Three ways to describe nuclear dynamics with energy density functional

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[7]Physics Department, Tennessee Technological University, Cookeville, USA

Why treating explicitly the dynamics ?

Two ways to tackle a quantum problem

$$H\psi = E\psi$$

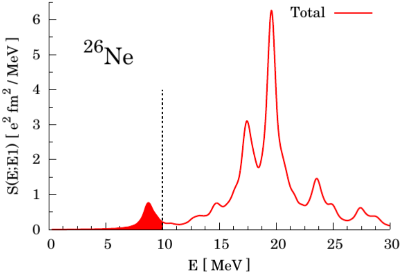
Costly full diagonalization $\Longrightarrow$ dynamics for any initial condition

$$i\hbar\partial_t\psi = H\psi$$

No need for the full Hilbert space $\Longrightarrow$ dynamics for one initial condition only

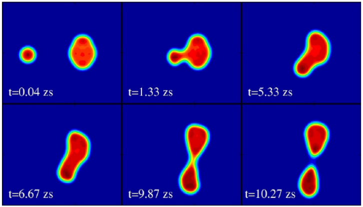
Sucessfull applications of dynamical approaches

- Vibration modes: gamma strength function
- Fission: yields, fragments observables
- Heavy ion collision: fusion barriers, nucleon transfer, fusion/fission versus quasi-fission

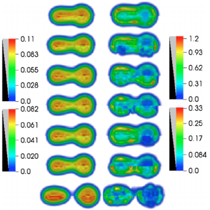


Ebata *et al.*, PRC 90 (2014)

Progress of the time dependent mean field approaches



Quasi-fission of ^{40}Ca+^{238}U, Oberacker *et al.*, PRC 90 (2014)



Scission of ^{240}Pu, Bulgac *et al.*, PRL 116 (2016)

Major improvements in the last few years:

- Unrestricted spatial symmetries
- Inclusion of the pairing correlations

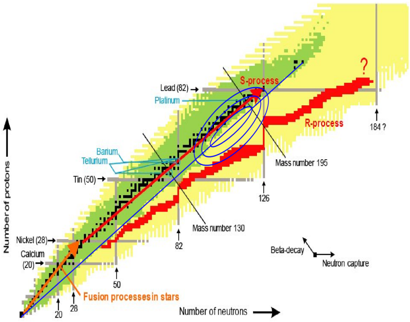
Method	Cost (10-20 zs)
TDHF	few days, few CPU
TDBCS	1 week, few CPU
TDHFB	10h, 1700 GPU

Recent achievements

- Understanding the role of quasi-fission in ^{40,48}Ca+^{238}U
- Prediction of the energy sharing between reaction products

Some general goals/challenges for dynamical approaches

- Fission yields of exotic system involved in the r-process
- Transfer reactions in sub-barrier heavy ion collisions
- Quest to super-heavy production
- Cluster radioactivity of super-heavy nuclei
- Dissipation of collective vibrations



What is the current status of time-dependent approaches based on energy density functionals ?

Two illustrative examples:

1. Fission dynamics
2. Collisions between two superfluid nuclei near the Coulomb barrier

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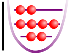
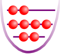
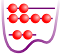
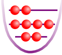
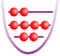
1: Choosing an *ansatz* for the many body state

- The nucleus is described by a quantum state $|\psi(t)\rangle$
- The degrees of freedom are the nucleons

	Single reference EDF Mean-field	Multi-reference EDF
Static	$\lvert\psi\rangle =$ |  $\rangle$	$\lvert\psi\rangle = f_1$ |  $\rangle + f_2$ |  $\rangle + \cdots$ $\lvert\psi\rangle = \int_q f(q)\lvert\phi(q)\rangle dq$
Time dependent	$\lvert\psi(t)\rangle =$ |  $(t)\rangle$	$\lvert\psi(t)\rangle = \int_q f(q,t)\lvert\phi(q,t)\rangle dq$ $\lvert\phi(q,t)\rangle = \lvert\bar{\phi}(q)\rangle \implies \text{TDGCM}$ $\lvert\phi(q,t)\rangle = \prod_i^A a_i^\dagger(t)\lvert 0\rangle \implies \text{MC-TDHF}$

\|  $\rangle$ = Slater determinant (HF)
Quasiparticule vacuum (HFB)

2: Getting the dynamics from a variational principle

The dynamics derives from the stationarity of the Dirac-Frenkel action:

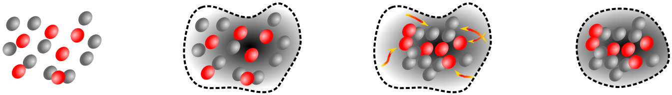
$$\delta S = 0, \quad S = \int_{t_0}^{t_\infty} \langle \psi(t) | \hat{H} - i\hbar\partial_t | \psi(t) \rangle dt \tag{1}$$

$\Longrightarrow$ optimal evolution given the *ansatz*

Example: TDHF, a set of coupled 1-body Shrödinger equations

$$i\hbar\frac{\partial}{\partial t}\begin{bmatrix} \phi_1(\mathbf{r},\sigma,t) \\ \dots \\ \phi_n(\mathbf{r},\sigma,t) \end{bmatrix} = \begin{bmatrix} h[\rho]\phi_1(\mathbf{r},\sigma,t) \\ \dots \\ h[\rho]\phi_n(\mathbf{r},\sigma,t) \end{bmatrix}$$

$\phi_i(\mathbf{r},\sigma,t)$: 1-body wave function
$h[\rho]$: mean field Hamiltonian



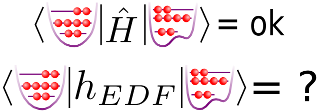
Comment on EDF versus Hamiltonian

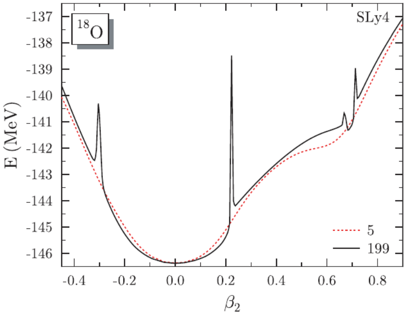
Using directly the bare n-n interaction is problematic:

- hard-core of the interaction
- huge numerical cost of 3-body forces

In practice: effective interaction / energy density functional (EDF) that accounts for the medium effects for a given *ansatz*: Skyrme, Gogny, Relativistic functionals.

