Dynamics of Spontaneous Fission

Collective Inertia

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OUTLINE

- Collective Inertia in Fission dynamics
- Time-Dependent Hartree-Fock-Bogoliubov (TDHFB) Theory
- Adiabatic TDHFB Theory
- Cranking Approximations
  - ATDHFB-Cranking
  - Perturbative Cranking
- Collective Inertia Results for Fermium Isotopes
- Summary and Outlook

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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*).

Time-Dependent Hartree-Fock Bogoliubov Theory

- *Approximation : wavefunction is a Slater determinant and stays such at all times*
- TDHFB equation (*Ring and Schuck, Page 488*)

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

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix} \text{ and } \mathcal{W} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$

- TDHFB cannot describe quantum tunneling process as the energy is conserved :

$$\frac{dE}{dt} = \mathrm{Tr}(\mathcal{W}\dot{\mathcal{R}}) = \imath\mathrm{Tr}(\mathcal{W}[\mathcal{R}, \mathcal{W}]) = 0 \qquad (1)$$

- Conceptual problem of non-linearity - superposition principle is violated

Adiabatic TDHFB

- *Approximation : Collective motion is slow (adiabatic) compared to the single-particle velocity of the nucleons*
- 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.
- Main emphasis of the ATDHFB formalism is to derive the phenomenological parameters appearing in the Bohr Hamiltonian microscopically and in order to achieve this, the densities are expanded up to quadratic terms only, i.e.,

$$\mathcal{R} = \mathcal{R}_0 + \mathcal{R}_1 + \mathcal{R}_2$$

  with $\mathcal{R}_1 = \imath[\chi, \mathcal{R}_0]$ and $\mathcal{R}_2 = \frac{1}{2}\imath^2[\chi, [\chi, \mathcal{R}_0]]$

Adiabatic TDHFB

- 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

- Trace in the collective mass expression is evaluated in the quasiparticle basis. Defining the transformation

$$\begin{aligned}\mathcal{R}_0 &= \sigma_z \mathcal{A}^\dagger \mathcal{G} \mathcal{A} \sigma_z \\ \mathcal{W}_0 &= \sigma_z \mathcal{A}^\dagger \mathcal{E} \mathcal{A} \sigma_z \\ \mathcal{R}_1 &= \sigma_z \mathcal{A}^\dagger \mathcal{Z} \mathcal{A} \sigma_z \\ \dot{\mathcal{R}}_0 &= \sigma_z \mathcal{A}^\dagger \mathcal{F} \mathcal{A} \sigma_z\end{aligned}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad \mathcal{A} = \begin{pmatrix} A^\dagger & B^\dagger \\ B^T & A^T \end{pmatrix}$$

- Derivative of $\mathcal{R}_0$ is given by the ATDHFB equation

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

and in quasiparticle representation can be expressed as

$$\imath \mathcal{F} = [\mathcal{E}, \mathcal{Z}] + [\mathcal{A} \sigma_z \mathcal{W}_1 \sigma_z \mathcal{A}^\dagger, \mathcal{G}]$$

Adiabatic TDHFB

- Matrix elements of the ATDHFB equation in the canonical basis is given by *(J. Dobaczewski and J. Skalski, Nucl. Phys. A369 (1981) 123)*

$$
\begin{aligned}
-\imath F_{\mu\nu} &= \sum_{\delta}(E^{0}_{\mu\delta}\, Z_{\delta\nu} + Z_{\mu\delta}\, E^{0\,*}_{\delta\nu}) \\
&+ \sum_{\delta\gamma}\left(\frac{1}{2} V^{pp}_{\delta\gamma\mu\nu}\, \zeta^{-}_{\delta\gamma}\zeta^{-}_{\mu\nu} + V^{ph}_{\bar{\mu}\delta\nu\bar{\gamma}}\, s^{*}_{\bar{\mu}} s_{\gamma}\eta^{-}_{\delta\gamma}\eta^{-}_{\mu\nu}\right) Z_{\delta\gamma}
\end{aligned}
$$

