Toward a microscopic calculation of induced fission cross sections

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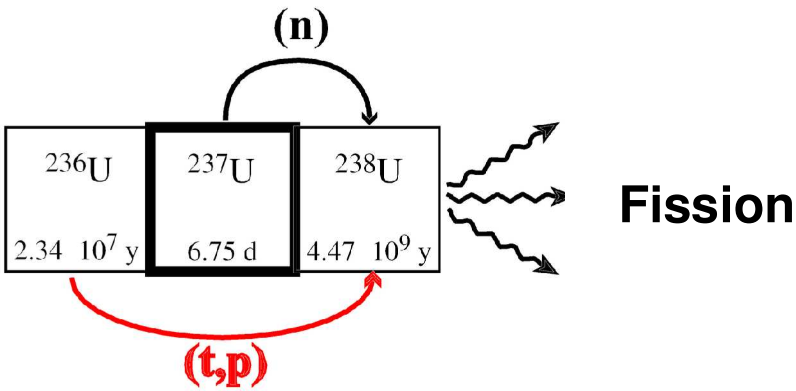
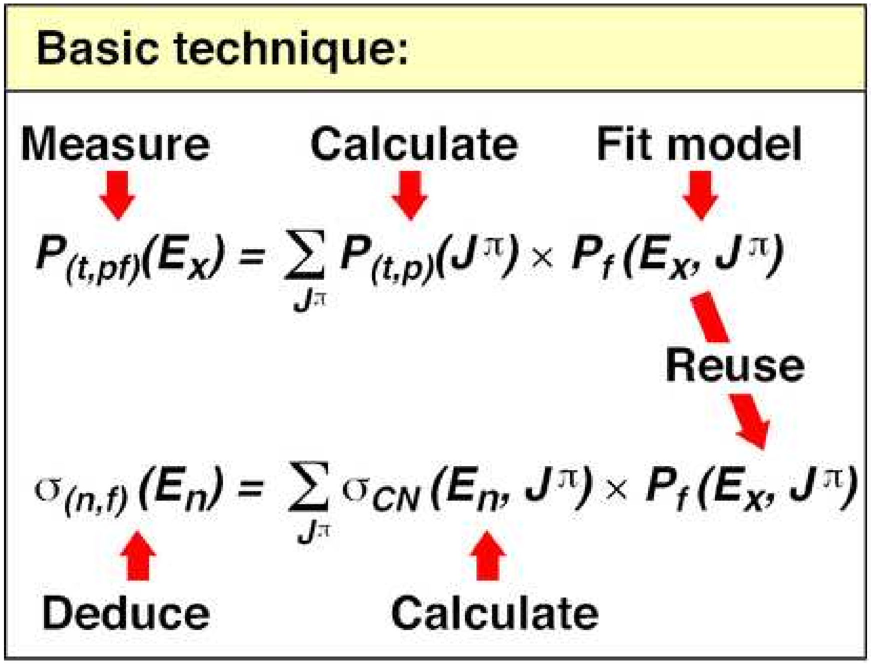
Introduction

- Surrogate technique for (n,f) reactions that can't be measured
  - use surrogate reactions, e.g., (t,p), to populate same compound nucleus
  - Use model to compensate between (t,p) and (n) reactions



  - Younes *et al*., 67 024610 (2003), ...
  - Phenomenological treatment of fission
  - Extend to E_n = 20 MeV
- Microscopic treatment of fission
  - Self-consistent barrier properties
    e.g., Bonneau *et al*., EPJA 21, 391 (2004)

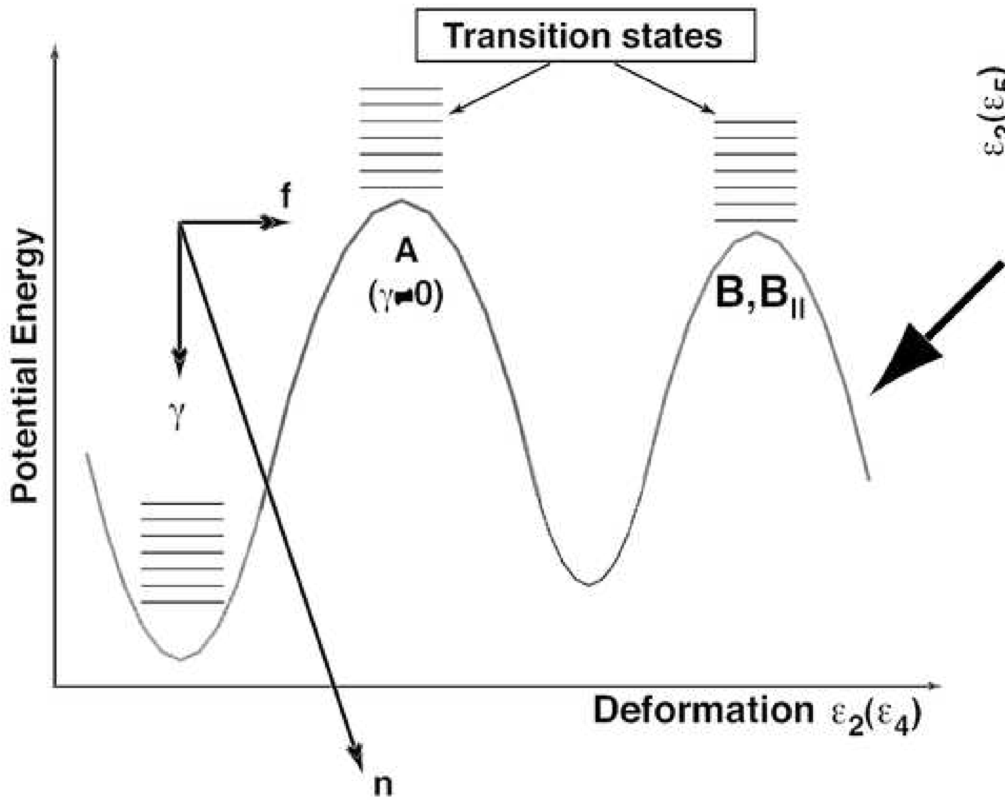
Surrogate-reaction technique: formalism I

