ATDHFB Collective Inertia and Fission Paths at Finite Temperature

Javid A. Sheikh

University of Tennessee / Oak Ridge National Laboratory
and University of Srinagar, India

- **Collective Inertia beyond Cranking approximation**
  A. Baran, W. Nazarewicz, J. Dobaczewski
- **Fission paths and barriers at Finite temperature**
  W. Nazarewicz, J.C. Pei, A.K. Kerman

Collective Inertia in Fission dynamics

- Spontaneous fission half-life (*M. Brack et al., Rev. Mod. Phys. 44 (1972) 320*)

$$\mathrm{T_{sf}} = \frac{\mathrm{In2}}{n}\frac{1}{P}$$

Penetration probability, P, is calculated in WKB approximation

$$P = [1 + exp\ S(L_{min})]^{-}1$$

where

$$S(L) = 2\int \sqrt{\frac{2}{\hbar^2}\mathcal{M}(q)\,[V(q) - E]}\ \ \mathrm{d}q$$

- To obtain kinetic energy and mass distributions of fission fragments, first collective Hamiltonian is derived and then re-quantized using Pauli prescription (*Goutte et al., Phys. Rev. C71 (2005) 024316*).

Perturbative Cranking Approximation

- Standard Cranking mass expression

$$\mathcal{M}_{ij} = 2\sum_{\mu\nu} \frac{\langle \nu | \partial \hat{h}/\partial q_i | \mu \rangle \langle \mu | \partial \hat{h}/\partial q_j | \nu \rangle}{(E_\mu + E_\nu)^3} (u_\mu v_\nu + u_\nu v_\mu)^2$$

where

$$\langle \mu | \frac{\partial \hat{h}}{\partial q} | \nu \rangle = \langle \mu | \hat{Q} | \nu \rangle \left[2 \sum_m \frac{\langle \phi_0 | \hat{Q} | m \rangle \langle m | \hat{Q}^* | \phi_0 \rangle}{\mathcal{E}_m - \mathcal{E}_0} \right]^{-1}$$

- Several approximations in the derivation of the above expression.

Adiabatic Time-dependent Hartree-Fock-Bogoliubov (ATDHFB) theory

- Density operator is expanded as *(Baranger and Veneroni, Ann. of Phys. 114 (1978) 123)*

$$\mathcal{R} = e^{\imath\chi}\mathcal{R}_0 e^{-\imath\chi}$$

$\mathcal{R}_0$ and χ are hermitian and time-even operators, and correspond to the classical variables of coordinate and velocity.

- Using the expansion of the density, total HFB energy can be separated into kinetic and potential terms, and the kinetic energy can be expressed as

$$\mathcal{K} = \frac{1}{2}\dot{q}_i\dot{q}_j\mathcal{M}_{ij}$$

where the collective inertia is given by

$$\mathcal{M}_{ij} = \frac{\imath}{2\dot{q}_i}\mathrm{Tr}\left(\frac{\partial\mathcal{R}_0^i}{\partial q_j}[\mathcal{R}_0, \mathcal{R}_1]\right)$$

Adiabatic TDHFB

- Time-odd ATDHFB equation

$$\imath\dot{\mathcal{R}}_0 = [\mathcal{W}_0, \mathcal{R}_1] + [\mathcal{W}_1, \mathcal{R}_0]$$

- Cranking approximation : Second-term on the right-hand side referred to as the Thouless-Valatin self-consistent term is neglected
- Perturbative Cranking : $\dot{\mathcal{R}}_0$ is evaluated using perturbation theory
- ATDHFB-Cranking : $\dot{\mathcal{R}}_0$ is evaluated explicitly

