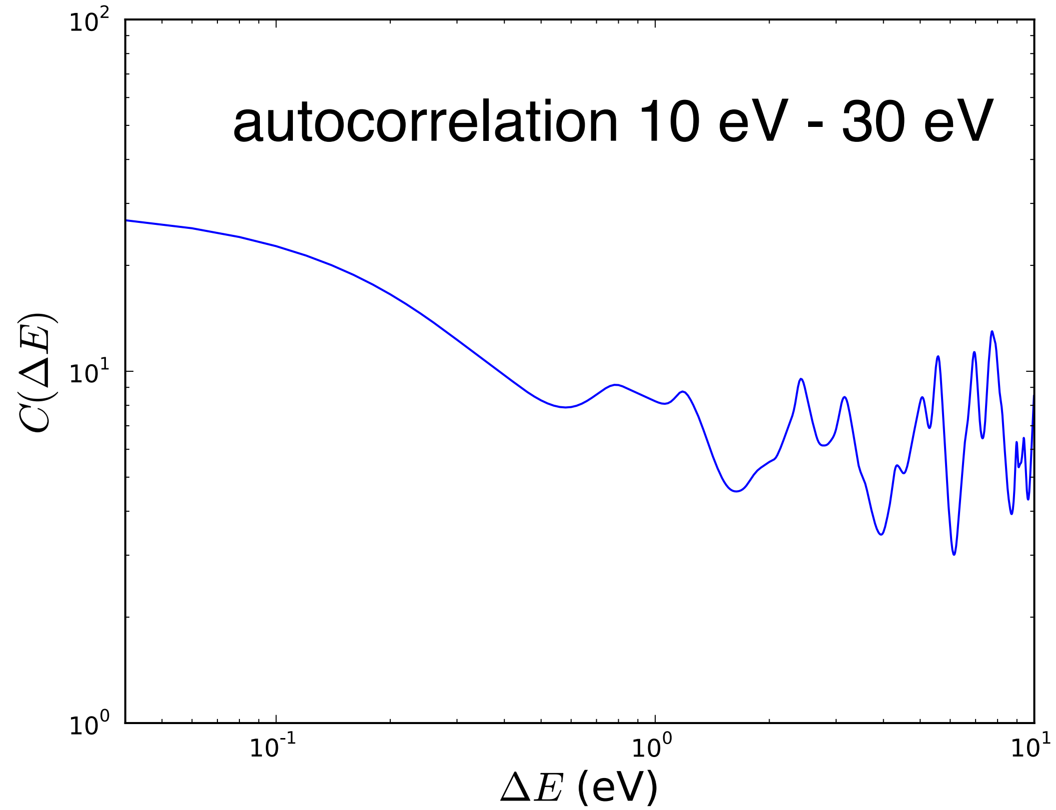
$$\alpha_{sts}^{-1} \approx 0.9$$

Hauser-Feshbach violation!

Adding transition states







Blue: capture; red: fission

$$\alpha_{3ts}^{-1} \approx 3$$

Two sources of Hauser-Feshbach violation   Text

Bertsch and Kawano, arXiv:1701.00276 (2017)

1) well-known in the evaluator community--”width fluctuation correction”

Moldauer, Phys. Rev. C 14 764 (1976).

$$\left\langle \frac{\Gamma_\alpha}{\Gamma_\alpha + \Gamma_0} \right\rangle_\alpha \Big/ \left\langle \frac{\Gamma_0}{\Gamma_\alpha + \Gamma_0} \right\rangle_\alpha < \left\langle \frac{\Gamma_\alpha}{\Gamma_0} \right\rangle_\alpha$$

2) In principle known, but forgotten: T<1. Need to solve explicitly for the S-matrix:

$$K = \pi \tilde{\gamma}^T \frac{1}{E - H} \tilde{\gamma} \qquad\qquad S = \frac{1 - iK}{1 + iK}$$

Future

Fluctuations:

1. When is Porter-Thomas violated?

   Claim in PRL 115 052501 (2015): properties of the entrance channel can produce violations of otherwise statistical distributions.

2. Validity of Ericson's treatment of compound-nucleus fluctuations

Autocorrelation function $$C(\epsilon) = \left\langle \frac{\sigma(E)\sigma(E+\epsilon)}{\bar{\sigma}^2} \right\rangle$$

Width of CN states $$C(\epsilon) = 1 + \frac{1}{N_c}\frac{1}{1+(\epsilon/\bar{\Gamma})^2}$$

E_B>> Gamma $$C(0) - 1 = \frac{1}{N}\frac{1}{1+(E_B/\pi\bar{\Gamma})}$$

P. Fessenden, et al., Phys. Rev. Lett. 15 796 (1965).