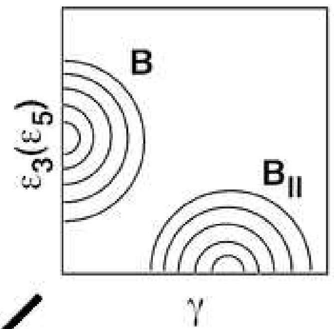


Basic ingredients:

- (t,p) reaction population
- (n) reaction cross section
- Fission model
  - → $P_f(E_x, J^\pi)$

Double-humped fission model





Discrete levels:
- based on experiment

Continuous level density:
- micro/macro model
+ grand-partition func

Width fluctuations

Non-resonant barrier coupling

No class-II states

Procedure:
– adjust barrier A & B heights to fit measured $P_{(t,pf)}$

Surrogate-reaction technique: formalism II

Basic technique:

Measure → $P_{(t,pf)}(E_x)$; Calculate → $P_{(t,p)}(J^\pi)$; Fit model → $P_f(E_x, J^\pi)$

$$P_{(t,pf)}(E_x) = \sum_{J^\pi} P_{(t,p)}(J^\pi) \times P_f(E_x, J^\pi)$$

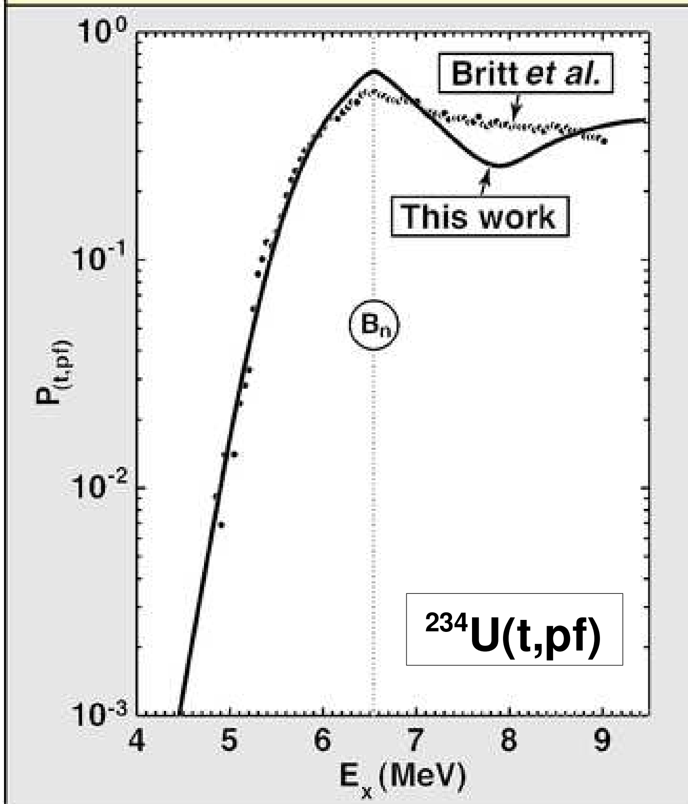
Reuse $P_f(E_x, J^\pi)$

$$\sigma_{(n,f)}(E_n) = \sum_{J^\pi} \sigma_{CN}(E_n, J^\pi) \times P_f(E_x, J^\pi)$$

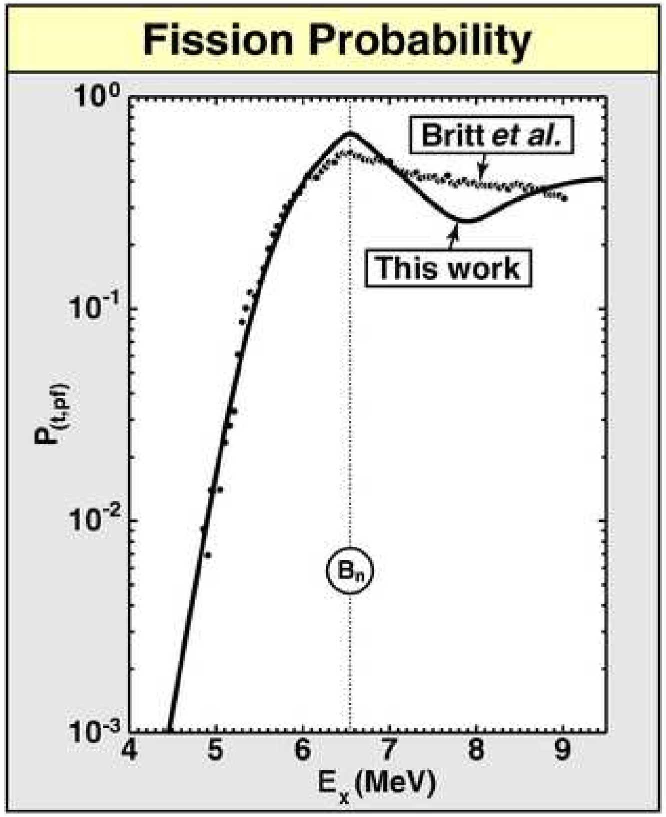
Deduce → $\sigma_{(n,f)}(E_n)$; Calculate → $\sigma_{CN}(E_n, J^\pi)$

