Collective aspects of microscopic mean-field evolution along the fission path

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Nuclear fission

• **Importance**
  – Energy production
  – Synthesis of super heavy elements
  – Astrophysical process
  – Production of radioactive isotopes
Nuclear fission

• **Importance**
  – Energy production
  – Synthesis of super heavy elements
  – Astrophysical process
  – Production of radioactive isotopes

• **Theoretical challenges**
  – Phenomenological models in terms of a few macroscopic degrees of freedom (elongation, mass asymmetry,...) have been developed
  – Successful microscopic models are still under development
  – Complicated dynamical process of quantum many-body system
    • Quantal treatments for both single-particle and collective DOFs
    • Dynamical and non-adiabatic effects
    • Different time scales
Microscopic models for fission

Static approach

- With energy density functional (EDF) theories (Skyrme, Gogny, RMF)
- Fission paths on the potential energy surface
  - Adiabatic (no excitation)
  - Dynamics is poorly treated
Our motivation:

- Dynamical approach to fission based on **time-dependent energy density functional** (TD-EDF) theory
- Mapping TD-EDF trajectory onto a selected set of collective variables

**TD-EDF ↔ collective space**

- Momenta
- Masses

for a given set of collective variables
To Bridge TD-EDF and collective motion

Collective variable(s): \( \hat{Q}_\alpha \)
ex: \( \hat{Q}_2 = 2z^2 - x^2 - y^2 \)

Mass and conjugate momentum associated with \( Q_\alpha \)?
To Bridge TD-EDF and collective motion

Collective variable(s): $\hat{Q}_\alpha$

ex: $\hat{Q}_2 = 2z^2 - x^2 - y^2$

Mass and conjugate momentum associated with $Q_\alpha$?

... We demand that

$$\frac{d\langle \hat{Q}_\alpha \rangle}{dt} = \frac{\langle \hat{P}_\alpha \rangle}{M_\alpha}$$

$$\text{Tr}(\rho(t)[\hat{Q}_\alpha, \hat{P}_\alpha]) = i\hbar$$

$$\frac{m_N}{M_\alpha} = \text{Tr}[\rho(t)\nabla Q_\alpha \cdot \nabla Q_\alpha]$$

$$P_\alpha = \frac{\hbar}{2i m_N} \frac{M_\alpha}{\hbar} \left( (\nabla Q_\alpha) \cdot \nabla + \nabla \cdot (\nabla Q_\alpha) \right)$$

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Application to $^{258}$Fm

- TDHF + BCS
  (Sly4d + constant pairing)
- Starting from a point on PEC
- No spontaneous fission for $Q_2(t=0) < 160$ b

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Symmetric fission of $^{258}$Fm with TDHF + BCS
1. Collective mass and momentum

\[ m_N \frac{M_2(Q_2) / M_2(\infty)}{M_\alpha} = \text{Tr}[\rho \nabla Q_\alpha \cdot \nabla Q_\alpha] \]

- \( Q_2 \) mass on dynamical path
- Deviation from static one around scission
- Scission happens more smoothly

\[ ^{258}\text{Fm} \quad E_x = 0.0 \text{ MeV}, \quad t = 0.00 \text{ fm/c} \]
1. Collective mass and momentum

\[ \frac{m_N}{M_\alpha} = \text{Tr}[\rho \nabla Q_\alpha \cdot \nabla Q_\alpha] \]

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\(^{258}\text{Fm} \quad E_x = 0.0 \text{ MeV}, \ t = 1187.18 \text{ fm/c} \]

\[ Q_2 \text{ mass on dynamical path} \]
1. Collective mass and momentum

\[ P_2 = M_2 \left( \frac{dQ_2}{dt} \right) \]

Dissipation before the scission (static)

Dissipation
before the scission
Assume a classical motion with dissipative force:

\[ \dot{Q}_2 = \frac{P_2}{M_2} \]

\[ \dot{P}_2 = -\frac{\partial V_{\text{coll}}}{\partial Q_2} + \frac{1}{2} \frac{\partial M_2}{\partial Q_2} \dot{Q}_2^2 + \gamma(Q_2) \dot{Q}_2 \]

\[ \dot{P}_2 - \frac{1}{2} \frac{\partial M_2}{\partial Q_2} \dot{Q}_2^2 = -\frac{\partial V_{\text{coll}}}{\partial Q_2} + \gamma(Q_2) \dot{Q}_2 \]

\[ F(Q_2) \sim \text{force coming from dynamical potential and friction} \]
2. More analysis of motion in $Q_2$ space

\[ \dot{P}_2 - \frac{1}{2} \frac{\partial M^2_2}{\partial Q_2} \dot{Q}_2^2 = - \frac{\partial V_{coll}}{\partial Q_2} + \gamma(Q_2) \dot{Q}_2 \]

$F(Q_2) \sim$ force coming from dynamical potential and friction

- Reduction of outward force compared to the static path
  - fragments stick together more
  - friction against separation (dissipation)

- Dissipation occurs before scission
2. More analysis of motion in $Q_2$ space

Define "dynamical potential" (work done by $F$ on $Q_2$)

$$V^{\text{dyn}}(Q_2) \equiv V_C(Q_2^{\text{max}}) + \int_{Q_2}^{Q_2^{\text{max}}} dQ_2' F(Q_2')$$
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Potential **along adiabatic path**

Work by $F$ **along dynamic path**

Difference = Dissipated Energy
3. Generalization to several DOFs

Diagonalize the inertia tensor:

\[
\frac{m_N}{M_{\alpha\beta}} = \text{Tr}[\rho \nabla Q_{\alpha} \nabla Q_{\beta}]
\]

\[
\frac{1}{M} \to \frac{1}{M'} = W \frac{1}{M} W^T
\]

\[
Q' \to WQ
\]

\[
(P/M)' \to W(P/M)
\]

\[
\Rightarrow \langle [Q'_{\alpha}, P'_{\beta}] \rangle = \delta_{\alpha\beta} i\hbar
\]
3. Generalization to several DOFs

Diagonalize the inertia tensor:

\[ \frac{m_N}{M_{\alpha\beta}} = \text{Tr}[\rho \nabla Q_\alpha \nabla Q_\beta] \]

\[ \frac{1}{M} \rightarrow \frac{1}{M'} = W \frac{1}{M} W^T \]

\[ Q' \rightarrow W Q \]

\[ (P/M)' \rightarrow W (P/M) \]

**Collective kinetic energy**

\[ E^{\{\alpha\}}_{\text{kin}} = \sum_{\alpha} \frac{P_{\alpha}^2}{2M'_{\alpha}} \quad \text{selected set} \]

\[ E^{\text{tot}}_{\text{kin}} = \int d^3r \frac{\dot{r}^2}{\rho} \quad \text{total} \]
Summary and perspectives

• We have developed a method to extract information in collective space from TD-EDF theory

• Our goal: **unified microscopic approach for fission**

• Next steps
  – beyond-mean-field effects with configuration mixing
    • mapping onto \( \{Q_\alpha, P_\alpha\} \) space
    • quantum/thermal fluctuation of collective DOFs
  – obtain physical observables
    ✓ fragment mass/charge distribution
    ✓ kinetic energy of fragments
    ✓ ...
  – compare them with data
    and other theoretical approaches