Importances of exit channel fluctuations in reaction branching ratios

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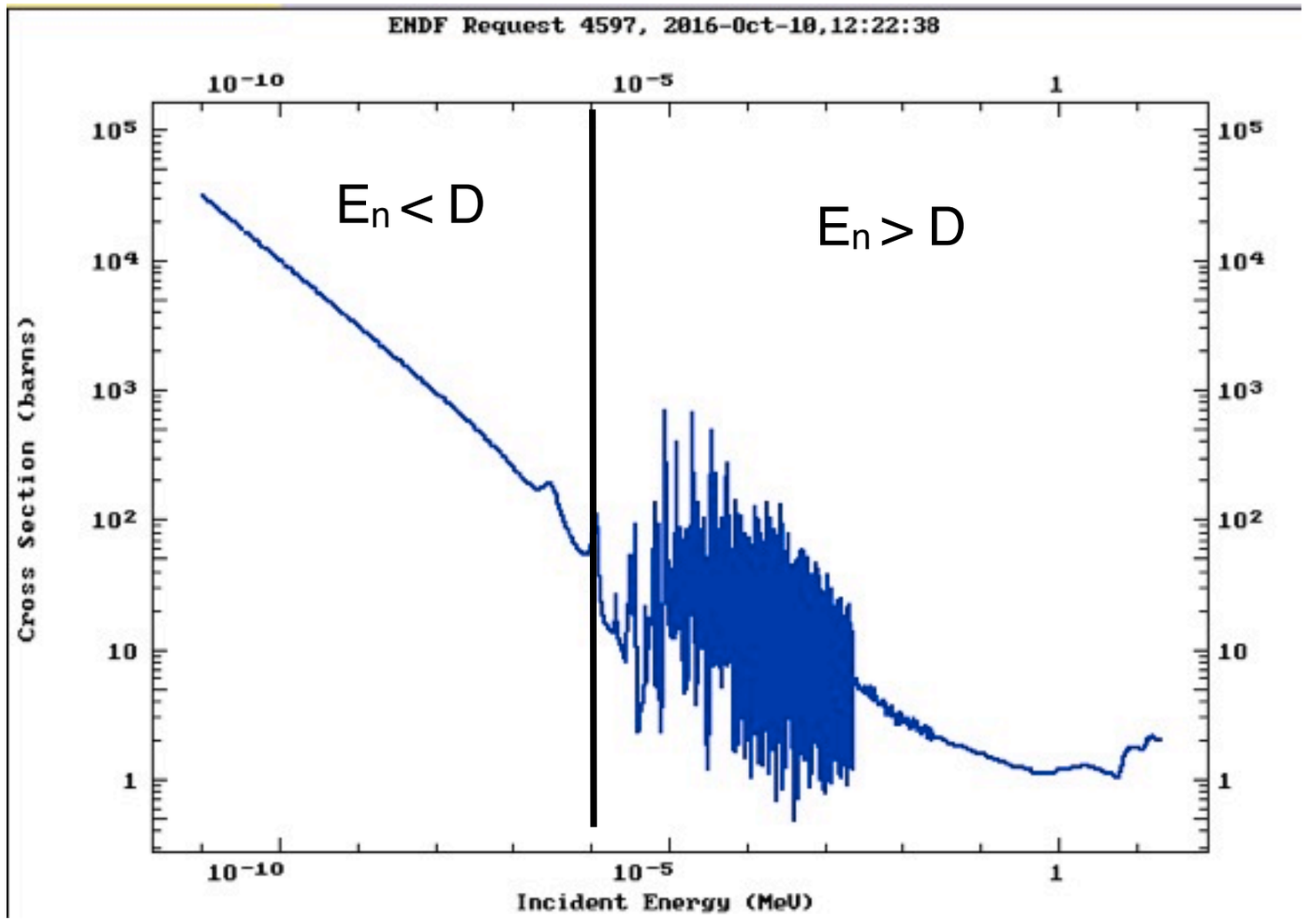
NMP17, MSU
March 7, 2017

Outline of my talk

1. Motivation: theory of nuclear fission, an open system
2. roadmap for a CI approach
3. Mazama: a flexible code to implement CI methods
4. Appliction to compound-nucleus branching ratios

Motivation

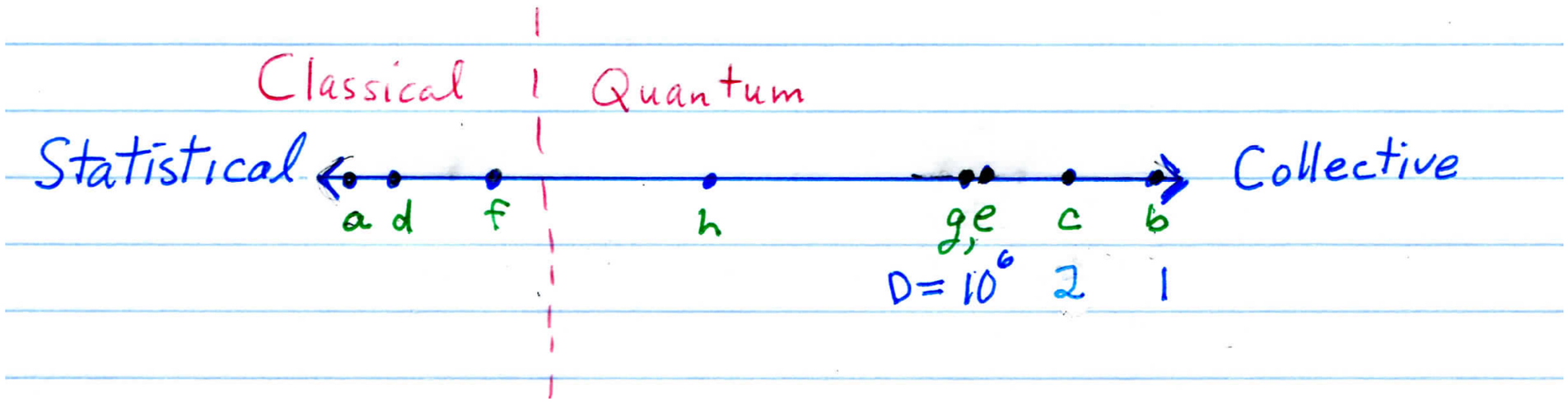
I would like an understanding of fission dynamics, based on a nucleonic Hamiltonian.



^{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)

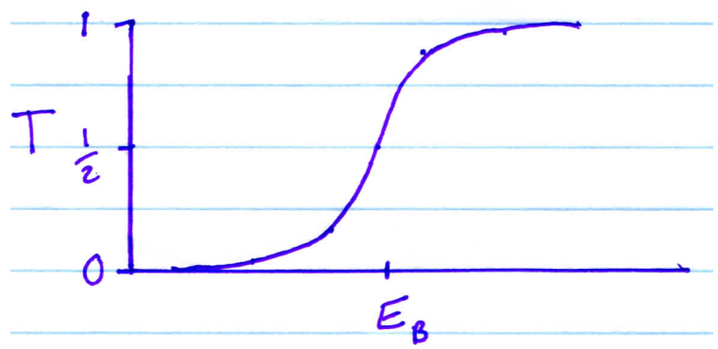
Only Guet et al. and Bulgac et al. dynamics relate to the nucleonic Hamiltonian.

The transmission coefficient, a key concept.

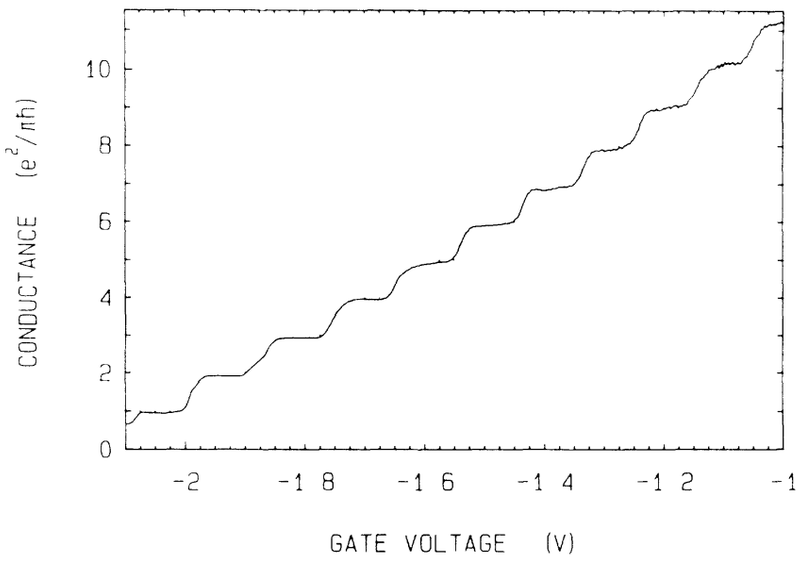
Wigner, Eyring (1930-1925) transition channels
Weisskopf (1937) detailed balance (microscopic reversability)

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: $$G = 1/R = \frac{e^2}{2\pi\hbar}\sum_c T_c$$
(See Bertsch, J. Phys. Condens. Matter 3 373 (1991).

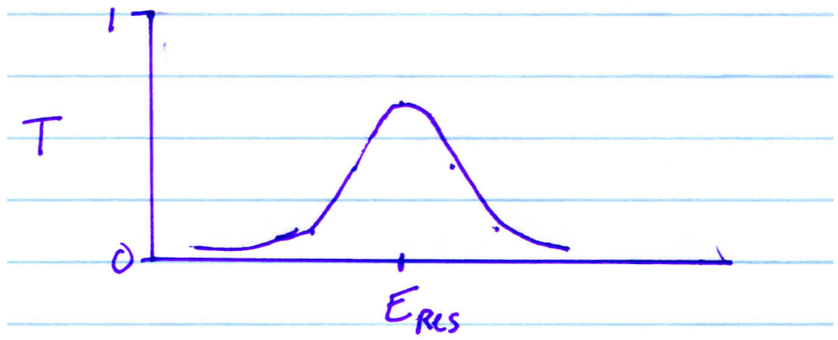


B.J. van Wees, et al. Phys. Rev. Lett. 60 848 (1988).

Transport through quantum dots (resonances)

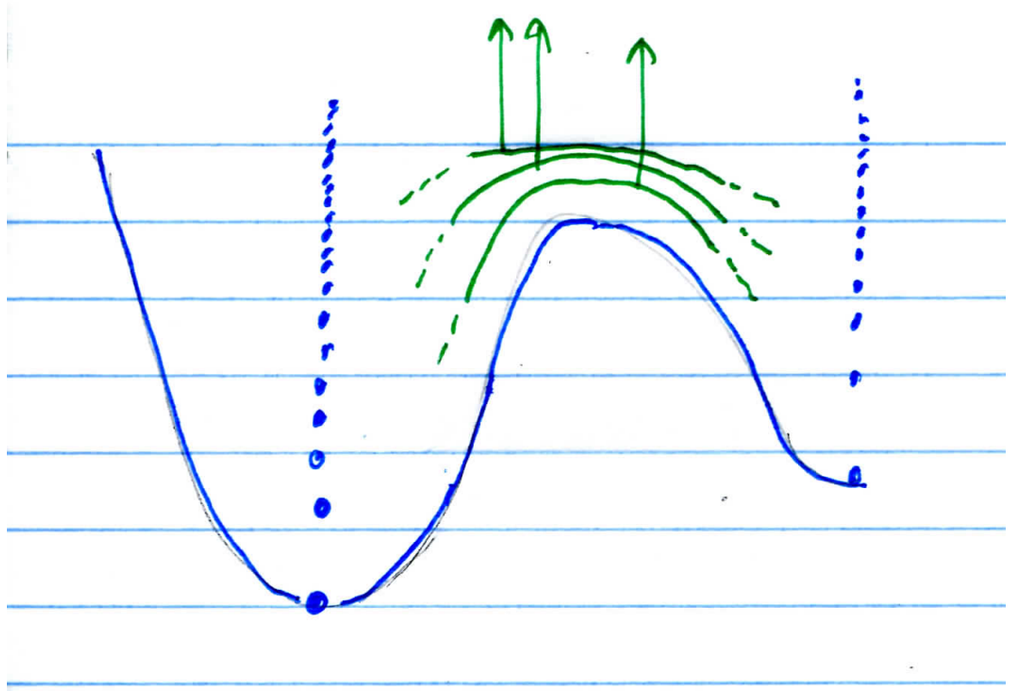
See Alhassid, RMP **72** 895 (2000)

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



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.

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

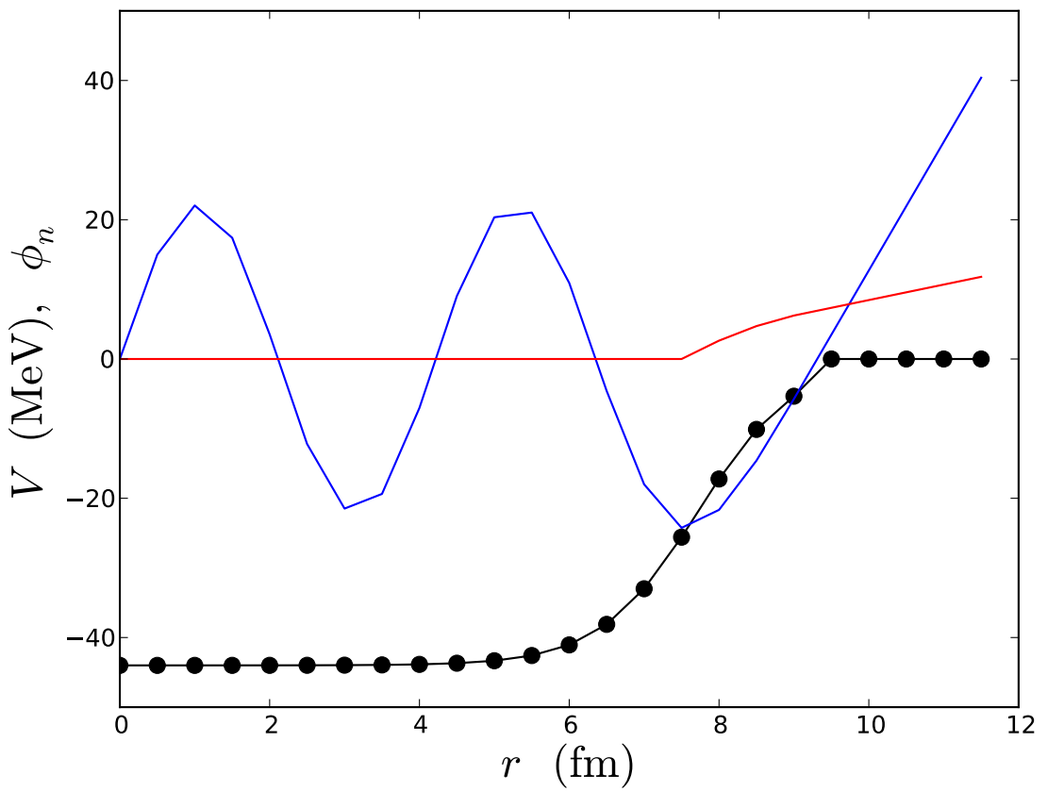
Remarks:

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 a discrete basis 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!