- Fit is not perfect
  - Model is over-constrained
  - Relative $P_f(E_x,J^\pi)$ are robust
- Renormalize to $P_{(t,pf)}$ data

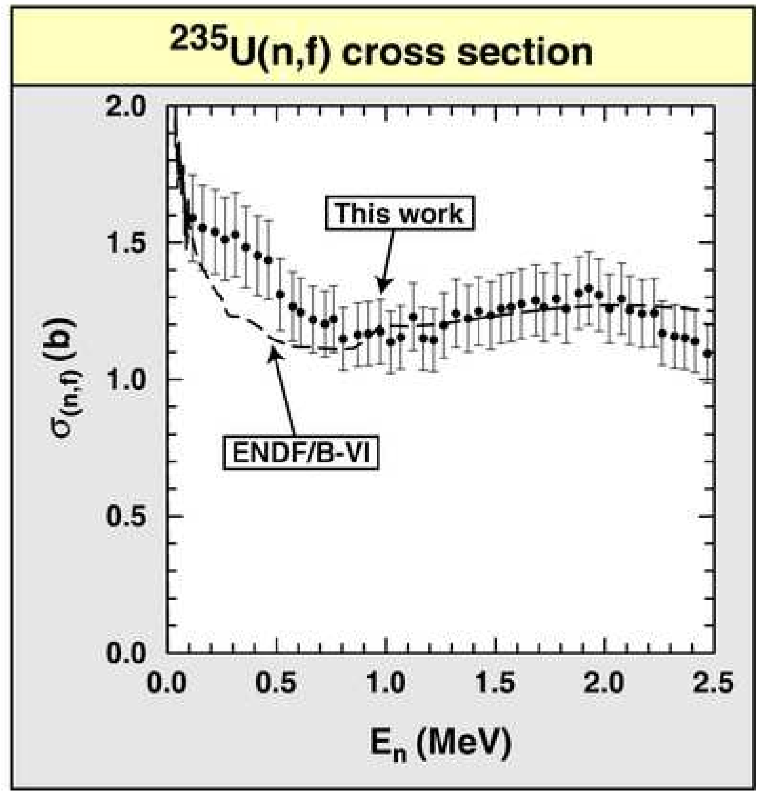
Best Fit to Fission Probabilities



Surrogate reaction technique: proof-of-principle



$$\sigma_{(n,f)}(E_n) \times \frac{P^{(expt)}_{(t,pf)}(E_x)}{P^{(calc)}_{(t,pf)}(E_x)}$$



Very good agreement, but limited to range of surrogate data

Surrogate technique: extension to E_n = 20 MeV

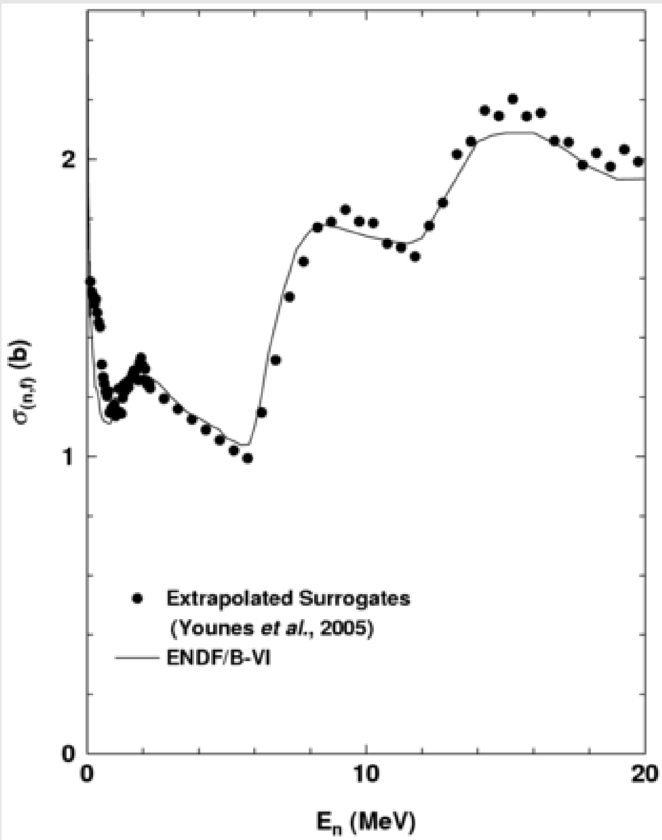
- 1^{st}-chance fission: $^{235}U(n,0nf)$
  - E_n ~ few MeV $\rightarrow$ use surrogate result
  - Higher E_n $\rightarrow$ smooth (linear) extrapolation

- 2^{nd}+higher-chance fission: $^{235}U(n,xnf)$ $x \geq 1$
  - Assume for 2^{nd} chance:
    P[fission, given $^{235}U^* = {}^{235}U(n,n')$] = P[fission, given $^{235}U^* = n + {}^{234}U$]
  - Then:
    Calculated $\sigma_{(n,n'f)}(^{235}U,E_n)$ is sum of two contributions
    - $\sigma_{(n,n'f)}(^{235}U,E_n)$ folded with EQ neutron distribution (Maxwell)
    - $\sigma_{(n,n'f)}(^{235}U,E_n)$ folded with PEQ neutron distribution (HMS calculation)

