Time dependent approaches in nuclear physics

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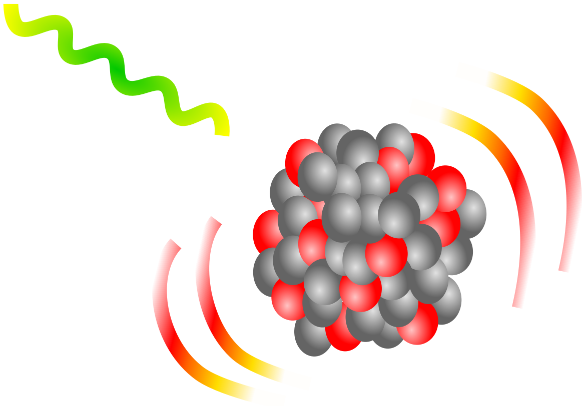
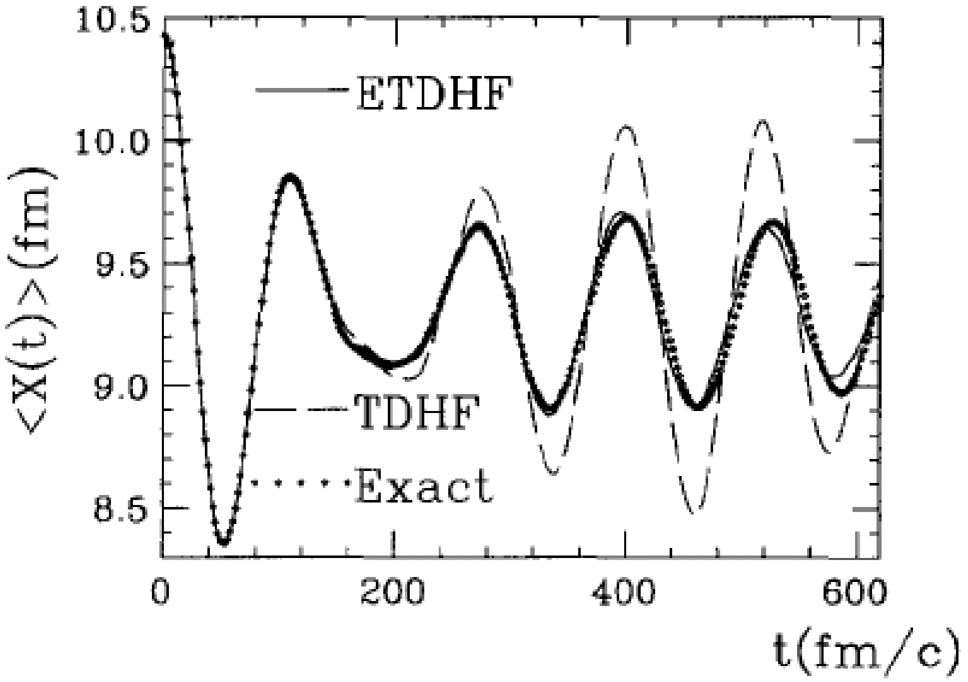
What is this course about ?

A survey of **theoretical approaches** that explicitly treat the **time evolution** of an atomic nucleus

Non equilibrium initial condition

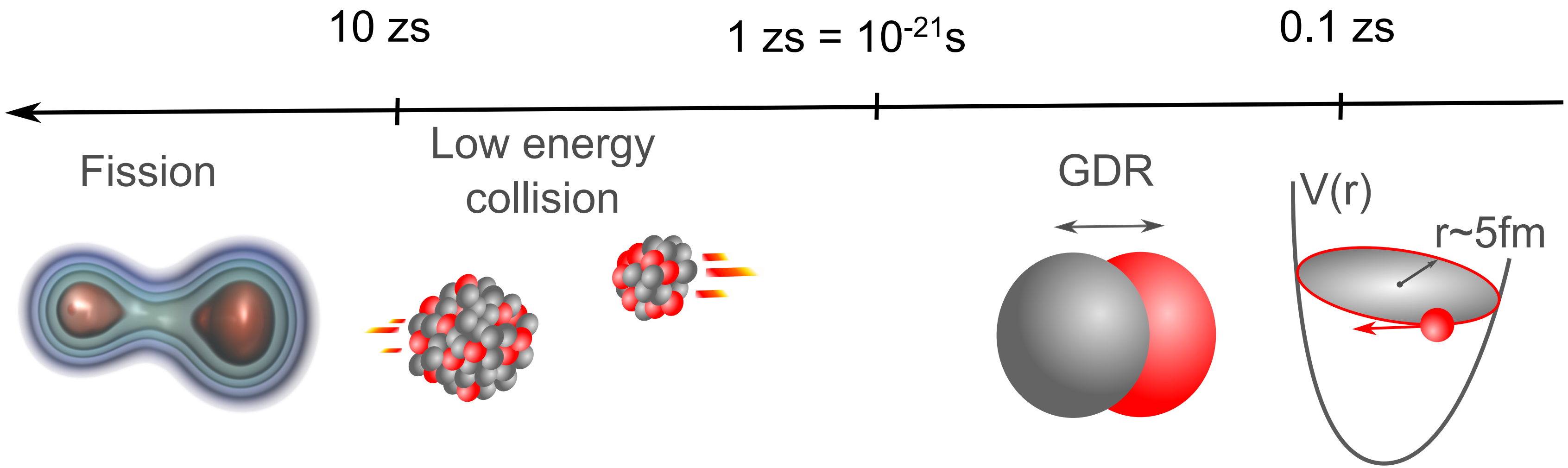


Evolution of the system in time



Nuclear time scales

- large molecule motion: 1 picosecond (10^{-12}s)
- electronic excitation: 1 femtosecond (10^{-15}s)
- shortest laser pulse: 1 attosecond (10^{-18}s)
- nuclear motion: 1 zeptosecond (10^{-21}s)



➡️ Direct measurement of a time dependent process not yet achieved

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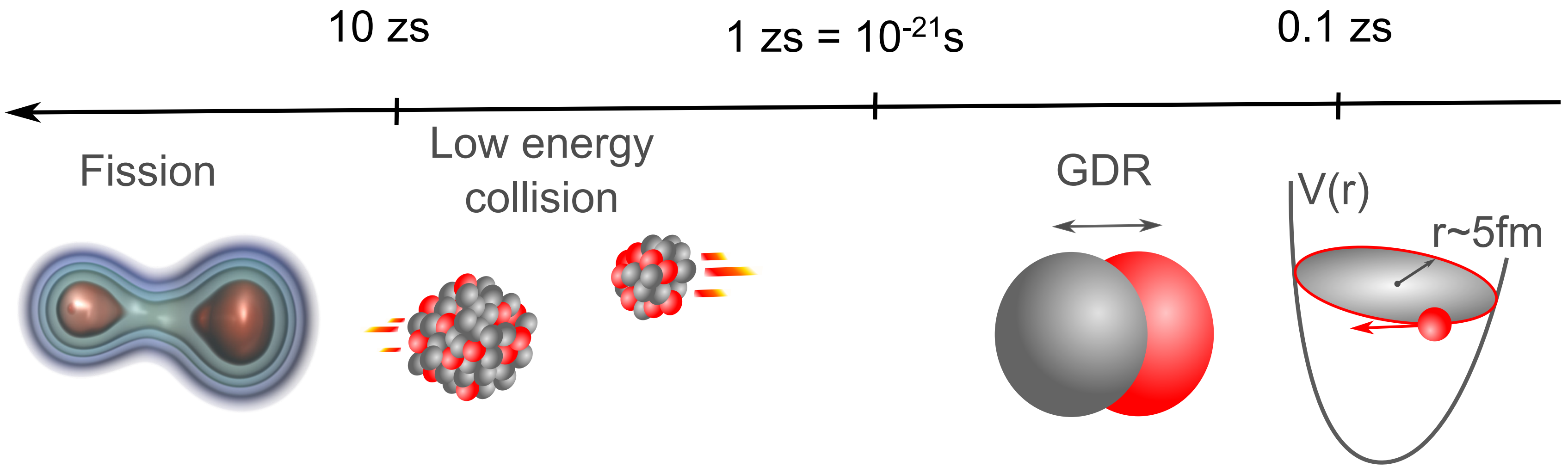

➡️ Direct measurement of a time dependent process not yet achieved

> Tip: 300 fm/c $\simeq$ 1 zs

Why treating explicitly the dynamics ?

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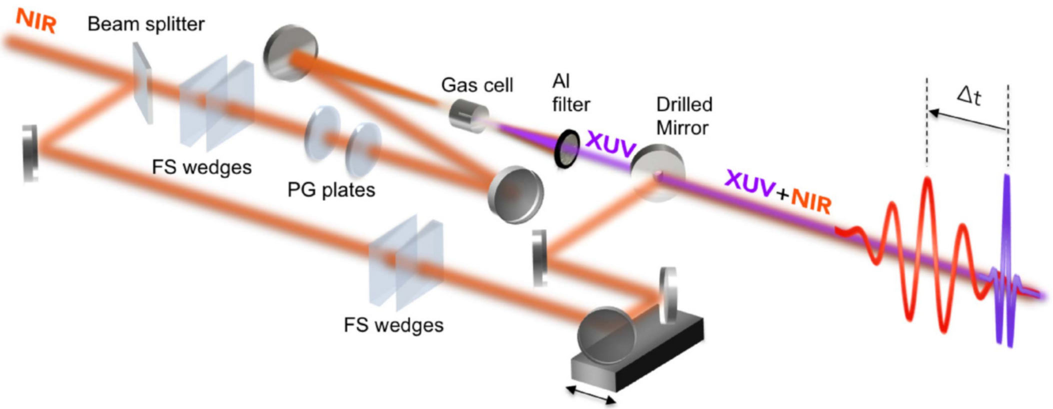
❌ To predict observables as a function of time

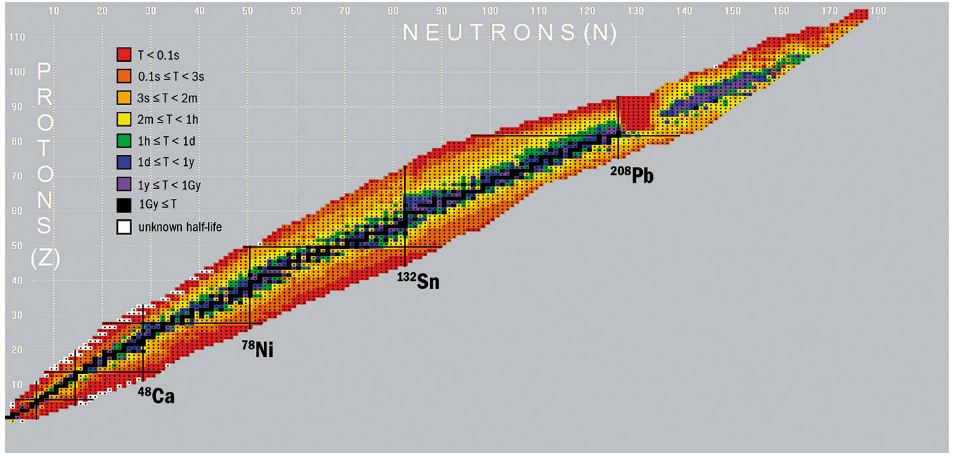
❌ To determine decay lifetimes

✅ To predict the output of reactions

- with large number of output channels,
- and collective behaviors.



Attosecond lasers, Q. Liu *et al.* J. Opt **20** (2018)



Nuclear half-lives

Static versus time-dependent Schrödinger equations

Static

$$\hat{H}\psi_n = E_n\psi_n$$

1. Full diagonalization
2. Dynamics for **any** initial condition

$$\psi(t=0) = \sum_n c_n\psi_n$$

$$\psi(t) = \sum_n c_n\psi_n e^{-i\frac{E_n}{\hbar}t}$$

Time-dependent

$$i\hbar\partial_t\psi = \hat{H}\psi$$

1. Numerical integration on time
2. Dynamics for **one** initial condition

$$\psi(t+dt) \simeq \psi(t) - \frac{i}{\hbar}\hat{H}\psi(t)$$

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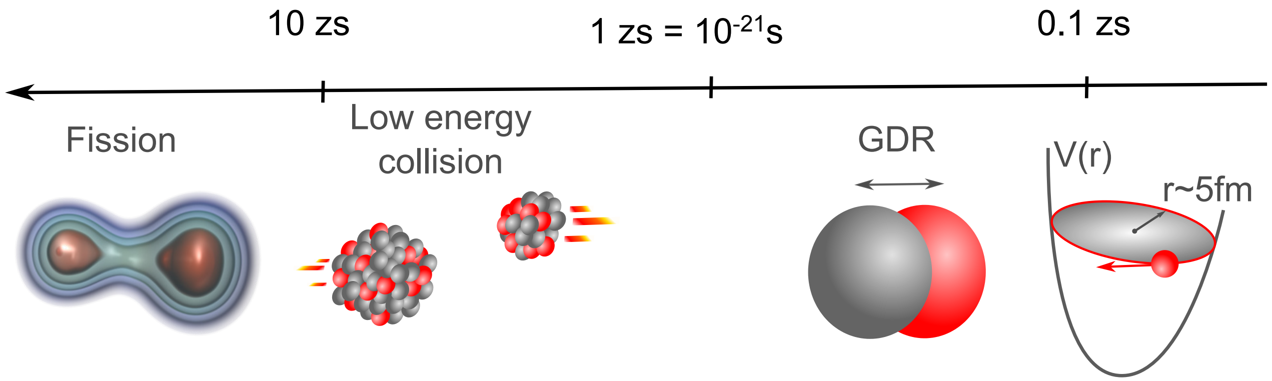
Cost $\simeq O(N_{\text{inital conditions}} \times N_{\text{steps}} \times \mathrm{dim}^2)$

- In practice, **dim >** 10^{200} (Eddington number: 10^{80} $\simeq$ **atoms in the univers**)
- Choose what **converges the fastest** to predict a specific set of observables

Which phenomena can we tackle whith dynamics ?

