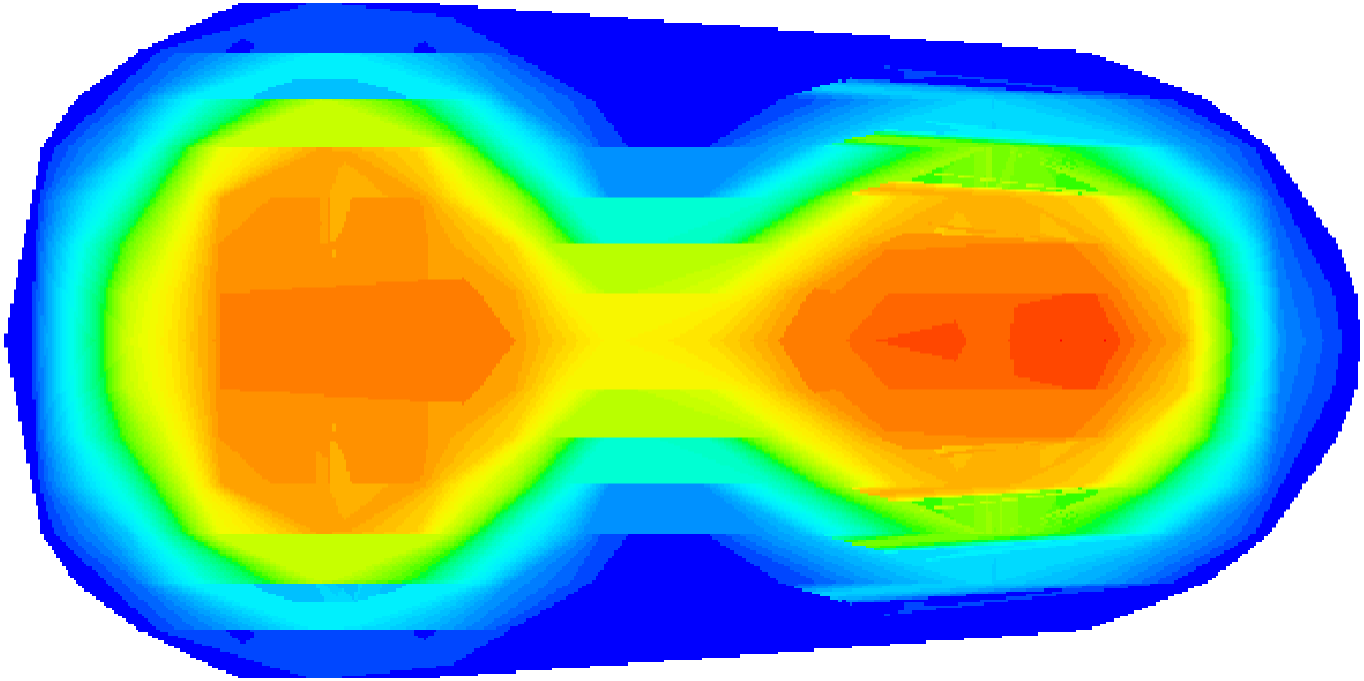
Microscopic Study of Fission in Two Collective Coordinates



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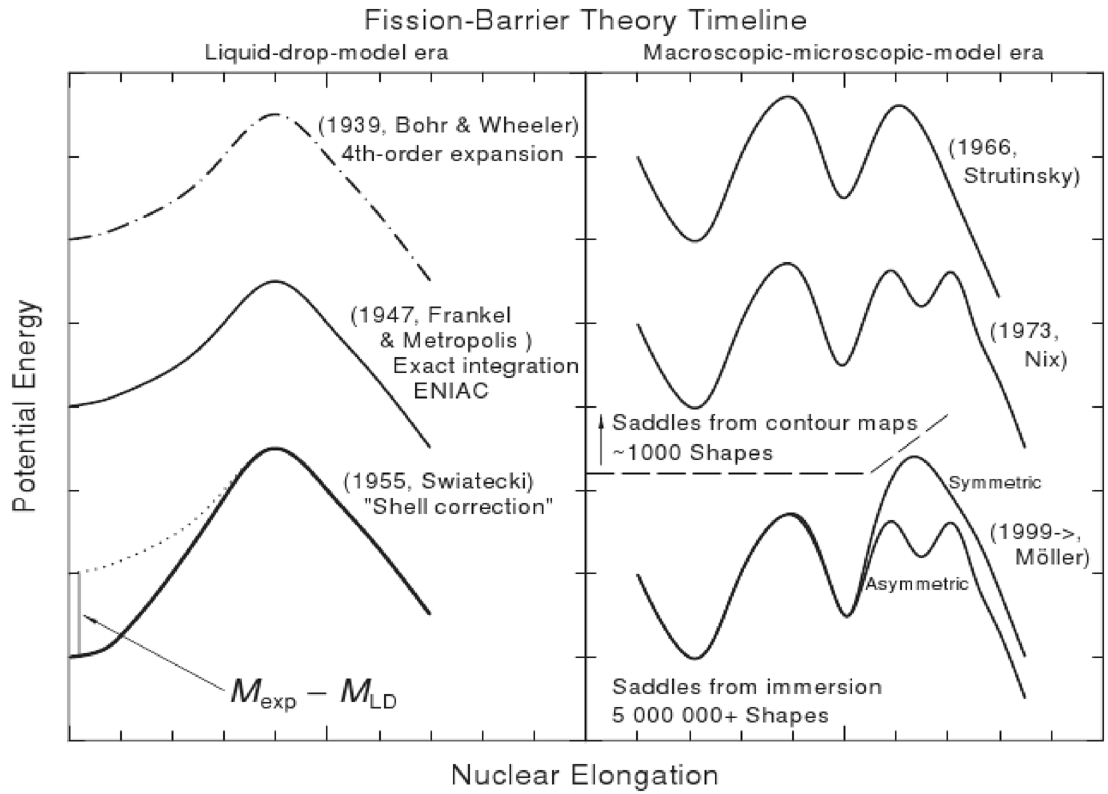
State of Fission

-Fission has been thoroughly studied experimentally and phenomenologically since the 1930s...