Only one free parameter for 2^{nd}-chance fission:
$\rightarrow$ Maxwell-distribution temperature

Extended surrogate technique: proof-of-principle

^{235}U(n,f) cross section



- **Excellent agreement with measured $\sigma_{(n,f)}$**
- **Slope of 1st-chance fission depends on**
  - **Fission barriers**
  - **Level densities**

$$\frac{\Gamma_n}{\Gamma_f} \propto \frac{\exp\left(2\sqrt{a_n\left(E-B_n\right)}\right)}{\exp\left(2\sqrt{a_f\left(E-B_f\right)}\right)}$$

(very roughly)

Need consistent calculations of barriers, level densities

Details of the HF+BCS calculations

- **Code:**
  - **HFODD v2.09i (Dobaczewski *et al*., CPC 1997-2005)**
  - **Modified to print out single-particle wave functions in cylindrical basis**
- **Force:**
  - **SKM* (standard)**
  - **Pure pairing BCS, G_p and G_n adjusted to match experimental gaps**
- **Basis:**
  - **Up to 31 oscillator quanta in cartesian directions**
  - **Up to 1140 basis states**

Check of the single-particle wave functions

- **Calculated ground-state <Q_{20}>:**

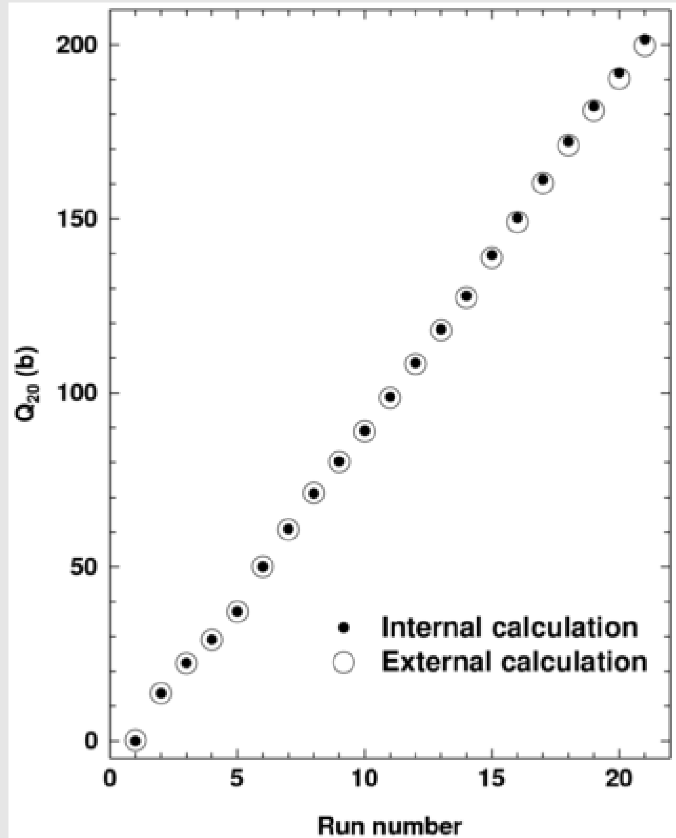
$$\left\langle \mathrm{G.S.} \left| \hat{Q}_{20} \right| \mathrm{G.S.} \right\rangle = 2 \sum_{i>0} \left\langle i \left| \hat{Q}_{20} \right| i \right\rangle v_i^2$$

$$|i\rangle = \sum_{j>0} C_{j,i} \left| N^{(j)}, n_z^{(j)}, \Lambda^{(j)}, \Sigma^{(j)} \right\rangle$$

- **Within HFODD (internal)**
- **From s.p. Wave functions (external)**

Very good agreement

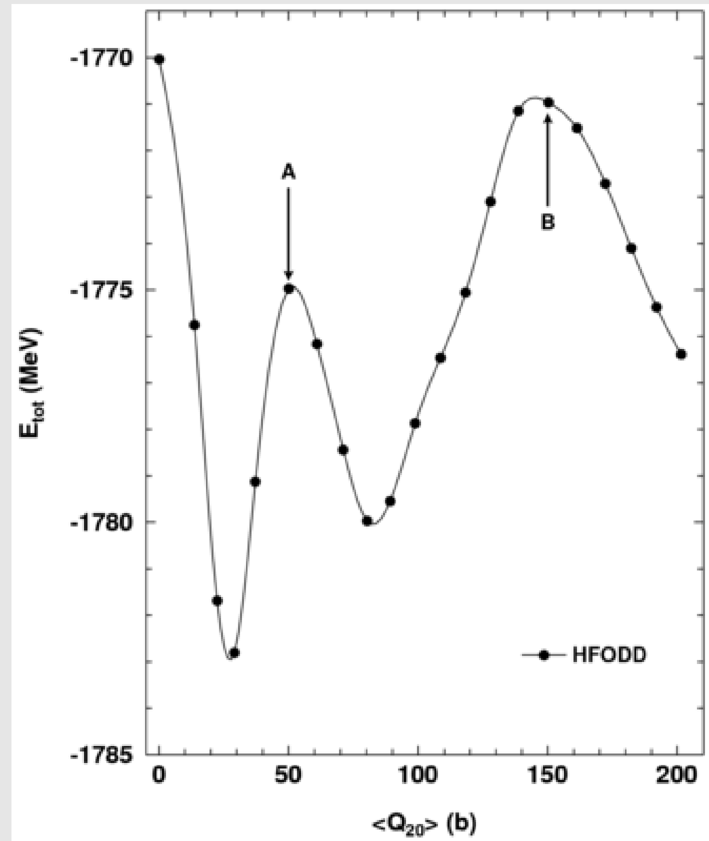
Calculation of Q_{20} for ^{236}U



^{236}U potential surface along the symmetric path

- **Barriers along symmetric path**
  - ➔ **$E_A \approx$ 7.8 MeV**
    (accepted ≈ 5.75 MeV)
  - ➔ **$E_B \approx$ 11.8 MeV**
    (accepted ≈ 5.75 MeV)