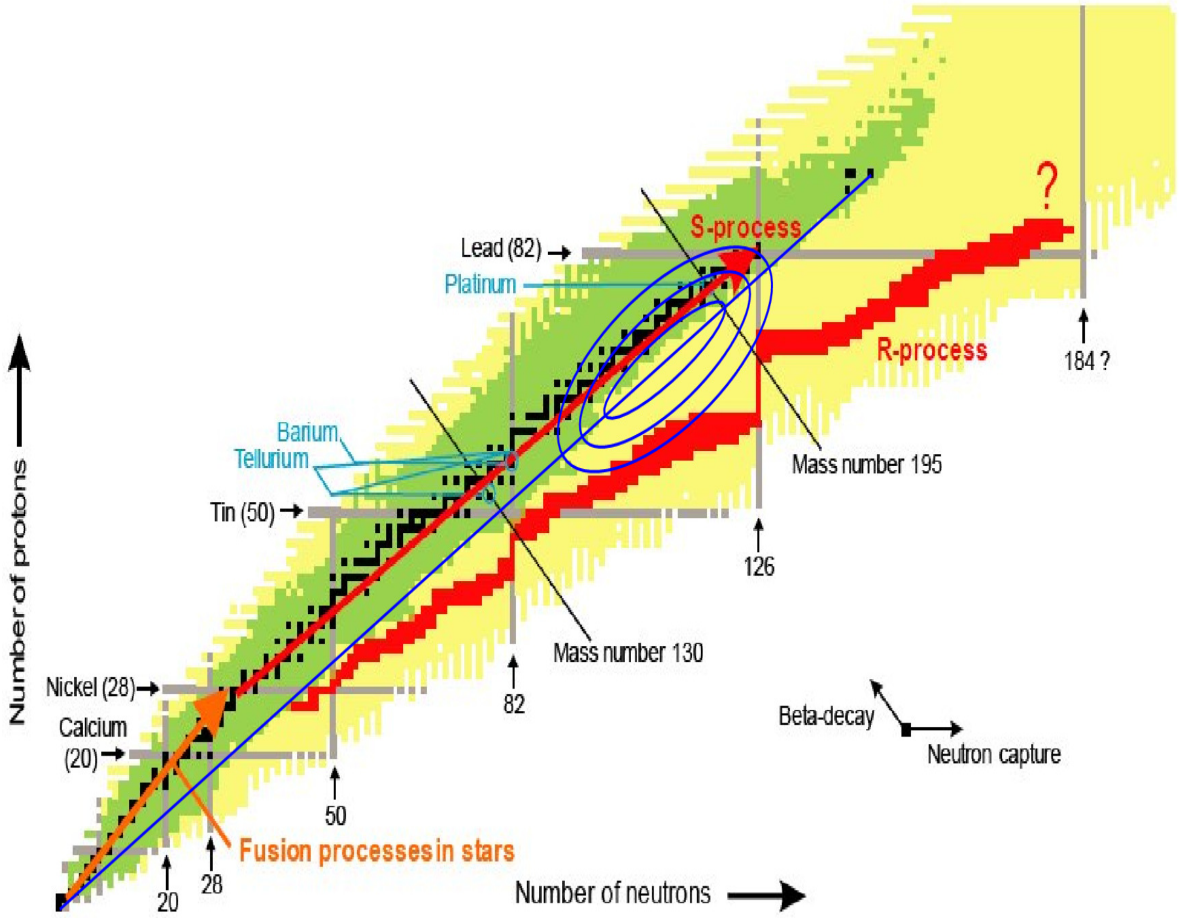
Sucessfull predictions in nuclear physics

- **Collective vibrations**:
  - response to a gamma excitation
  - cross section for (n, γ) reactions
- **Fission**:
  - mass and charge yields
  - fragments characteristics
- **Heavy ion collision (low energy)**:
  - fusion barriers
  - nucleon transfer
  - fusion/fission versus quasi-fission



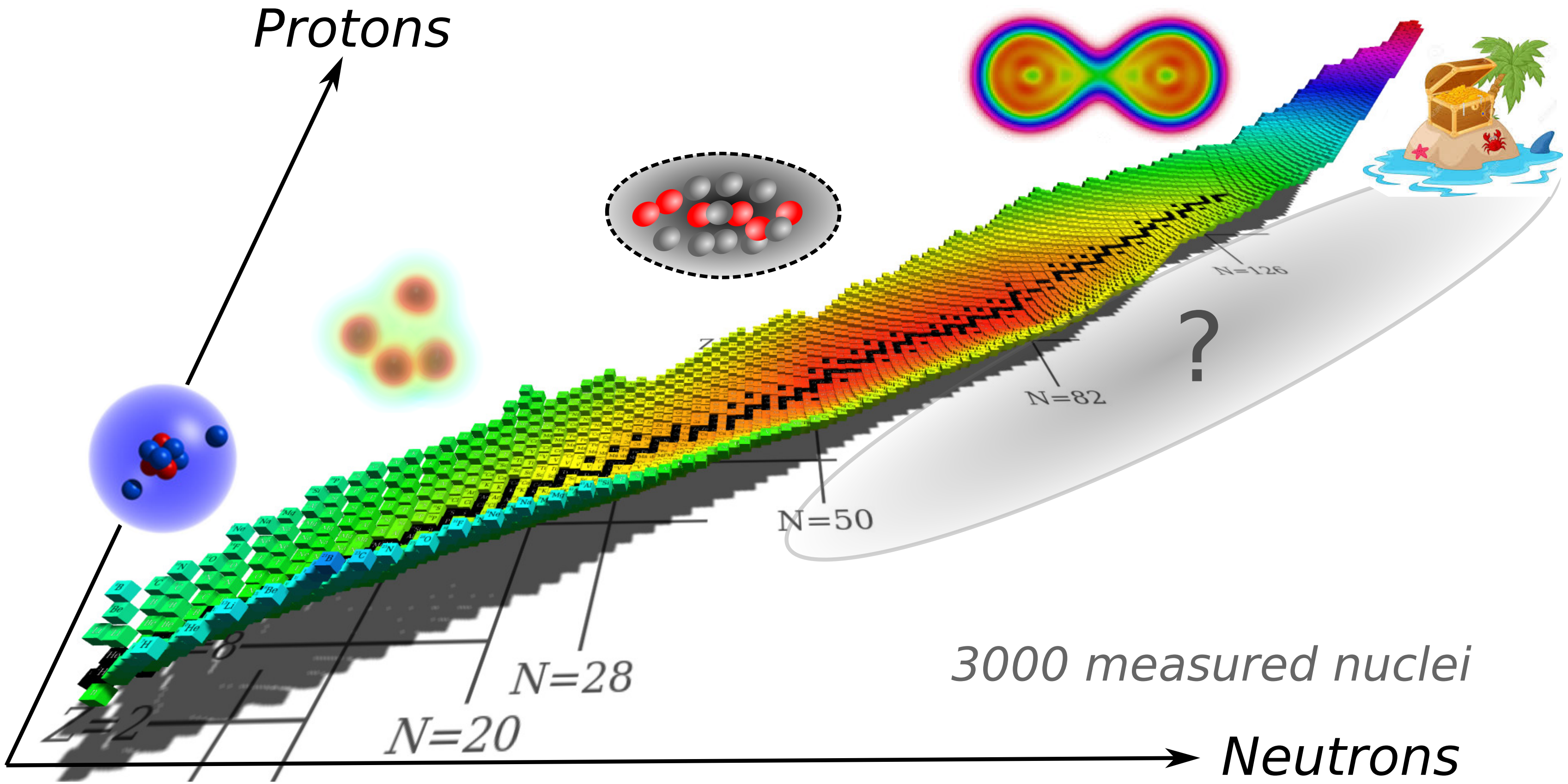
Related fundamental questions

How were the heavy elements synthetized ?

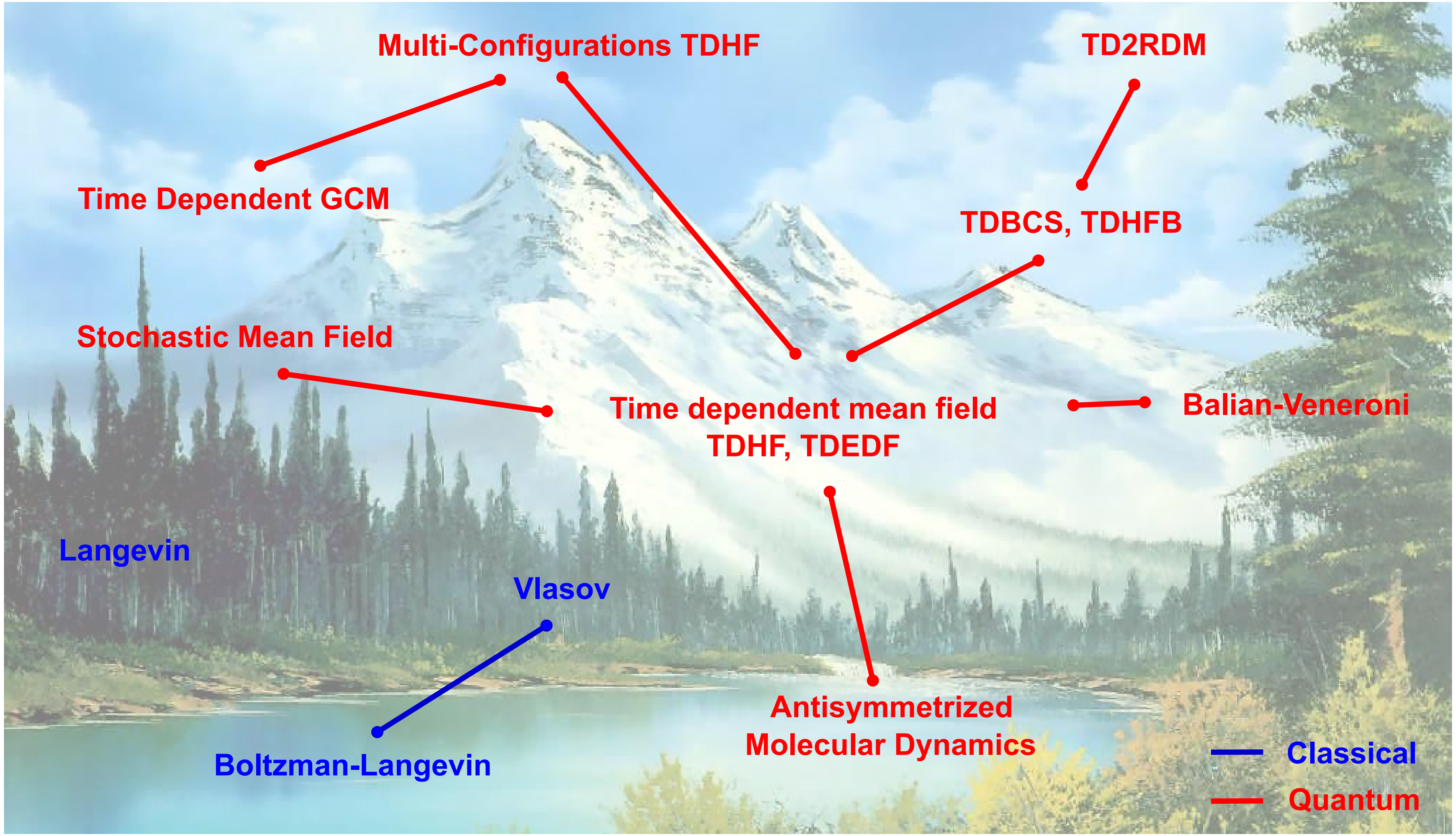


Related fundamental questions

Is there a superheavy island of stability ?



How to approximate the dynamics ?