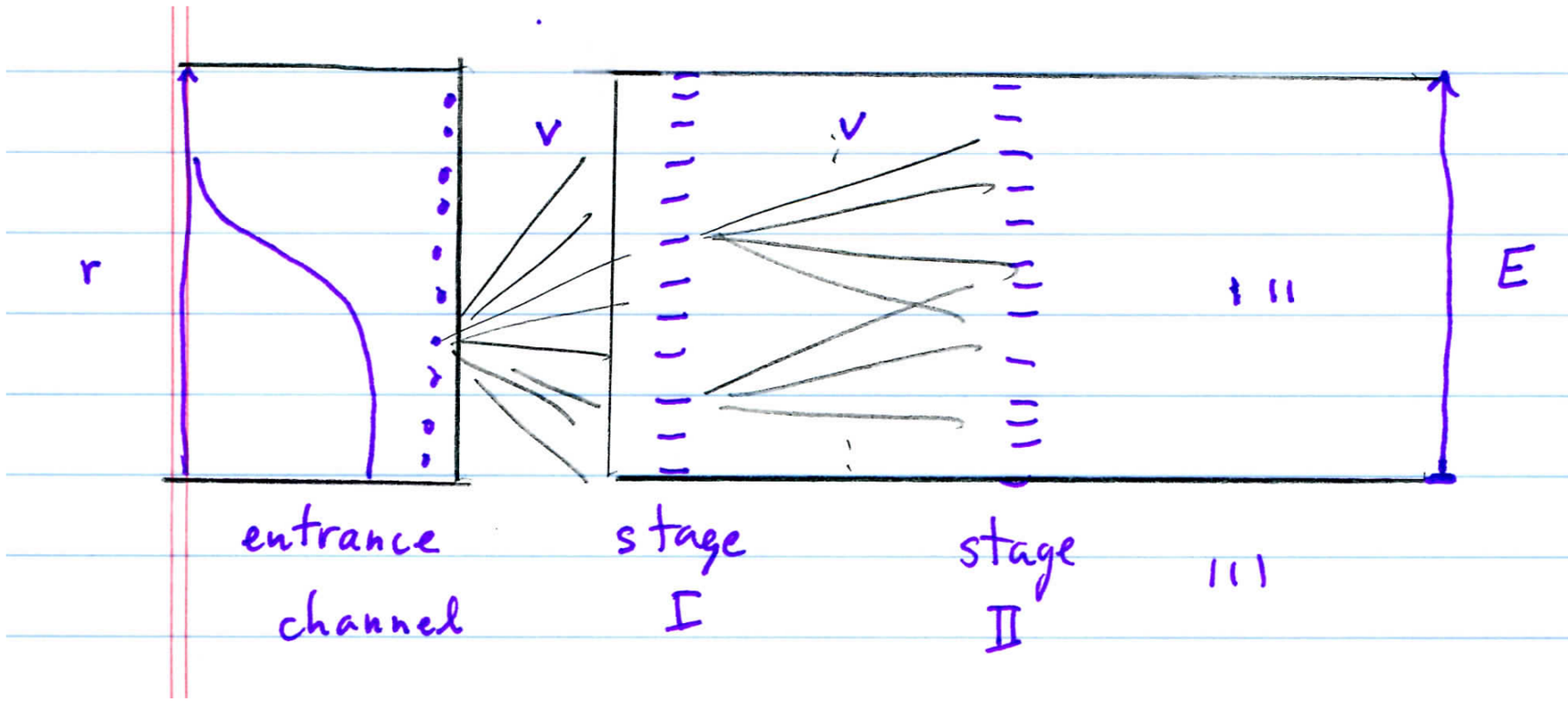


black: V
blue: phi_n.real
red: phi_n.imag

Other stages are described by a spectrum of levels with space either uniform or following the GOE ensemble.

```
m1=numpy.random.randn(N,N)
m2=m1+numpy.transpose(m1)
eigs,U = numpy.linalg.eigh(m3)
```

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).



The Hauser-Feshbach formula

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

(prefactor modified by symmetries)

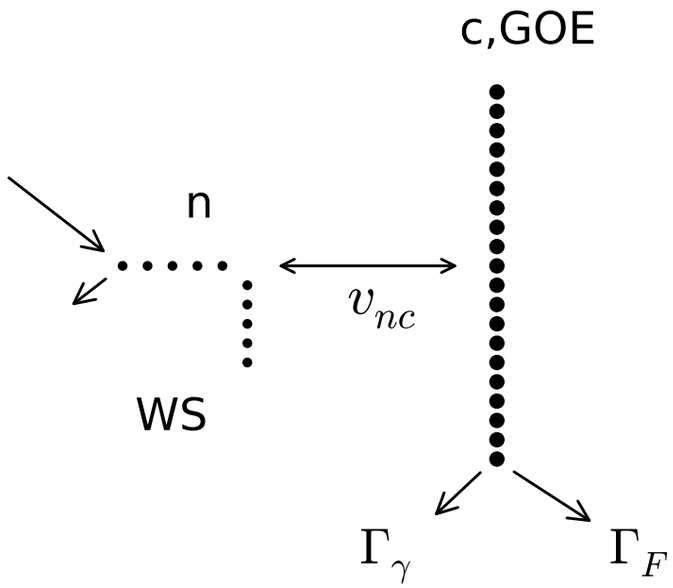
Definition of compound nucleus

1) level spacing follows GOE spectrum

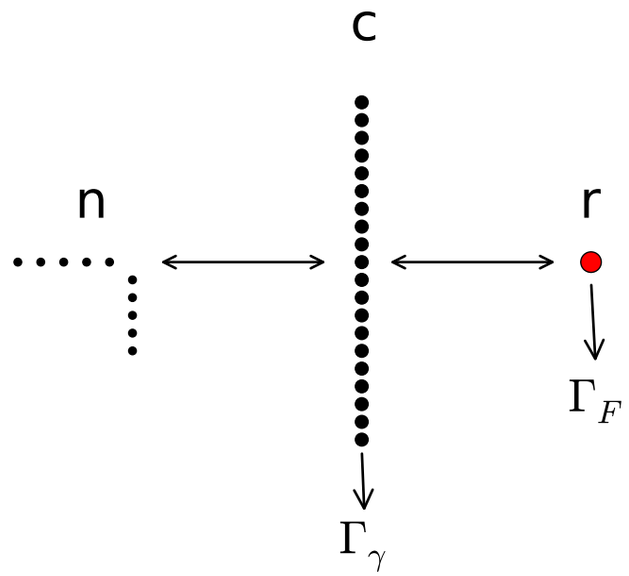
2) matrix elements $\langle\alpha|v|x\rangle$ follow Porter-Thomas distribution

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

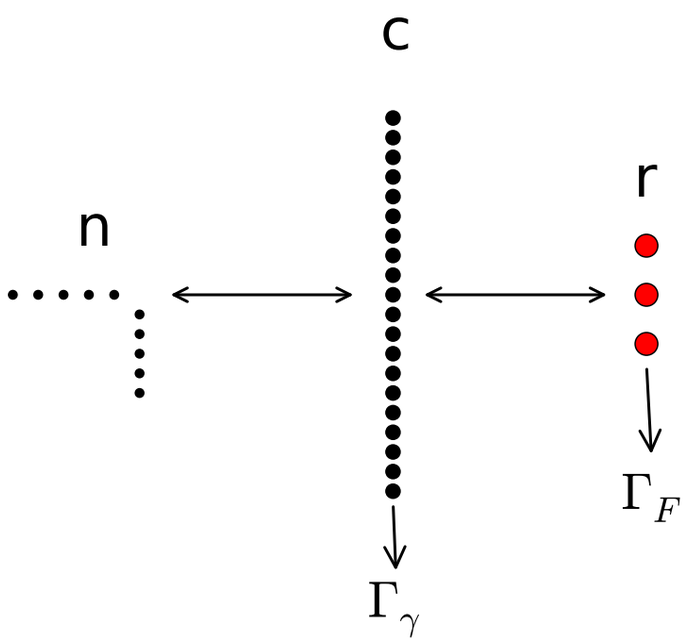
Examples of models that can be analyzed with Mazama.



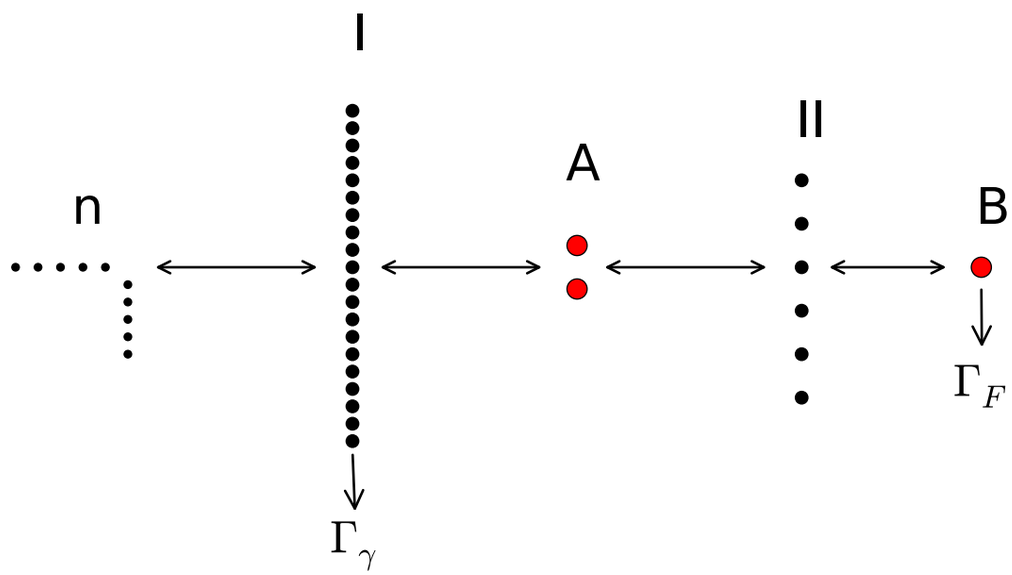
Hauser-Feshbach



Simple barrier model



More transition states

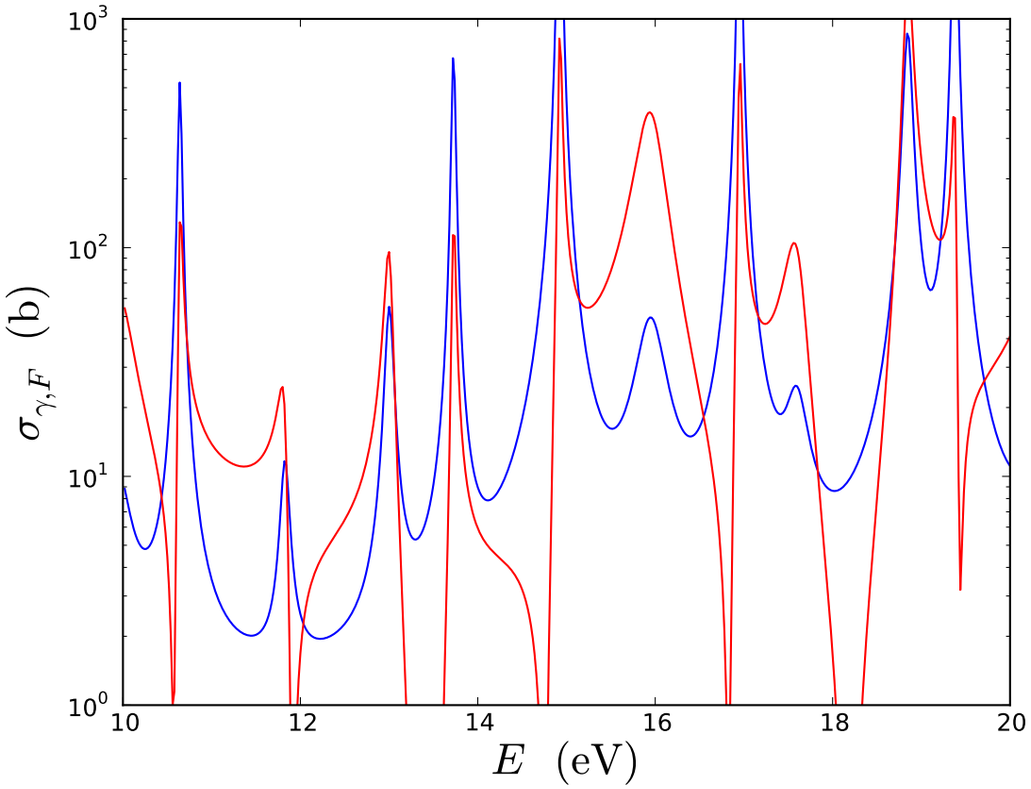


Double-barrier dynamics

How far can we get with the simpler barrier model?

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

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



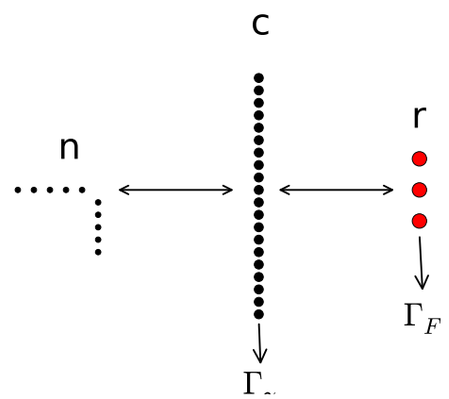
Blue: capture; red: fission

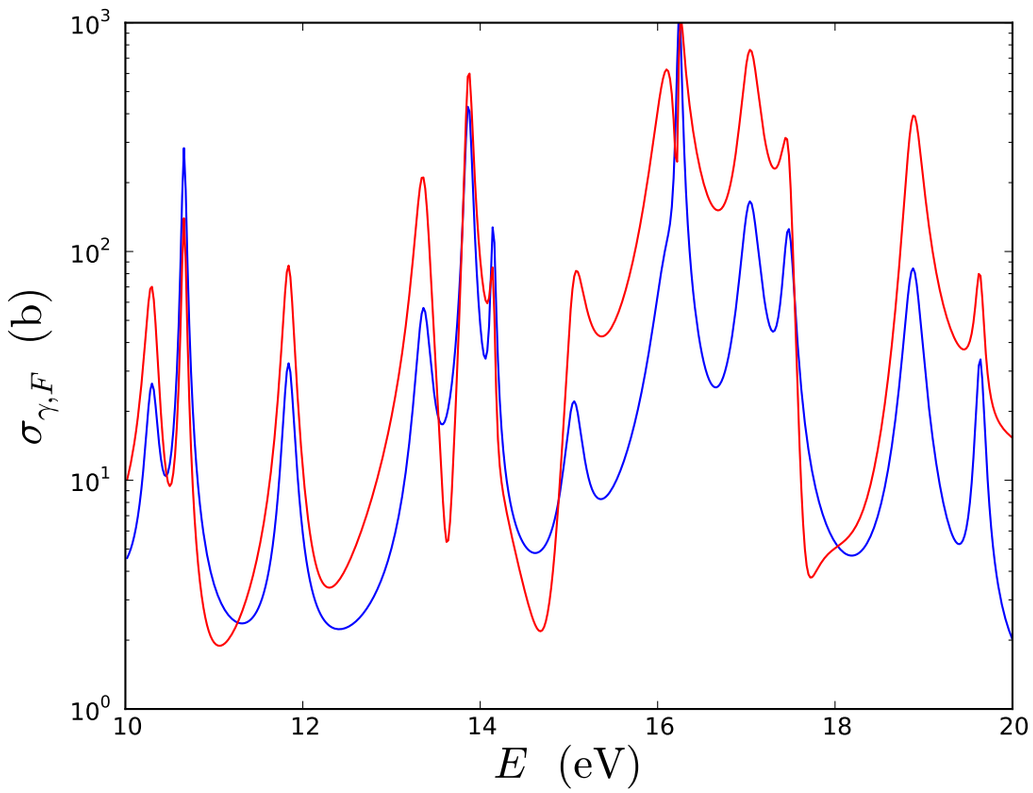
Single transition state

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

Hauser-Feshbach violation!