- Hermiticity property of $\mathcal{Z}$ and $\mathcal{F}$ matrices allows to write

$$
\mathcal{Z} = \begin{pmatrix} 0 & -Z^{*} \\ Z & 0 \end{pmatrix} \quad \text{and} \quad \mathcal{F} = \begin{pmatrix} 0 & -F^{*} \\ F & 0 \end{pmatrix}
$$

  where $Z^{*} = -Z^{\dagger}$ and $F^{*} = -F^{\dagger}$.
- Collective mass tensor in terms of F and Z

$$
\mathcal{M}_{ij} = \frac{\imath}{\dot{q}_i \dot{q}_j} \mathrm{Tr}\left(Z^{i*} F^{j} - Z^{i} F^{j*}\right)
$$

Adiabatic TDHFB

- Evaluation of the collective inertia needs F and Z matrices. F matrix is simply derivative of the ρ_0 and is given by

$$F^{i*}_{\mu\bar{\nu}} = \frac{-s_{\bar{\nu}}}{(u_\mu v_\nu + v_\mu u_\nu)} \dot{q}_i \left(\frac{\partial \rho_0}{\partial q_i}\right)_{\mu\nu}$$

- Taking the derivative of the static HFB equation, above equation can also be written as

$$F^{i*}_{\mu\nu} = \frac{\dot{q}_i}{(E_\mu + E_\nu)} \Bigg[(u_\mu v_\nu + v_\mu u_\nu) s_\nu \left(\frac{\partial h}{\partial q_i}\right)_{\mu\bar{\nu}} - (u_\mu u_\nu + v_\mu v_\nu) \left(\frac{\partial \Delta}{\partial q_i}\right)_{\mu\nu} \Bigg]$$

ATDHFB-Cranking

- *Approximation : Two-body terms are neglected in ATDHFB equation*

$$-\imath F_{\mu\nu} = \sum_{\delta} (E^0_{\mu\delta}\, Z_{\delta\mu} + Z_{\mu\delta}\, E^0_{\delta\nu}{}^{*})$$

where HFB energy matrix, $E^0_{\mu\nu}$, is given

$$E^0_{\mu\nu} = \zeta^+_{\mu\nu}\, h_{\mu\nu} + \eta^+_{\mu\nu}\, \Delta_{\mu\bar{\nu}}\, s^*_{\bar{\nu}}$$

$$\eta^{\pm}_{\mu\nu} = u_\mu v_\nu \pm u_\nu v_\mu \quad \text{and} \quad \zeta^{\pm}_{\mu\nu} = u_\mu u_\nu \mp v_\mu v_\nu$$

- In HF+BCS approximation, $E^0_{\mu\nu}$ matrix is simply a vector of BCS quasiparticle energies and Z is simply given by

$$Z_{\mu\nu} = -\imath F_{\mu\nu}/(E_\mu + E_\nu)$$

ATDHFB-Cranking

- In the complete HFB framework, $E^0_{\mu\nu}$ matrix is non-diagonal and in order to evaluate Z, we need to find the inverse of $E^0_{\mu\nu}$ matrix.
- As an approximation, equivalent BCS energies can be calculated *(J. Dobaczewski, W. Nazarewicz, T.R. Werner, J.-F. Berger, C.R. Chinn, and J. Dechargé, Phys. Rev. C53 (1996) 2809)*

$$E_\mu = E_{\mu\mu} = \sqrt{(h_{\mu\mu} - \lambda)^2 + \Delta^2_{\mu\bar{\mu}}}$$

Above equation is quite similar to the BCS quasiparticle energy expression, but involves quantities $h_{\mu\mu}$ and $\Delta_{\mu\bar{\mu}}$, which are obtained by transforming the HFB particle-hole and the pairing fields to the canonical basis.

Perturbative Cranking

- *Approximation : Perturbation theory is employed to evaluate the derivatives*
- The standard 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

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

and is obtained by considering the quadrupole constraint as an external field.