Main references

Review papers

- Time-dependent density-functional description of nuclear dynamics
  T. Nakatsukasa *et al.*, Rev. Mod. Phys, **88** (2016)
- Heavy-ion collisions and fission dynamics with the time-dependent hartree-Fock theory and its extensions
  C. Simenel, A.S. Umar, Prog. Part. Nucl. Phys. **103** (2018)
- The time-dependent generator coordinate method in nuclear physics
  M. Verriere, D. Regnier, Front. Phys. **8** (2020)

Books

- Quantum theory of finite systems
  J.-P. Blaizot, G. Ripka, MIT Press (1985)
- The nuclear many-body problem
  P. Ring, P. Schuck, Springer science (2004)

Lectures

- Microscopic approaches for nuclear Many-body dynamics
  C. Simenel *et al.*, arXiv:0806.2714v2 (2009)

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Time dependent variational principle(s)

A state $|\psi(t)\rangle \in [t_i, t_f] \to \mathcal{H}$ is solution of the time dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle,$$

'if and only if' it makes an action $S[|\psi(t)\rangle] : [t_i, t_f] \times \mathcal{H} \to \mathbb{C}$ stationary:

$$\delta S \Big|_{|\psi(t)\rangle} = 0.$$

The simplest possible action of the system for normalized states is:

$$S[|\psi(t)\rangle, \langle\psi(t)|] = \int_{t_i}^{t_f} \langle\psi(t)|i\hbar\frac{d}{dt} - \hat{H}|\psi(t)\rangle dt.$$

Remarks:

- Stationary $\neq$ extremal or minimal
- Several choices of action yield the time dependent Schrödinger equation
- Some variational principle do not give any information on the phase or the norm of the state

P. Kramer, M. Saraceno, Geometry of the Time-Dependent Variational Principle in Quantum Mechanics (1981)

Variational principle(s) as an approximation

We build an approximation of the solution of the Shrödinger equation by:

1. defining a subspace $[t_i, t_f] \times \Omega \subset [t_i, t_f] \times \mathcal{H}$,
2. defining the action $\tilde{S}[|\tilde{\psi}(t)\rangle] : [t_i, t_f] \times \Omega \to \mathbb{C}$,
3. deriving the equation of motion from the condition that $\tilde{S}$ is stationary,
4. solving the equation of motion.

$\implies$ Schrödinger evolution under the constraint that the state stays in Ω at all time (infinite potential in directions perpendicular to Ω).

Usual cases:

- Ω is a sub-vector space of $\mathcal{H}$

$$i\hbar \frac{\partial}{\partial t} |\tilde{\psi}(t)\rangle = (\hat{P}_\Omega \hat{H} \hat{P}_\Omega^\dagger) |\tilde{\psi}(t)\rangle$$

- We know a real/complex parameterization of Ω:

$$|\tilde{\psi}(t)\rangle = |\tilde{\psi}(x_1(t), \cdots, x_k(t))\rangle$$

V. I. Arnold, Mathematical method of classical mechanics (1989)

Time Dependent Hartree-Fock

We look for the equation of motion under the constraint that:

- the state is a normalized N-fermions **Slater determinant** at all times.

$$\psi(r_1, \cdots, r_N, t) = \frac{1}{\sqrt{N!}} \sum_{\sigma \in \{\text{N-permutation}\}} \text{sign}(\sigma) \prod_{i=1}^{N} \phi_{\sigma(i)}(r_i, t)$$

with

$$\langle \phi_i(t) | \phi_j(t) \rangle = \delta_{ij}.$$

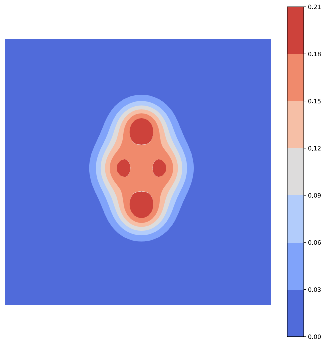
Remarks on Slater determinants:

- One body density matrix:

$$\rho(r, r') = \sum_{i=1}^{N} \phi_i(r) \phi_i^*(r')$$

- One body local density:

$$\rho(r) = \rho(r, r' = r)$$



Local density of ^{20}Ne

Derivation of the TDHF equation

The action of interest reads:

$$S[\phi_1(r,t)\cdots\phi_N(r,t)] = \int_{t_i}^{t_f} dt \left[i\hbar \sum_{i=1}^{N} \langle \phi_i | \dot{\phi}_i \rangle - \langle \psi(t) | \hat{H} | \psi(t) \rangle - \sum_{ij}^{N} \lambda_{ij} \langle \phi_i | \phi_j \rangle \right]$$

We consider here:

$$\hat{H} = \int_{r_i r_j} t_{r_i r_j} c^\dagger(r_i) c(r_j) + \frac{1}{4} \int_{r_i r_j r_k r_l} \bar{v}_{r_i r_j r_k r_l} c^\dagger(r_i) c^\dagger(r_j) c(r_l) c(r_k),$$

where $c^\dagger(r)$ creates a single particle at position r.

The energy of the Slater reads

$$\langle \psi(t) | \hat{H} | \psi(t) \rangle = \int_{r_1 r_2} t_{r_1 r_2} \rho_{r_2 r_1} + \frac{1}{2} \int_{r_1 r_2 r_3 r_4} \rho_{r_3 r_1} \bar{v}_{r_1 r_2 r_3 r_4} \rho_{r_4 r_2}.$$

Derivation of the TDHF equation

Making the action stationary consists here in finding the single particle states $\phi_i(r)$ and the λ_{ij} such that $\forall i, j \leq A$:

$$\frac{\partial S[\phi]}{\partial \phi_i(r,t)} = 0, \qquad \frac{\partial S}{\partial \phi_i^*(r,t)} = 0, \qquad \langle \phi_i(t) | \phi_j(t) \rangle = \delta_{ij}$$

This yields the system

$$i\hbar \dot{\phi}_i(rt) = \hat{h}[\rho]\phi_i(rt) + \sum_j \lambda_{ij}\phi_j(rt)$$

$$\langle \phi_i(t) | \phi_j(t) \rangle = \delta_{ij}$$

Using the first equation we notice that

$$i\hbar \frac{\partial}{\partial t} \langle \phi_i | \phi_j \rangle = \sum_k \left[\langle \phi_i | \phi_k \rangle \lambda_{kj} - \lambda_{ik} \langle \phi_k | \phi_j \rangle \right]$$

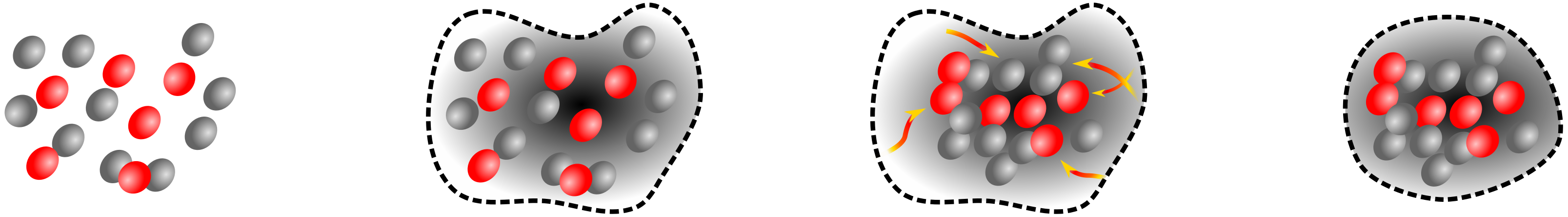
Taking $\lambda_{ij} = 0$ and starting with orthonormal states gives one solution.

The usual equation of motion

A system of A non linear coupled equations:

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

A picture of this first order evolution:



The mean field Hamiltonian reads in this case

$$\hat{h}_{rr'}[\rho] = \frac{\partial E}{\partial \rho_{r'r}} = t_{rr'} + \int_{r_1 r_2} \bar{v}_{rr_2r'r_1}\rho_{r_2r_1}$$

Break: Let us write down a pseudo-code that solves TDHF for N spinless particles

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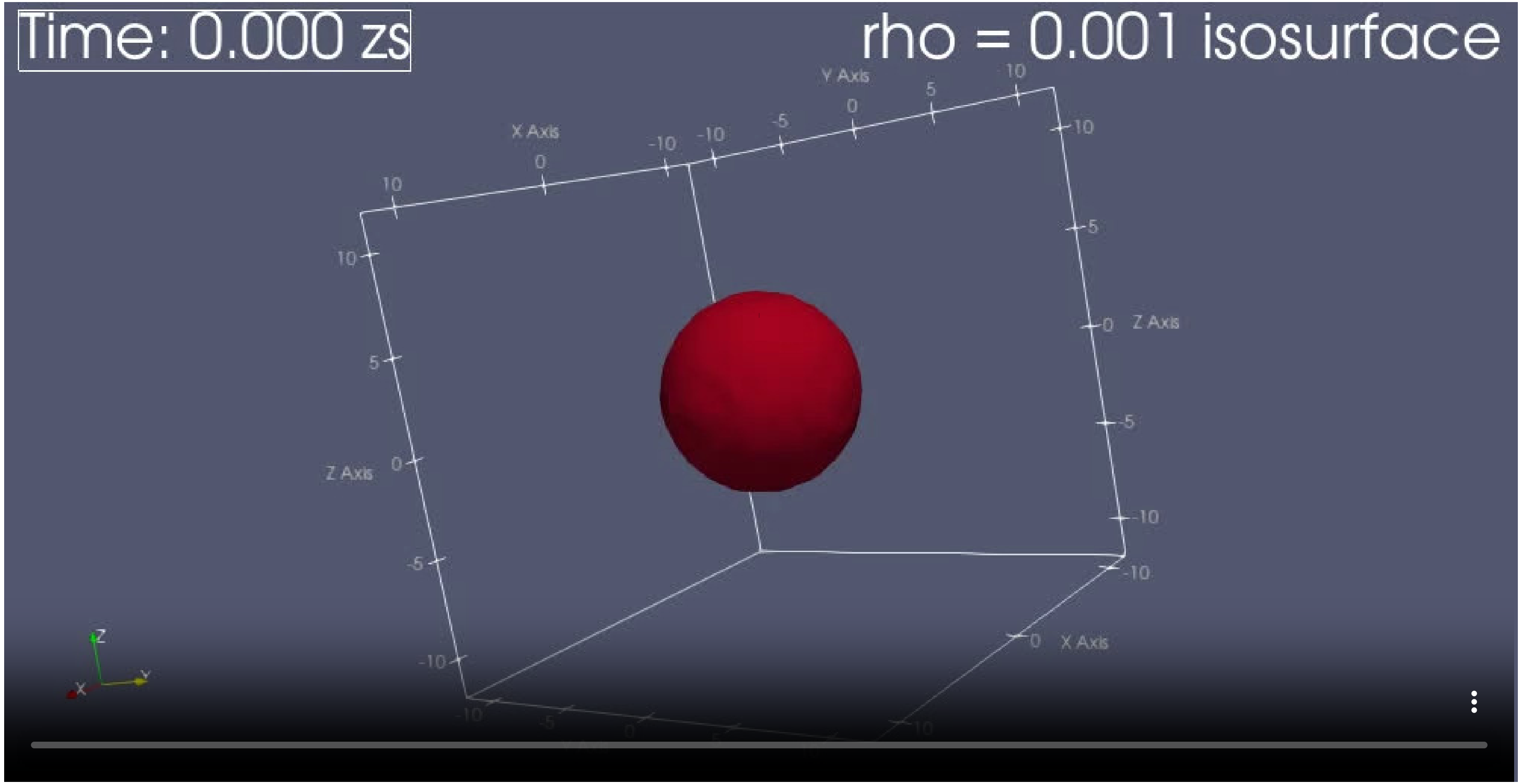
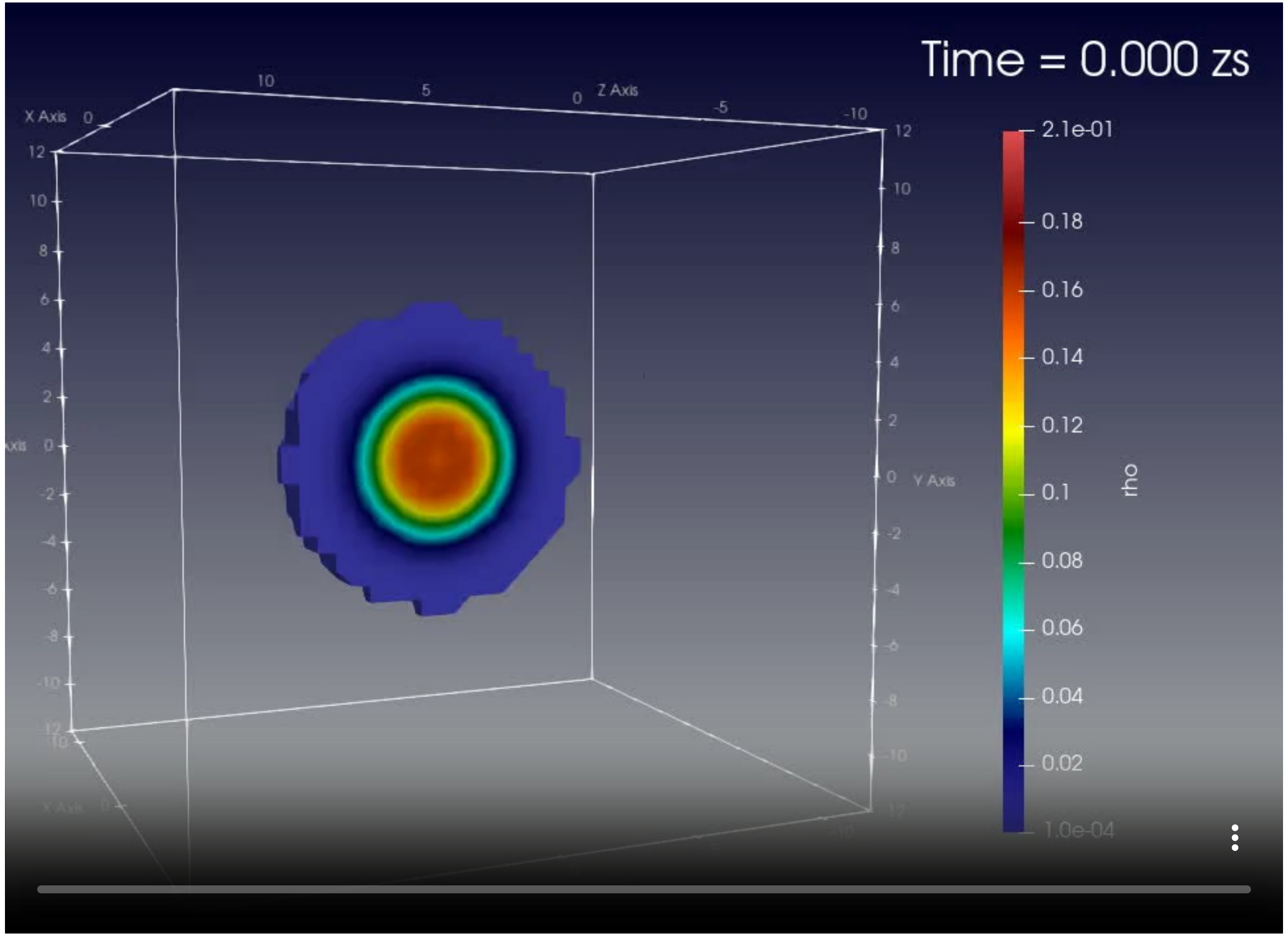
Application to collective vibrations