Adding transition states





Blue: capture; red: fission

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

Two sources of Hauser-Feshbach violation

Bertsch and Kawano, arXiv:1701.00276 (2017)

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

Moldauer, Phys. Rev. C **14** 764 (1976)
T. Kawano, et al., Phys. Rev. C **92** 044617 (2015).

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

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

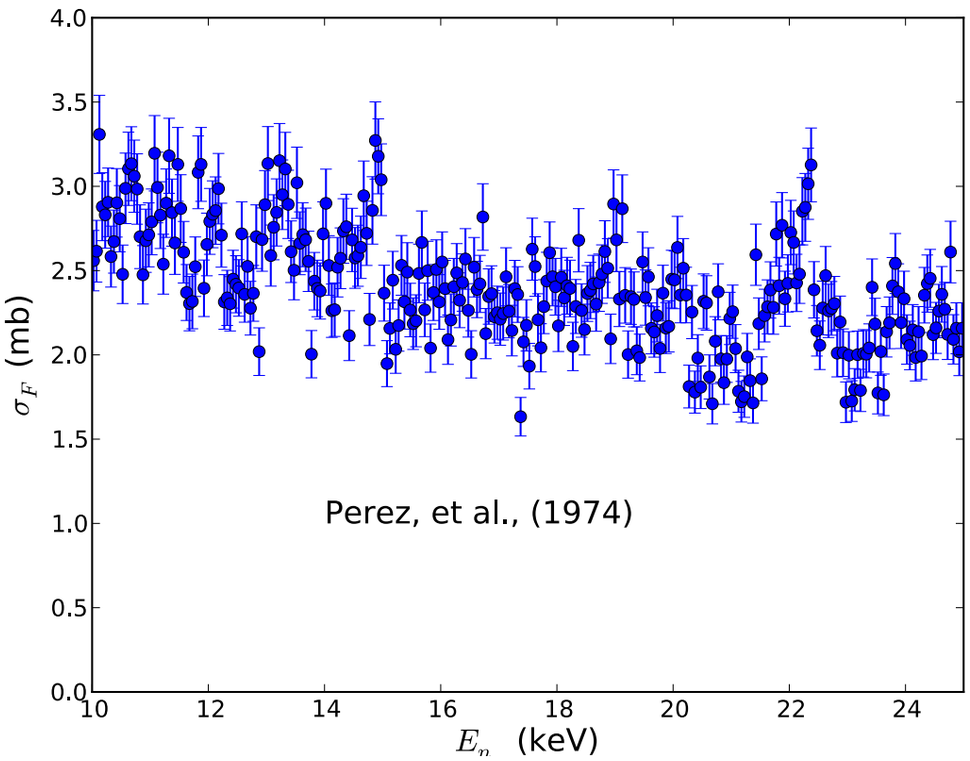
Width of CN states $$C(\epsilon) = 1 + \frac{1}{N_c} \frac{1}{1+(\epsilon/\bar{\Gamma})^2}$$

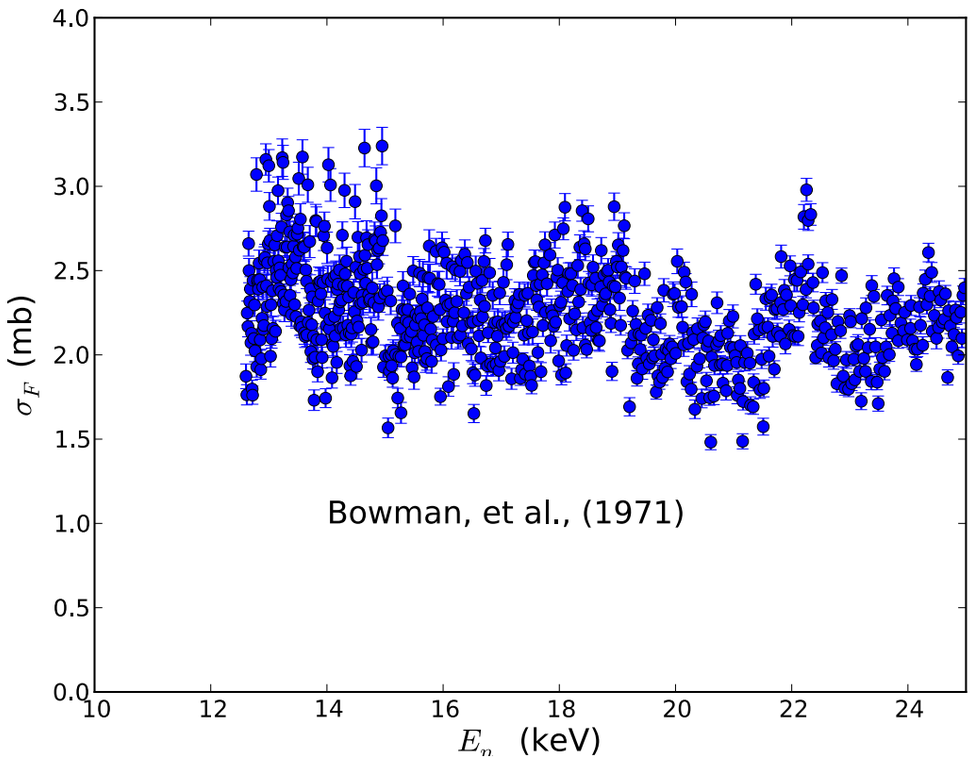
E_B>> Gamma $$C(0) - 1 = \frac{1}{N} \frac{1}{1+(E_B/\pi\bar{\Gamma})}$$

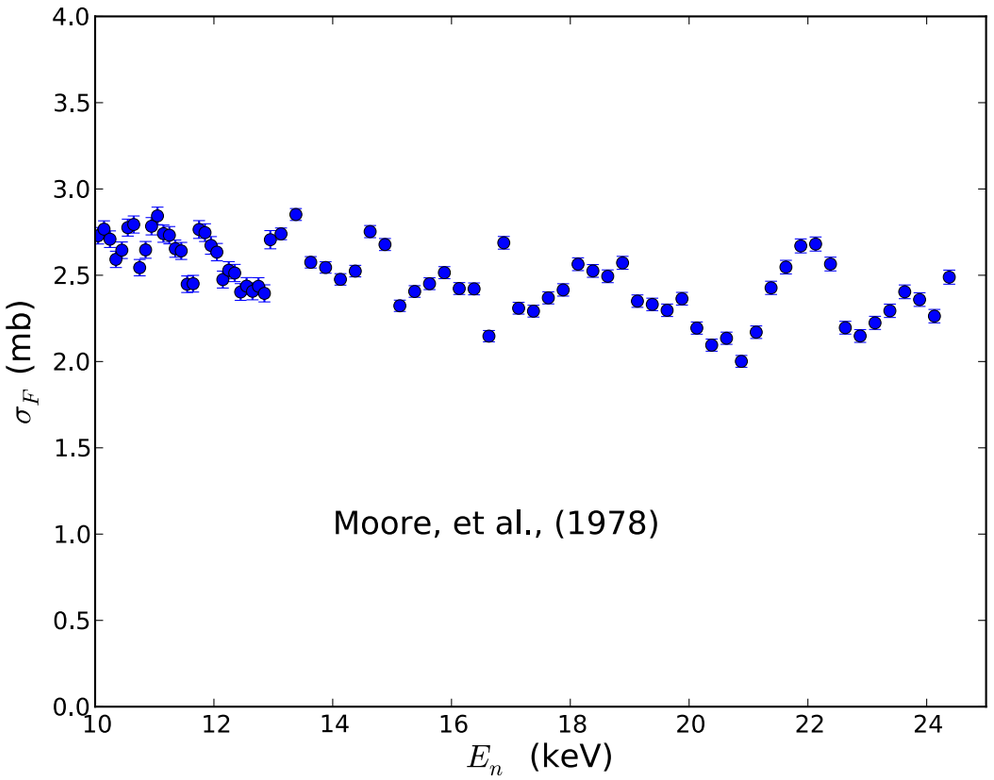
P. Fessenden, et al., Phys. Rev. Lett. 15 796 (1965).

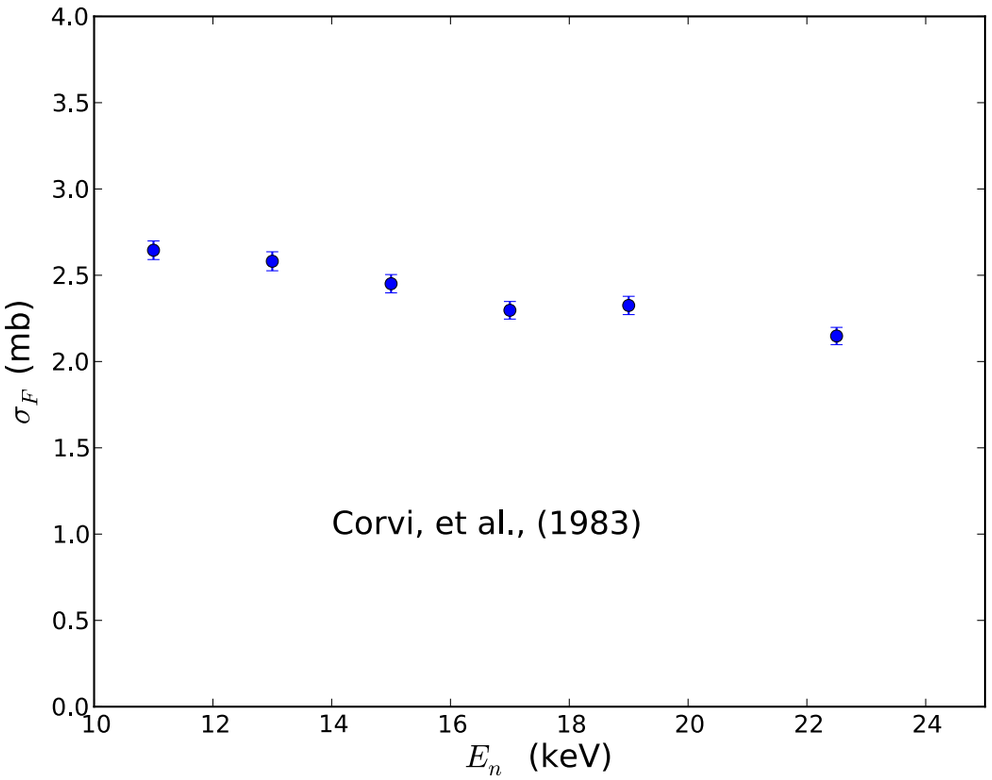
Some of the original data ^{235}U(n,f)

Many thanks to David Brown (BNL) for tracking down the data!









Fluctuation measures

1. Autocorrelation function

$$C(\delta E) = \frac{\int_{E_0}^{E_1} dE\,(\sigma(E) - \bar{\sigma})\,(\sigma(E+\delta E) - \bar{\sigma})}{E_1 - E_0}$$

Measures CN lifetimes in overlapping resonance region.

Ericson, Ann. Phys. **23** 390(1963).
Richter, in *Nuclear Spectroscopy and Reactions*, ed. Cerny

2. Fourier transform

$$\sigma(t) = \int_{E_0}^{E_1} dE e^{-itE}\sigma(E)$$

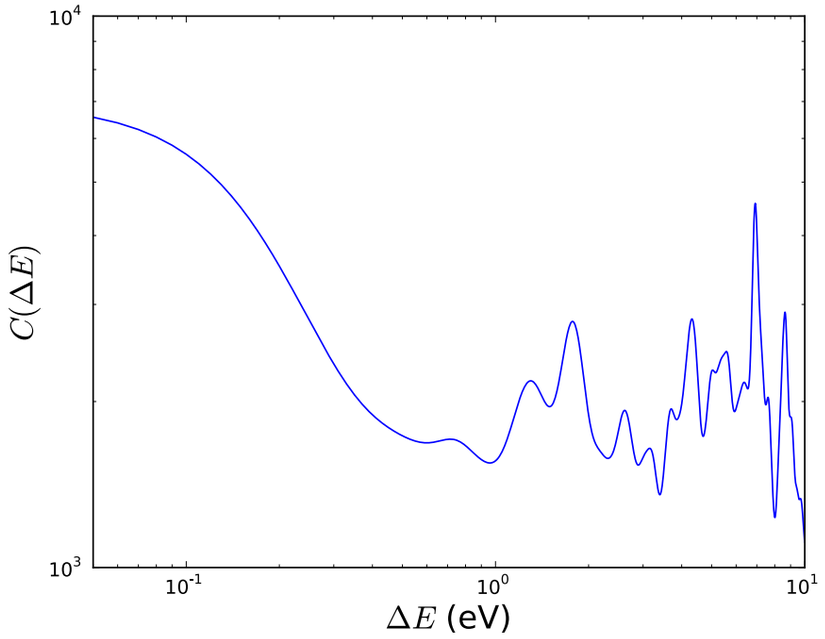
$$\sigma(t_i) = FFT_{ij}[\sigma(E_j)]$$

3. Chi-squared

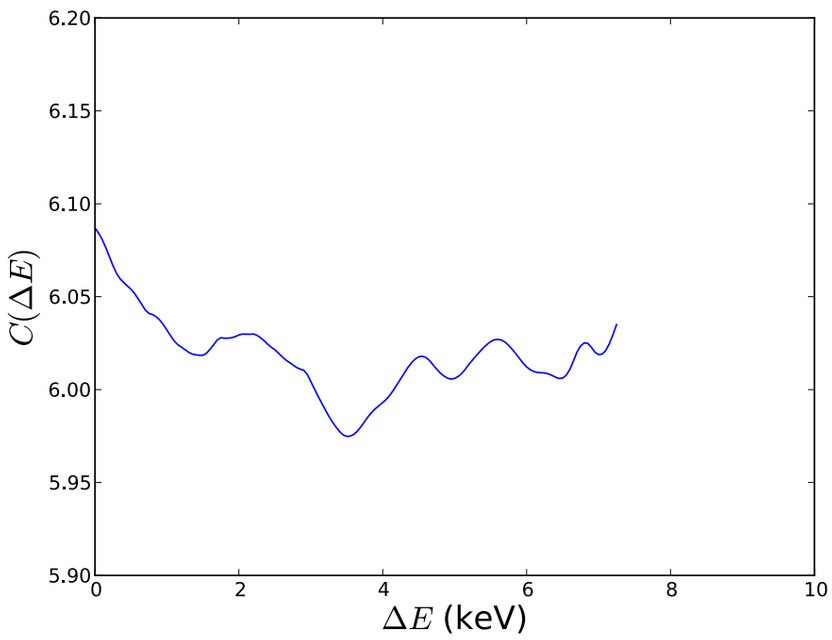
$$\chi^2 = \frac{1}{N}\sum_{i}^{N}\left(\frac{(\sigma(E_i) - <\sigma>)^2}{\sigma_{err}^2}\right)$$

Examples of autocorrelation functions

^{235}U(n,f) 10 eV - 30 eV



Moore et al 10 keV - 25 keV



$$\chi^2 = 26$$

$$\left\langle \left(\frac{\sigma - \bar{\sigma}}{\bar{\sigma}} \right)^2 \right\rangle^{1/2} \approx 0.08$$

Conclusion on 12.5 - 15.0 keV data:

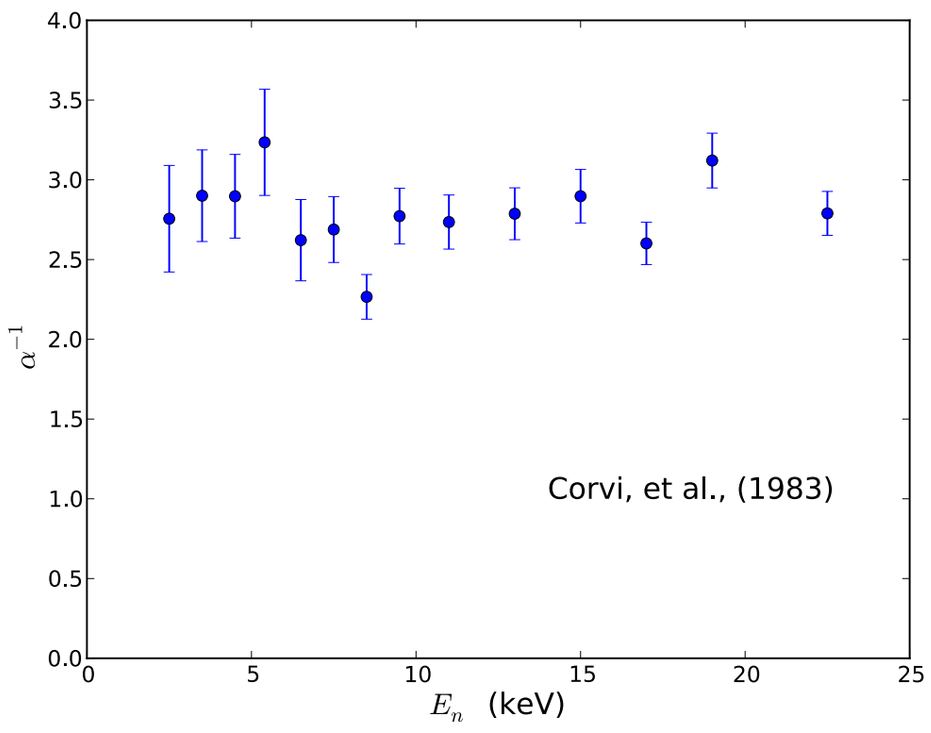
There is good evidence for fluctuations in (n,f) cross section on the scale of 1 keV; amplitude is +/- 15-20%.