^{236}U energy, Q_{22} = 0, Q_{30} = 0



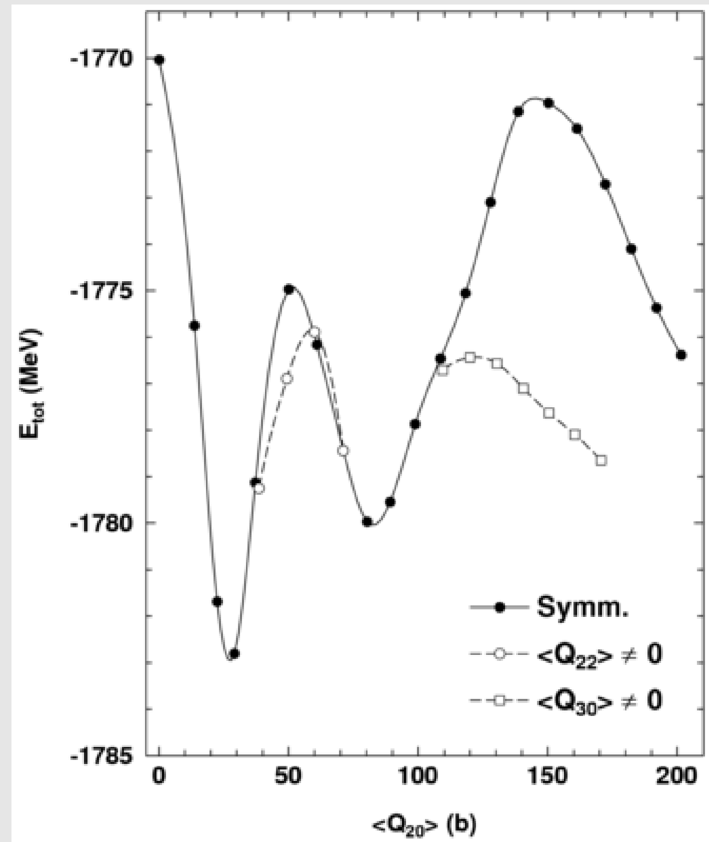
Next: Explore Q_{22}, Q_{30}

Barriers with Q_{22}, Q_{30} degrees of freedom

- Barriers
  - ➔ $E_A \approx 6.92$ MeV
    (accepted ≈ 5.75 MeV)
  - ➔ $E_B \approx 6.37$ MeV
    (accepted ≈ 5.75 MeV)

Next: zero-point corrections

^{236}U total energy



ATDHF + Belyaev cranking

- Libert *et al.*, PRC 60, 054301 (1999)

- Parameterize
  - Nuclear shape

$$q_0 \equiv \left\langle 2z^2 - x^2 - y^2 \right\rangle$$
$$q_2 \equiv \left\langle x^2 - y^2 \right\rangle$$

Not used presently

  - Nuclear orientation

$$q_1 \equiv \langle -2iyz \rangle$$
$$q_{-1} \equiv \langle -2xz \rangle$$
$$q_{-2} \equiv \langle 2ixy \rangle$$

- Study response to slowly-varying field

Zero-Point-Energies from ATDHF + cranking

- **Define:**

$$\Delta V_{ij} \equiv \frac{M_{ij}^{(-2)}}{M_{ij}^{(-3)}}$$

$$M_{ij}^{(-k)} \equiv \sum_{\mu\nu} \frac{\left|\left\langle \phi \left| \hat{Q}_i \right| \mu\nu \right\rangle \left\langle \mu\nu \left| \hat{Q}_j \right| \phi \right\rangle\right|}{(E_\mu + E_\nu)^k}$$

- **Zero-point vibrational energy:**

$$\Delta V_{vib} = \Delta V_{0,0}, \qquad \hat{Q}_0 \equiv \hat{Q}_{20}$$

- **Zero-point rotational energy:**

$$\Delta V_{rot} = \Delta V_{-2,-2} + \Delta V_{-1,-1} + \Delta V_{1,1}$$

$$\hat{Q}_{-2} \equiv 2ixy, \quad \hat{Q}_{-1} \equiv -2xz, \quad \hat{Q}_1 \equiv -2iyz$$

Zero-Point-Energies from ATDHF + cranking

- **Define:**

$$\Delta V_{ij} \equiv \frac{M_{ij}^{(-2)}}{M_{ij}^{(-3)}}$$

$$M_{ij}^{(-k)} \equiv \sum_{\mu\nu} \frac{\left|\left\langle \phi \left| \hat{Q}_i \right| \mu\nu \right\rangle \left\langle \mu\nu \left| \hat{Q}_j \right| \phi \right\rangle\right|}{(E_\mu + E_\nu)^k}$$