Quadrupole excitation of ^{16}O



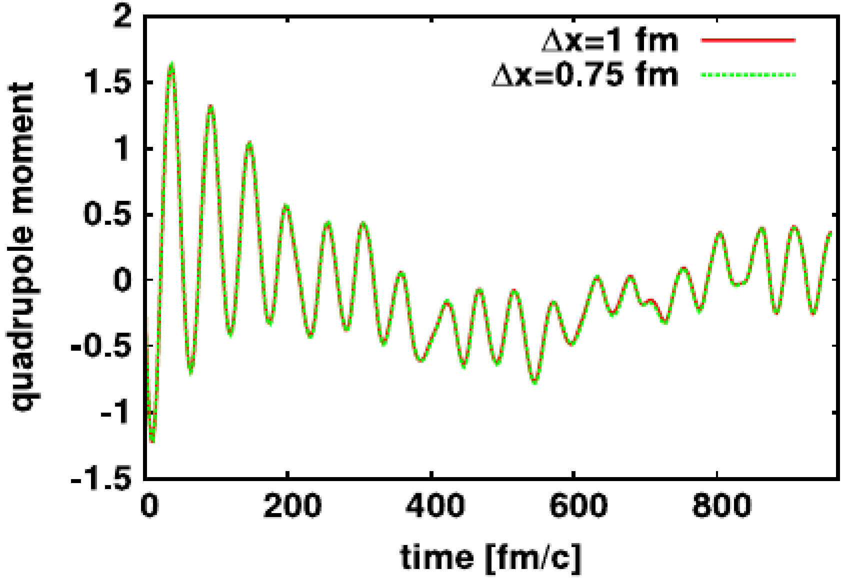
Application to collective vibrations

Monopole excitation of ^{16}O

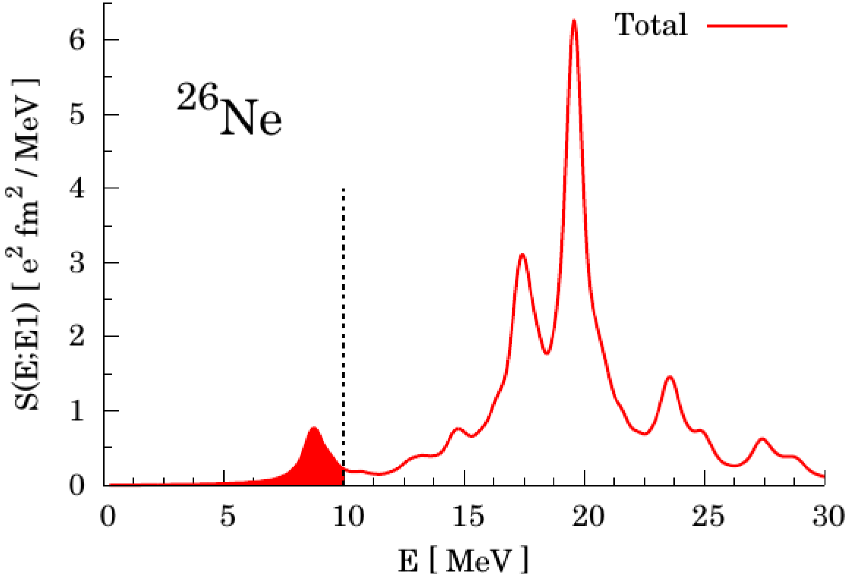


Mean field evolution of multipole moments

Quadrupole moment of ^{16}O from TDHF



Strength function of ^{26}Ne



For a given multipol excitation:
The associated strength function is the **Fourier transform** of the time evolution of the expectation value of the multipol observable after the excitation.

Don't forget: 300 fm/c $\simeq$ 1 zs

How to build the initial state for these calculations ?

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Solution 1:
Perform a constrained mean field calculation at a non equilibrium point.

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Perform a constrained mean field calculation at a non equilibrium point.

Solution 2:
Boosting the mean field ground state for a specific one body observable:

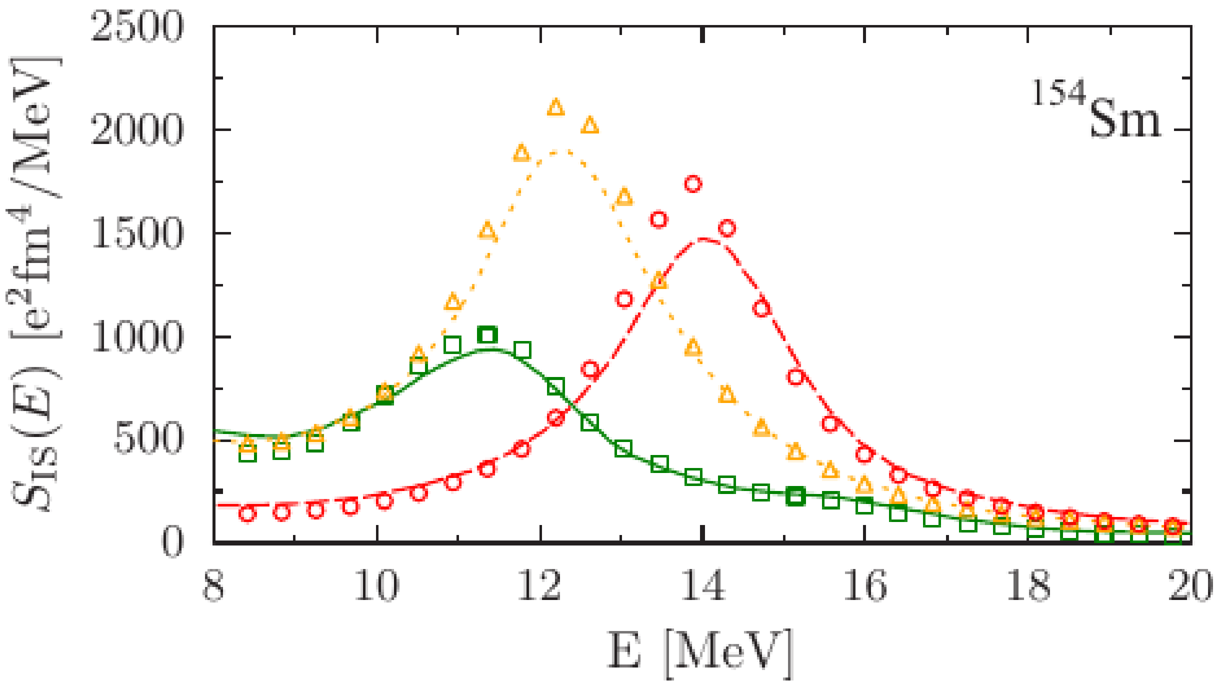
$$|\psi(t=0)\rangle = e^{-ip\hat{Q}}|\psi_{\mathrm{GS}}\rangle.$$

In the TDHF case it reduces to applying the operator on all single particle states:

$$\forall i : \quad |\phi_i(t=0)\rangle = e^{-ip\hat{Q}}|\phi_{i,\mathrm{GS}}\rangle.$$

Comparison to linear response (RPA)

Random Phase Approximation (RPA) $\simeq$ TDHF in the limit of
small fluctuations in the neighborhood of the Hartree-Fock ground state

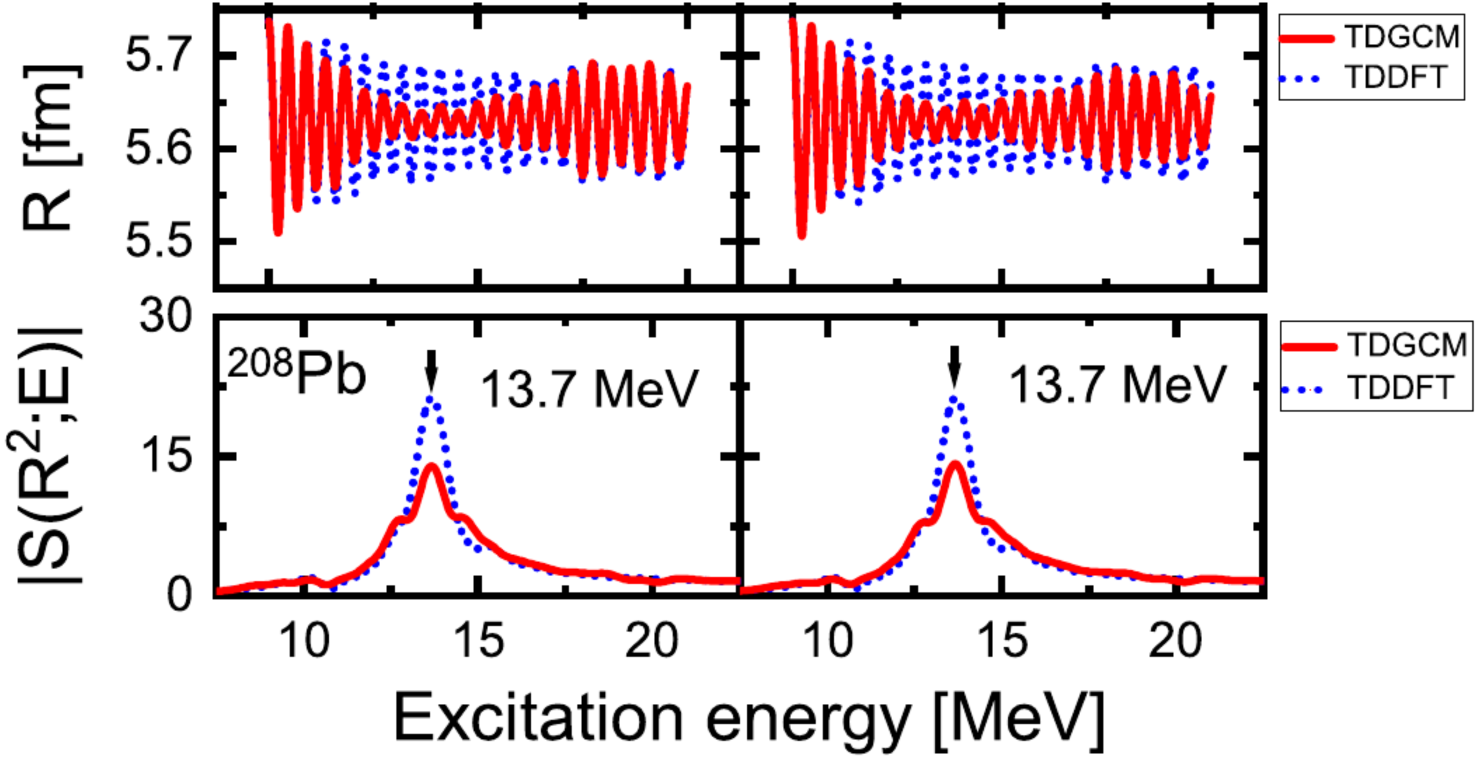


Strength function of the isoscalar quadrupol giant resonance of Sm154.
TDBCS (symbols) is compared to QRPA (lines).