There is no evidence for fluctuations on a narrower energy scale.

A sensitive observable for barrier-related fluctuations:

$$\alpha^{-1} = \frac{\sigma_F}{\sigma_\gamma}$$

But the data is not precise enough:



Conclusions

1. Fluctuations are present above the barrier.

2. They cannot be explained by channel openings.

3. A discrete-basis formalism offers promise to describe them.

4. The compound-nucleus ansatz can seriously overestimates the channel conductance.

5. We are still far from a predictive theory anchored to the nucleon-nucleon interaction.

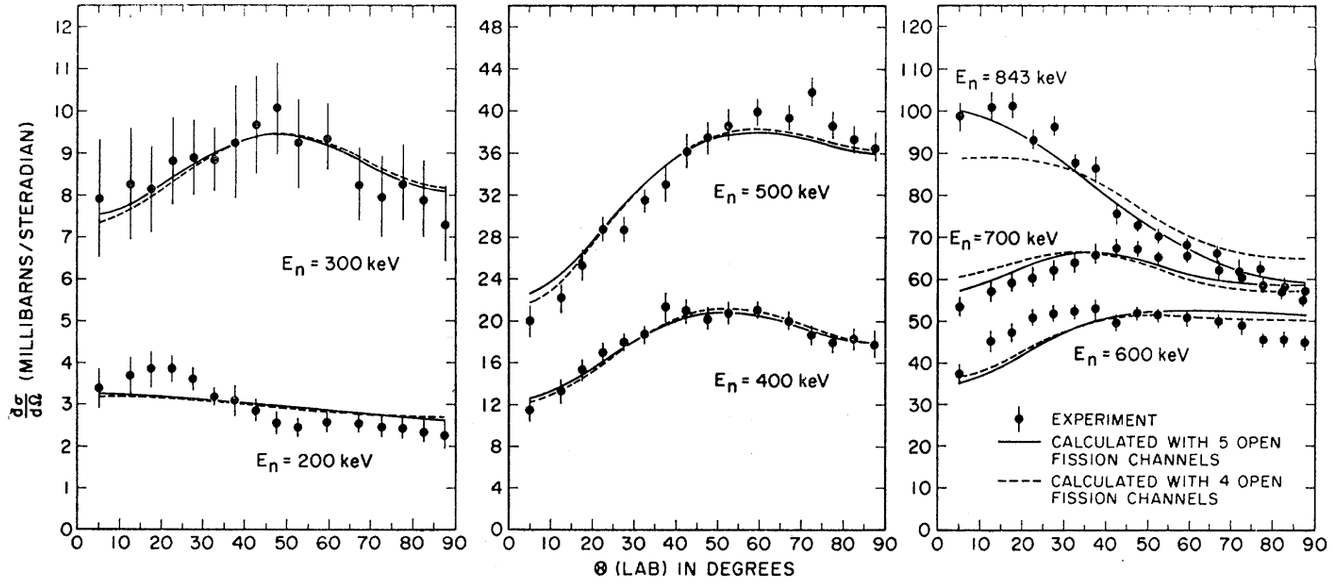
Other fluctuations: angular distributions

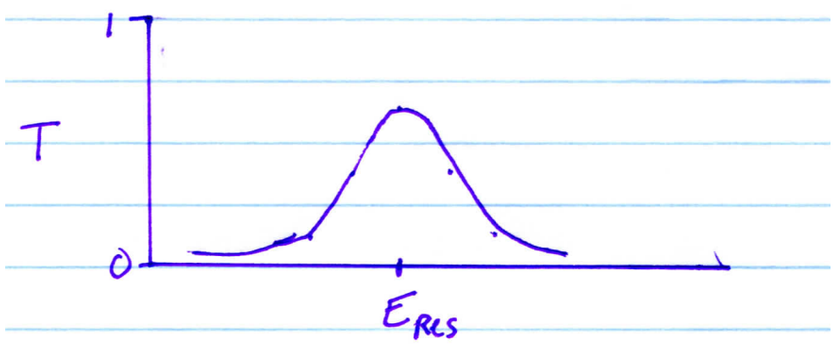
1) (gamma,f) well understood at threshold with opening K-pi identified channels. (Little K-mixing at E = 5.5 MeV)

2). (X,f) well understood at higher energy by thermal distribution of K-pi channels.

3). Not so clear at energies just above the barriers.

A. Behkami, et al., Phys. Rev. 171 1267 (1969).

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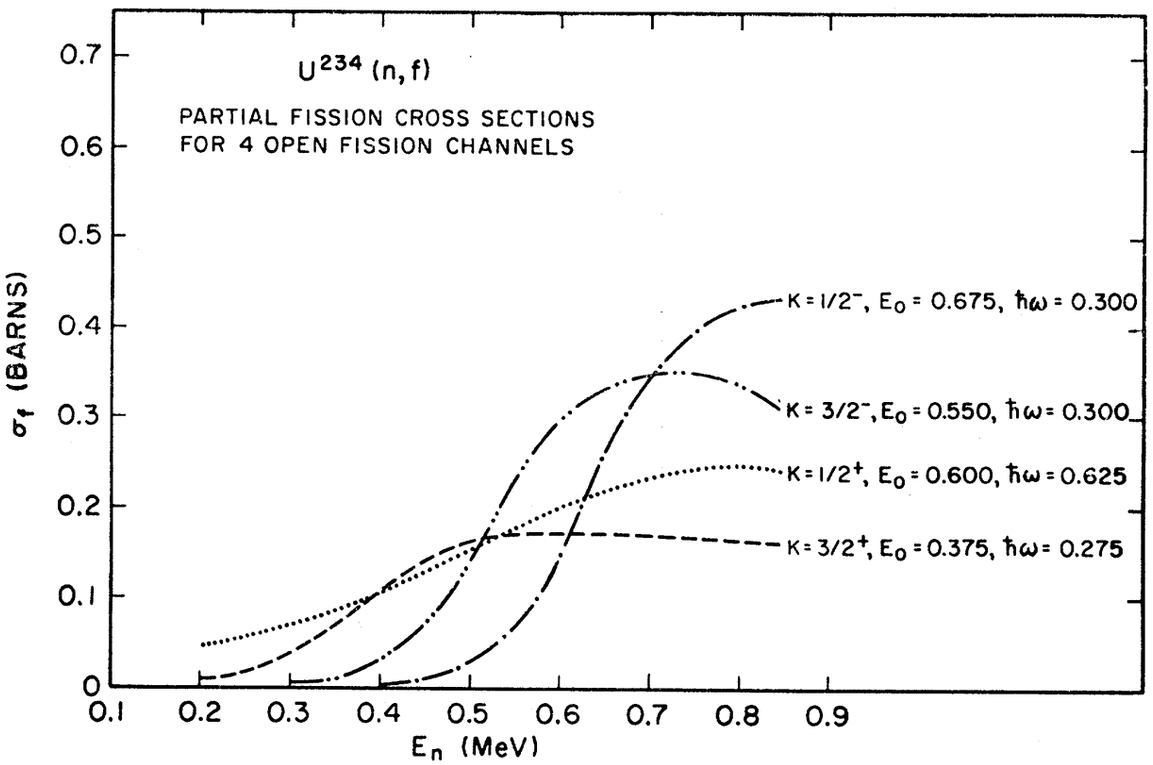


FIG. 8. Summary of the parameters describing the accessible states of the transition nucleus and the partial fission cross section associated with each state as a function of the incident neutron energy. The energies are given in MeV. A possible fourth state in the transition nucleus is also shown.

hypotheses involving weakly excited states which will fit the data. We simply cannot say anything about them.

Beginning with the case of the data from two neutron energies, $E_n=200$ and 300 keV, and two accessible states of the transition nucleus, we found, after extensive searching, that we could reject all hypotheses not assigning values of $\frac{1}{2}+$ and $\frac{3}{2}+$ for the K, π of these two states. A few sample fits to the angular distributions are shown in Fig. 5. We found that the data at 400 and 500 keV could be adequately described by adding a third accessible state in the transition nucleus and assigning values of $(K,\pi)=\frac{3}{2}-$. The fits to the 400- and 500-keV angular distributions and the total fission cross section[12] are shown in Figs. 6 and 7. Detailed calculations revealed that the values of E_0 and $\hbar\omega$ given in Table III should be regarded as uncertain to at least $\pm$50–100 keV. The partial fission cross sections are shown in Fig. 8.

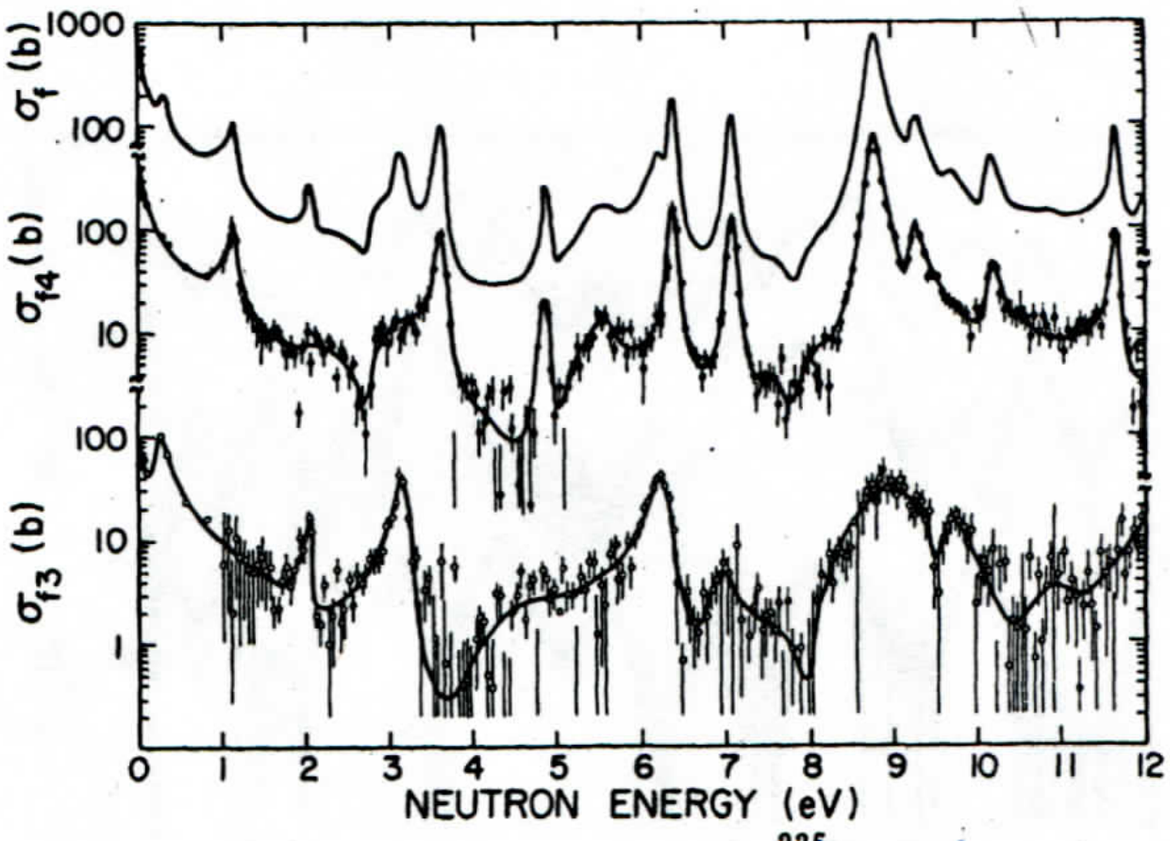
Further attempts to fit the data from $E_n=200$ keV to $E_n=843$ keV by adding a fourth and fifth accessible state in the transition nucleus were unsuccessful. The best attempts at fitting this data are shown in Figs. 9 and 10, although it should be understood that these are not satisfactory fits to the data when judged by a χ^2 criterion. About all that can be said is that there must be at least one more accessible state of the transition nucleus with $K=\frac{1}{2}$ coming into play before $E_n=843$ keV.

Do we understand the fluctuations in (n,f) cross sections?