Few details of the mean-field calculations

- HFODD program : Solves HF or HFB equations self-consistently using Cartesian 3D deformed harmonic-oscillator basis (*J. Dobaczewski and J. Dudek, Comp. Phys. Comm. 102 (1997) 166*)
- Breaking of most of the symmetries is allowed in HFODD : crucial in the fission studies
- Lowest 1140 single-particle basis states - corresponding to 17 oscillator shells at the spherical point
- Energy cutoff for quasiparticle states : 60 MeV
- No. of Hartree Fock or canonical states : twice the neutron/proton particle number
- Standard center of mass correction : multiplying kinetic energy term by $(1 - 1/A)$

Few details of the mean-field calculations

- Skyrme interaction : SkM* in the particle-hole channel
- HFB : density-dependent delta-interaction in particle-particle channel

$$\mathcal{V}_{pair}(\vec{r}_1 - \vec{r}_2) = v_{0t}\, \delta(\vec{r}_1 - \vec{r}_2) \left(1 - \alpha \, \frac{\rho(\vec{r}_1)}{\rho_0}\right)$$

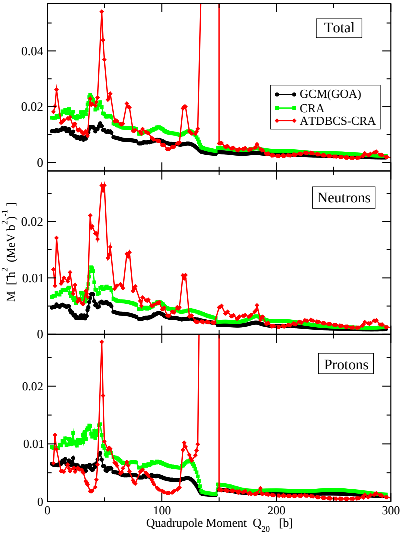
where $\alpha = 1/2$ (mixed pairing), $\rho_0 = 0.16$ fm^{-3}, v_{0n} = -425.5 MeV fm^3 and v_{0p} = -448.5 MeV fm^3 (fitted to reproduce the empirical odd-even mass difference in ^{252}Fm).

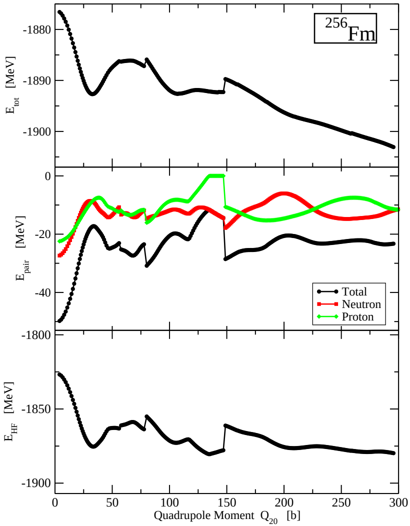
- HF+BCS : seniority pairing force

$$\begin{aligned} G_n &= [24.70 - 0.108(N-Z)]/A \\ G_p &= [14.76 + 0.241(N-Z)]/A \end{aligned}$$

Comparison of various mean-field models for ^{256}Fm

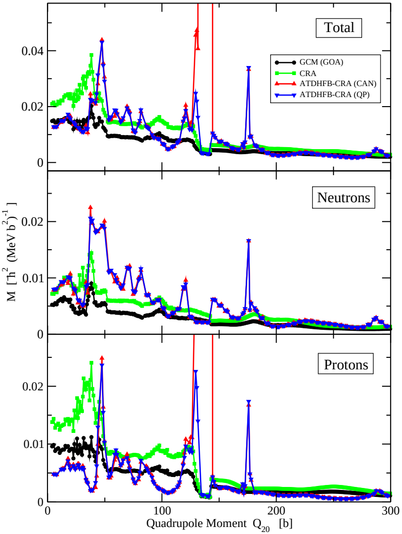
BCS study

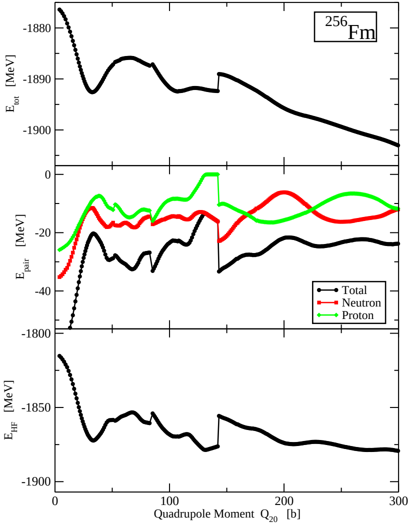




Comparison of various mean-field models for ^{256}Fm

HFB study





Experimental Observations :