G. Scamps *et al.*, PRC 89 (2014)

(Very) recent highlights

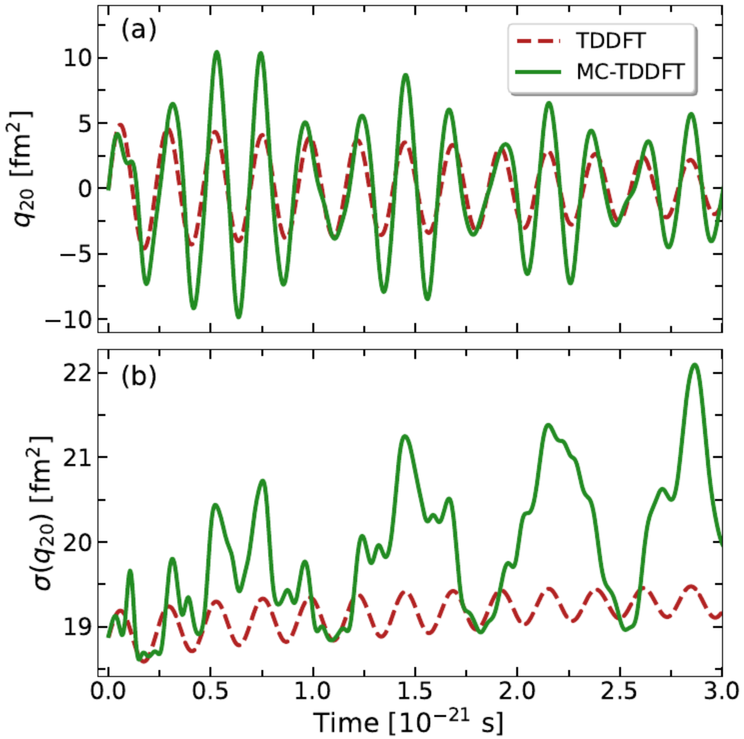
Generalized time-dependent generator coordinate method for small and large amplitude collective motion
B. Li, *et al.*, arXiv:2304.13369v1, (**April 26 2023**)

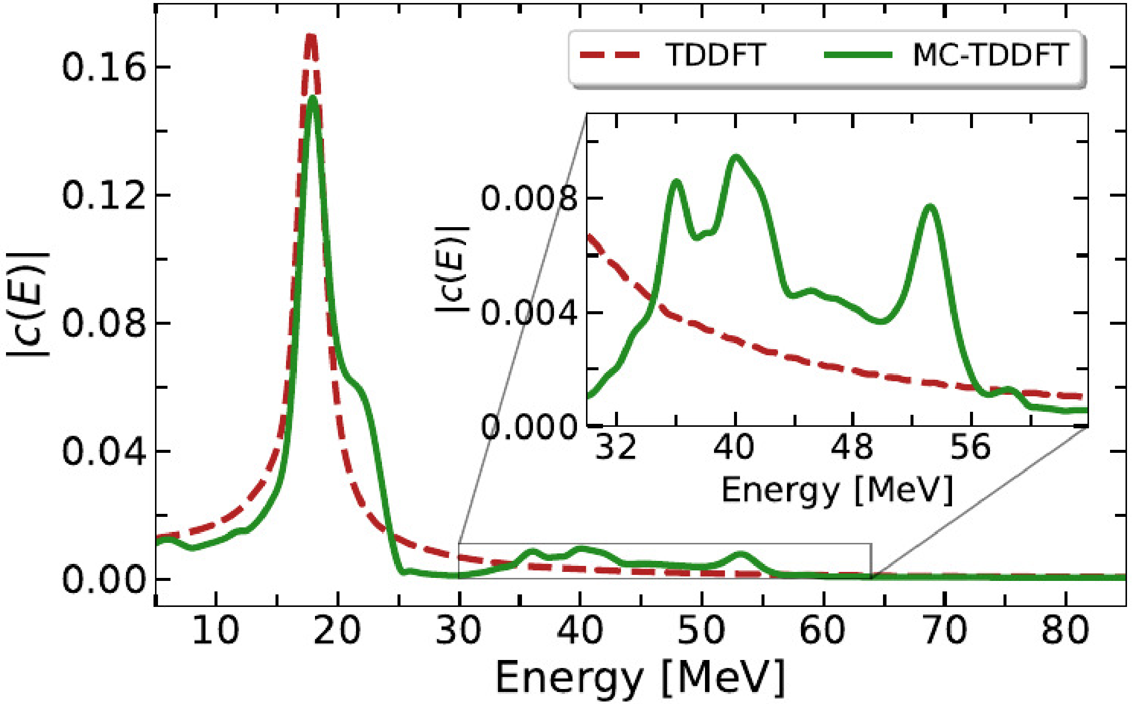


➡️ Time-dependent Hartree-Fock underestimates the **damping** of the oscillation

(Very) recent highlights

Quantum fluctuations induce collective multi-phonons in finite Fermi liquids
P. Marevic, *et al.*, arXiv:2304.0738v1, (**April 14 2023**)





➡️ Time-dependent Hartree-Fock misses **multi-phonons**

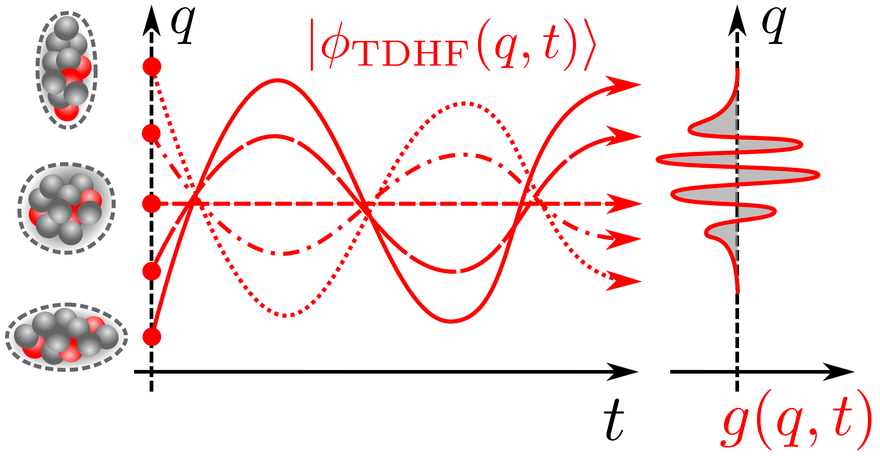
Take away messages

Small amplitude collective vibrations in nuclei

- Comparison dynamics vs static approaches

State-of-the-art

- Time-dependent Bardeen-Cooper-Schrieffer
  $\rightarrow$ giant resonance frequency
- Some current limitations:
  - underestimate damping
  - missing multi-phonons



On going work

- Approximation on a larger variational space (MC-TDDFT)
- Second RPA
- ...

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Some properties of the TDHF equation

- Equation of motion of the one body density:

$$i\hbar\frac{\partial}{\partial t}\rho = [\hat{h}[\rho];\rho]$$

- Conservation of the norm:

$$i\hbar\frac{\partial}{\partial t}\langle\psi(t)|\psi(t)\rangle = 0$$

- Conservation of energy:

$$\begin{aligned}\frac{\partial}{\partial t}\langle\hat{H}\rangle &= \int_{rr'}\frac{\partial E}{\partial\rho_{r'r}}\dot{\rho}_{r'r}\\ &= Tr(\hat{h}[\rho]\dot{\rho})\\ &= \frac{i}{\hbar}Tr(\hat{h}[\rho]\left[\rho;\hat{h}[\rho]\right]) = 0\end{aligned}$$

We used here $Tr(ABC) = Tr(BCA)$

Some more properties of the TDHF equation

- Ehrenfest theorem for one body observables:

$$\hat{O} = \int_{rr'} O_{rr'} c^\dagger(r) c(r'), \qquad \langle \hat{O} \rangle = Tr(O\rho) \qquad i\hbar \frac{\partial}{\partial t} \langle \hat{O} \rangle = \left\langle [\hat{h}[\rho]; \hat{O}] \right\rangle$$

Observables that **commute** with the mean field Hamiltonian are **constants of the motion** (e.g. Number of particles, spatial symmetries).

- Equation of continuity:
  If $\hat{H} = \text{Kinetic 1 bdy} + \text{zero-range 2 bdy interaction},$

$$\frac{\partial \rho(r)}{\partial t} = -\nabla \cdot \boldsymbol{j}(r)$$

  with the current density of particles

$$\boldsymbol{j}(r) = \frac{\hbar}{2im} \sum_{k=1}^{A} [\phi_k^* \nabla \phi_k - \nabla \phi_k^* \phi_k]$$

Including pairing correlation / superfluidity

TDHF ➡️ TDBCS, TDHFB, TDSLDA

- Exactly the same methods as in static calculations
- Can be treated:
  - at the Bardeen-Cooper-Schrieffer level (numerical cost $\simeq \times 4$)
  - at the Hartree-Fock-Bogoliubov level (numerical cost $\simeq \times$ **dim(one-body basis)**)
- Is crucial to make simulation of fission !

Blackboard explanation ?

⚠️ The continuity equation is not satisfied with BCS
⚠️ The system has not a good particle number anymore

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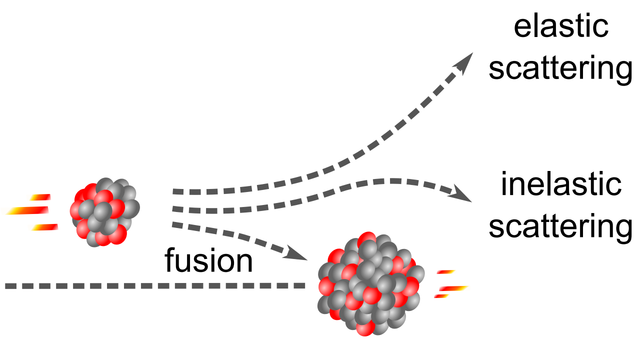
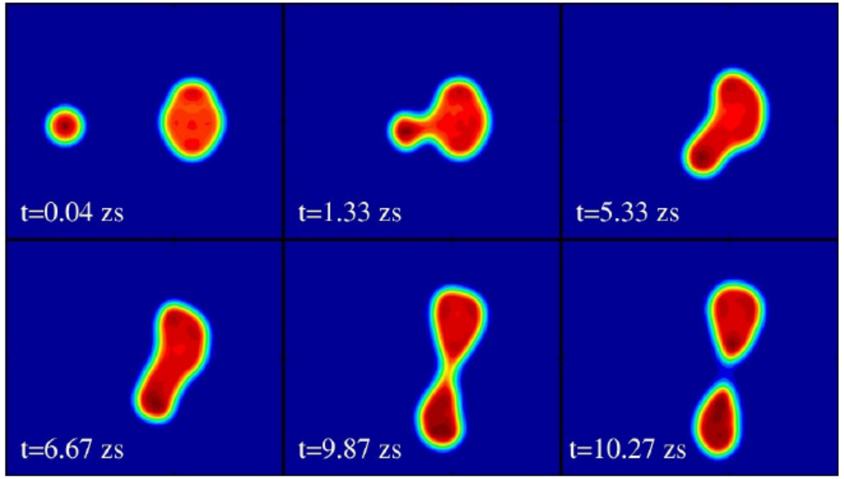
Predicting heavy-ion collisions with TDHF



Let us focus on **low energy** heavy-ion collisions

$$E_k \simeq B_{\text{Coulomb}}$$

Major improvement of the TDHF codes in the last decade: **unrestricted spatial symmetries**