-Great strides in studies via density functional theory (DFT) incorporating different nucleon-nucleon interaction models (Skyrme, Gogny...).



Möller *et al*, Phys. Rev. C **79**, 064304 (2009)

State of Fission

-Presently, our colleagues are working on new interaction models and functionals arising from the underlying QCD and its low-energy renormalizations – the “other end” of the UNEDF effort

-We want to use that UNEDF functional to produce a predictive theory of fission for real observables

$$
\begin{aligned}
E^F \approx \sum_q \int d\mathbf{R} \Big\{ & A^{\rho\rho}\, \rho_q(\mathbf{R})\, \rho_q(\mathbf{R}) + A^{\rho\tau}\, \rho_q(\mathbf{R})\, \tau_q(\mathbf{R}) + A^{\rho\Delta\rho}\, \rho_q(\mathbf{R})\, \Delta\, \rho_q(\mathbf{R}) + A^{\rho\nabla J}\, \rho_q(\mathbf{R})\, \nabla \cdot \mathbf{J}_q(\mathbf{R}) \\
& + A^{\nabla\rho J}\, \nabla\rho_q(\mathbf{R}) \cdot \mathbf{J}_q(\mathbf{R}) + A^{JJ} \sum_{\mu\nu} J_{q,\mu\nu}(\mathbf{R})\, J_{q,\mu\nu}(\mathbf{R}) \\
& + A^{J\bar{J}} \Big[\Big(\sum_{\mu} J_{q,\mu\mu}(\mathbf{R}) \Big) \Big(\sum_{\mu} J_{q,\mu\mu}(\mathbf{R}) \Big) + \sum_{\mu\nu} J_{q,\mu\nu}(\mathbf{R})\, J_{q,\nu\mu}(\mathbf{R}) \Big] \Big\} \\
+ \sum_{\bar{q}} \int d\mathbf{R} \Big\{ & B^{\rho\rho}\, \rho_q(\mathbf{R})\, \rho_{\bar{q}}(\mathbf{R}) + B^{\rho\tau}\, \rho_q(\mathbf{R})\, \tau_{\bar{q}}(\mathbf{R}) + B^{\rho\Delta\rho}\, \rho_q(\mathbf{R})\, \Delta\, \rho_{\bar{q}}(\mathbf{R}) + B^{\rho\nabla J}\, \rho_q(\mathbf{R})\, \nabla \cdot \mathbf{J}_{\bar{q}}(\mathbf{R}) \\
& + B^{\nabla\rho J}\, \nabla\rho_q(\mathbf{R}) \cdot \mathbf{J}_{\bar{q}}(\mathbf{R}) + B^{JJ} \sum_{\mu\nu} J_{q,\mu\nu}(\mathbf{R})\, J_{\bar{q},\mu\nu}(\mathbf{R}) \\
& + B^{J\bar{J}} \Big[\Big(\sum_{\mu} J_{q,\mu\mu}(\mathbf{R}) \Big) \Big(\sum_{\mu} J_{\bar{q},\mu\mu}(\mathbf{R}) \Big) + \sum_{\mu\nu} J_{q,\mu\nu}(\mathbf{R})\, J_{\bar{q},\nu\mu}(\mathbf{R}) \Big] \Big\},
\end{aligned}
$$

A Skyrme-like DME exchange energy functional from Gebremariam *et al*, arXiv:0910.4979v3

Outline

I. Method and Motivation

II. Triple-Humped Barriers in Actinides

III. Results for Excited Nuclei

IV. Future and Conclusions

Method and Motivation

HFODD – symmetry-unrestricted, iterative-diagonalization nuclear DFT solver

A. SkM* in particle-hole channel, BCS with δ-pairing in particle-particle
   1. Pairing parameters fit to experimental pairing energys

B. One-center, Cartesian harmonic oscillator basis
   1. 31 major shells, to cover full range of shapes

   *** A major driver in campaign to parallelize the program

   2. Densities obtained in coordinate space (Gauss-Hermite points)
   3. Current computational power requires we keep a simplex symmetry

Method and Motivation

HFODD – symmetry-unrestricted, iterative-diagonalization nuclear DFT solver [Dobaczewski *et al*, CPC 180, 2361 (2009).]

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} E_k$$

C. Constrained Hartree-Fock

1. Quadratic penalty functions to drive deformation - Elongation (Q_{20}), triaxiality (Q_{22}), and reflection asymmetry (Q_{30})
2. Augmented Lagrangian method gives precise control over deformation, but convergence requires a long time

$$\mathcal{E}^{mult} = \sum_{\lambda\mu} C_{\lambda\mu} \left(\left\langle \hat{Q}_{\lambda\mu} \right\rangle - \bar{Q}_{\lambda\mu} \right)^2 + a^i_{\lambda\mu} \left(\left\langle \hat{Q}_{\lambda\mu} \right\rangle - \bar{Q}_{\lambda\mu} \right)$$

$$a^{i+1}_{\lambda\mu} = a^i_{\lambda\mu} + 2C_{\lambda\mu} \left(\left\langle \hat{Q}_{\lambda\mu} \right\rangle - \bar{Q}_{\lambda\mu} \right)$$

D.P. Bertsekas, *Constrained Optimization and Lagrange Multiplier Methods*, (Athena Scientific, Belmont, MA), 1996.

