Real time description of fission

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Outline

- Overview of the fission process
- Dynamic models for fission
- Time-dependent density functional theory (TDDFT)
- Fission results from TDDFT
- Overview and outlook
Goals

- Understand fission from a microscopic model
- Estimate the validity of different approximations used in more phenomenological approaches
- Obtain trends of different observables that cannot be measured

Not a goal: perfect agreement with experiment at this point
Fission process


All the information about fission (FF, prompt neutrons and gammas) comes after neutron emission.

Goennenwein, talk at FIESTA 2014
Model and experiment: excitation energy dependence

Excitation energy sharing between fragments varies with excitation energy in the fissioning system.

- No much experimental information
- Directly connected with the average spin in the FF
- No direct connection with the excitation energy

New experimental results presented at FIESTA2017

Navqi et. al., PRC 34 (1986) 218
Fission observables goals

Fission fragment distributions of:

- mass
- charge
- TKE

Direct comparison with experiment (where available)

- angular momentum distribution
- sharing of excitation energy

Input into CGMF and comparison with prompt neutron and gamma-ray emission data

At the moment: averages of one-body observables only (extensions possible)
Fission models

- **Scission point model**
  - Static model, based on the structure of the energy surface
  - $Y(A)$
  - Low computational cost

- **Macro-micro + Langevin**
  - Based on a random walk on the energy surface
  - Classical dynamics, analog to classical model of diffusion
  - Collective Coordinate $\rightarrow$ Generalized coordinate $\rightarrow$ Conjugate momenta
  - Adiabatic approximation $\rightarrow$ "cold" FFs
  - $Y(A, \text{TKE})$
  - Low computational cost

- **DFT + TDGCM**
  - Based on DFT
  - Adiabatic approximation
  - $Y(A, \text{TKE})$
  - Moderate-high computational cost

- **TD-SLDA**
  - Based on a time-dependent formulation of the superfluid-local-density approximation
  - $Y(A, \text{TKE}, E^*_L, E^*_H, J_L, J_H)$
Density functional theory

For any Hamiltonian

\[ H = \sum_i^A T(i) + \sum_{i<j}^A V_{ij} + \sum_{i<j<k}^A V_{ijk} + \ldots + \sum_i^A V_{ext}(i) \]

There is an **exact** one to one correspondence between the many-body wave function, the external field and the density. The ground-state energy of the system can be obtained by minimizing a **universal** EDF

\[ E_0 = \min_{\rho(\vec{r})} \int d^3r \left( \frac{\hbar^2}{2m} \tau(r) + \mathcal{E}[\rho(\vec{r})] + V_{ext}(\vec{r})\rho(\vec{r}) \right) \]

The DFT we use is phenomenological and **local**

\[ \left( -\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) + V_{ext}(\vec{r}) \right) \phi_n(\vec{r}) = \epsilon_n \phi_n(\vec{r}) \]

\[ \tau(\vec{r}) = \sum_n |\nabla \phi_n(\vec{r})|^2 \]

\[ \rho(\vec{r}) = \sum_n |\phi_n(\vec{r})|^2 \]

For superfluid systems, we use a local pairing field \( \Delta(\vec{r}) = -g(r) \nu^*(\vec{r}) \) and the equations are formally equivalent to HFB/BdG.
Time-dependent density functional theory implementation for local functionals

\[
\begin{align*}
&i\hbar \frac{\partial}{\partial t} \begin{pmatrix}
  u_\uparrow \\
  u_\downarrow \\
  v_\uparrow \\
  v_\downarrow
\end{pmatrix} = \\
&\begin{pmatrix}
  h_{\uparrow\uparrow} - \mu & h_{\uparrow\downarrow} & 0 & \Delta \\
  h_{\downarrow\uparrow} & h_{\downarrow\downarrow} - \mu & -\Delta & 0 \\
  \Delta^* & 0 & -h^*_{\uparrow\uparrow} & -h^*_{\downarrow\downarrow} \\
  0 & -\Delta^* & -h^*_{\downarrow\downarrow} & -(h^*_{\uparrow\downarrow} - \mu)
\end{pmatrix} \begin{pmatrix}
  u_\uparrow \\
  u_\downarrow \\
  v_\uparrow \\
  v_\downarrow
\end{pmatrix}
\end{align*}
\]

- Lattice implementation on a 3D special lattice (continuum well represented)
- Fully self consistent
- No symmetry restrictions
- Requires somewhat large computational resources:
  - Adams-Bashforth-Milne fifth order predictor-corrector-modifier
  - FFTW for derivatives
  - Number of equations solved ~ number of lattice points (from thousands to 1-2 million)

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General applications of TD-DFT

- Description of structure, creation and decay of quantized vortices in Fermi superfluids
- Microscopic description of incipient phases of quantum turbulence in Fermi superfluids, crossing and recombination of vortices
- Creation of domain walls, quantized vortices and vortex rings, their dynamics and decay; quantum shock waves
- Microscopic description of quantized vortices in neutron matter
- Interaction of quantized vortices with nuclei in neutron star crust
- Coulomb excitation of nuclei
- **Nuclear fission**
- Collisions of heavy nuclei
Fission fragments from TDSLDA for $^{240}$Pu*

- Large number of initial conditions, but small dispersion (focusing effect)
- Different energy sharing mechanism for neutron-induced and spontaneous fission (mass yields significantly different)

Comparison with TDHF+BCS

- Our calculation does not support the large width of the mass distribution due to initial conditions

Tanimura et. al, PRL 188, 152501 (2017)
**Strong one-body dissipation**

- Saddle-to-scission: viscous fluid, with the trajectory following predominantly the steepest descent => microscopic justification of the overdamped Brownian motion approach (Moller and Randrup)

- Langevin dynamics should be driven by force given by the gradient of the free energy:

\[ F_Q = -\nabla (E_{int} - TS(Q, T)) \]

(generalization of the work by Ward et. al., PRC 95, 024618 (2017))
Evidence for neutron emission during scission/acceleration

Robust independence of the initial conditions and nuclear energy density functional used

$^{240}\text{Pu}$
Summary and outlook

- In nuclear physics, TD-SLDA applied to the description of
  - Linear response: IVGDR
  - LACM: Relativistic Coulomb Excitation of a heavy nucleus and FISSION
- Encouragingly accurate description of fission observables (not perfect)
- The spread in initial conditions are not enough to explain the observed widths in mass yields
- Strongly overdamped motion, strong one-body dissipation
- Evidence for emitted neutrons at scission and during the acceleration

- Investigation of other observables (e.g., angular momenta)
- Fluctuations
Additional slides
Yields in \((n,f)\) vs. \((sf)\)

- Both model (Möller) and data show wider \(Y(A)\) in \((n,f)\)
- \(Y(A)\) for \((sf)\) are sharply peaked near \(N=82\) closure!

Avg. \(E_\gamma\) increase is a property of products \(\rho\), \(J^{\pi}\), and \(U^*\)

Courtesy P. Jaffke