Fission of Highly Excited Nuclei: a Finite Temperature Description

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Outline

What are we going to do?

- An attempt to study the temperature dependence of fission in heavy nuclei using a microscopic theory. Application to two test nuclei.
  - Gogny force.
  - Reasonably big configuration space
  - Axially deformed base.
  - Breaking of reflection symmetry allowed: octupole deformation.

Specifics: Gogny Force

- D1S set.
- Pairing automatically included.
- D1S set has not been adjusted to finite temperature, although it has adjusted the surface energy term, hence it has been successful with fission barriers at zero temperature and high angular momentum.

Specifics: Calculation Basis

- Configuration space with 15 major shells. Checked for convergence with 17 shells in selected cases.
- Axially deformed basis: we are going to put a constraint on $<\hat{Q}_2>=q_2$.
- Standard truncation condition:

$$N_{\perp}+\frac{n_z}{q}<N_0$$

where $N_{\perp}, n_z$ are the HO quantum numbers and q is the nuclear axis ratio. A value $q=1.5$ is used.

  - i.e: N_0 shells in the perpendicular direction and up to $1.5N_0$ in the axial (z) direction.

Finite Temperature HFB

- For a system at constant T and average number of particles N, the equilibrium state is obtained by minimizing the grand canonical potential

$$\Omega = F - \mu N \text{ with } F = E - TS$$

By solving

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

with h the HF hamiltonian and Δ the pairing potential, U, V and E_i are obtained.

FTHFB (II)

- This in turn allows for the calculation of the density matrix and pairing tensor:

$$\begin{aligned} \rho &= UfU^{+} + V^{*}(1-f)V^{t} \\ \kappa &= UfV^{+} + V^{*}(1-f)U^{t} \end{aligned}$$

$$\text{with } f_i = \frac{1}{1+e^{\beta E_i}} \text{ and } \beta = 1/kT$$

- From this, expected values of an observable $\hat{O}$ are obtained as thermal averages

$$O = \mathrm{Tr}(\hat{D}\hat{O}) \quad \text{where}$$

$$\hat{D} = Z^{-1}\exp(-\beta(\hat{H}-\mu\hat{N})) \quad \text{and} \quad Z = \mathrm{Tr}\left[\exp(-\beta(\hat{H}-\mu\hat{N}))\right]$$

An additional constraint

- In order to study the barriers as the nucleus elongates, we add a constraint on the quadrupole deformation. Minimize:

$$\Omega = E - TS - \mu N - \lambda_{Q_{20}} q_2$$

- Once done this, thermal fluctuations come for free. The probability of obtaining a given value q of the constrained magnitude is given by the Free energy as

$$P(q) \propto e^{-F(q)/T}$$

  Ensemble averages of the observable $\hat{O}$ are obtained by means of its thermal expectation value $O(q)$:

$$\left\langle \hat{O} \right\rangle = \frac{\int O(q) e^{-F(q)/T} \mathrm{d}q}{\int e^{-F(q)/T} \mathrm{d}q}$$

Collective Masses

- To include dynamical effects, collective masses in the quadrupole degree of freedom are calculated using the ATDHFB framework at finite temperature.
- As usual, the residual interaction is neglected and the masses are:

$$M(q_{20}) = \frac{1}{2} \sum_{\mu\nu} \frac{\mathbb{Q}_{\mu\nu}\mathbb{Q}_{\mu\nu}}{|\mathbb{E}_{\mu} - \mathbb{E}_{\nu}|^3} |\mathbb{F}_{\mu} - \mathbb{F}_{\nu}|$$

- This approximation gives trouble when two levels cross or their quasiparticle energies are almost equal. An extra, constant, value added to the denominator avoids numerical divergence and simulates the residual interaction.
- Values in the 0.5-1.0 range were tested, and the results do not show a qualitative difference being quantitatively close.