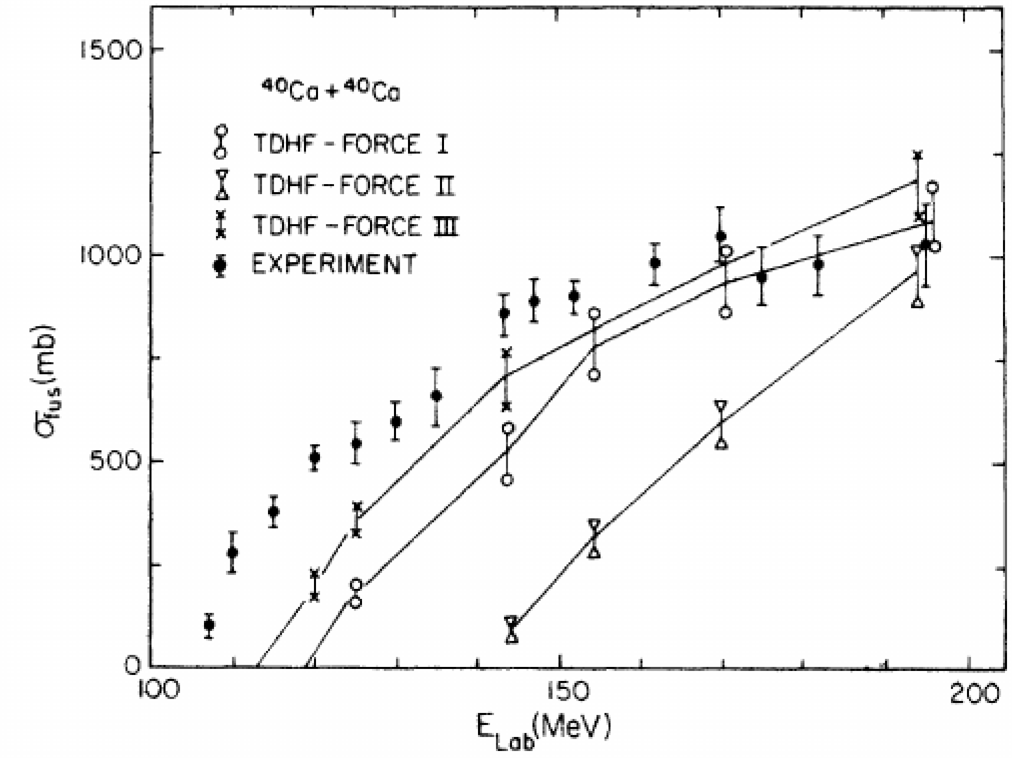


Quasi-fission of ^{40}Ca + ^{238}U, with the Sky3D code, $\simeq$ few days.CPU

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

Fusion cross section

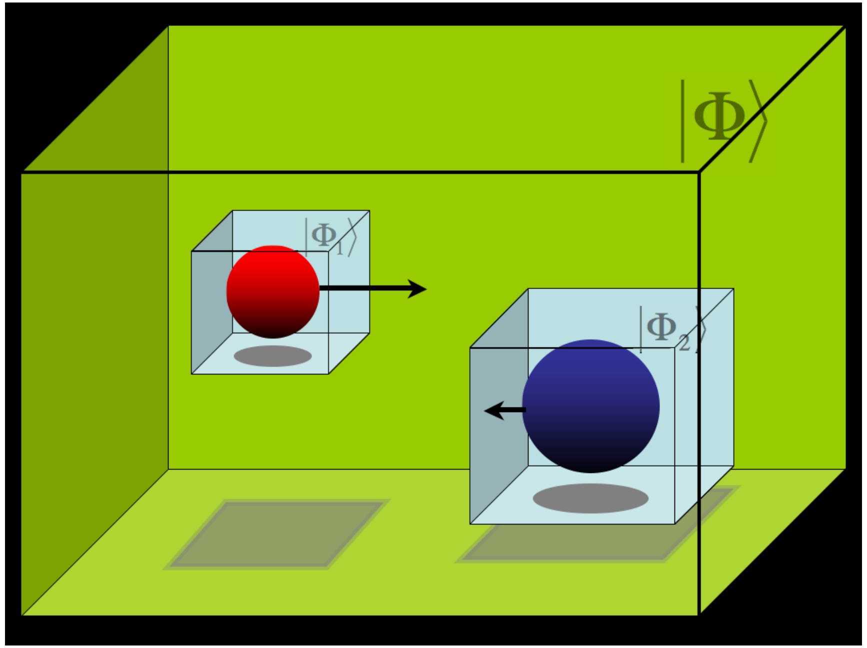
One of the first applications of TDHF in nuclear physics in the 1970's.



P. Bonche *et al.*, PRC 17 (1978)

How to predict this quantity from TDHF dynamics ?

The starting point



C. Simenel *et al.*. arXiv:0806.2714v2 (2009)

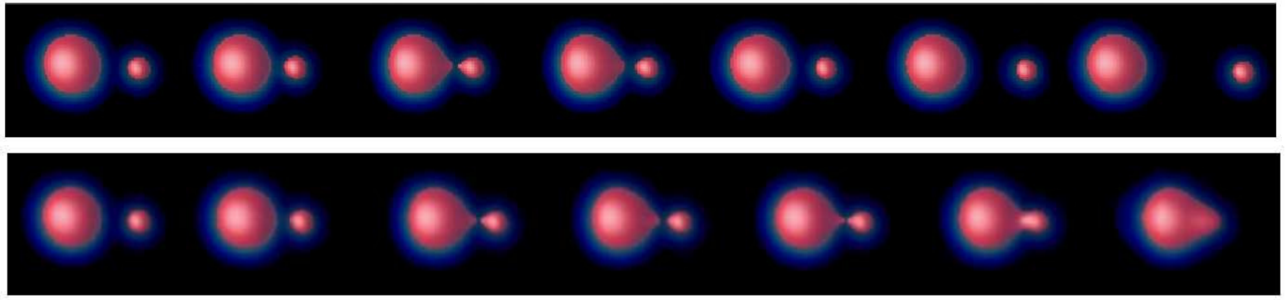
1. Compute static HF states for the two reaction partners
2. Place them in the simulation box for the collision simulation
3. Increase their relative momentum by applying a boost

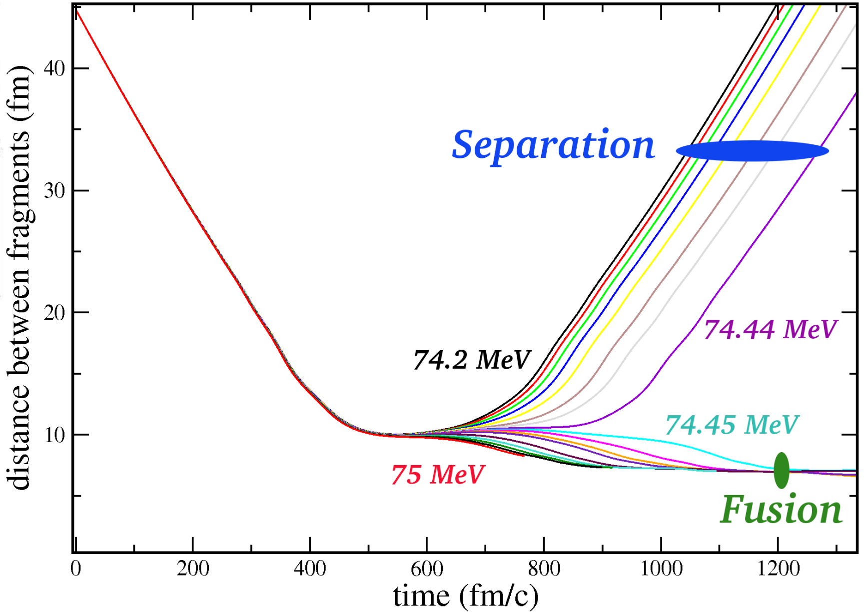
$$\forall i \in [1, A_1] : \quad \phi'_i(r) = e^{im\mathbf{v_1}\cdot\hat{\mathbf{r}}}\phi_i(r)$$
$$\forall i \in [1, A_2] : \quad \phi'_i(r) = e^{im\mathbf{v_2}\cdot\hat{\mathbf{r}}}\phi_i(r)$$

Determination of the fusion barrier

Case of a head on collision ^{16}O + ^{208}Pb

(from C. Simenel *et al.*Joliot Curie School (2008))





Top: Center of mass energy 74.44 MeV.
Bottom: Same with 74.45 MeV

Note:

The fusion barrier depends on the initial impact parameter

Reconstruction of the fusion cross section

1. Find the fusion barrier for various impact parameters with TDHF
2. Reconstruct the cross section as a sum over the impact parameters that can fuse for a given energy

$$\sigma_{\text{fus}}(E_{\text{lab}}) = \frac{2\pi}{k^2} \sum_l (2l+1) \tag{4a}$$

$$\approx \frac{\pi\hbar^2}{\mu E_{\text{lab}}} \left[(l_> + 1)^2 - (l_< + 1)^2 \right]. \tag{4b}$$

C. Simenel *et al.*. arXiv:0806.2714v2 (2009)

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C. Simenel *et al.*. arXiv:0806.2714v2 (2009)

Take away messages:

- TDHF has a **classical behavior for** the expectation values of **one-body observables** (here the distance between the two fragments)
- We need to add **collective fluctuations** to reproduce cross sections

For recent applications see: K. Sekizawa, Front. in Phys., Mini Review (2019)

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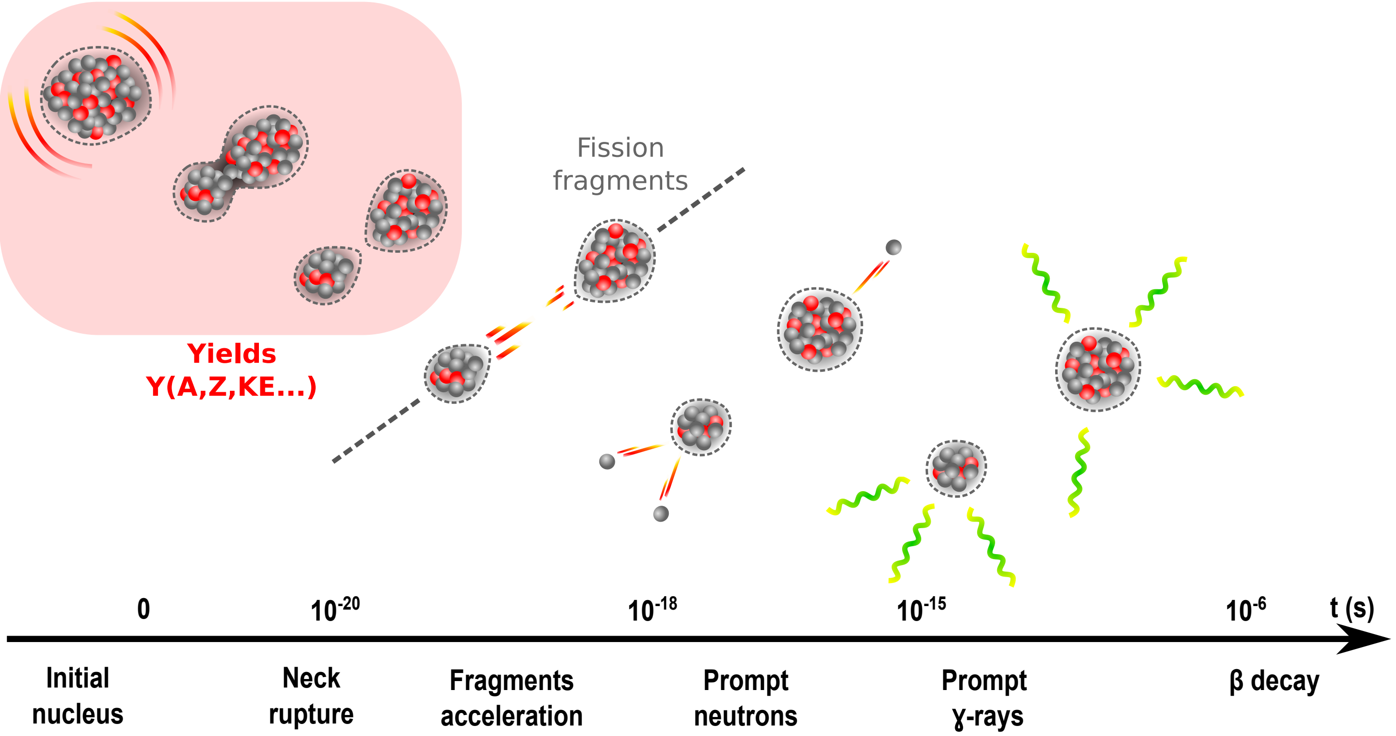
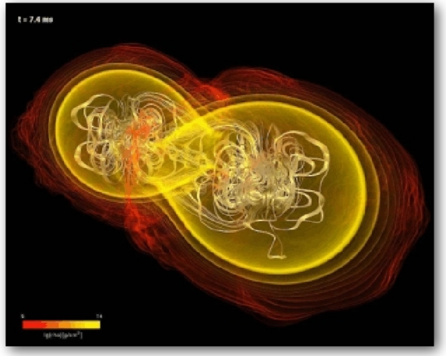
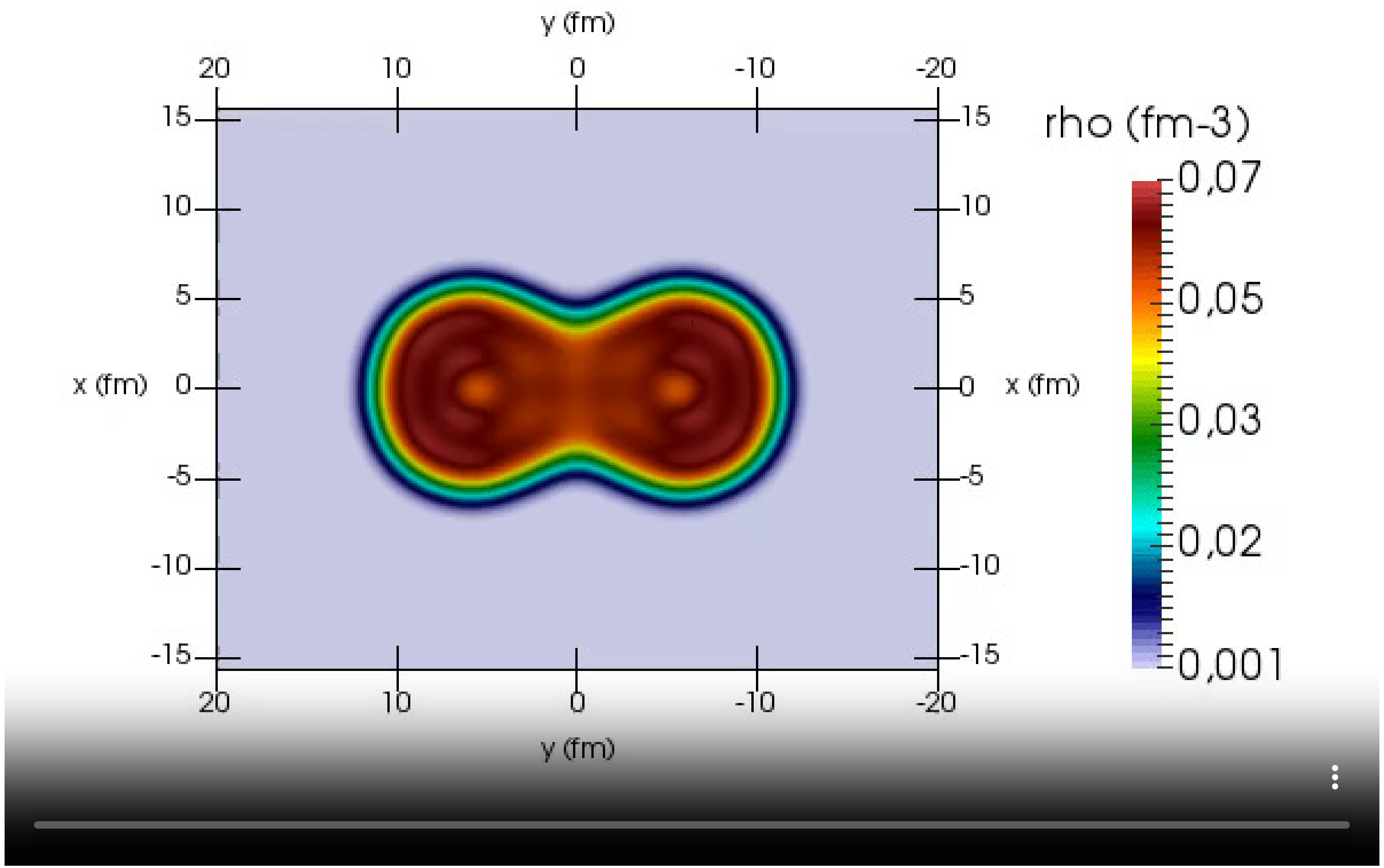
Simulating the fission dynamics





