Microscopic phase-space exploration of nuclear fission


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Outline

• Introduction
• Overview of theories for fission
• Stochastic mean-field (SMF) theory
• Spontaneous fission of $^{258}$Fm
• Summary
Nuclear fission

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

• Theoretical challenges
  – Large-amplitude process of quantum many-body system
  – Quantum tunneling of many-degrees of freedom
  – Coupling between collective and internal (single-particle) degrees of freedom
Theories for fission

- **Conventional strategy**
  1. select a set of relevant collective degrees of freedom (DOF) $Q$ 
     *ex. elongation, mass asymmetry, etc.*
  2. construct potential energy $V(Q)$ and collective inertia parameters
  3. solve the equations of motion of $Q$ to get fission observables 
     *lifetime, fragment mass/charge distribution, etc.*

- Approaches based on the **macroscopic** model + shell correction have been successful
- **Microscopic** models are still under development
- With microscopic approaches
  - energy density functional (EDF) theory is employed
  - less phenomenological assumptions
Theories for fission

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**We aim to establish a microscopic theory for description of the fission process**
Microscopic models

1. Static approach → talk by S.A. Giuliani

- With energy density functional theory (Skyrme, Gogny, RMF)
- Fission paths on the potential energy surface given by constrained mean-field calculations
- Relevant DOF? Mass parameter?
- Dynamics is not fully treated
2. Dynamical approaches

TDHF (Time-dependent Hartree-Fock)

- No need to select collective DOFs and compute mass parameters
- Fully non-adiabatic
- Collective motions are nearly classical
- No spontaneous symmetry breaking

TDGCM (Time-dependent generator coordinate method)

- Quantum treatment of collective degrees of freedom
- Relevant DOF? Mass?
- Numerical cost rises rapidly with number of collective DOFs


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Our method

TDHF $\rightarrow$ Stochastic mean field (SMF) theory

- No need to select collective DOFs
- Fully non-adiabatic
- Quantum fluctuations by initial-state sampling
- Symmetry breaking

$\rightarrow$ microscopic and dynamical description of fission

S. Ayik, PLB658, 174 (2008)
Stochastic mean-field theory

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- Quantum fluctuation at $t = 0$ is taken into account by random sampling of one-body density matrix $\{\rho^{(n)}\}$

$$\rho^{(n)}(t = 0) = \rho^{(n)}(t = 0) + \delta \rho^{(n)} = \frac{1}{N} \sum_{n=1}^{N} \rho^{(n)}(t = 0) + \delta \rho^{(n)}$$

- Evolution of a quantum wave packet is simulated by an ensemble of classical (TDHF) trajectories

$$i\hbar \dot{\rho}^{(n)} = [h[\rho^{(n)}], \rho^{(n)}]$$

- Expectation values and dispersions of one-body observables

$$\langle Q \rangle \rightarrow \overline{Q^{(n)}} = \overline{\text{Tr}[\rho^{(n)}Q]}$$
$$\langle Q^2 \rangle - \langle Q \rangle^2 \rightarrow \overline{Q^{(n)2}} - \overline{Q^{(n)}}^2$$
Stochastic mean-field theory

- Quantum fluctuation at $t = 0$ is taken into account by random sampling of one-body density matrix $\{\rho^{(n)}\}$

$$
\rho^{(n)}(t = 0) = \rho^{(n)}(t = 0) + \delta \rho^{(n)}
$$

If the initial many-body state is a Slater determinant:

- Configuration-mixing effect
- Symmetries breaking

$$
\delta \rho_{i,j}^{(n)} = 0
$$

$$
\frac{\delta \rho_{i,j}^{(n)} \delta \rho_{i',j'}^{(n)}}{\delta \rho_{i,j}^{(n)} \delta \rho_{i',j'}^{(n)*}} = \frac{1}{2} \delta_{ii'} \delta_{jj'} [n_i (1 - n_j) + n_j (1 - n_i)]
$$

$$
\rho_{i,j}^{(n)}(t = 0) = \delta_{i,j} n_i + \delta \rho_{i,j}^{(n)}
$$
Stochastic mean-field theory

An application to an exactly solvable model

\[ H = \varepsilon J_z - \frac{V}{2} (J_+^2 + J_-^2) \]

\[ J_z = \frac{1}{2} \sum_{p=1}^{N} \left( c_{+p}^\dagger c_{+p} - c_{-p}^\dagger c_{-p} \right) \]

\[ J_\pm = \sum_{p=1}^{N} c_{\pm p}^\dagger c_{\mp p} , \]

Lacroix, Ayik, and Yilmaz, PRC 85, 041602(R) (2012)

Quasi-spin of Lipkin model with SMF

TDHF: nothing happens
Application to spontaneous fission of $^{258}$Fm

- Interaction: SLy4d + pairing
- $\delta \rho_{ij}$ is truncated within a window $\Delta \varepsilon$ around $\varepsilon_F$

$$\rho_{ij}^{(n)}(t = 0) = \delta_{ij} n_i + \delta \rho_{ij}^{(n)}$$
Total kinetic energy and fragment mass

- Width of distribution is reasonably reproduced
- Peak position is shifted from TDHF value
- Does not reproduce the asymmetric shape of TKE distribution

Wilkins et al., PRC14, 1832 (1976)
Deformation of fragments

“Projection” of motion of wavepacket onto certain collective subspace

- Quadrupole deformation is relaxed after scission
- Octupole deformation oscillates after scission
Summary and perspectives

- **Aim:** Fully microscopic and dynamical description for fission
- **We applied the SMF theory to take into account the quantum fluctuations missing in TDHF**
  - fluctuation of $\rho_{ij}$ is introduced at $t = 0$ by random sampling
  - spontaneous fission of $^{258}\text{Fm}$: possible to obtain realistic TKE and fragment-mass distributions

- Induced fission
- Initial fluctuation determined from GCM calculation
- Systematic calculations
With and without dynamical pairing
Evaporation of particles

![Graph showing the probability of neutron and proton evaporation](image)

- **Neutron**
- **Proton**

**Axes:**
- **$P(N_{\text{fin}})$ (%)**
- **$N_{\text{fin}}$**

**Legend:**
- Pink bars: Neutron
- Blue bars: Proton
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