An issue with the multi-reference EDF formalism





M. Bender et. al., PRC 79 (2009)

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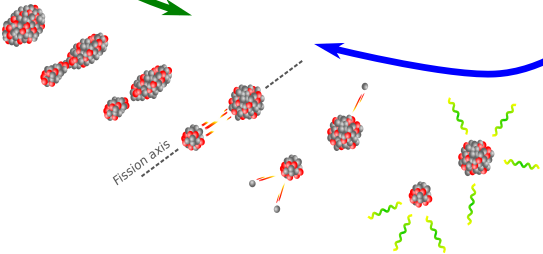
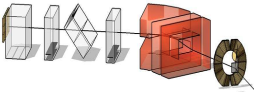
Probing the fission dynamics

Many-body calculations based on energy density functional

Fission time scale ?
Scission neutron ?
Fragments characteristics ?
Fragments deexcitation ?



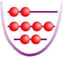
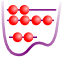
VAMOS@GANIL
SOFIA@GSI
SPIDER@LANL
Fission@ALTO
...



0	10^{-20}	10^{-18}	10^{-15}	10^{-6}	t (s)
Scission	90% KE	Prompt n emission	Prompt γ and internal conversion	β^- decay, delayed n and γ	

Time Dependent Generator Coordinate Method (TDGCM)

A multi-reference EDF ansatz

$|\psi(t)\rangle = f_1(t)\,|$  $\rangle + f_2(t)\,|$  $\rangle + \cdots$

Constrained HFB solutions with ≠ shapes,
time independent

A two step process:

1. Generate an ensemble of deformed quasi-particule vacua $|\phi_q\rangle$
2. Solve the evolution equation for the mixing function $f(q,t)$
   - Here we use the Gaussian overlap approximation
     $\Longrightarrow$ a local Schrödinger like equation

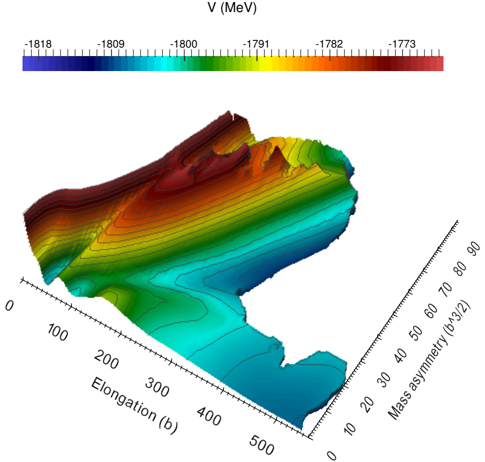
A fully quantum-mechanical description of the time evolution

Gives the amplitude of probability for the nucleus to have a given shape at time t.

Time Dependent Generator Coordinate Method (TD-GCM)

Example of a n + ^{239}Pu fission

1. Choose the collective variables:
   - elongation (Q_{20} in b),
   - mass asymmetry (Q_{30} in $b^{3/2}$)
2. Calculate potential energy surface and inertia tensor
3. Define initial wave packet for the probability amplitude
4. Compute time evolution of probability amplitude
5. Extract fission fragment distribution by computing the flux of the probability amplitude across the scission line



Potential energy surface for (n+^{239}Pu) fission

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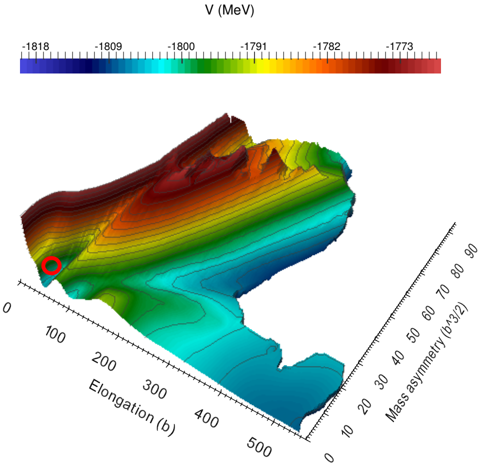

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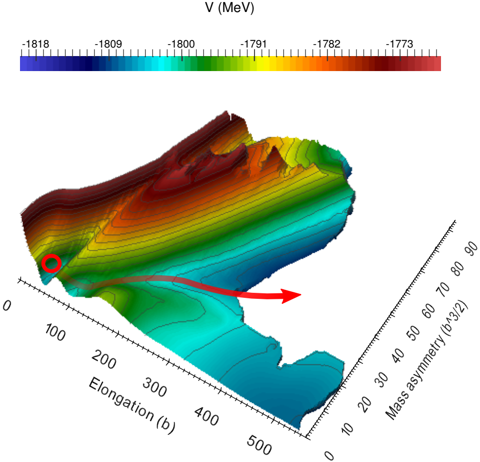