Fission Half-life

- Spontaneous fission half-life is computed as:

$$T_{sf} = \frac{\ln 2}{\nu}\frac{1}{P}$$

- The assault frequency is set to $1\text{MeV}/\hbar$ and the penetration probability is calculated using the WKB approximation as:

$$P = \frac{1}{1 + \exp(2G)}$$

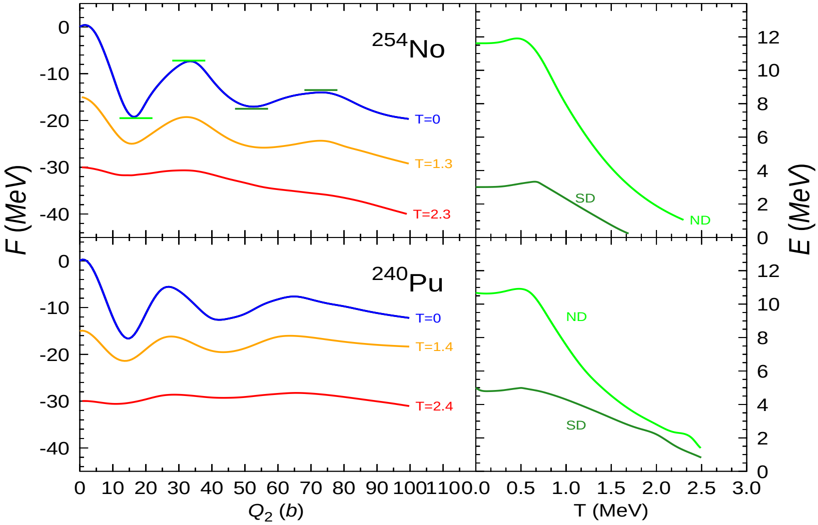
- and the action: $G = \int_{q_2 min}^{q_2 max} \sqrt{2M(q_2)\Delta F}\mathrm{d}q_2$ where $\Delta F = F(q_2) - E_0$ is the free energy above the ground state. The q_2 limits are set to span the barrier of interest. $F(q_2) = E(q_2) - TS(q_2)$, where $E(q_2)$ is obtained by substracting the zero-point energy correction for q_2 to the corrected (kinetic energy and rotational energy) HFB energy.

Test Nuclei

Calculations have been performed on two well known nuclei:

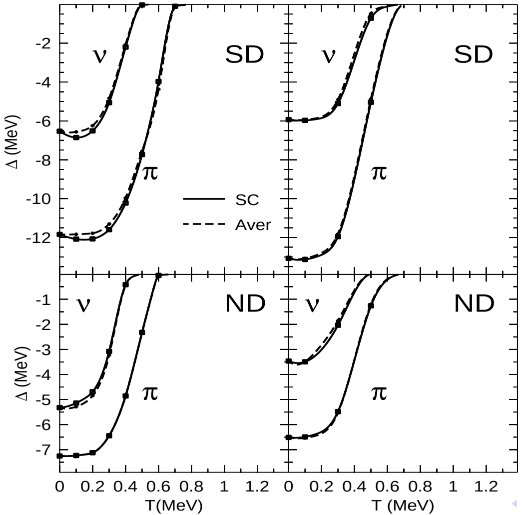
- ^{240}Pu, typical benchmark case.
- ^{254}No, also extensively studied. High spin D1S calculations (T=0) available. Shell stabilized ('magic' N=152). Appearance of octupole deformation in its path to fission.

Free Energy Curves and Fission Barriers.

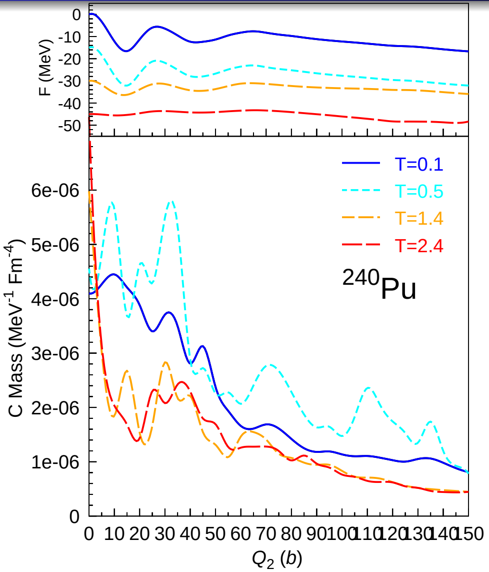


Pairing energy.