- Cold-fusion experiment at GSI
  $({}^{70}Zn + {}^{208}Pb)\ {}^{278}112 \rightarrow {}^{277}112 + n$
  S. Hofmann and G. Munzenberg, Rev. Mod. Phys. **72**, *733(2000)*
- Hot-fusion experiment at Dubna
  $({}^{48}Ca + {}^{244}Pu)\ {}^{292}114 \rightarrow {}^{288}114 + 4n$
  Y. Oganessian, Pure Appl. Chem. **78**, *889(2006)*
- Highly excited experiment at GANIL
  ${}^{208}Pb + Ge,\quad {}^{238}U + Ni,\quad {}^{238}U + Ge$
  with lifetimes $> 10^{-18}$s for Z=120, 124 and much shorter lifetimes for neutron-deficient nuclei with Z=114
  M. Morjean, et al., Phys. Rev. Lett. **101**, *072701(2008)*

Mean-field Theory at Finite Temperature

- Equilibrium state of a physical system at constant temperature, T and chemical potential, μ is obtained from the minimization of the grand canonical potential

$$\Omega = E - TS - \mu N$$

$$E = \mathrm{Tr}(\hat{D}\hat{H}) \ , S = -k\mathrm{Tr}(\hat{D}\mathrm{In}\hat{D}) \ , N = \mathrm{Tr}(\hat{D}\hat{N})$$

- Density operator and the grand partition function are defined as

$$\begin{aligned} \hat{D} &= e^{-\beta(\hat{H}-\mu\hat{N})}/Z \\ Z &= \mathrm{Tr}(e^{-\beta(\hat{H}-\mu\hat{N})}) \end{aligned}$$

- Variation of the grand canonical potential using one-body density operator leads to the following HFB equations

$$\mathcal{H}\begin{pmatrix} U_i \\ V_i \end{pmatrix} = E_i \begin{pmatrix} U_i \\ V_i \end{pmatrix}$$

$$\mathcal{H} = \begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix}$$

- Finite temperature generalizations of the particle and pairing density density matrices are given by

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

  where the quantity "f" stands for the Fermi function, defined as,

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

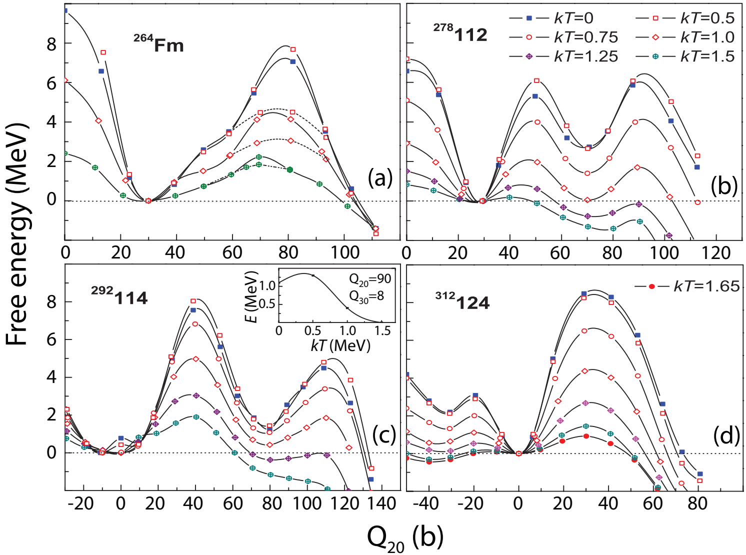
  Kinetic densities and spin-currents are also modified analogous to the above normal densities.