$^{235}U + n$ --> fission, resolved into J= 3 vs. J=4

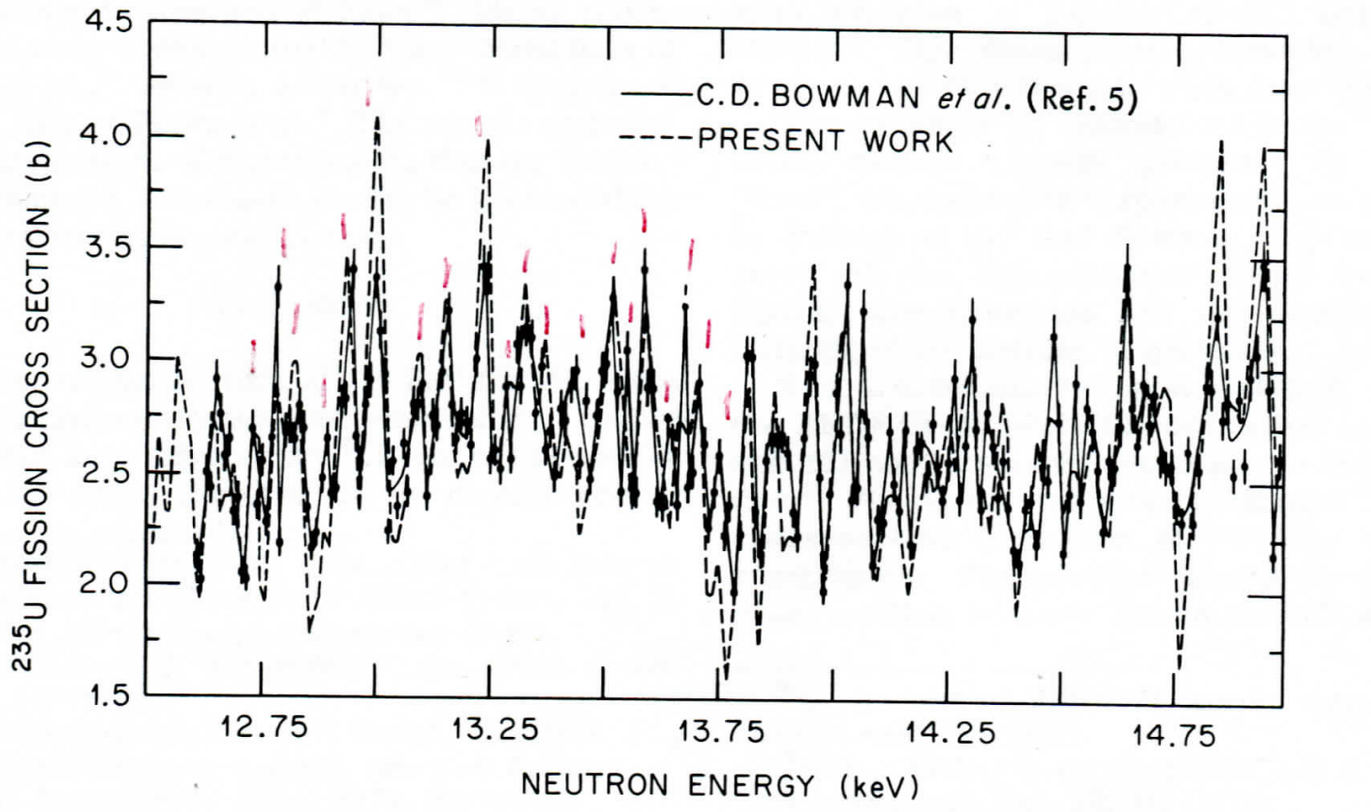
M.S. Moore, et al., Phys. Rev. C 18 1328 (1978).

On the smallest energy scale, compound nucleus statistics with D=0.45 eV



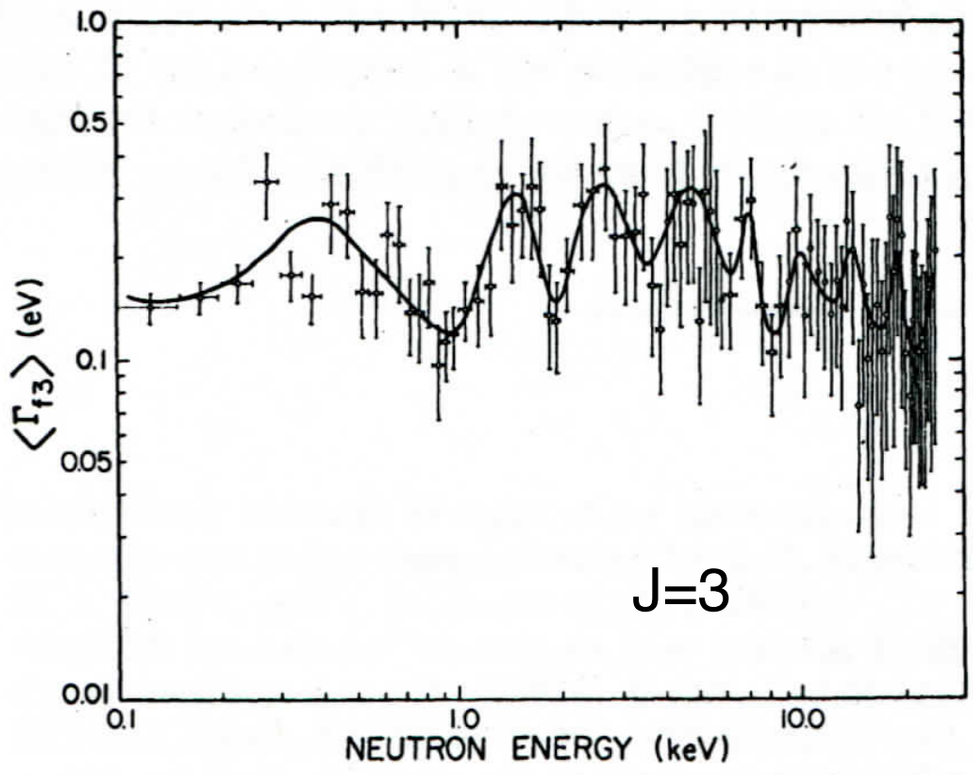
On the 100 eV scale, level density of class II states

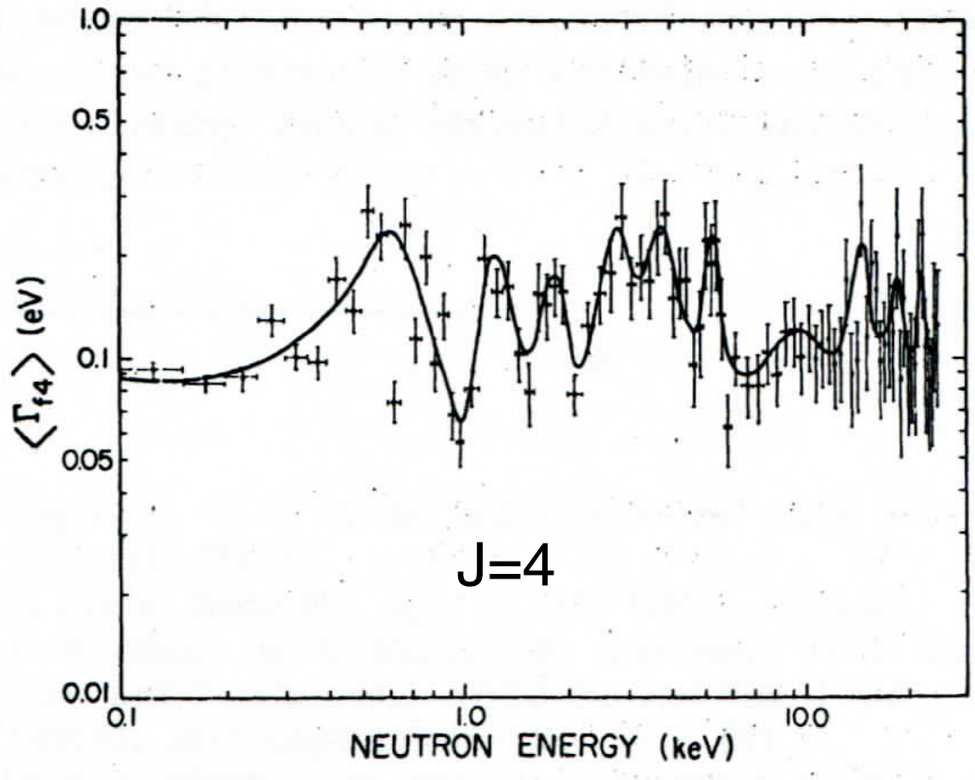
$^{235}U + n$ --> fission



R.B. Perez, et al., Nuclear Science and Engineering **55** 203 (1974)

But what about fluctuations on a 1 keV scale?





Channels or Resonances?

Bohr-Wheeler framework $$W = \frac{1}{2\pi\hbar\rho_I}\sum_c T_c$$

Typical channel $$T_c(E) \approx \frac{1}{1+\exp(2\pi(B_c - E)/\omega_c)}$$

Typical resonance $$T_r = \frac{\Gamma_R\Gamma_L}{E_b^2 + (\Gamma_R+\Gamma_L)^2/4}$$

Questions:

1. How to calculate transmission coefficients at the channel interface?
2. What is the bandwidth of the channels?
3. How to calculate mixing between channels?

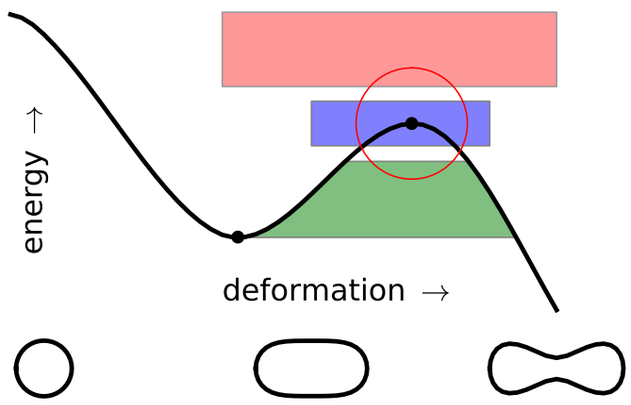
Answers from the literature:

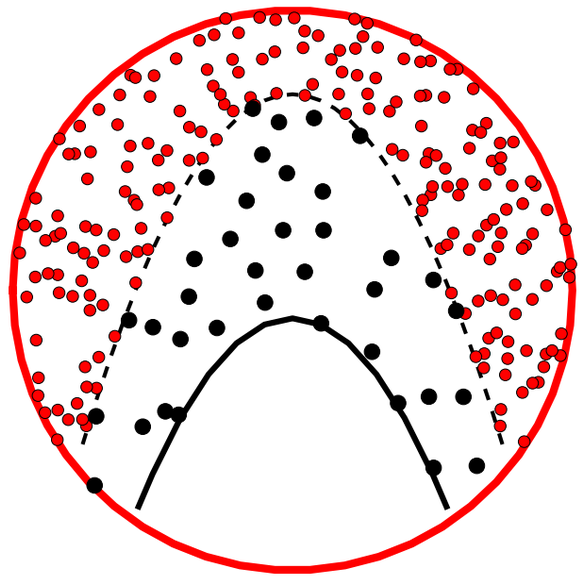
1. None
2. None
3. R. Bernard, H. Goutte, D. Gogny and W. Younes, Phys. Rev. C 84 044308 (2011)

Problems with the channel picture:

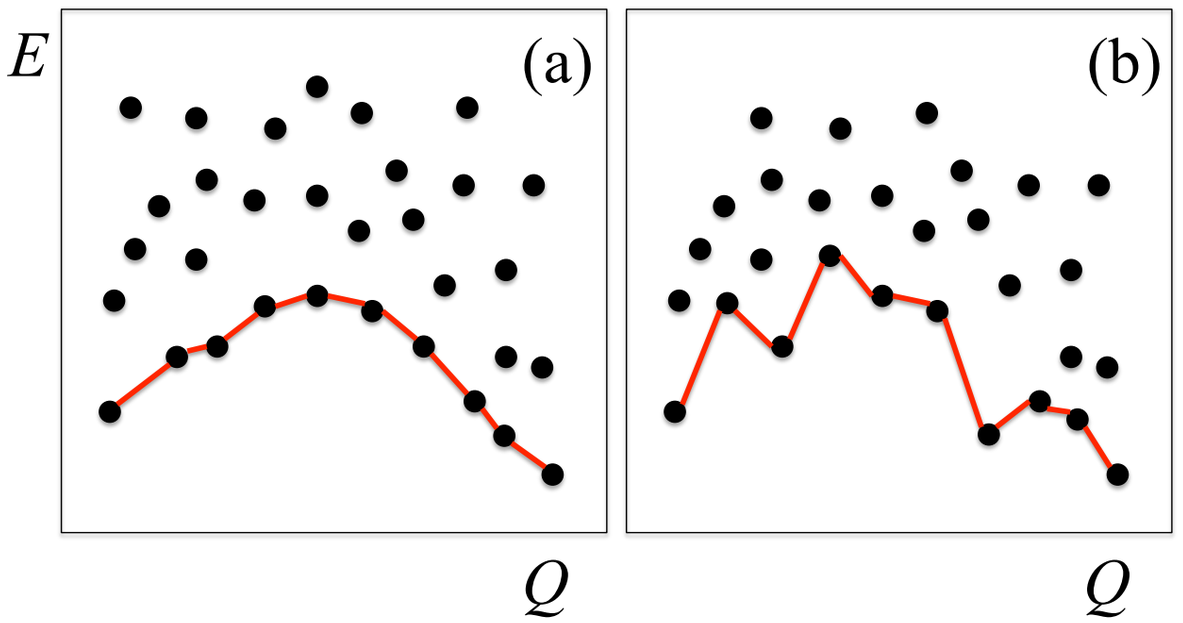
1. Nonorthogonality
2. Separation of collective and intrinsic energy scales (unlike the Born-Oppenheimer separation in chemistry).

My picture

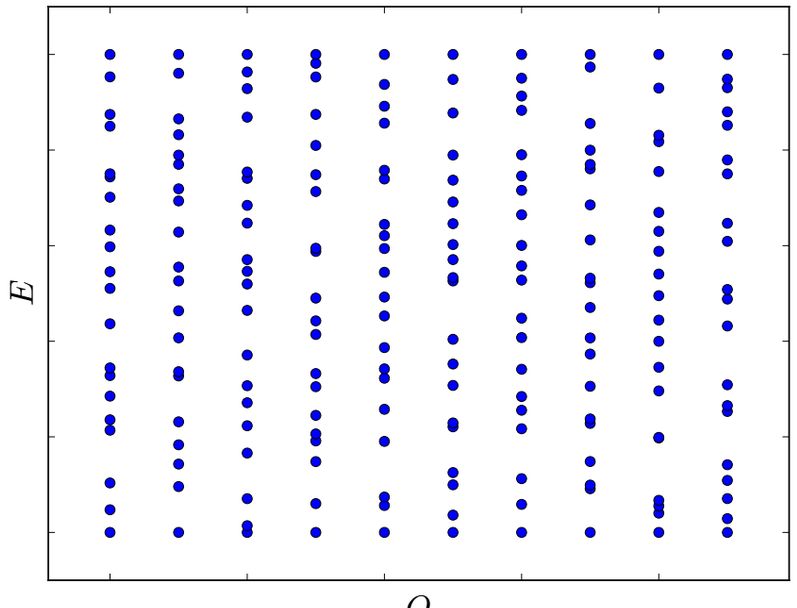


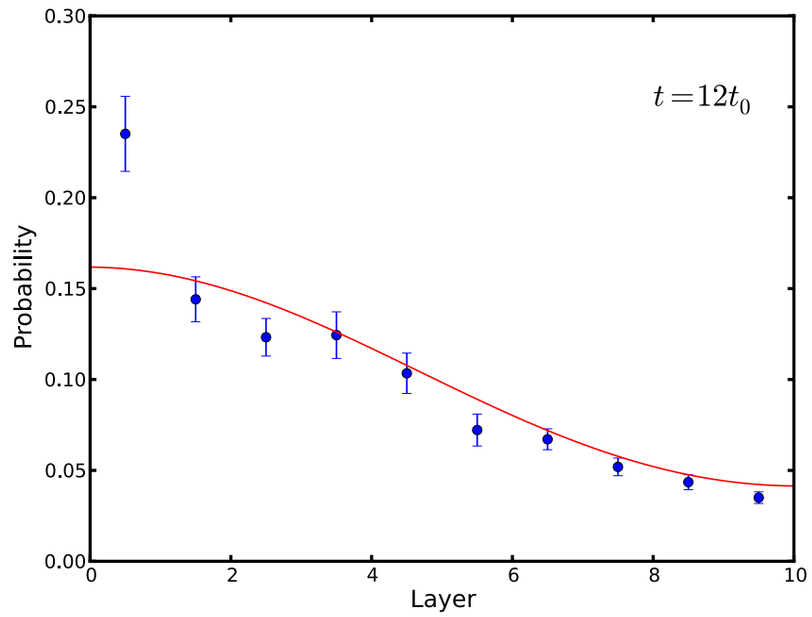


Start with a discrete representation of the many-body wave functions



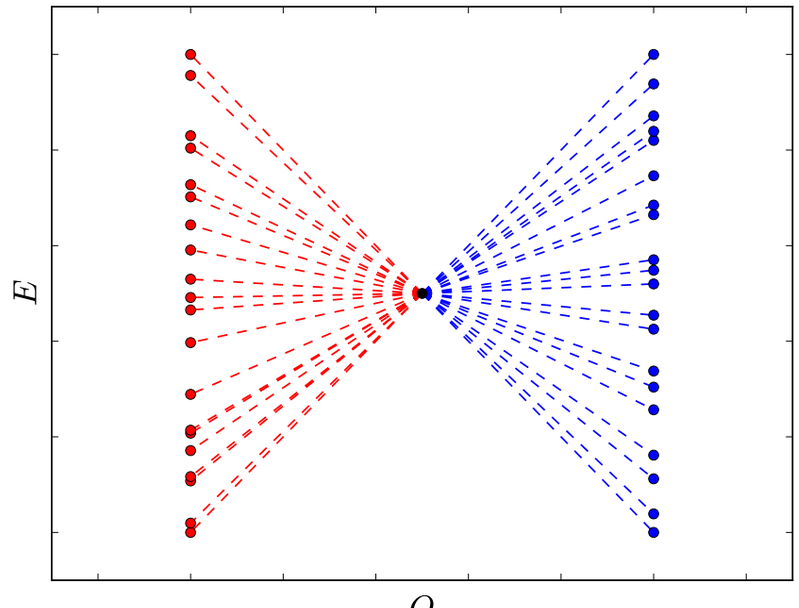
Diffusive limit $$\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial q^2}$$





$$D = 2\pi\rho(E)\overline{(q_\alpha - q_\beta)^2\langle\alpha|v|\beta\rangle^2}$$