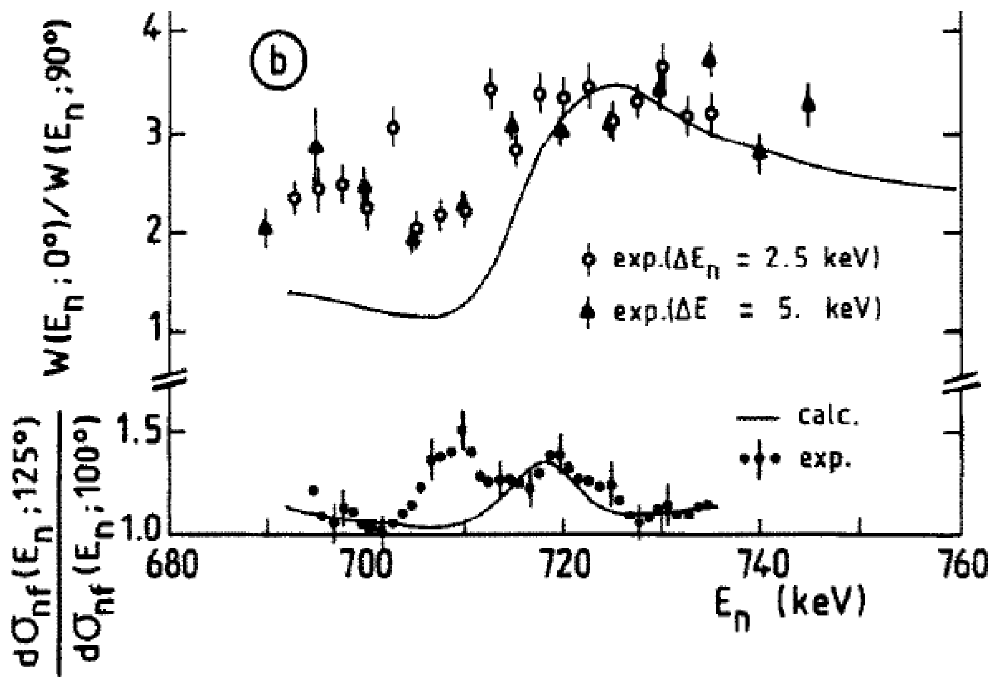
Method and Motivation

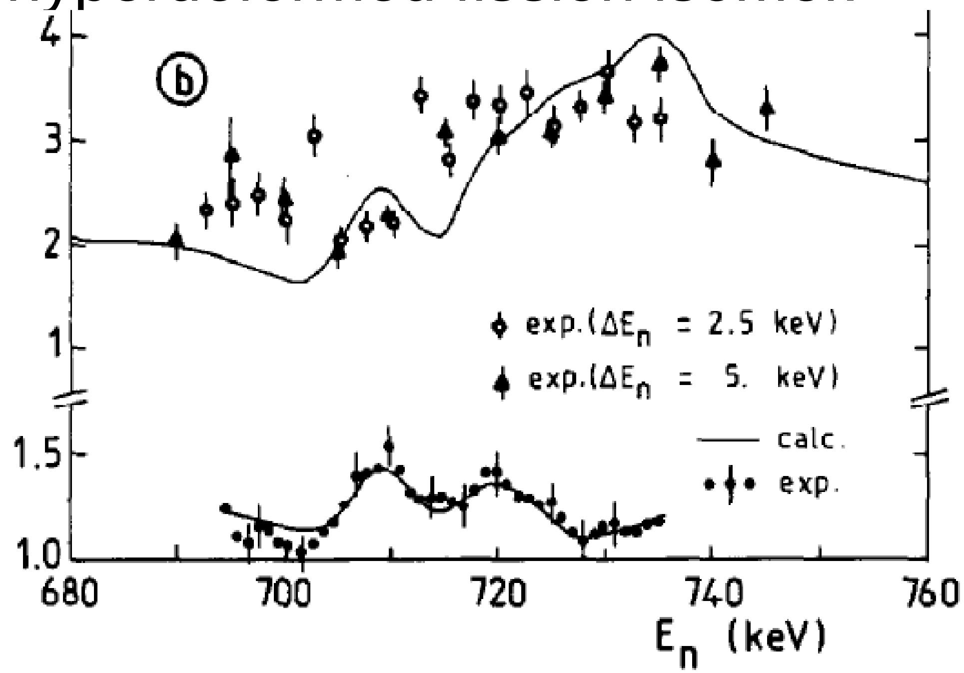
Q: Why multiple constraints?
A: It is frequently taken for granted that a symmetry-unrestricted Hartree-Fock solver will “automatically” find the optimal solution, accounting for every relevant degree of freedom. It turns out that such an approach is highly prone to sinking into false minima, adding numerical noise that must rather be dealt with by controlling the constraints manually (Möller *et al*, Phys. Rev. C **79**, 064304 (2009)).

Q: What does our method offer?
A: Fission has been heavily studied by phenomenological methods, but it remains an unconquered peak for first-principles, self-consistent methods.