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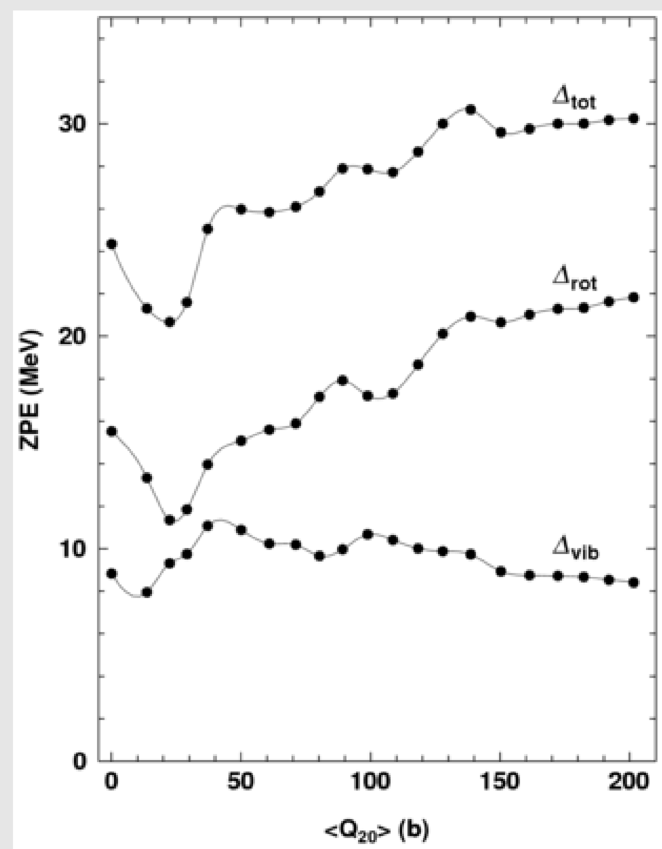
$$\Delta V_{vib} = \Delta V_{0,0}, \qquad \hat{Q}_0 \equiv \hat{Q}_{20}$$

- **Zero-point rotational energy:**

$$\Delta V_{rot} = \Delta V_{-2,-2} + \Delta V_{-1,-1} + \Delta V_{1,1}$$

$$\hat{Q}_{-2} \equiv 2ixy, \quad \hat{Q}_{-1} \equiv -2xz, \quad \hat{Q}_1 \equiv -2iyz$$

^{236}U, along symmetric path



Calculated ZPEs are too large!

Zero-point energies at the barriers

- Assume 1D motion in Q_{20} only at
  - 1st barrier ($<Q_{22}> \neq 0$)
  - 2nd barrier ($<Q_{30}> \neq 0$)

	1st min	1st barrier	2nd barrier
ΔV_{vib} (MeV)	9.75	10.32	8.78
ΔV_{rot} (MeV)	11.85	15.88	17.84
ΔV_{tot} (MeV)	21.60	26.20	26.62

- Yields ZPE corrections
  - At 1st barrier: 4.60 MeV
  - At 2nd barrier: 5.02 MeV

Barriers are lowered too much!

Collective mass from ATDHF + cranking

- **For Q_{20} only:**

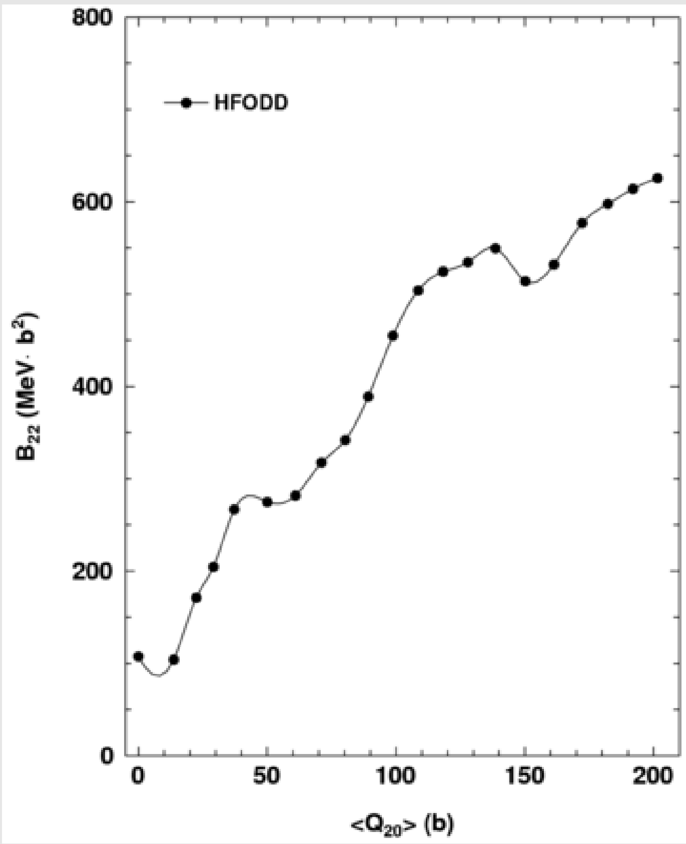
$$\mathcal{M}_{22} \equiv \frac{M^{(-3)}}{\left[M^{(-1)}\right]^2}$$

$$M^{(-k)} \equiv \sum_{\mu\nu} \frac{\left|\left\langle \mu\nu \left| \hat{Q}_{20} \right| \phi\left(q_{20}\right)\right\rangle\right|^2}{\left(E_\mu + E_\nu\right)^k}$$