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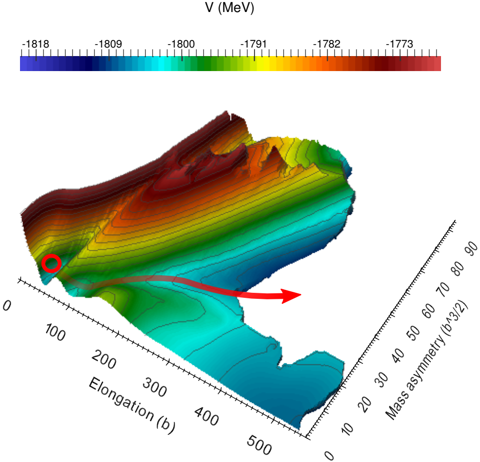

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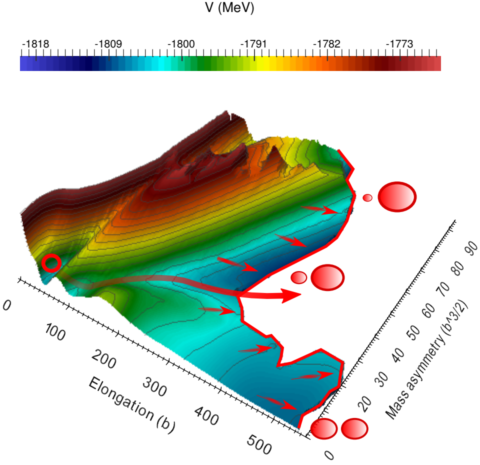


Potential energy surface for (n+^{239}Pu) fission

Development of this microscopic approach

2005: First calculation for ^{238}U

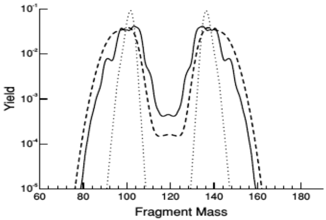
H. Goutte *et al.*, PRC **71**, 024316 (2005)

2012: Fission yields of ^{236}U and ^{240}Pu

W. Younes *et al.*, LLNL-TR-586678 (2012)

- Promising results
- High numerical costs

2D PES	40000 HFB states
Dynamics	10 zs ($10^{-21}s$)



Pre-neutron mass yields for ^{238}U at 2.4 MeV above the fission barrier (H. Goutte *et al.*).
solid line: dynamics calculation
dashed line: Whal evaluation (2002)

Upgrade numerical methods

Gaussian process to speed up HFB solver

FELIX-1.0

D. Regnier *et al.*, CPC **122**, 350-363 (2016)

FELIX-2.0

D. Regnier *et al.*, CPC **225**, 180-191 (2018)

Recent applications

Fission of ^{240}Pu, ^{252}Cf, ^{226}Th, Fm

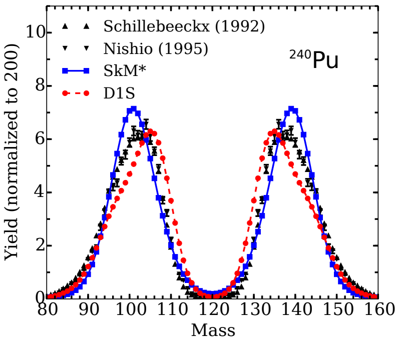
A. Zdeb *et al.*, PRC **95**, 054608 (2017)

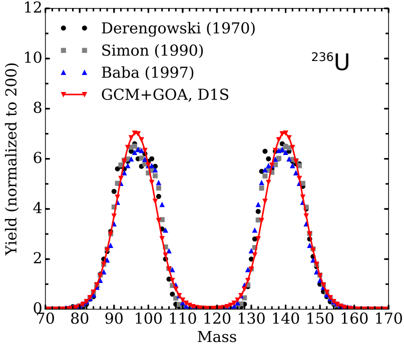
H. Tao *et al.*, PRC **96**, 024319 (2017)

J. Zhao *et al.*, PRC **99**, 014618 (2019)

D. Regnier *et al.*, PRC **99**, 024611 (2019)

Primary fragments mass yields for low energy fission of actinides

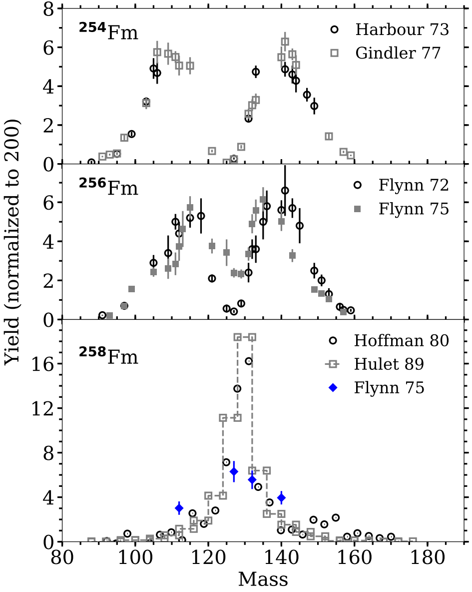




- The initial energy is taken 1 MeV above the fission barrier.
- The raw flux results are convoluted with a Gaussian of width $\sigma = 4$.

- The qualitative reproduction of the asymmetric fission of actinides is robust.
- A better modeling of several physics effects (initial state, fragment separation) is necessary to reach a $\simeq$10% accuracy.