Resonance-mediated conductance limit



$$T_r = \frac{\Gamma_R\Gamma_L}{E_b^2 + (\Gamma_R + \Gamma_L)^2/4}$$

See:

Bertsch, arXiv:1407.1899.pdf (2014)

Alhassid, RMP 72 895 (2000)

Advantages of a discrete basis representation

--Close connection to microscopic Hamiltonians

--Well-known CI computational methods are applicable

--Conceptual bridge to condensed matter theory (quantum transport)

--Different dynamical limits are accessible
- --channel limit
- --diffusive limit
- --resonance-mediated conductance limit

Possible implementation: the axial basis

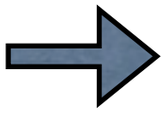
Instead of using a generator coordinate to distinguish states, use the filling of orbitals by the K quantum number.

Example ^{16}O in shell model: $s_{1/2}$, $p_{3/2}$,$p_{1/2}$

K	1/2	3/2	5/2	7/2	9/2	11/2	13/2
p^+	2						
p^-	4	2					
n^+	2						
n^-	4	2					

A toy model for fission

	1/2	3/2	5/2
p^+	6	2	2
p^-	4	2	
n^+	6	2	2
n^-	4	2	



	1/2	3/2	5/2
p^+	4	2	
p^-	2		
n^+	4	2	
n^-	2		

+

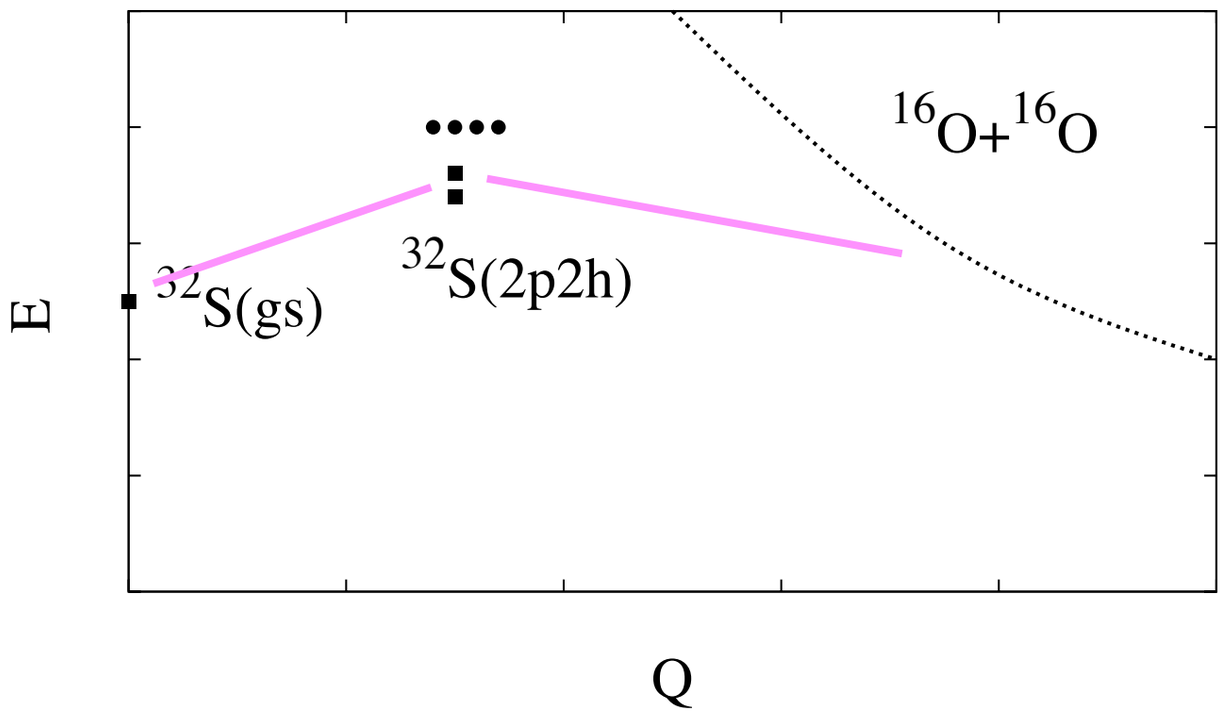
	1/2	3/2	5/2
p^+	2		
p^-	4	2	
n^+	2		
n^-	4	2	

=

	1/2	3/2	5/2
p^+	6	2	
p^-	6	2	
n^+	6	2	
n^-	6	2	

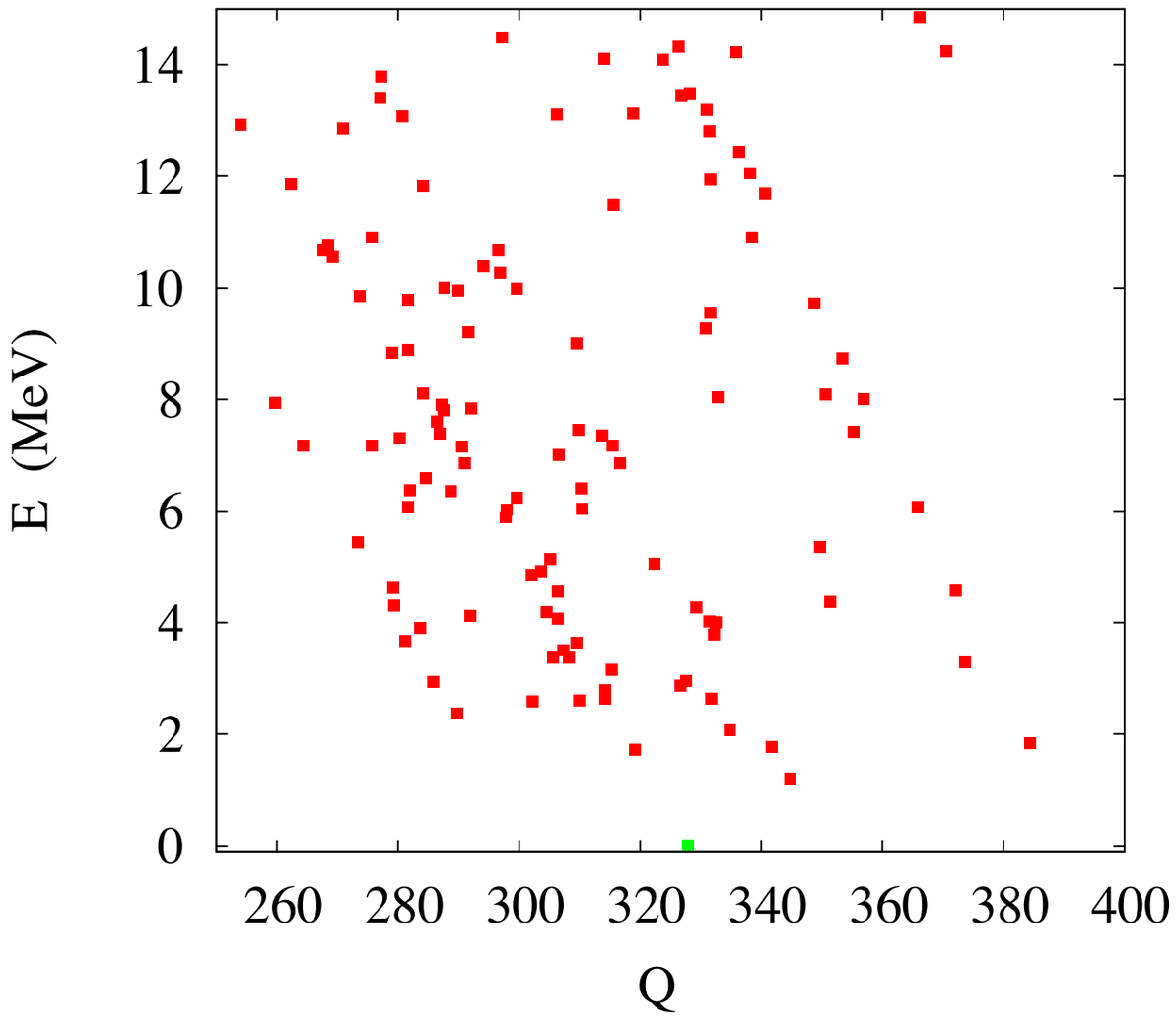
^{32}S ^{16}O ^{16}O

$^{16}O + {}^{16}O$



Construct the basis by HF minimization constraining only the K partition.

Example: partition-defined states in ^{162}Dy

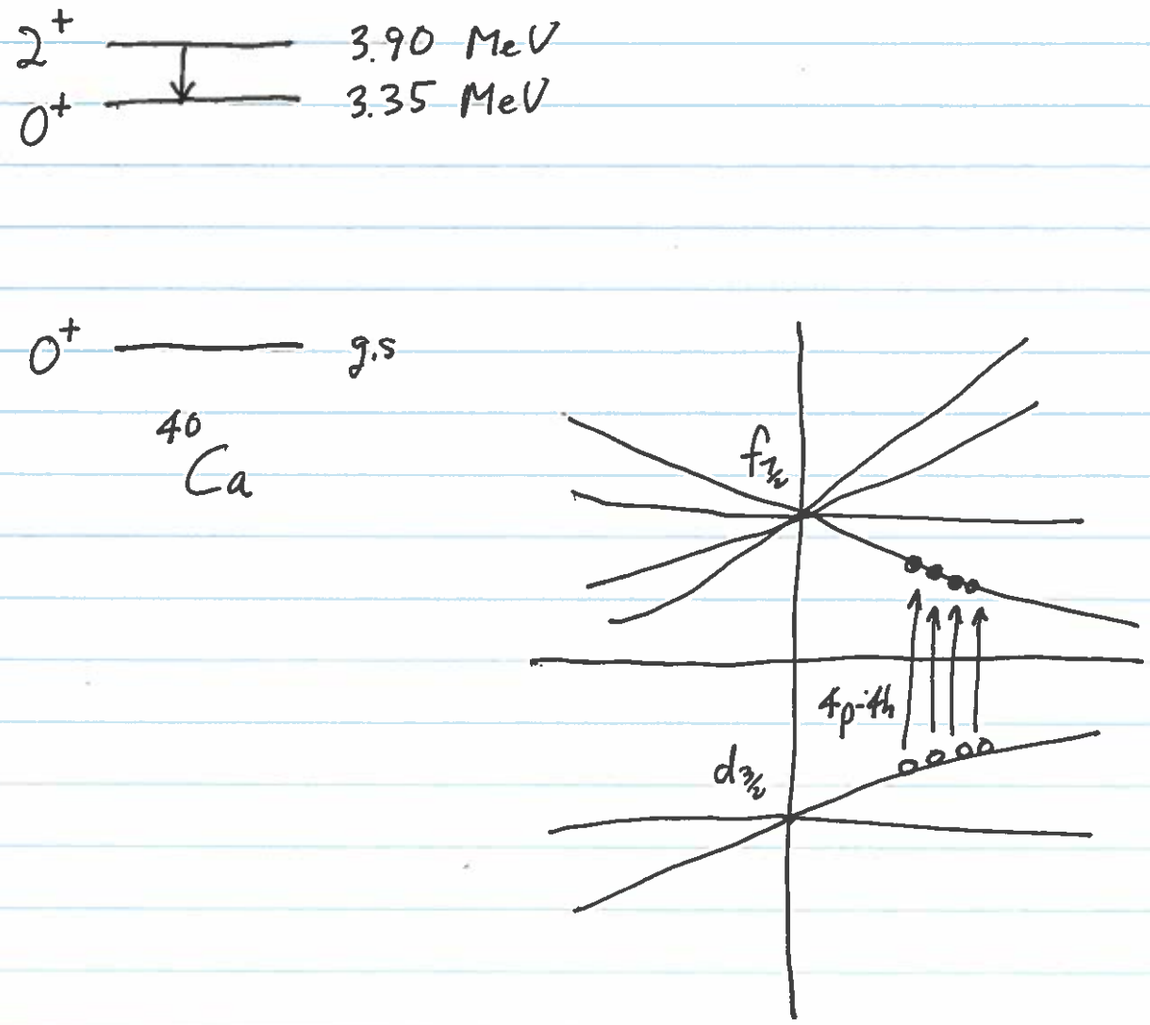


$$H = \sum \varepsilon_i a_i^\dagger a_i + \sum v_{ij,kl} a_i^\dagger a_j^\dagger a_l a_k$$

H from Y. Alhassid, et al. PRL 101 082501 (2008).