$$B_{22} = \frac{1}{\mathcal{M}_{22}}$$

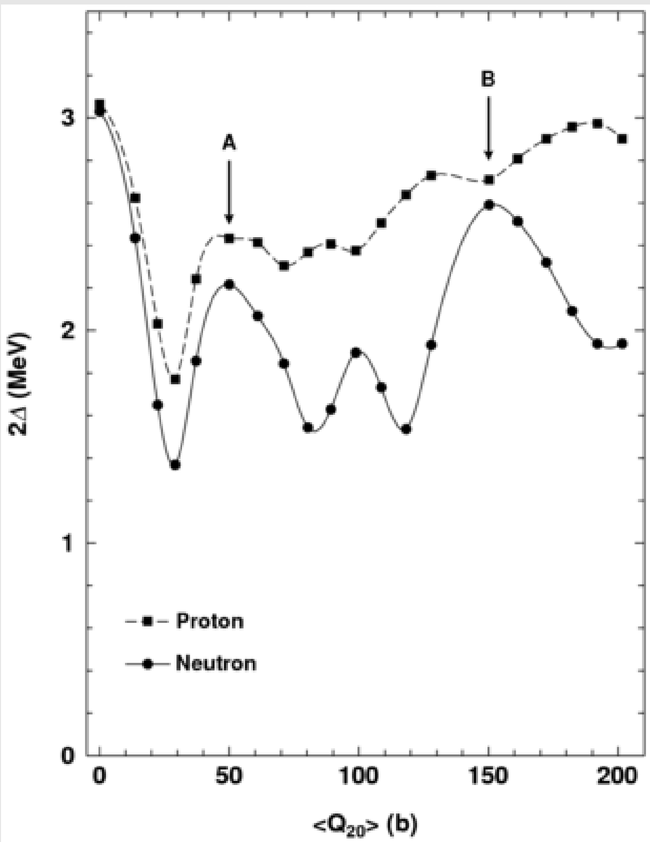
- **At 1st barrier ($\langle Q_{22}\rangle \neq 0$):**
  - → B_{22} = 280.24 MeV b^2
- **At 2nd barrier ($\langle Q_{30}\rangle \neq 0$):**
  - → B_{22} = 408.95 MeV b^2

^{236}U, along symmetric path

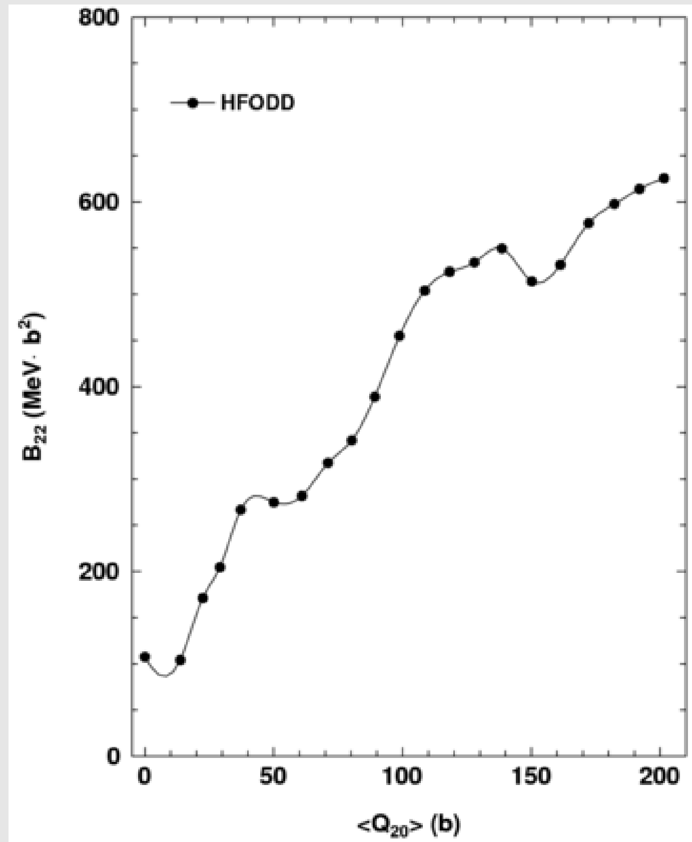


Collective mass and pairing gaps

^{236}U, along symmetric path



^{236}U, along symmetric path



Calculated barrier properties for ^{236}U

- **Barrier heights:**
  - $E_A \approx 6.92 - 4.60 = 2.32$ MeV (compared to 5.75 MeV)
  - $E_B \approx 6.37 - 5.02 = 1.35$ MeV (compared to 5.75 MeV)

Too low!

- **Barrier curvatures:**

$$V(q) = E_i - \frac{1}{2}\mu(q)(\hbar\omega_i)^2(q-q_i)^2$$

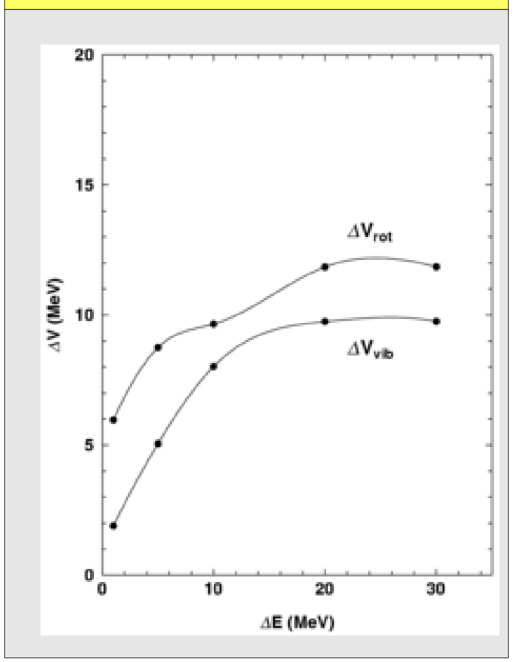
  - $\hbar\omega_A \approx 2.89$ MeV (compared to 0.90 MeV)
  - $\hbar\omega_B \approx 1.22$ MeV (compared to 0.50 MeV)

Too large!