Triple-Humped Barriers in Actinides

We have selected ^{232}Th as a typical light actinide whose fission barrier exhibits three humps and three minima. This nuclide has a particularly thoroughly studied third, hyperdeformed fission isomer.





The seminal experimental reports [e.g. Blons *et al*, NPA414 (1984) 1-41] exhibit the inadequacy of double-humped barriers for the fragment angular distribution of $^{230, 232}$Th (left), while a triple-humped barrier model successfully fits the data (right).

Results at Finite Temperature

Does a discussion of "temperature" make sense for a system of only ~10^2 particles? With the rapid increase of the density of states, statistical mechanics does prove viable [Egido *et al*, *Nuc. Phys.* **A451**, 77 (1986)].

Self-consistent HFB...

$$h = \epsilon + \Gamma$$

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} E_k$$

$$\Gamma_{\mu\nu} = \sum_{\alpha\beta} v_{\mu\beta\nu\alpha}\rho_{\alpha\beta}$$

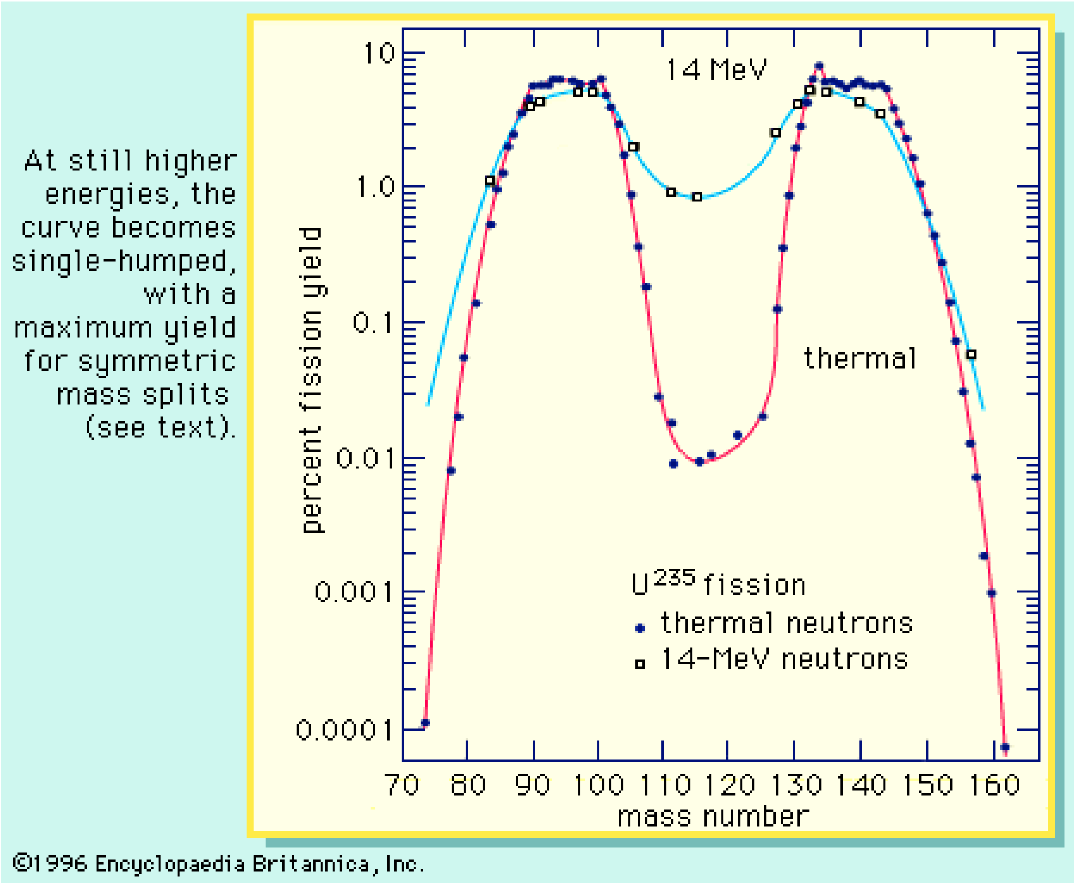
$$\Delta_{\mu\nu} = \frac{1}{2}\sum_{\alpha\beta} v_{\mu\nu\alpha\beta}\kappa_{\alpha\beta}$$