Fission yields in neutron rich Fermium isotopes



- **Open symbols:** Spontaneous fission
- **Full symbols:** Thermal n-induced fission
- **D1S:** Our calculation starting from 1 MeV above the fission barrier
  D. Regnier et al., PRC **99**, (2019)

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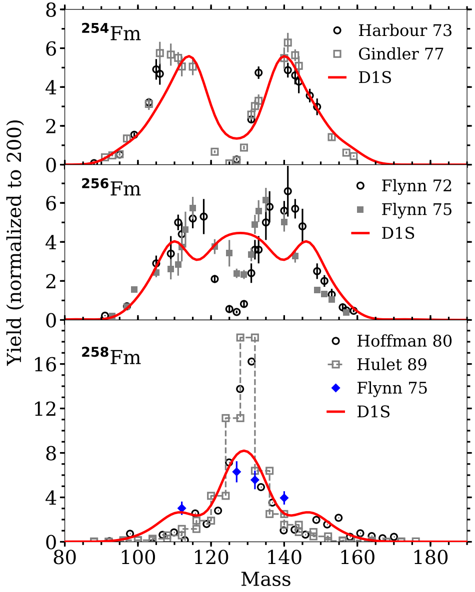

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Results

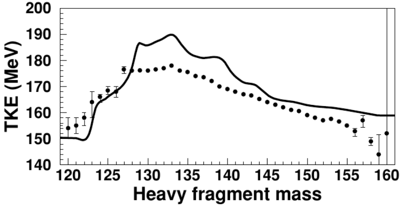
- Transition reproduced
- Difficulty with ^{256}Fm

Limitations of the current implementation of TDGCM

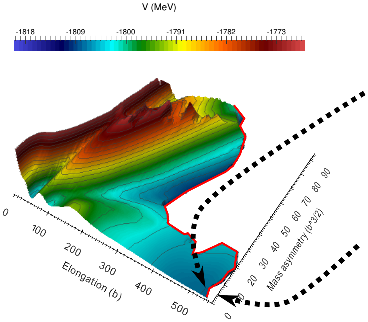
1. A mostly adiabatic dynamics
2. Lacuna in our set of generator states

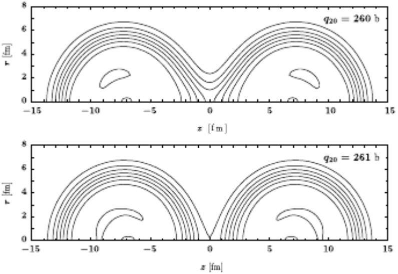
$\Longrightarrow$ Consequences:

- Missing the dynamics through scission
- Estimation of the fragments properties before complete separation

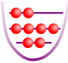


H. Goutte et al., PRC *71*, 024316 (2005)





Recovering the diabatic motion with time dependent mean-field

$$|\psi(t)\rangle = \Big|$$  $$(t)\Big\rangle$$

Recent developments:

2014: ^{258}Fm ^{264}Fm (no pairing)

C. Simenel *et al.*, PRC **89**, 031601(R) (2014)

2015: ^{258}Fm with pairing (TDBCS)

G. Scamps *et al.*, PRC **92**, 011602(R) (2015)

$\simeq$ 1 week on a few CPU

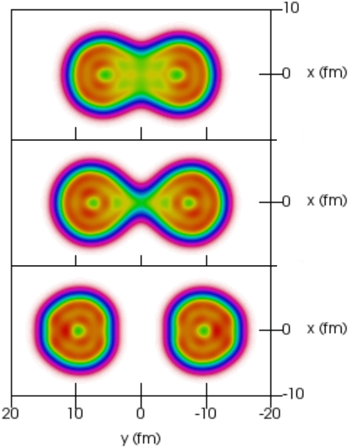
- 60 to 80% of the TXE is generated during the rapid descent to scission

2016: ^{240}Pu with pairing (full TDHFB)

A. Bulgac *et al.*, PRL **116**, 122504 (2016)

$\simeq$ 10h on 1700 GPU

- TKE reproduction within 3% for a few possible fragmentations



Density of protons for a symmetric fission of ^{258}Fm from TDBCS

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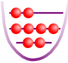
$$|\psi(t)\rangle = \Big|$$  $$(t)\Big\rangle$$

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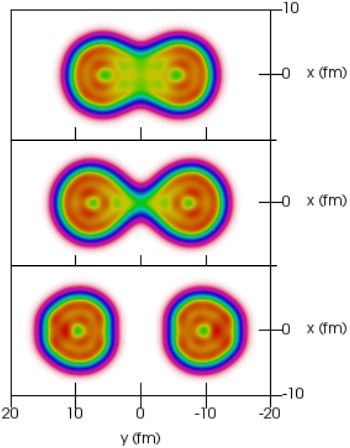

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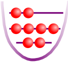
$$|\psi(t)\rangle = |$$  $$(t)\rangle$$

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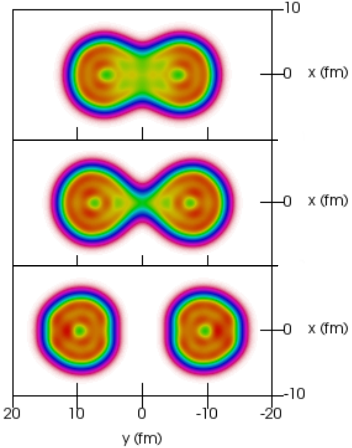


Density of protons for a symmetric fission of ^{258}Fm from TDBCS

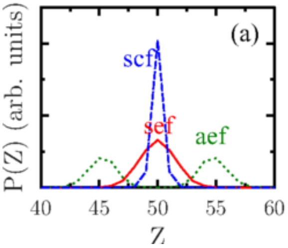
Perspectives and limitations of the time dependent mean-field picture

Up to now, only a few applications of this method to fission.
Some interesting perspectives:

- Scission neutrons
- Fragments spin

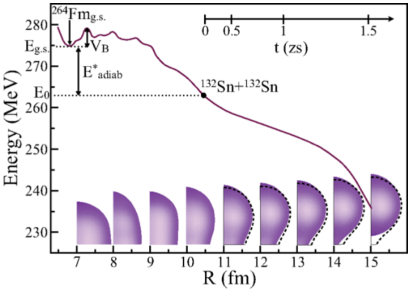
Major limitation for fission:

1. Too sharp distributions for the fragment observables (no yields)
2. No tunneling through the fission barrier



Particle distribution in the fragments for 3 TDBCS simulations of ^{258}Fm fission

G. Scamps *et al.*, PRC **92**, 011602(R) (2015)

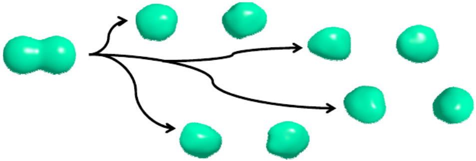


C. Simenel *et al.*, PRC **89**, 031601(R) (2014)

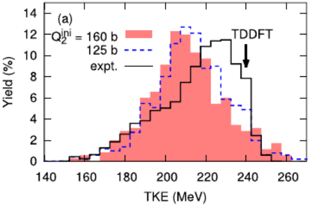
More fluctuations with the stochastic mean-field approach

Idea:

1. Generate an ensemble of one body-densities that mimic some initial quantum fluctuation
2. Evolve each density with the TDHFB equation
3. Recover distributions of final observables by classical average



Y. Tanimura *et al.*, PRL **118** (2017)



Total kinetic energy distribution of ^{258}Fm (SF)

- Possibility to compute fission fragments yields
- No tunneling through the fission barrier
- Formal issues: representativity problem, fluctuation cut off

To put it in a nutshell...

State of the art EDF methods to tackle fission dynamics:

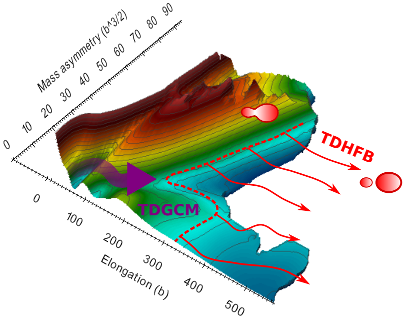
1. Time dependent mean-field with pairing
2. Stochastic mean-field
3. Time dependent GCM

Difficulty to tackle both

1. the dissipation/diabatic aspects
2. and the large quantum fluctuations.

Attempts and projects to move forwards:

- 2 quasi-particules exciated states in TDGCM
- Temperature in TDGCM
- Hybrid TDGCM + TD mean field approach ?



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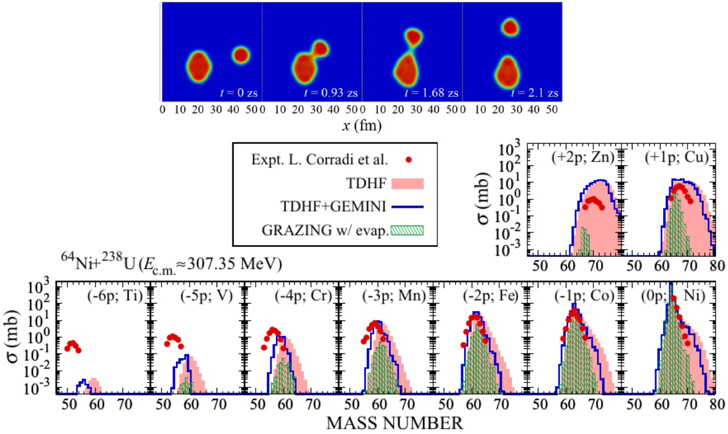
Time dependent mean-field for collisions



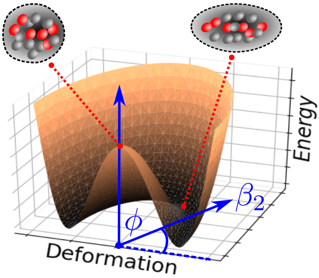
Fragment production cross section for ^{64}Ni + ^{238}U from K. Sekizawa, PRC 96 (2017)

- No need for empirical ion-ion potential
- All channels already included at the mean-field level

A mini-review: K. Sekizawa, arXiv:1902.01616

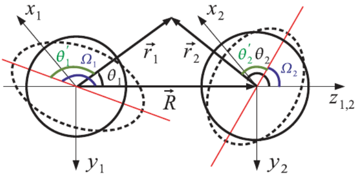
Spontaneous breaking of the rotational symmetry

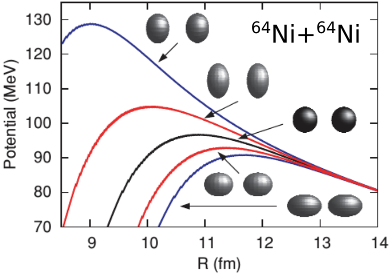
One system at the mean-field level



The physics does not depend on the orientation in space

Collision at the mean-field level



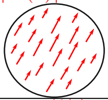
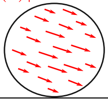


The physics strongly depends on the relative orientation

Collision between superfluid nuclei

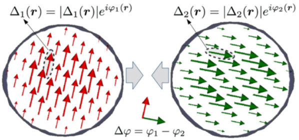
Treatment at the TDHFB level which

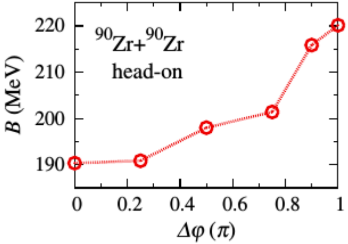
1. introduces the pairing gap $\Delta(\boldsymbol{r})$,
2. breaks the number of particle symmetry.