Mean-field Models at Finite Temperature

Finite temperature formalism has been implemented in two Skyrme-DFT codes

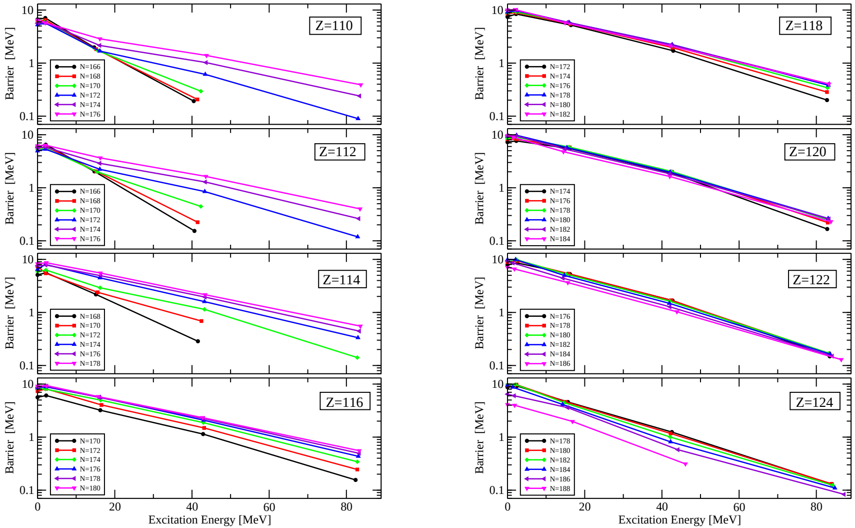
- HFB-AX
  J.C. Pei et al., Phys. Rev. C **78**, *064306 (2008)*
  Solves HFB equations with axial symmetry in coordinate space using B-spline functions
- HFODD
  J. Dobaczewski and J. Dudek, Comp. Phys. Comm. **102**, *166 (1997)*
  Solves HFB equations using oscillator basis in three-dimensions

Fission Barriers of Superheavy Elements using HFB-AX



J.C. Pei, W. Nazarewicz, JAS and A.K. Kerman, arXiv:0901.0901

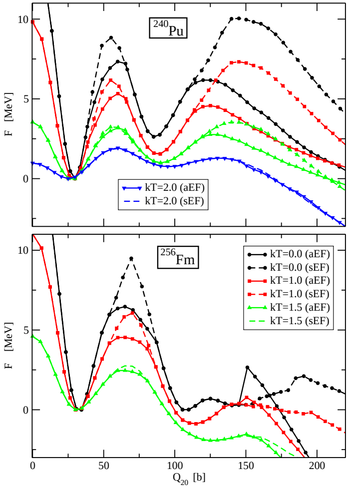
Barrier Heights of Superheavy Nuclei using HFODD



JAS, W. Nazarewicz and J.C. Pei (in preparation)

Transition from Asymmetric to Symmetric Path using HFODD

- Comprehensive experimental data available from radio-chemical work of secondary fragments in neutron-induced reactions for rare-earth and actinides, which clearly demonstrates a transition from asymmetric to symmetric fission
- Mass yield depicts a valley along with two humped structures at low neutron energies and the valley becomes shallow with increasing excitation energy
- *C. Wagemans, The Nuclear Fission Process (CRC Press,*



JAS, W. Nazarewicz and J.C. Pei

Summary and Outlook

Summary

- Collective masses derived from ATDHFB-Cranking approach are about 10% higher than the perturbative cranking masses for ^{256}Fm. It is expected that these differences will change half-lives by 1-2 orders of magnitude.
- Finite temperature Skyrme-DFT is able to provide an understanding of the synthesis of superheavy elements produced in hot and cold fusion experiments.

Outlook

- Evaluate collective inertia in the full ATDHFB approach by including time-odd fields.
- Evaluation of the fission half-lives and energy and mass distributions.
- Collective inertia and half-lives at finite temperature.