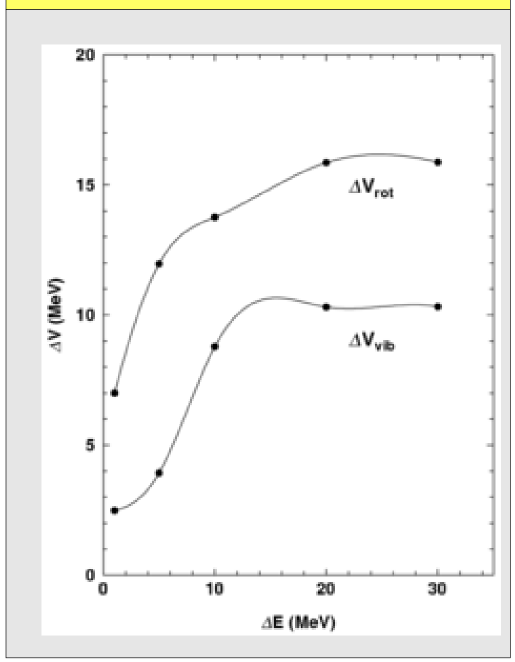
What's wrong?

- Mistake (phases?)
- Wrong prescription for pairing interaction
  - Test: vary energy cutoff (ΔE) in calculation of moments

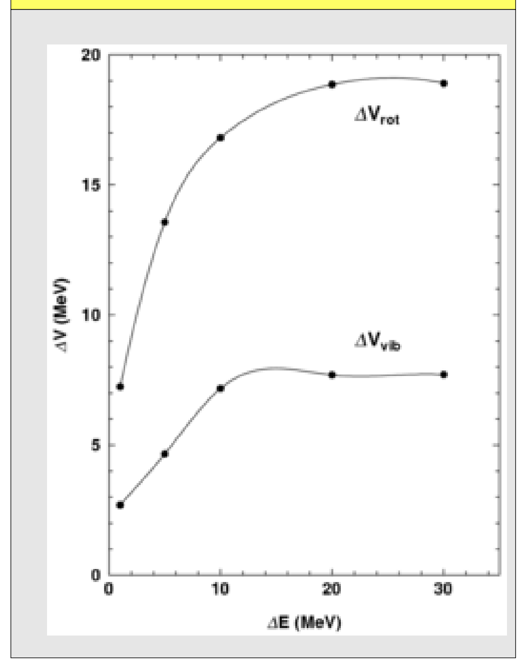
ZPE at 1st min



ZPE at 1st barrier



ZPE at 2nd barrier



  - Note slow convergence
- G_n, G_p, not constant with deformation

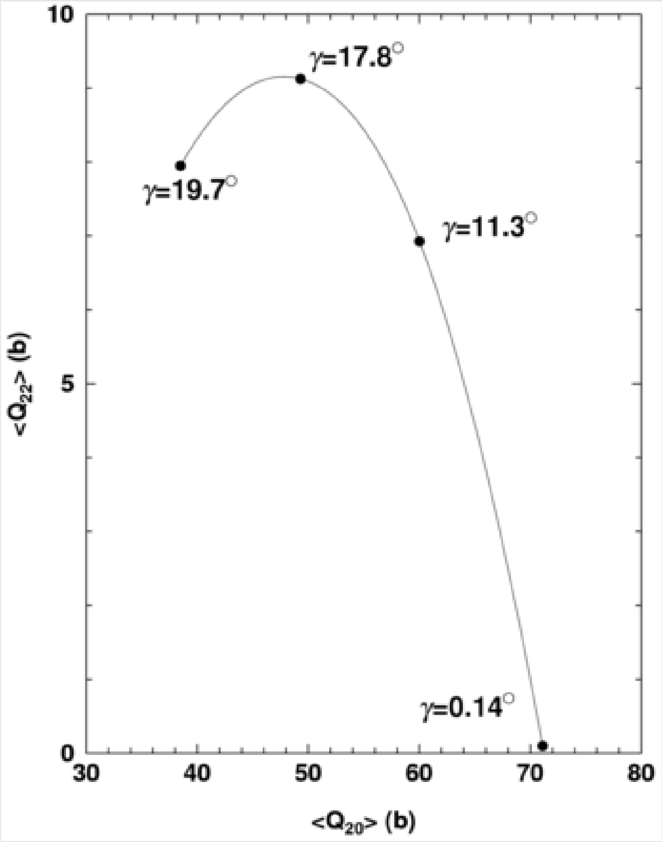
Conclusion

- Calculated
  - Microscopic energy surface
- Need to fix
  - Zero-point corrections
  - Collective mass
- Next:
  - Level densities
  - Fission probabilities $\Rightarrow$ (n,f) cross sections

Thanks to A. Staszczak, H. Goutte, D. Gogny, J. Dobaczewski

Evolution of $\langle Q_{22} \rangle$ and $\langle Q_{30} \rangle$

Triaxiality



Mass asymmetry