...in the grand canonical ensemble

$$\rho = UfU^\dagger + V^*(1-f)V^T$$

$$\kappa = UfV^\dagger + V^*(1-f)U^T$$

$$f_i = \frac{1}{1+e^{\beta E_i}}$$

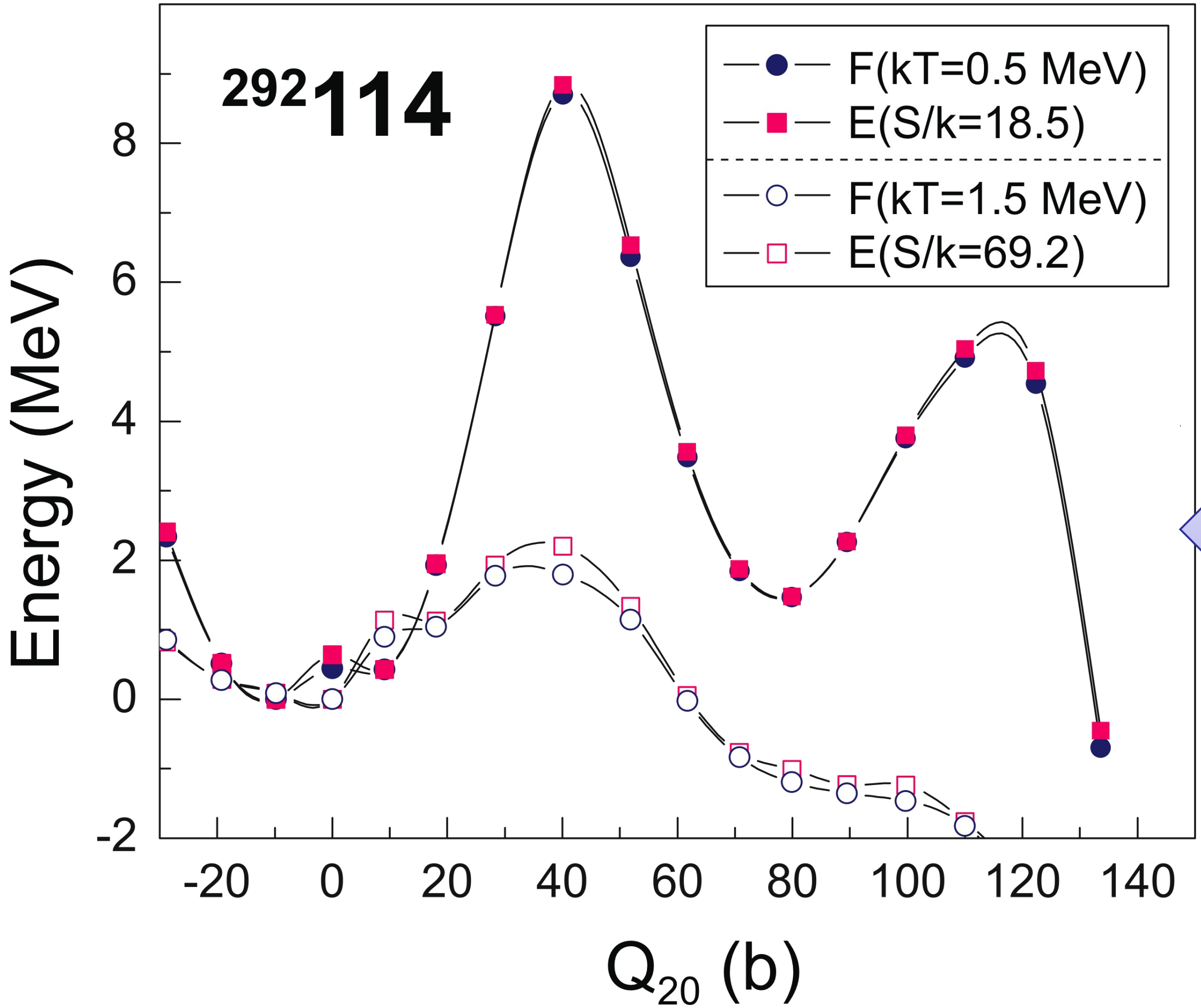


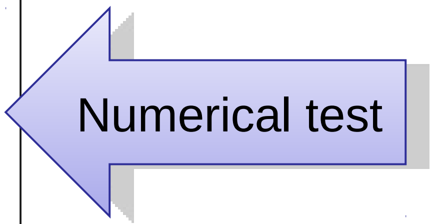
Results at Finite Temperature

We assume that fission is not isothermal, but adiabatic (isentropic). As found by Diebel and recently demonstrated numerically J.C. Pei *et al*, calculation of internal energy at constant entropy is equivalent to calculation of free energy at constant temperature.

$$\left(\frac{\partial E}{\partial Q_{20}}\right)_S = \left(\frac{\partial F}{\partial Q_{20}}\right)_T$$

Diebel *et al*, Nuc. Phys. **A355**, 66 (1981).