HFB state	Energy	Pairing field
$\|\Psi\rangle$	E_ψ	$\|\Delta(\mathbf{r})\|e^{i\theta(\mathbf{r})}$ 
$e^{i\theta_0 \hat{N}}\|\Psi\rangle$	E_ψ	$\|\Delta(\mathbf{r})\|e^{i(\theta(\mathbf{r})+2\theta_0)}$ 

The physics does not depend on the orientation in gauge space

Collision at the TDHFB level





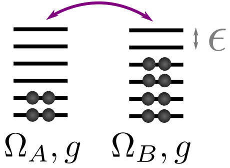
P. Magiersi *et. al* PRL 119, 042501 (2017)

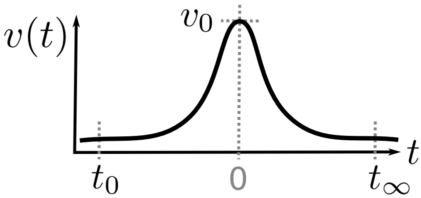
The fusion barrier varies by 30 MeV with the relative orientation

$\Longrightarrow$ How to remove this spurious effect ?

Toy model: interaction between two superfluid levels

$$V(t) = v(t) \sum_{k>0}^{\Omega_A} \sum_{l>0}^{\Omega_B} \left(a_k^\dagger a_{\bar{k}}^\dagger b_{\bar{l}} b_l + b_l^\dagger b_{\bar{l}}^\dagger a_{\bar{k}} a_k \right)$$





Hamiltonian: $H = H_A + H_B + V(t)$

- Pairing Hamiltonian $H_{A/B}$ in each system
- $\Omega_{A/B}$ twice degenerated levels in each system
- Coupling term $V(t)$ to simulate a short interaction

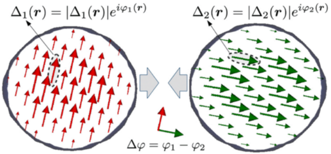
Initial state (exact)

1. Find the exact ground state for A and B with good particle number

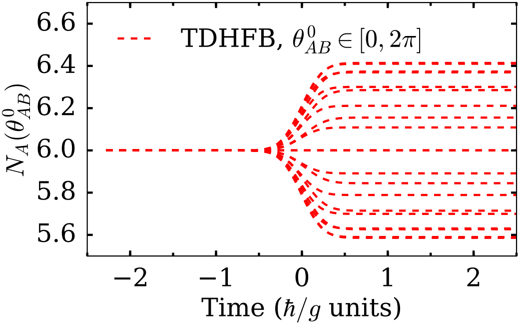
Initial state (BCS)

1. Solve the BCS equation for A and B
2. Scale the interaction (g_A, g_B, v_0) to recover the exact energy
3. Rotate one system by an angle θ^0_{AB} in the gauge space

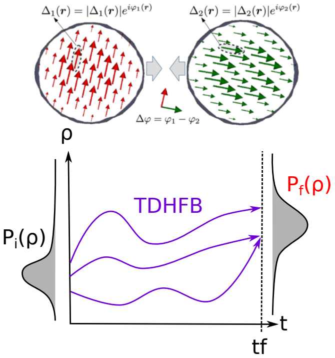
Treatment at the TDHFB level



Spurious dependency with the relative gauge angle



Transfer from a phase space averaging approach [1]



No relative gauge angle should be favored $P(\theta_{AB}) = \frac{1}{2\pi}$

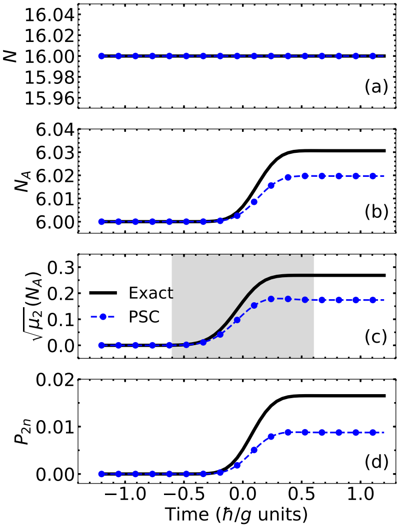
1. Initial distribution of mean field states $P_i(\rho(\theta_{AB}, t_0))$
2. Independent evolution of trajectories $\mathcal{O}[\rho(\theta_{AB}, t)] = \langle O(t) \rangle$
3. Statistical average over the final observables

$$\overline{O^k} \equiv \frac{1}{2\pi} \int_0^{2\pi} \mathcal{O}[\rho(\theta_{AB}), t]^k d\theta_{AB}$$

- No spurious components from initial fluctuation on N_A, N_B
- Fluctuations on θ_{AB} included
- No interference between trajectories (classical picture)

[1] D. Regnier *et al.*, PRC **97**, 034627 (2018)

Results with phase space averaging (PSC)



In the perturbative regime:

- semi-classical estimation of the first moments:

$$\mu_0 = 1, \quad \mu_1^{sc} \simeq \mu_1^{exa}, \quad \mu_2^{sc} \simeq \mu_2^{exa}$$

- Weak coupling:

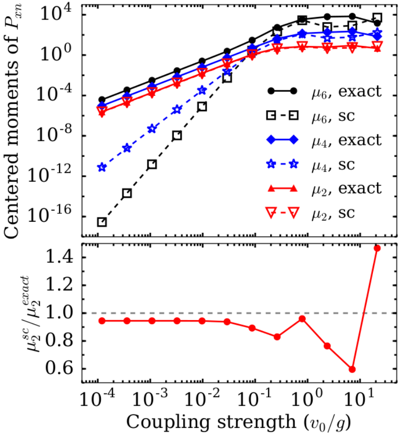
$$P_{0n} \gg (P_{2n}, P_{-2n}) \gg (P_{4n}, P_{-4n}) \cdots$$

Simple estimate for one pair transfer:

$$\begin{cases} P_{2n} \simeq \dfrac{\mu_2 + 2\delta N_A}{8} \\ P_{-2n} \simeq \dfrac{\mu_2 - 2\delta N_A}{8} \end{cases}, \qquad (2)$$

P_{2n}, P_{-2n} from independent TDHFB trajectories

Higher moments of $P(N_A)$ from phase space averaging



Moments of the probability distribution $P(N_A)$ at final time as a function of the coupling strength v_0/g.