Fission with TDBCS



Fission of a ^{258}Fm

Fission with TDHF: the need for pairing

2014: First fission simulations ^{258}Fm, ^{264}Fm (no pairing)
C. Simenel *et al.*, PRC **89** (2014)

2015: ^{258}Fm with pairing (TDBCS)
G. Scamps *et al.*, PRC **92** (2015)

- 60 to 80% of the fragments excitation energy is generated during the rapid descent to scission

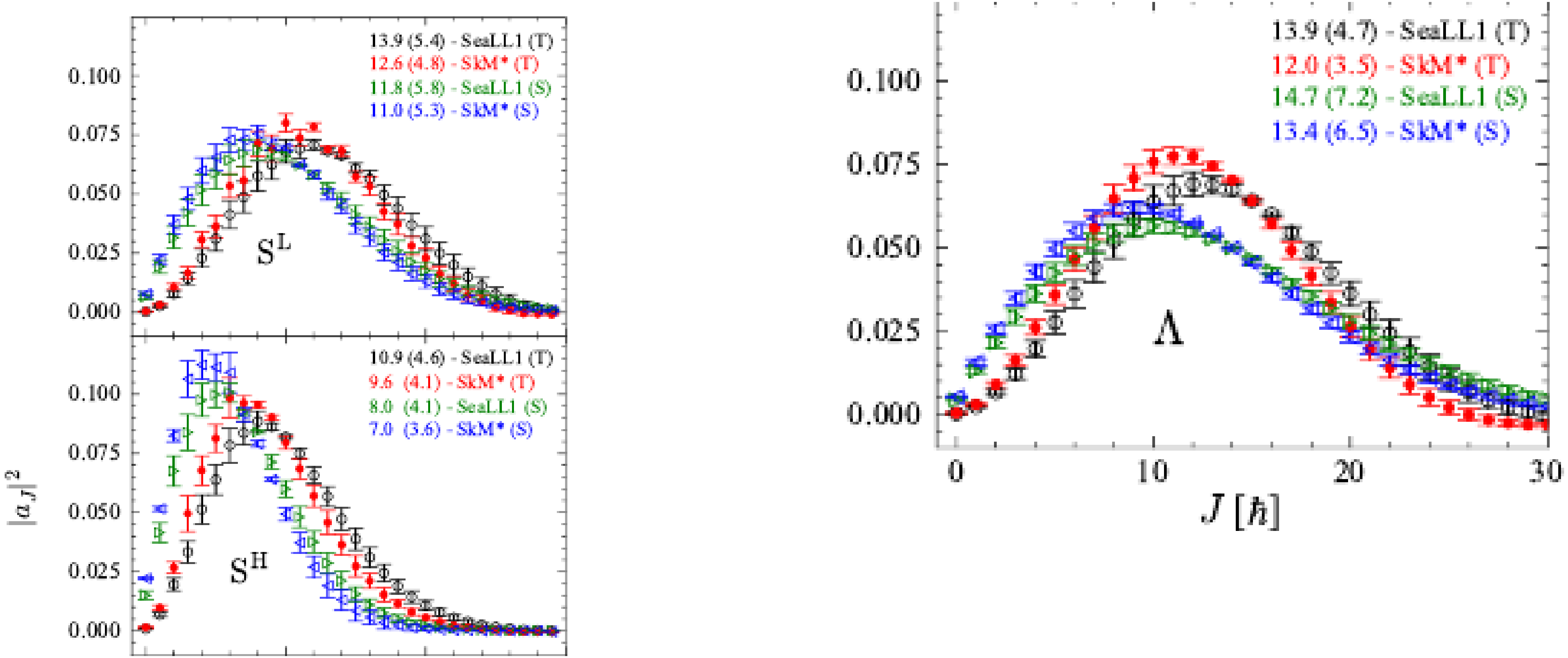
2016: ^{240}Pu with pairing (full TDHFB)
A. Bulgac *et al.*, PRL **11** (2016)

- Reproduction of the experimental total kinetic energies within 3%

2021-2022: First prediction of the fragments spins and orbital moment
A. Bulgac *et al.*, PRL **126** (2021)
A. Bulgac *et al.*, PRL **128** (2022)

Method	Numerical cost for 10-20 zs
TDHF	few days, few CPU
TDBCS	1 week, few CPU
TDHFB	10h, 1700 GPU

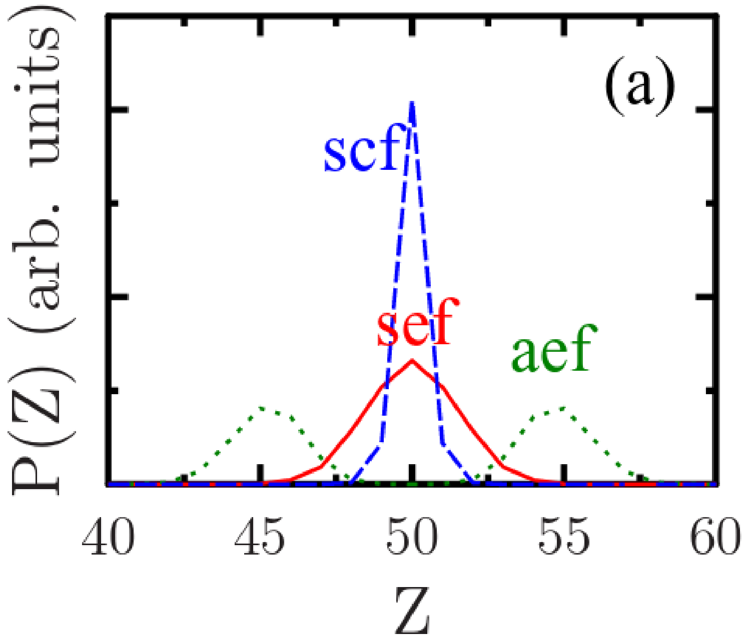
Recent highlight with TDHFB



First prediction of the distribution of intrinsic and orbital spin distribution of a fission of ^{252}Cf
A. Bulgac *et al.*, PRL 128 (2022)

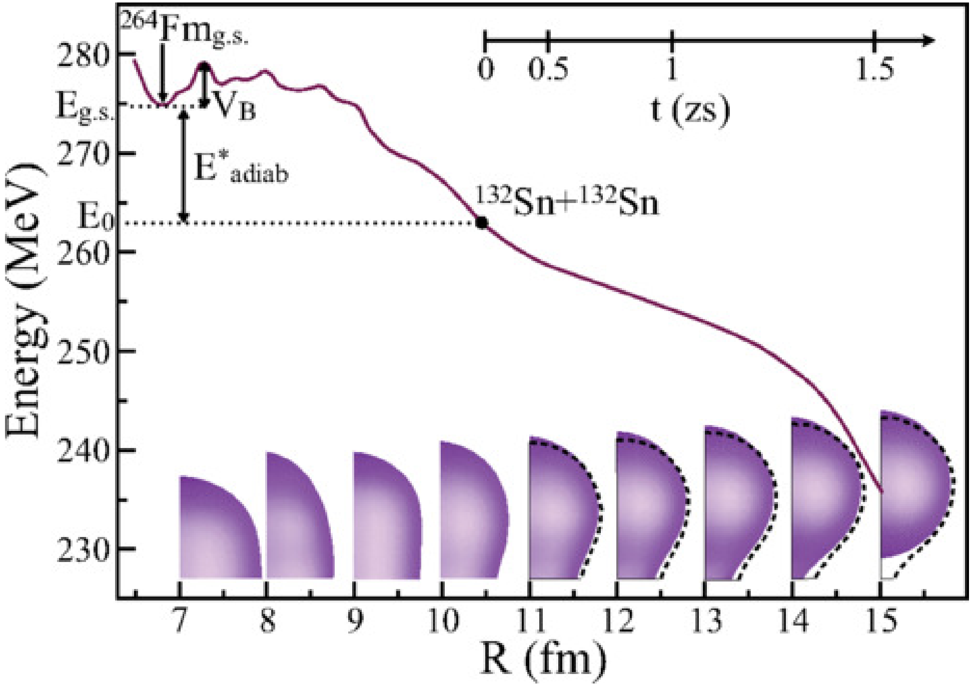
Limitations of the time dependent mean-field picture

Too sharp distributions for the fragment observables



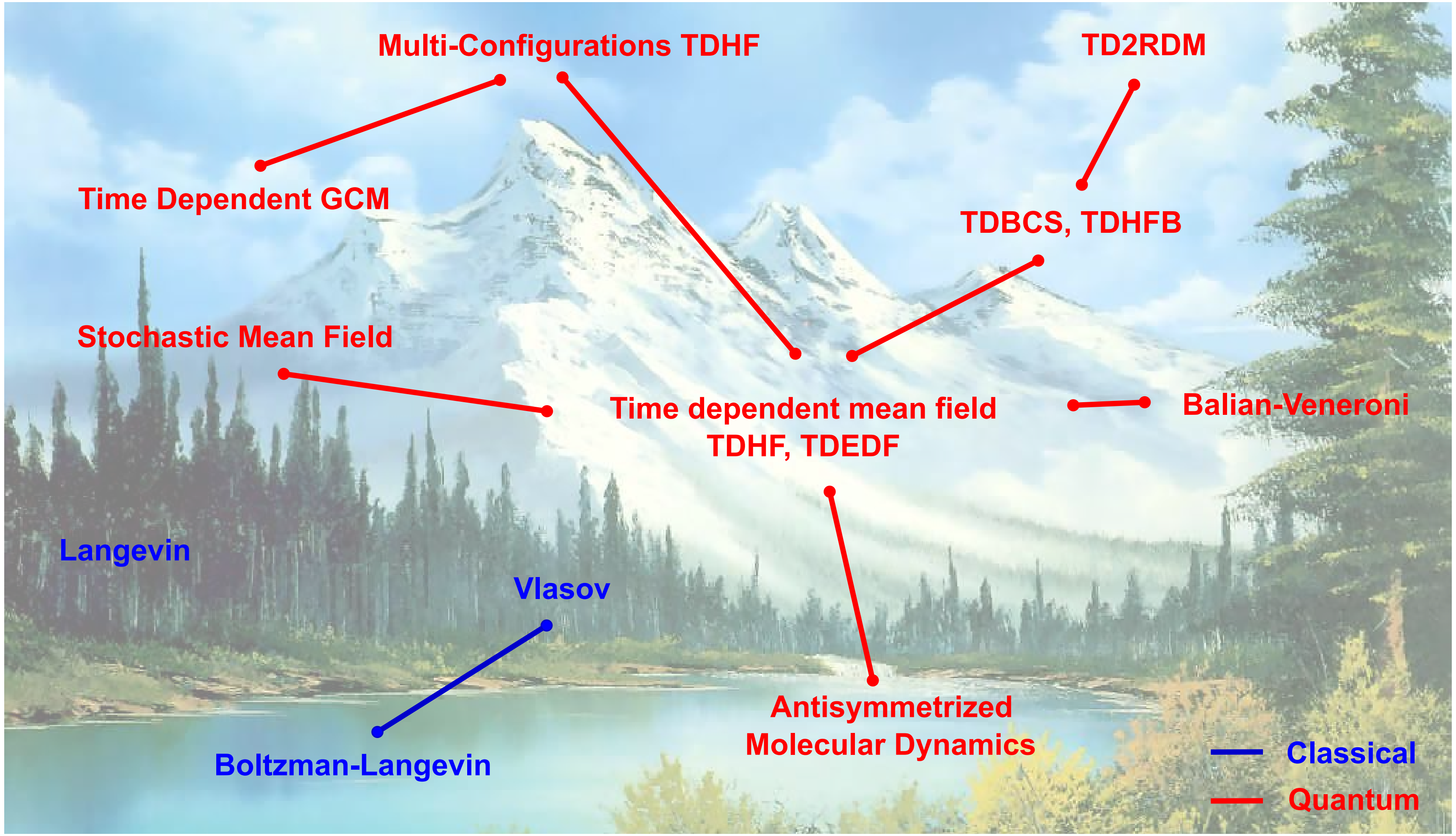
Charge distribution in one fragment for 3 TDBCS simulations of ^{258}Fm fission
G. Scamps *et al.*, PRC **92** (2015)

No tunneling through the fission/Coulomb barrier



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

A side step toward TDGCM



Another variational approach tailored for fission !