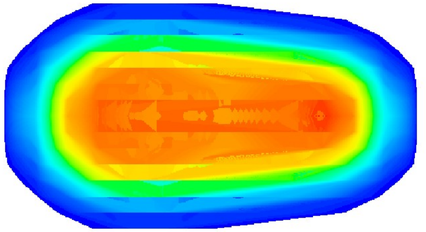


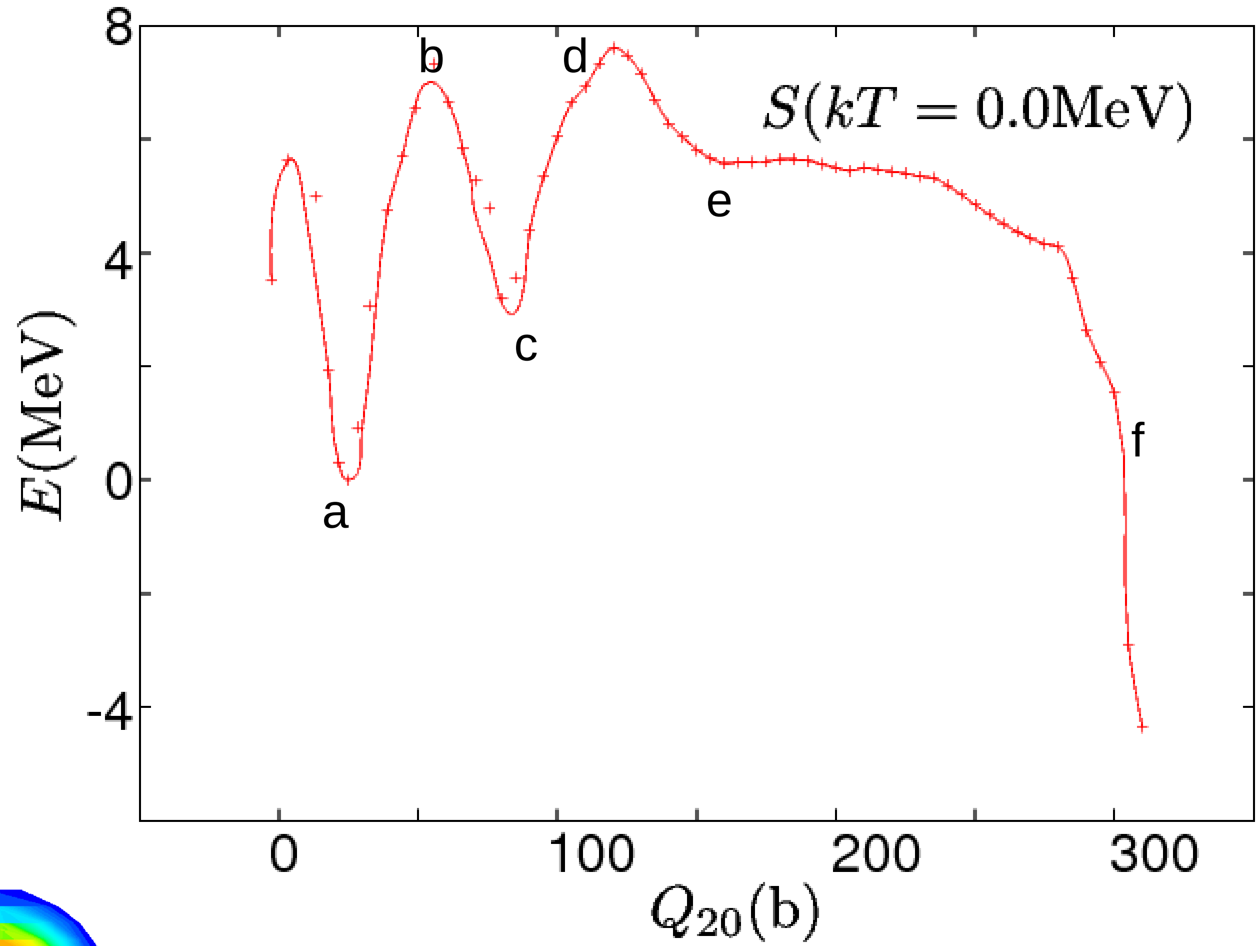
From J.C. Pei *et al*, Phys. Rev. Lett. 102, 192501 (2009).

Results for Excited Nuclei

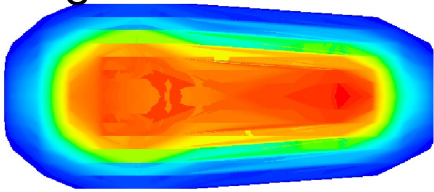
The optimal fission path exhibits its full range of shapes for zero-temperature: triaxial at inner barrier (a-b), and breaking reflection symmetry at the second barrier and beyond (d-f).