In the perturbative regime:

- Moment of order 2 matches the exact solution
- Higher moments underestimate the exact solution

This semi-classical approach fails to predict the probabilities of multi-pairs transfer

Another method: Multi-configuration TDHFB

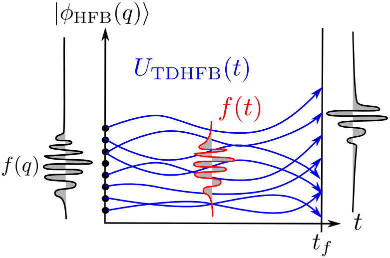
Projecting the initial state on the good number of particles in A and B:

$$|\psi(t_0)\rangle = \int_{\theta_1\theta_2} f(\theta_1,\theta_2)|\phi_{HFB}(\theta_1,\theta_2)\rangle d\boldsymbol{\theta}$$

The idea is to use the ansatz:

$|\psi(t)\rangle = f_1(t)\Big|$  $(t)\Big\rangle + f_2(t)\Big|$  $(t)\Big\rangle + \cdots$

TDHFB evolution from ≠ initial relative angles

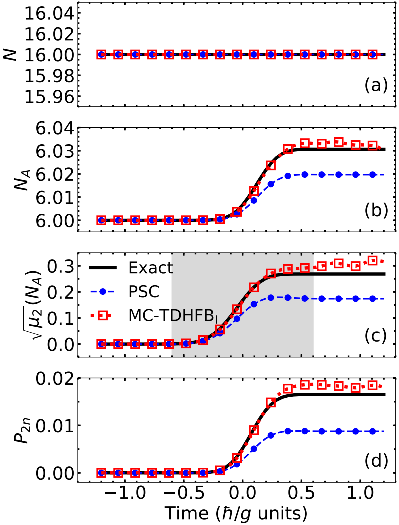


Variational determination of $f(\theta_1,\theta_2,t)$ in the ansatz:

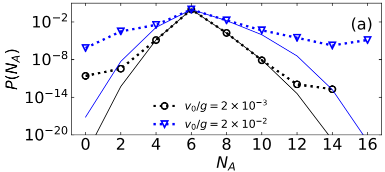
1. Projected initial wave function
2. Independent evolution of trajectories $|\phi_{HFB}(\theta_1,\theta_2,t)\rangle$
3. Evolution of the mixing function f
4. Quantum expectation of any N-body observable

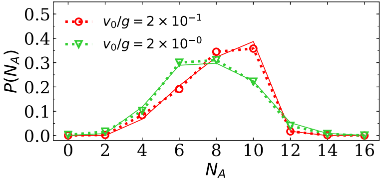
Quantum interferences between independent TDHFB trajectories

Results with Multi-configuration TDHFB



Full $P(N_A)$ distribution:





D. Regnier, et al. arXiv:1902.06491 (2019)

- Better P_{2n} in the perturbative regime
- Results hold for stronger interaction between nuclei

To put it in a nutshell...

State of the art method to tackle heavy-ion collisions:

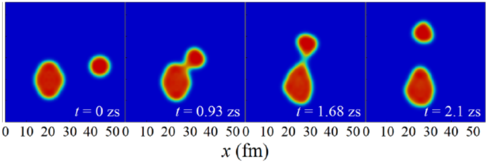
1. Time dependent mean-field (+ pairing),

Symmetry breaking introduces spurious behavior:

- Phase-space averaging to cure this issue
  - misses 40% of P_{2n}
  - fails for multi-particle transfer as well as in the non-perturbative regime

Attempts and projects to move forwards:

- Multi-configuration mixing to recover the quantum interferences
- Balian-Veneroni variational principle to recover fluctuations



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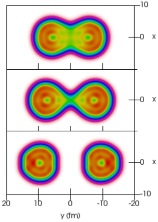
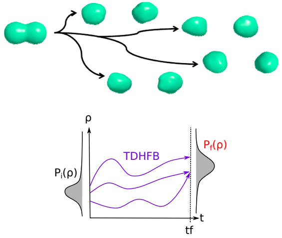
Overview of the time-dependent methods

Single reference EDF



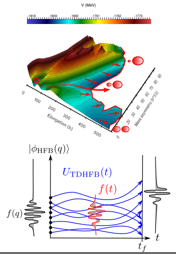
- Diabatic dynamics
- Misses collective fluctuations
- Breaks symmetries
- No collective tunnelling

Semi-classical ensemble



- More collective fluctuations (standard deviation of 1-body observables)
- Low cost, parallel algorithms
- Misses quantum interferences

Multi-configuration



- Quantum fluctuations, probability distribution
- Difficulty to get both fluctuations and diabatic motion
- High cost, parallel algorithms in some cases
- Formal issue with EDF

Thank you for your attention !