Evaluation of Collective Inertia using ATDHFB-Cranking

- Derivatives are calculated explicitly and using Lagrange three point formula the derivative of the density matrix, for instance, is given by

$$
\begin{aligned}
\left(\frac{\partial\rho}{\partial q}\right)_{\mu\nu} \approx\ & \frac{-\delta q'}{\delta q(\delta q+\delta q')}\sum_{n_1 n_2} D^*_{n_1\mu}(\rho(q_0-\delta q))_{n_1 n_2} D_{n_2\nu} \\
& + \frac{\delta q-\delta q'}{\delta q\,\delta q'}\sum_{n_1 n_2} D^*_{n_1\mu}(\rho(q_0))_{n_1 n_2} D_{n_2\nu} \\
& + \frac{\delta q}{\delta q'(\delta q+\delta q')}\sum_{n_1 n_2} D^*_{n_1\mu}(\rho(q_0+\delta q))_{n_1 n_2} D_{n_2\nu}
\end{aligned}
$$

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

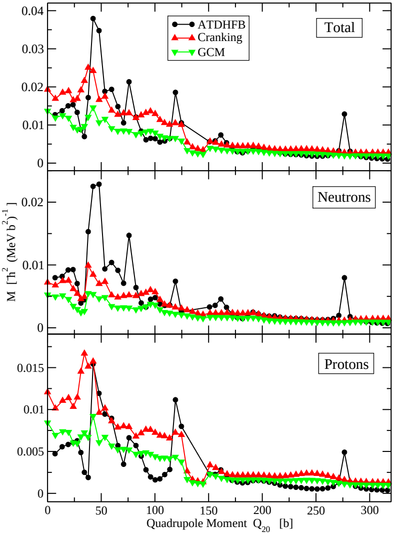
$$\mathcal{V}_{pair}(\vec{r}_1 - \vec{r}_2) = v_{0t}\ \delta(\vec{r}_1 - \vec{r}_2)\left(1 - \alpha\ \frac{\rho(\vec{r}_1)}{\rho_0}\right)$$

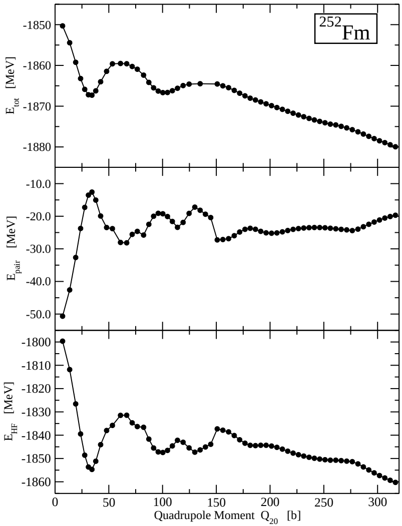
where $\alpha = 1/2$ (mixed pairing), $\rho_0 = 0.16$ fm^{-3}, v_{0n} = -425.5 MeV fm^3 and v_{0p} = -448.5 MeV fm^3 (fitted to reproduce the empirical odd-even mass difference in ^{252}Fm).

- 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 ^{252}Fm

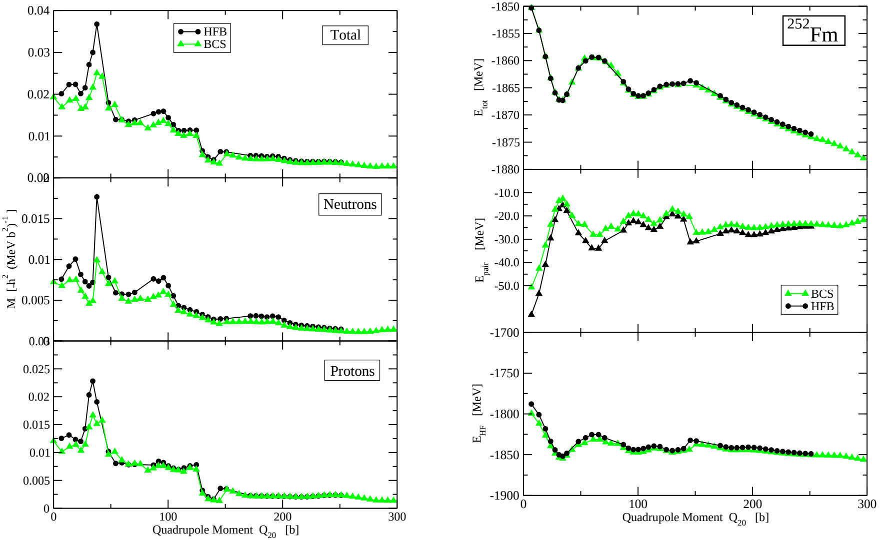




Comparative study of HF+BCS and HFB approaches

- In most of the fission analysis, HF+BCS approach is employed rather than HFB and has been justified by comparing the fission barriers.
- A systematic comparison of HF+BCS and HFB approaches has been performed not only for fission barriers, but also for masses and other properties.
- Masses have been calculated using “Equivalent BCS” procedure.