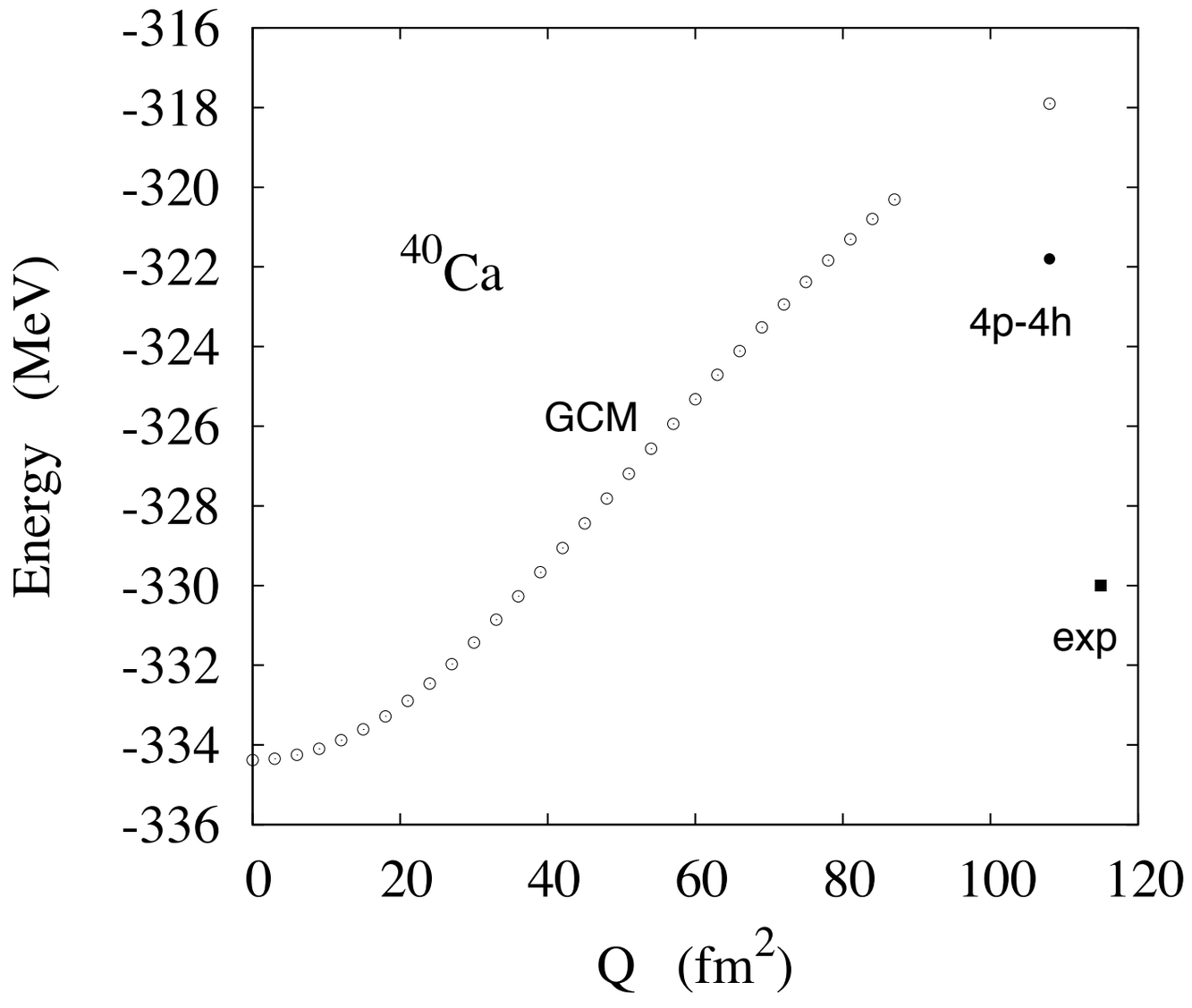
Comparison of GCM with discrete basis construction for the excited band in 40-Ca.

The spectrum

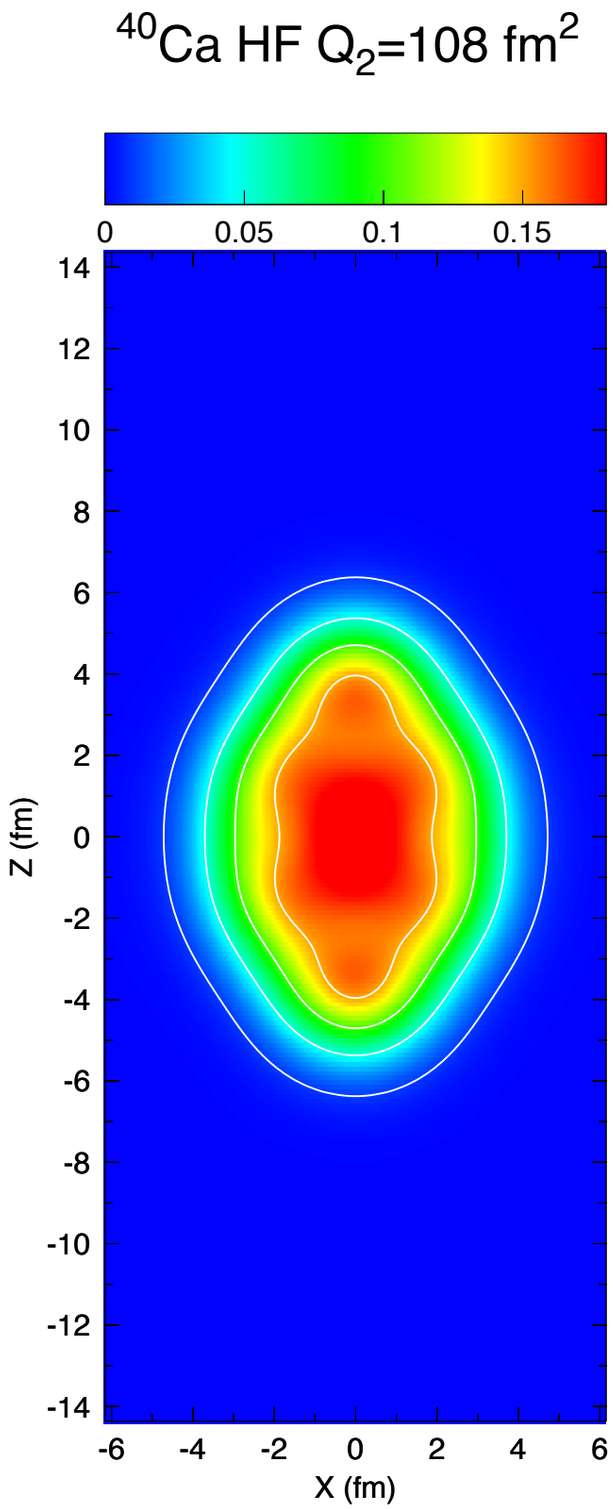


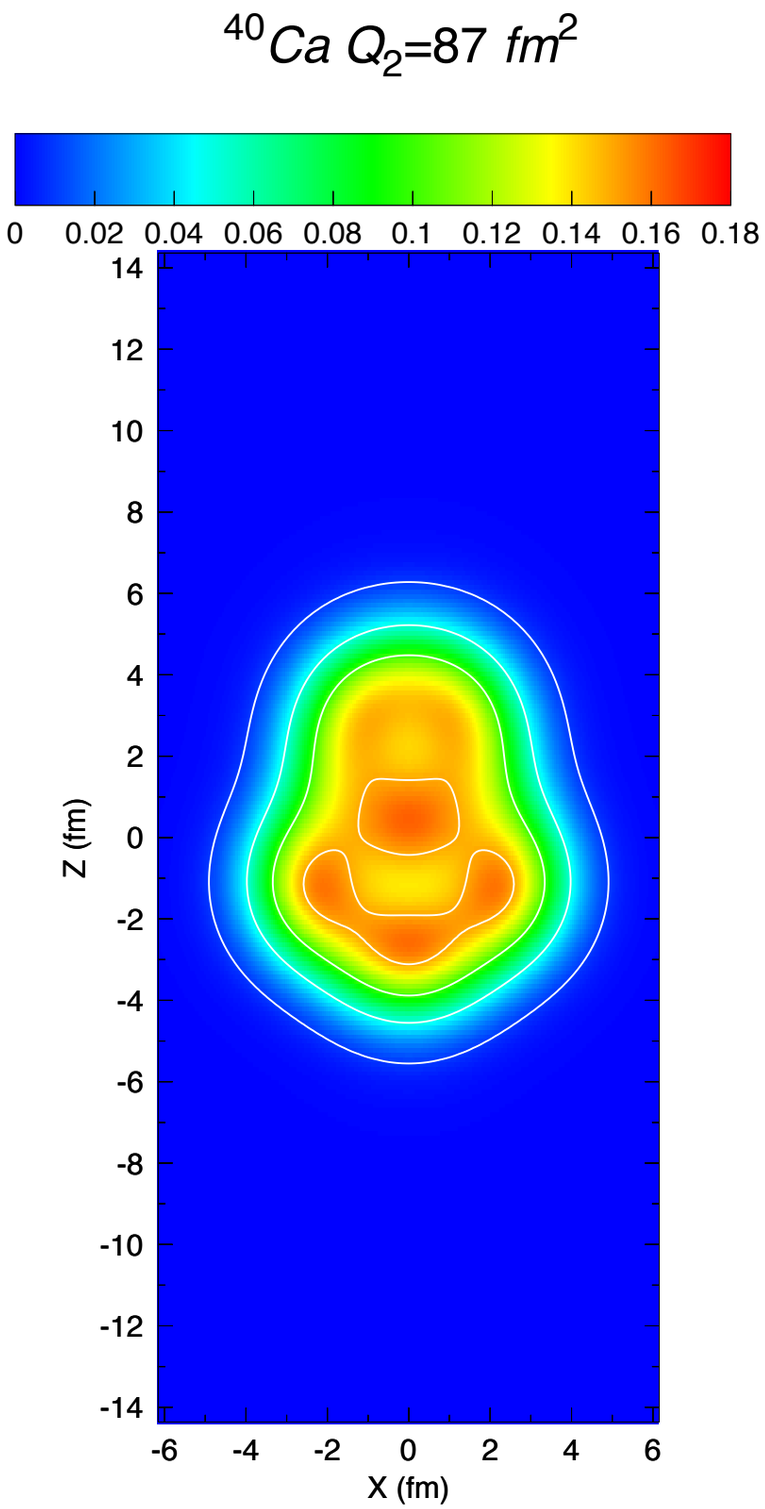
Constructing the K-pi constrained state

Comparison of GCM with discrete basis construction for the excited band in 40-Ca.

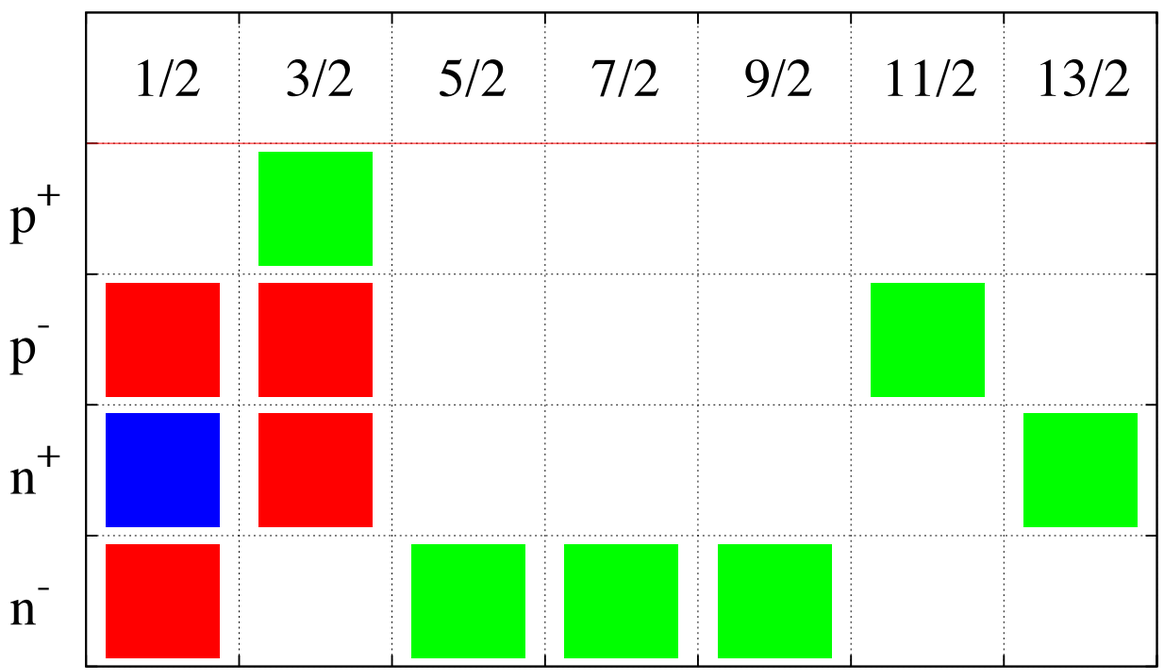


K-pi-constrained method might be more reliable to find the PES.


^{40}Ca HF Q_2=108 fm^2
0
0.05
0.1
0.15
14
12
10
8
6
4
2
0
-2
-4
-6
-8
-10
-12
-14
Z (fm)
-6
-4
-2
0
2
4
6
X (fm)

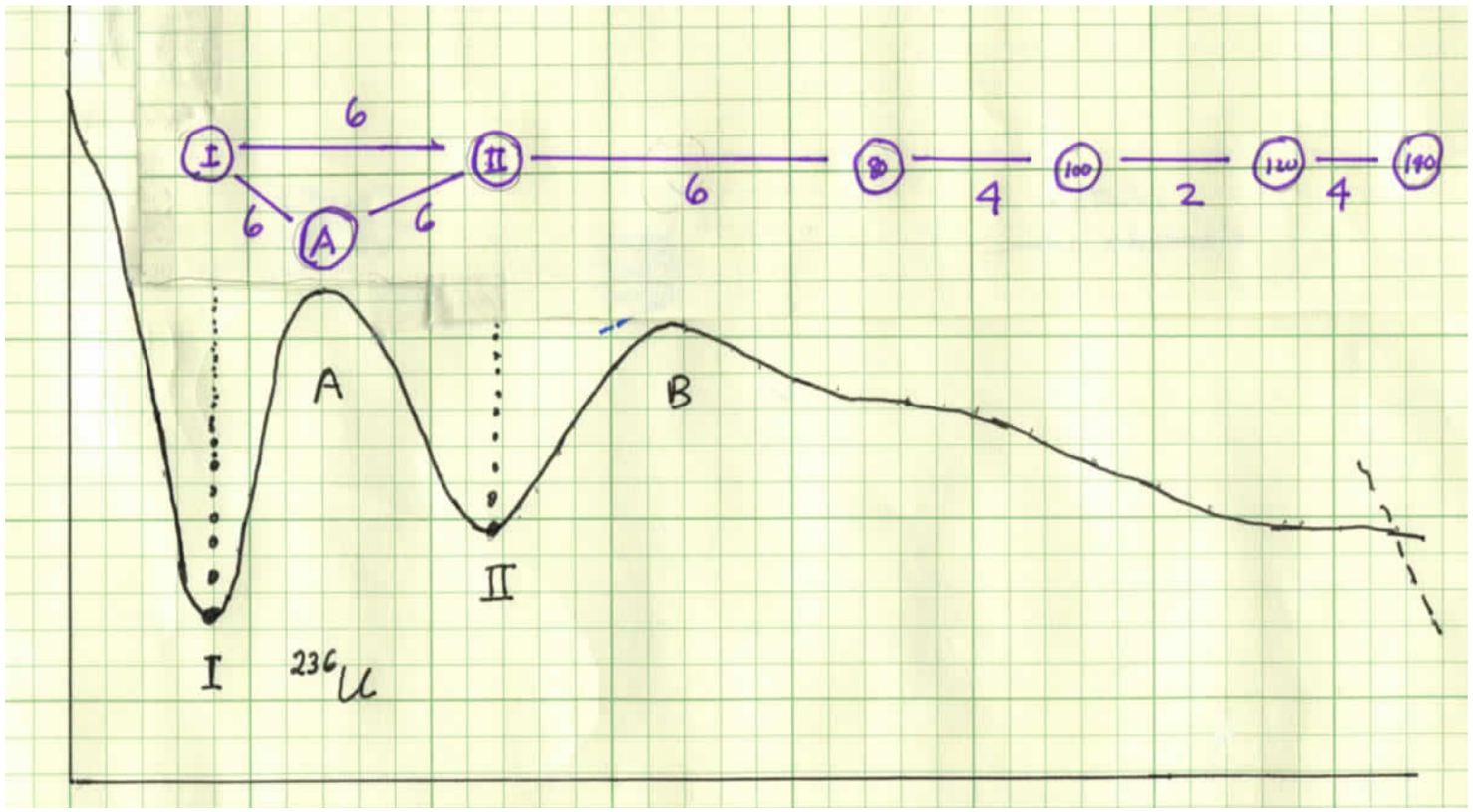

^{40}Ca Q_2=87 fm^2
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
14
12
10
8
6
4
2
0
-2
-4
-6
-8
-10
-12
-14
Z (fm)
-6
-4
-2
0
2
4
6
X (fm)

The landscape for U-236 fission, from class I to class II states



Green: Class I gs occupancy one unit higher
Red: Class II gs occupancy one unit higher
Blue: Class II gs occupancy two units higher

The hopscotch fission path for ^{236}U



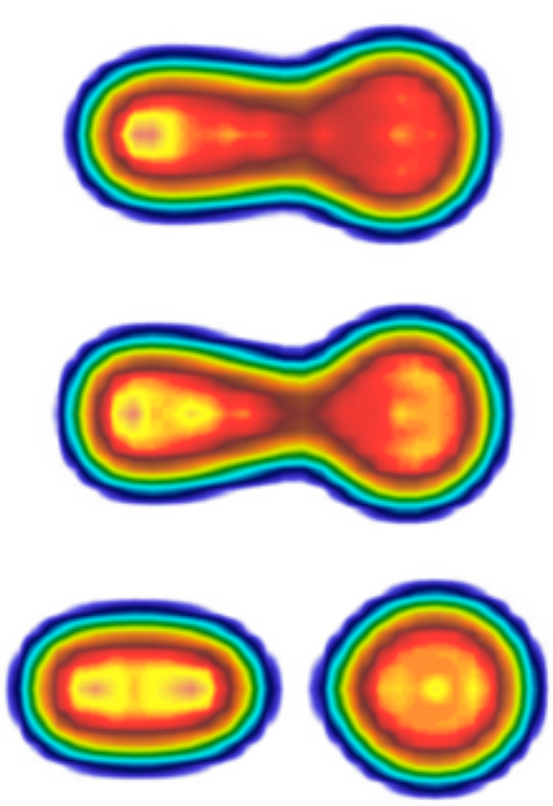
Wave functions calculated by the code HFBaxial. See Rodriguez-Guzman and L.M. Robledo, PRC 89 054310 (2014).