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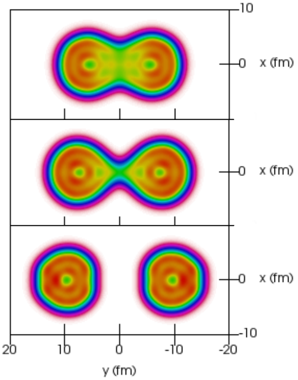
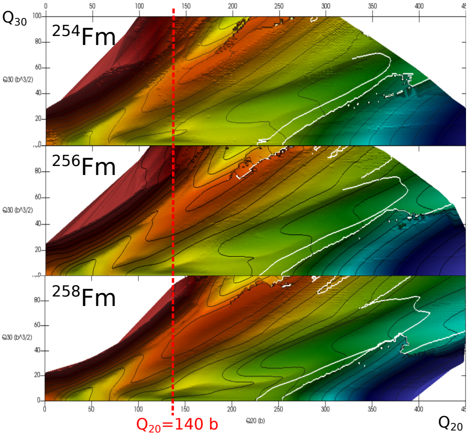
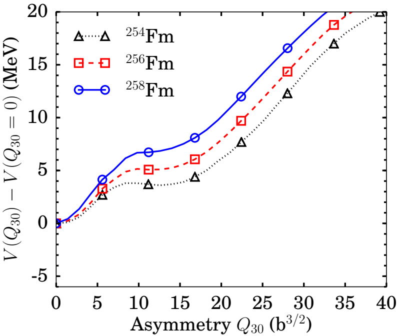
Lawrence Livermore National Laboratory

筑波大学 University of Tsukuba

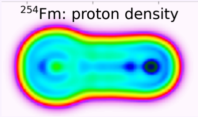


Competition between collective potential valleys



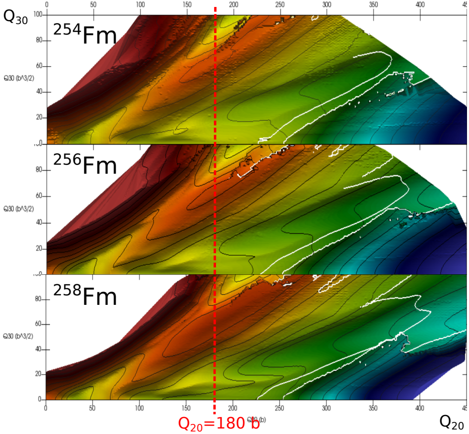


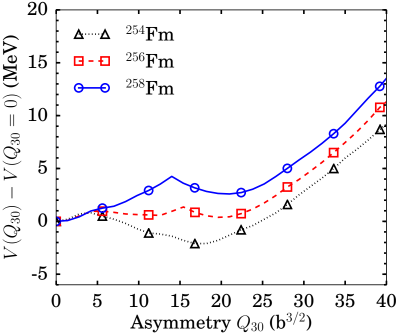
- Main fission modes driven by the static potential energy
- Dominant mode decided at rather low elongation $Q_{20} \simeq 180$ b



$Q_{20} = 180$ b, $Q_{30} = 20$ b$^{3/2}$

Competition between collective potential valleys





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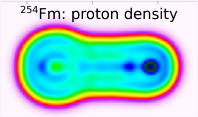

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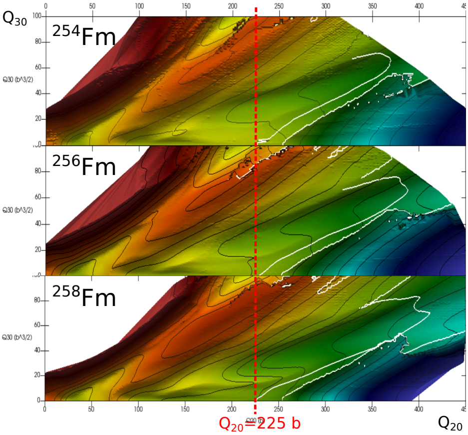

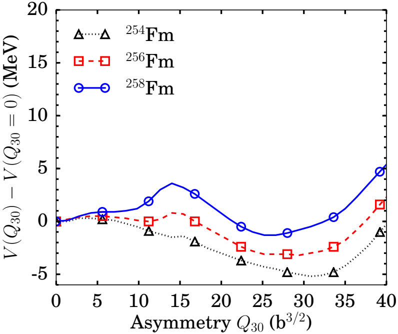

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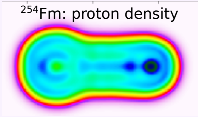
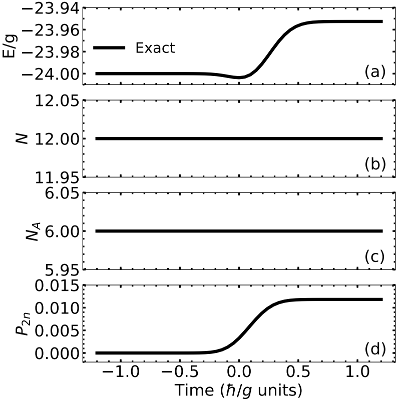


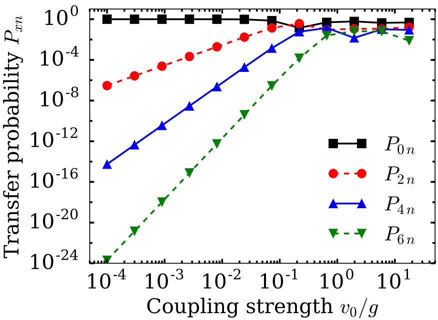
$Q_{20} = 180$ b, $Q_{30} = 20$ b$^{3/2}$

Exact transfer probabilities

Case of a symmetric reaction: $\Omega_A = \Omega_B = 6$, $N_A^0 = N_B^0 = 6$.



Evolution of some observables for a weak coupling between A and B ($v_0 = 2 \times 10^{-2} g$)



Probability of n particle transfer after the interaction, as a function of the coupling strength v_0

$\Longrightarrow$ Perturbative regime for $v_0 \leq 5.10^{-2} g$