Comparison of HF+BCS and HFB results



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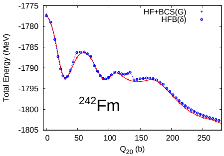

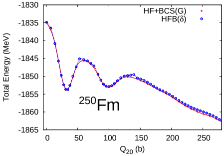

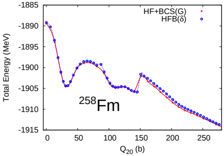

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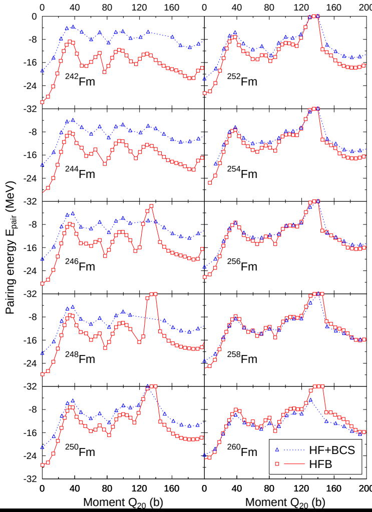

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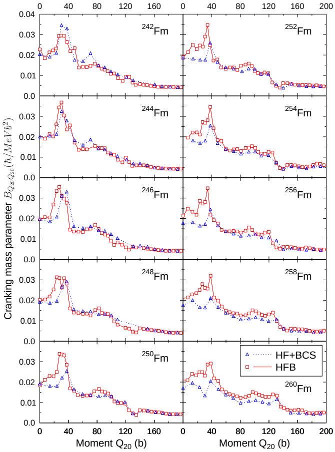

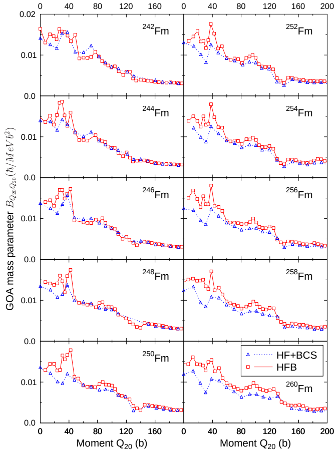

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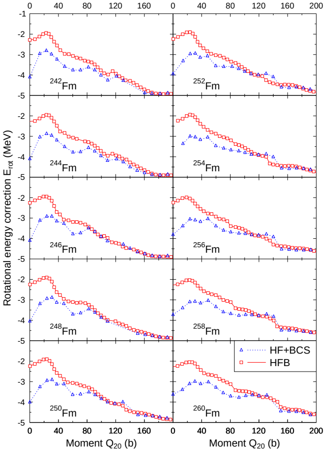

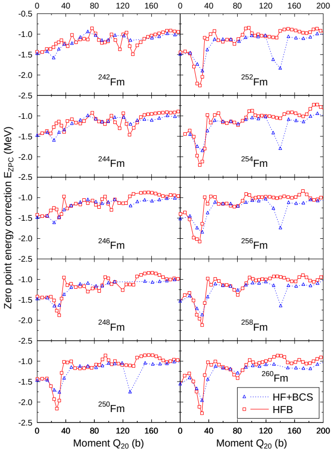

Summary and Outlook

Summary

- Collective masses derived from ATDHFB-Cranking approach are about 10% higher than the perturbative cranking masses for ^{252}Fm. It is expected that these differences will change half-lives by 1-2 orders of magnitude.
- HF+BCS and HFB approaches lead to similar barrier distributions and average pairing properties. However, the collective masses calculated in the two approaches are different.

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.