d

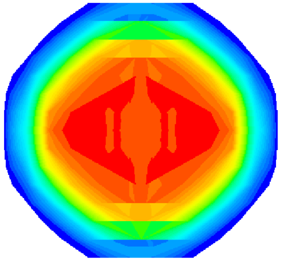




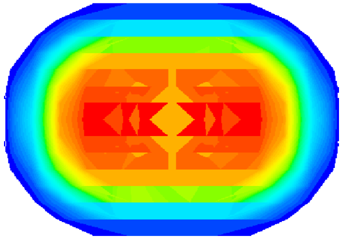
e



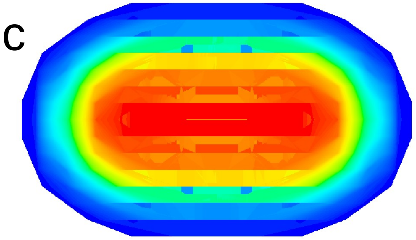
a



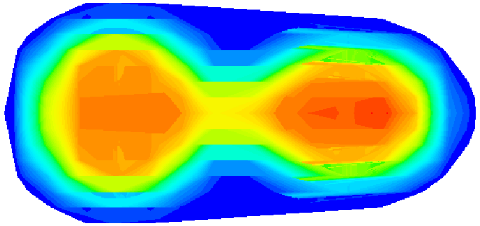
b



c

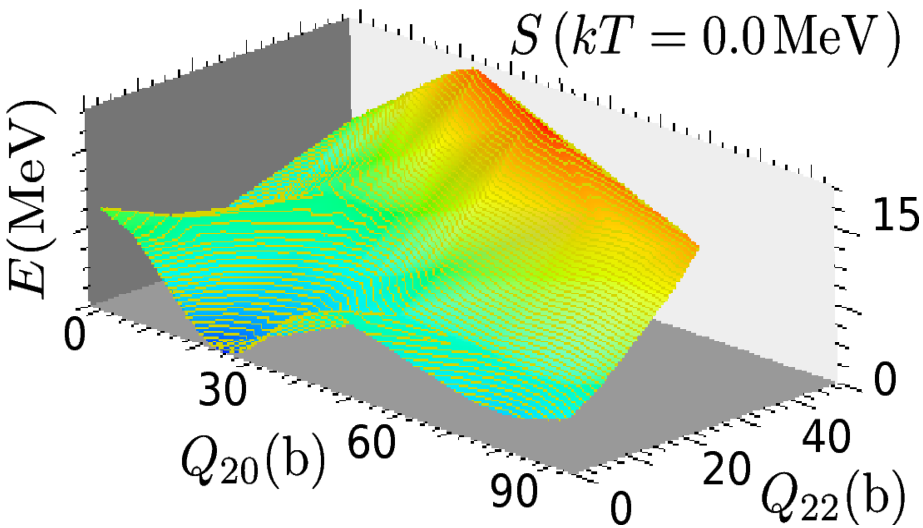


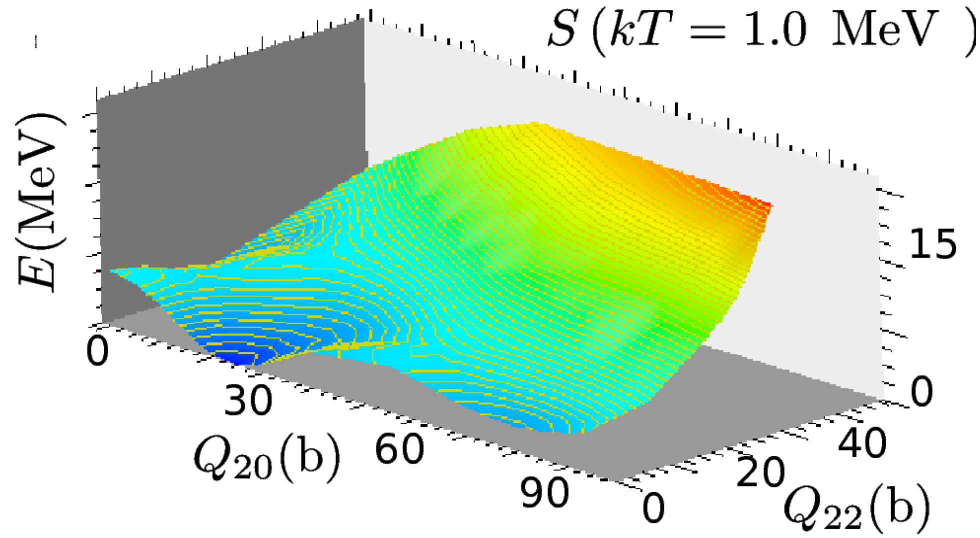
f

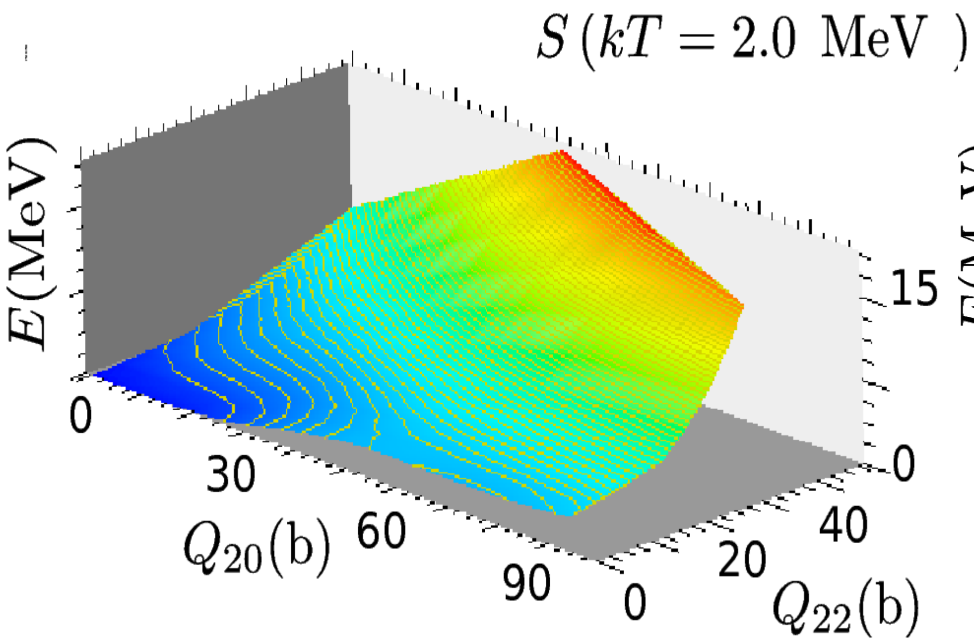


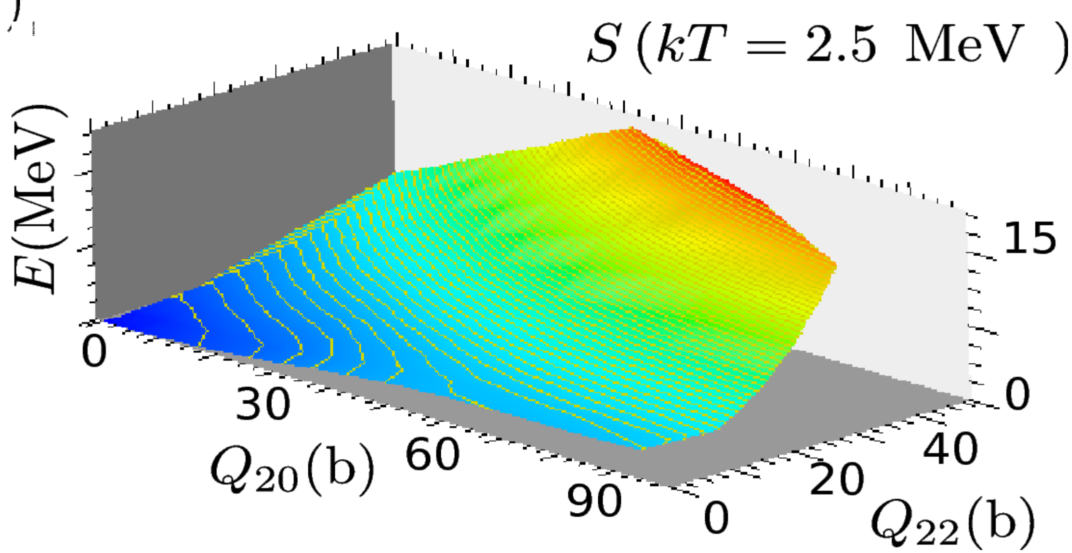
Results for Excited Nuclei – Inner Barrier