A completely different approach to dynamics: time-dependent mean-field theory

PRL 116, 122504 (2016) PHYSICAL REVIEW LETTERS week ending 25 MARCH 2016

Induced Fission of ^{240}Pu within a Real-Time Microscopic Framework

Aurel Bulgac,[1] Piotr Magierski,[1,2] Kenneth J. Roche,[1,3] and Ionel Stetcu[4]

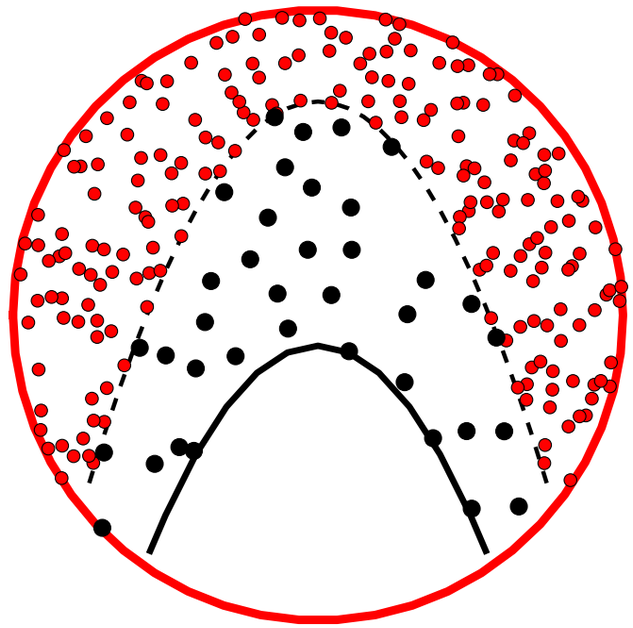


Near-term goals

1. Code for partition-constrained DFT (Skyrme or Gogny)

2. Calculate $\rho(q, E)$

3. Estimate diffusion coefficient $D(q, E)$

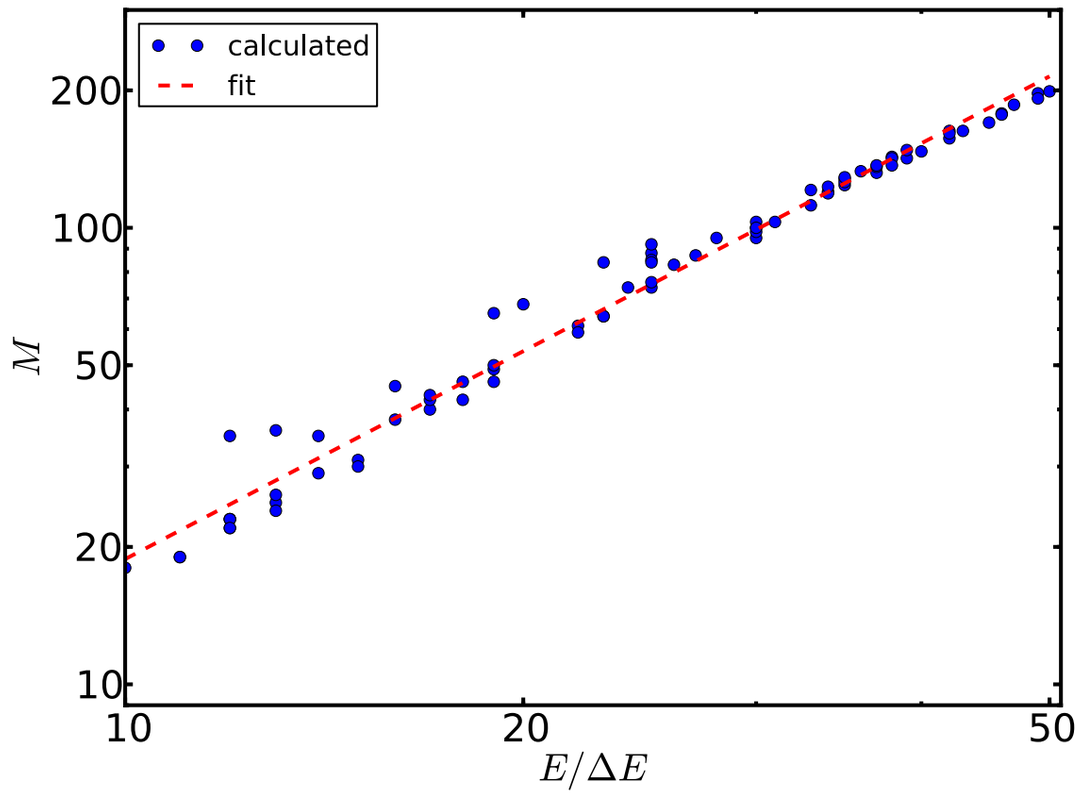


The interaction between configurations

$$\langle \alpha | v | \beta \rangle = \langle pp | v | pp \rangle \det | \langle \phi_i^\alpha | \phi_j^\beta \rangle |$$

See A. Arima and S. Yoshida, Nucl. Phys 12 139 (1959).

A qualitative result: $\overline{\langle \alpha | v | \beta \rangle^2} \sim E^{3/2} / \rho(E)$ B.W. Bush et al., Phys. Rev C 45 1709 (1992).



Shows that the interaction becomes stronger with excitation and thus the dynamics approach the diffusive limit.

A well-studied model has four stages beyond the entrance channel:

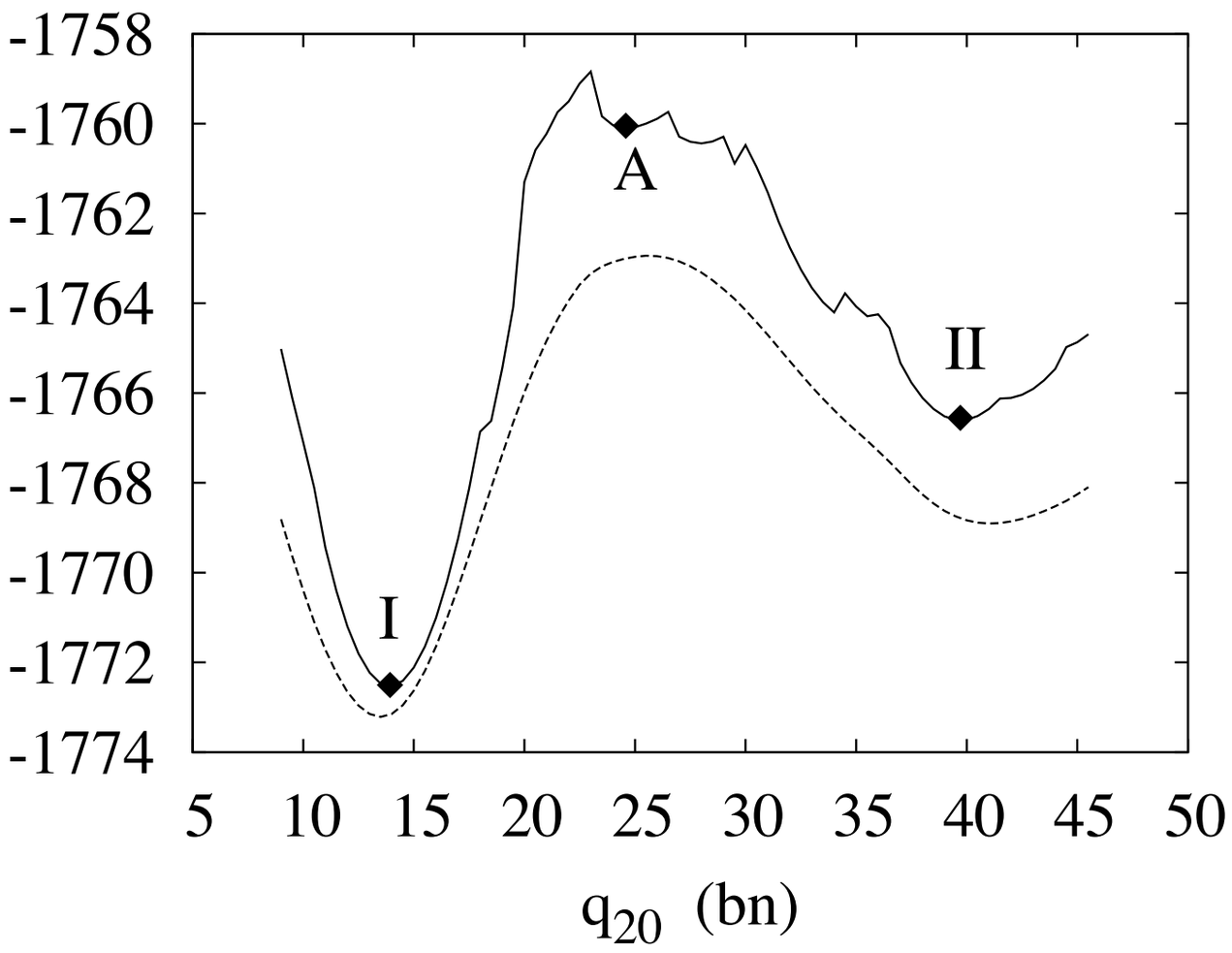
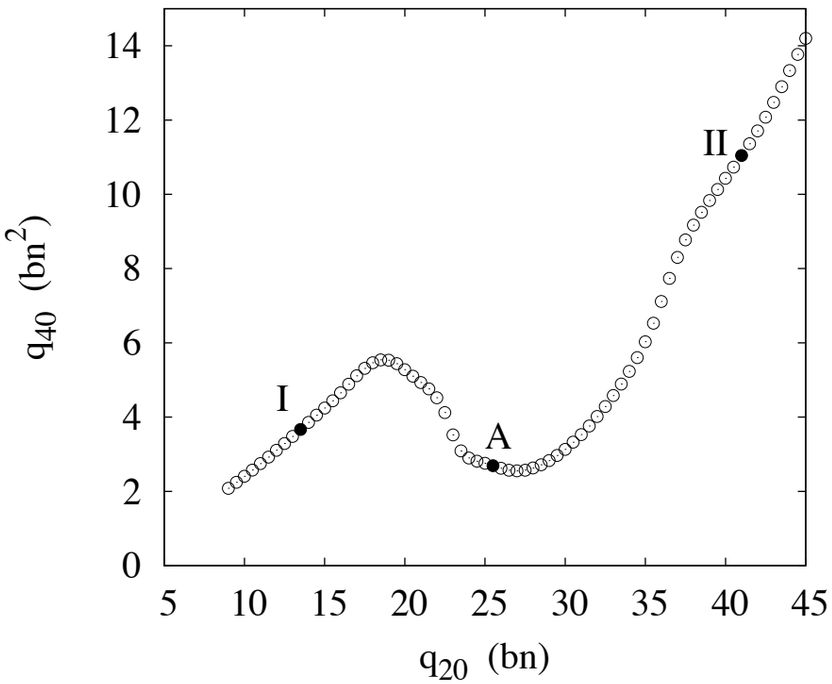
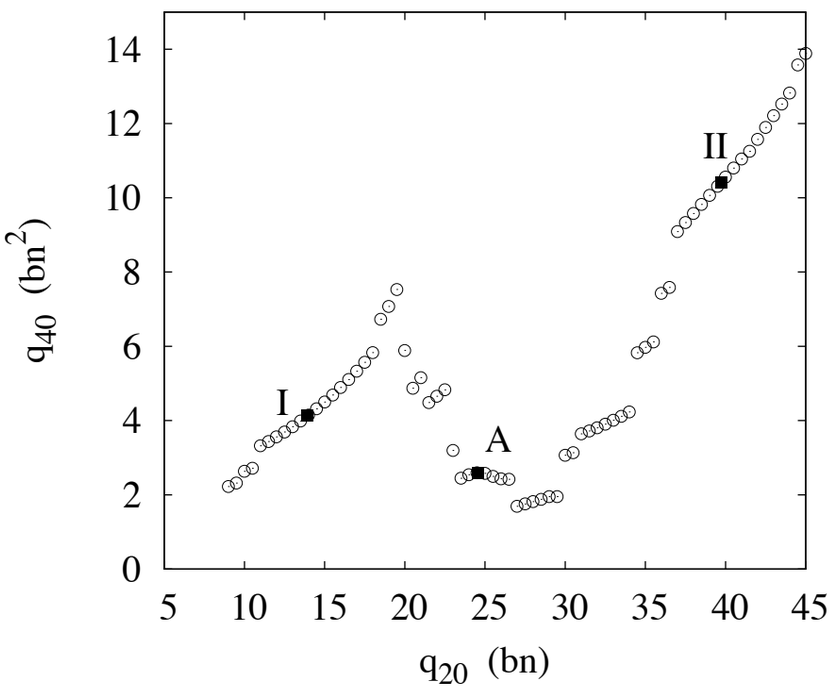
I usual compound nucleus
A first barrier
II second well
B second barrier.

Parameters:
-Woods-Saxon potential for entrance channel
-E_min, E_max, D= <Delta E>, Gamma for each stage
- <ilv^2Ij> for each stage-stage coupling.

Some of the parameters we know well, eg. the Woods-Saxon parameters, D and Gamma_gamma for the compound nucleus.

Can the other parameters be plausibly tuned to fit the 1 keV-scale (n,f) fluctutations? If so, is there some combination that is well-constrained by data?

Can one define a discrete basis around the barrier top?



DFT (Gogny) for ^{236}U between the first and second minimum. Solid line: HF; dashed line: HFB.