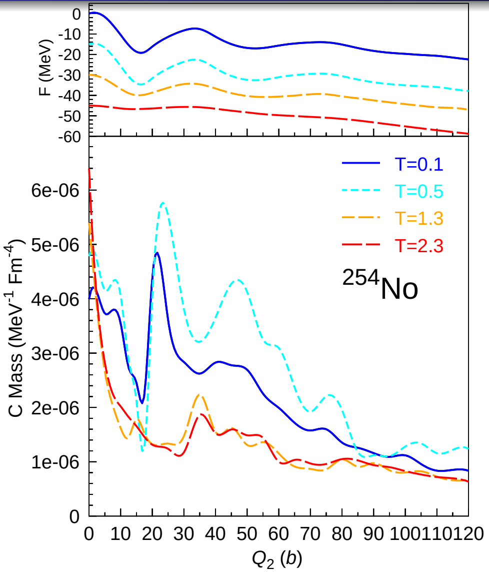
^{240}Pu ^{254}No



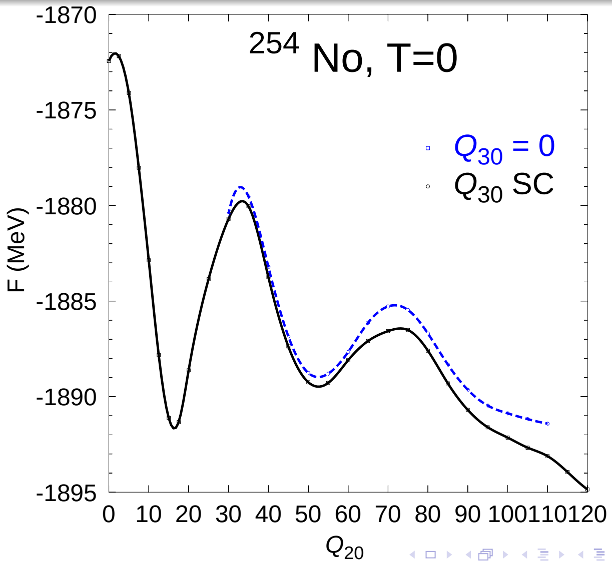
^{240}Pu Collective Mass



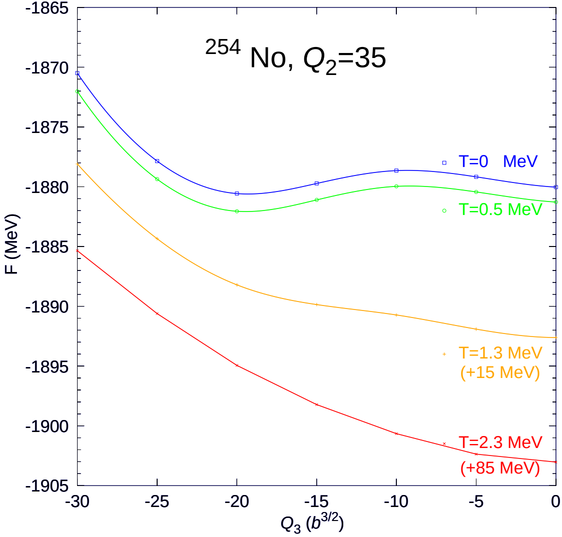
^{254}No Collective Mass



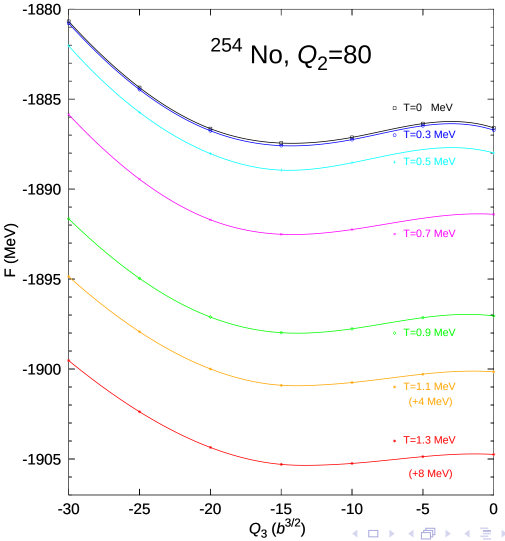
Q3 effect on ^{254}No fission barrier



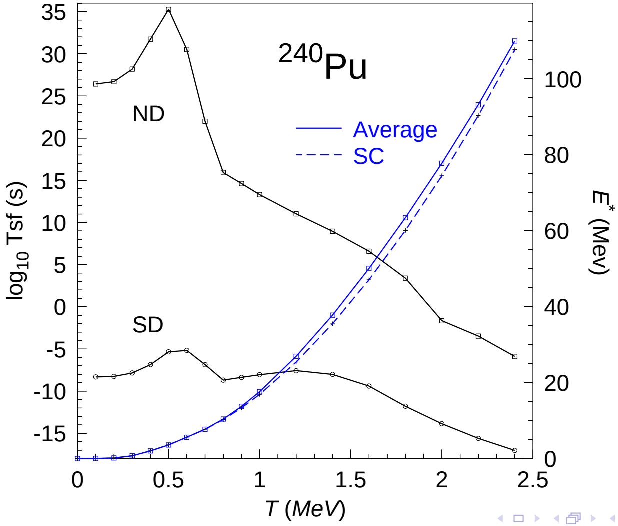
Q3 effect on ^{254}No first barrier, T$\neq$ 0



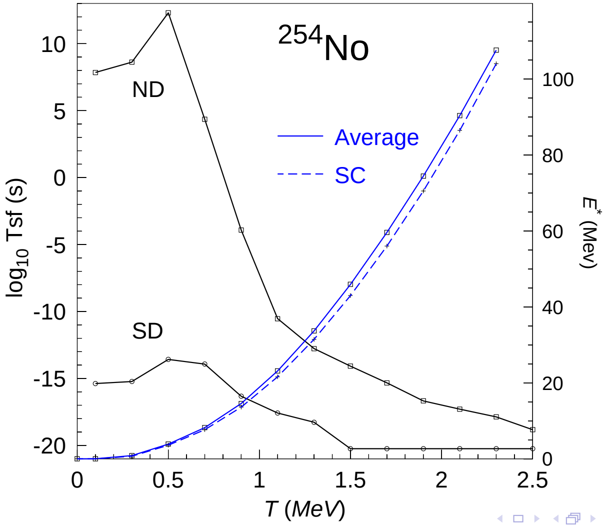
Q3 effect on ^{254}No second barrier, T$\neq$ 0



^{240}Pu Fission half-life



^{254}No Fission half-life



Conclusions

- Gogny D1S force used in FTHFB fission calculations with two typical test nuclei. Axial symmetry, octupole shapes allowed.
  - Fission barriers, as expected, go to zero with temperature. First and second barriers dissappear around the same temperature in ^{240}Pu.
  - A small increase in the height of the barriers is seen correlated with the pairing collapse. This is reflected in that spontaneous half-lives are bigger at around T=0.5 MeV.
  - Mass parameters behave as expected: smaller around the free energy minima and bigger near the top of the barriers. An overall increase of its value when pairing collapses.
  - Reflection assymetry also dissapears with temperature, although it is still relevant at pretty high temperatures.
- Future work.
  - Incoporate triaxial shapes. Fluctuations.