At zero temperature, the fission trajectory breaks the nucleus' axial symmetry in the vicinity of the first barrier. At higher excitation energies, the nucleus retains axially symmetric shape.



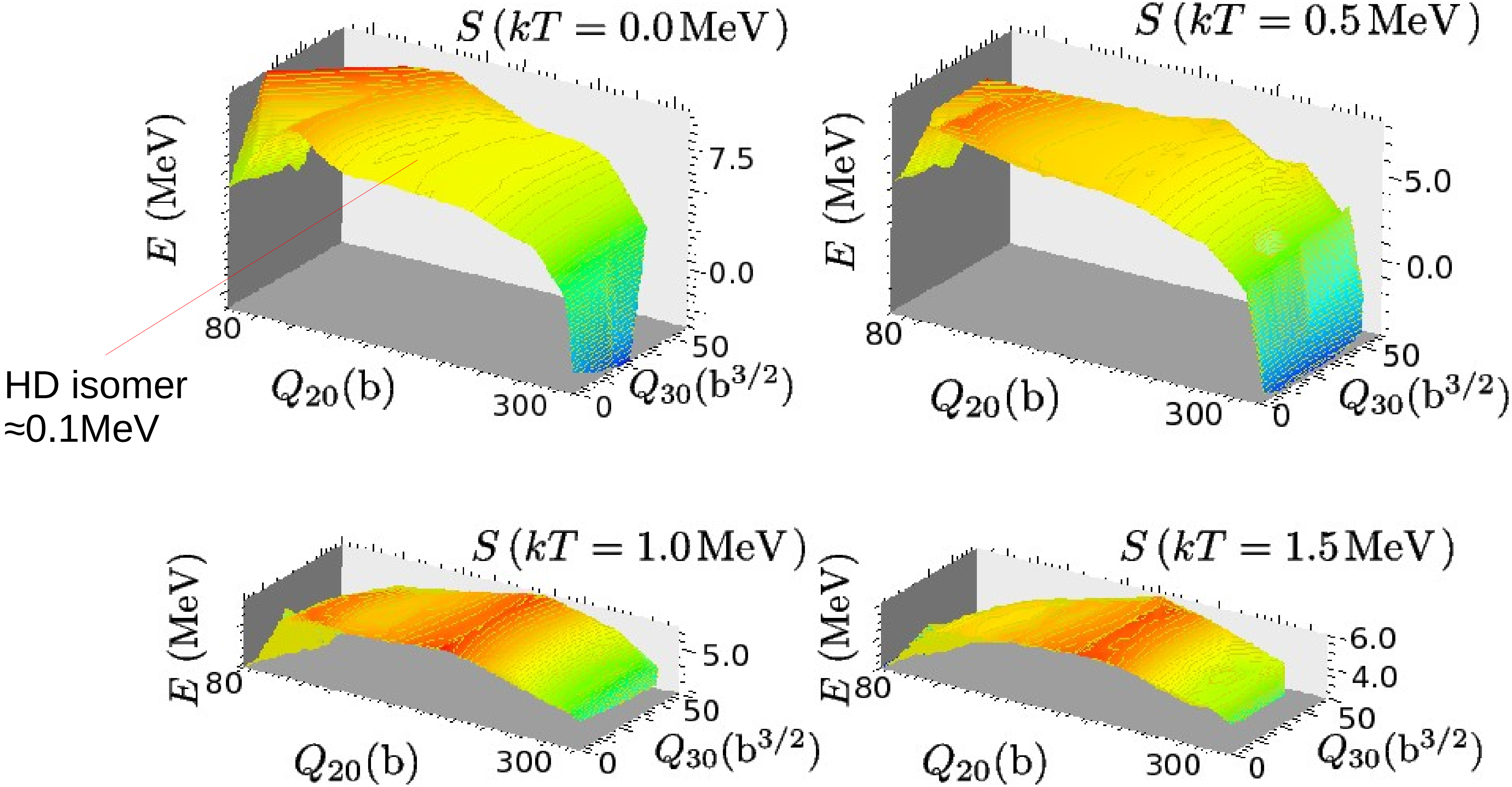






Results for Excited Nuclei – Outer Barrier(s)

At zero temperature, the fission path takes the nucleus to highly deformed, reflection asymmetric shapes – visiting the third isomer.



With the increase of temperature, the system's symmetry is restored. Further, the third isomer is dissolved by kT = 0.7MeV (with the quenching of pairing).

Future and Conclusions

-Strides are being made to understand fission from microscopic first principles.

-Turning up the heat has the general effect of yielding more symmetric configurations on fission path. The restoration of reflection symmetry beyond outer barriers is associated with more symmetric mass yields at higher excitation energy.

-Next step toward observables: fully dynamic calculations with ATDHFB