Time Dependent Generator Coordinate Method

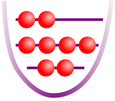
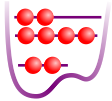
A multi-reference ansatz

$$|\psi(t)\rangle = \int_q f(q,t)|\phi(q)\rangle$$

A two step process:

1. Generate an ensemble of deformed quasi-particule vacua $|\phi_{\boldsymbol{q}}\rangle$
2. Solve the evolution equation for the mixing function $f(\boldsymbol{q},t)$

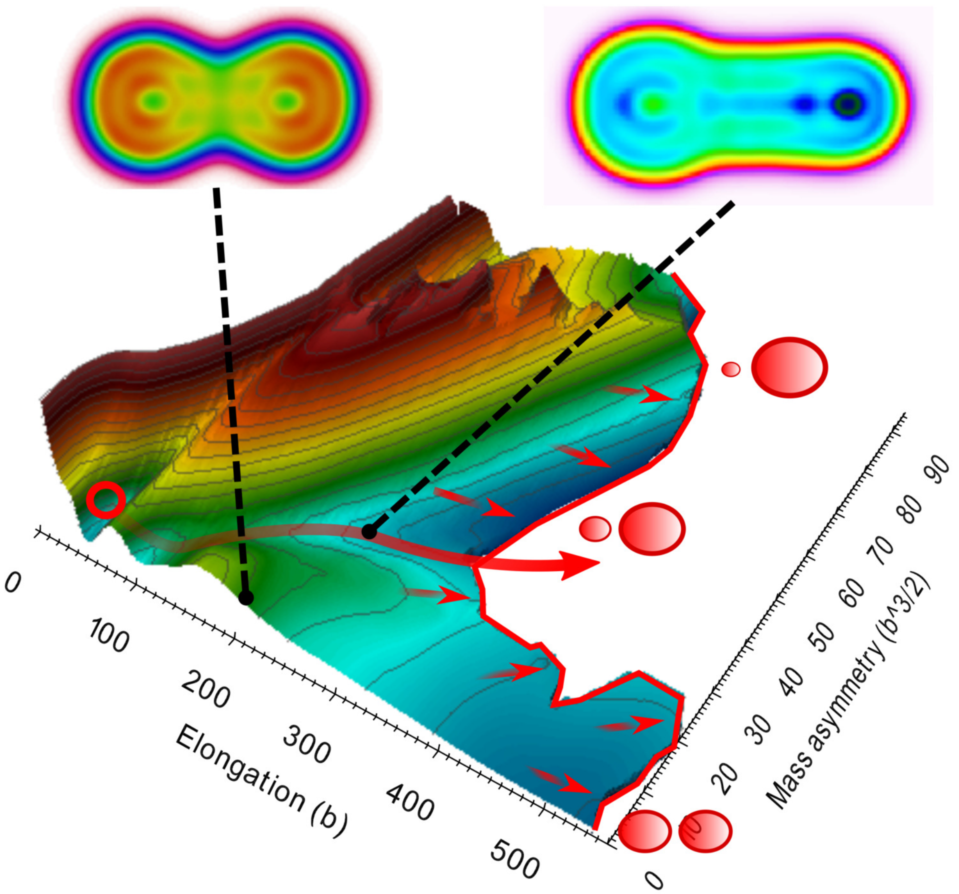
$f(\boldsymbol{q},t)$ follows a time dependent Schrödinger equation !

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

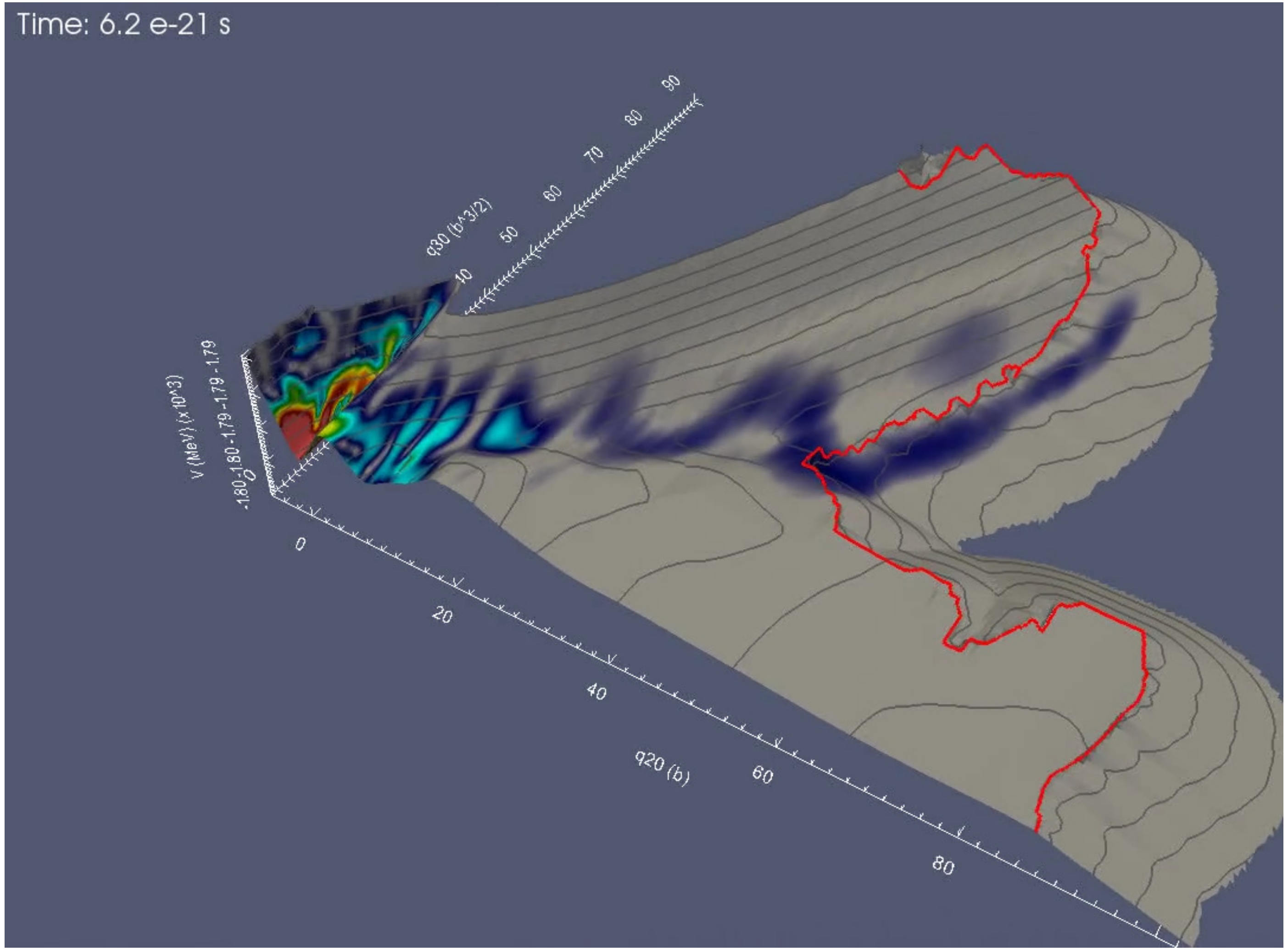
Constrained HFB solutions with ≠ shapes,
time independent

Example of a n + ^{239}Pu fission

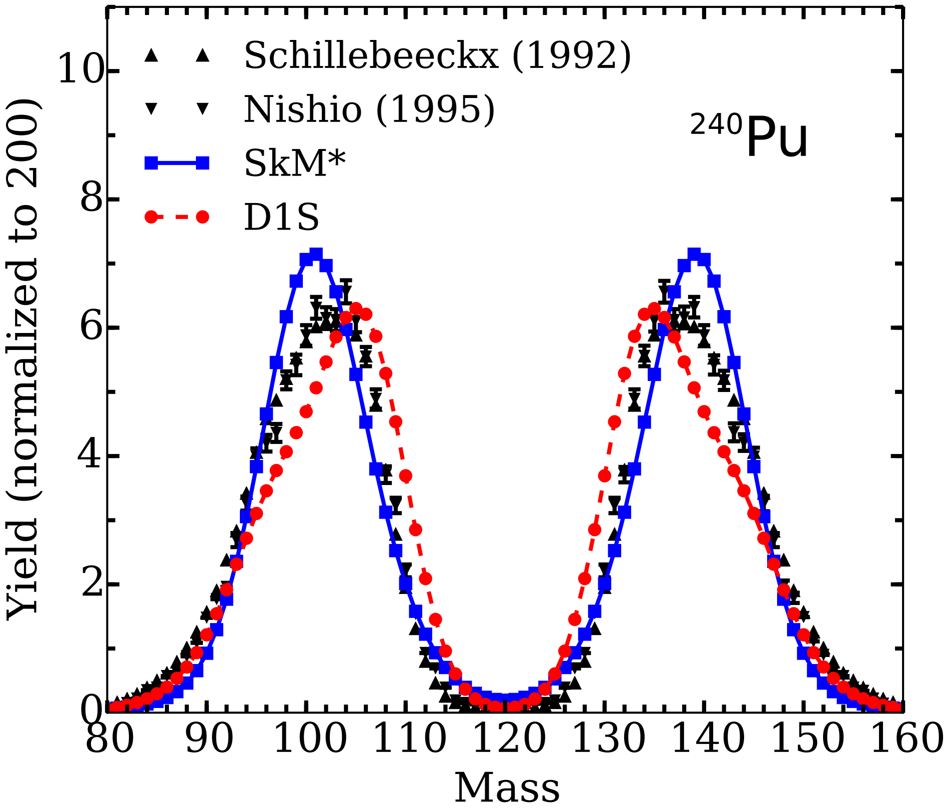
1. Choose the collective variables:
   - elongation (Q_{20} in b),
   - mass asymmetry (Q_{30} in b$^{3/2}$)
2. Calculate potential energy surface and inertia tensor
3. Define initial wave packet
4. Compute its **time evolution**
5. Extract probability to have a certain split

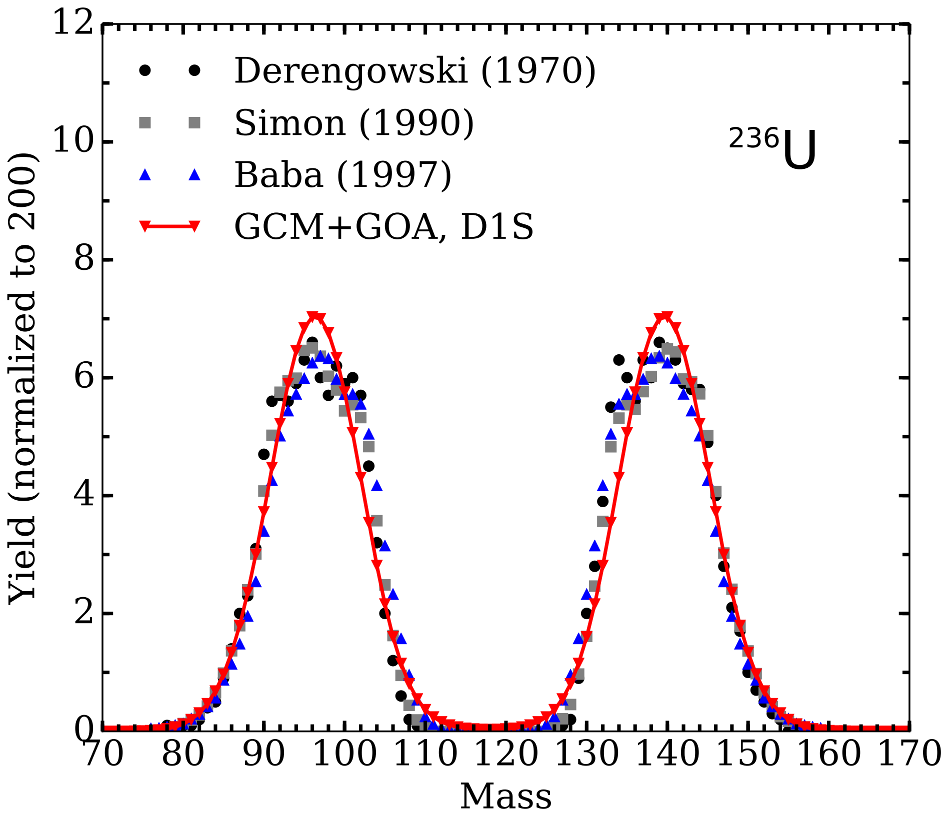


Evolution of the collective wavepacket $f(q,t)$



Large shape fluctuations





✅ Correct width of the fission fragment mass distribution for actinides !
⚠️ Pb with the energy balance
➡️ no perfect approach yet...

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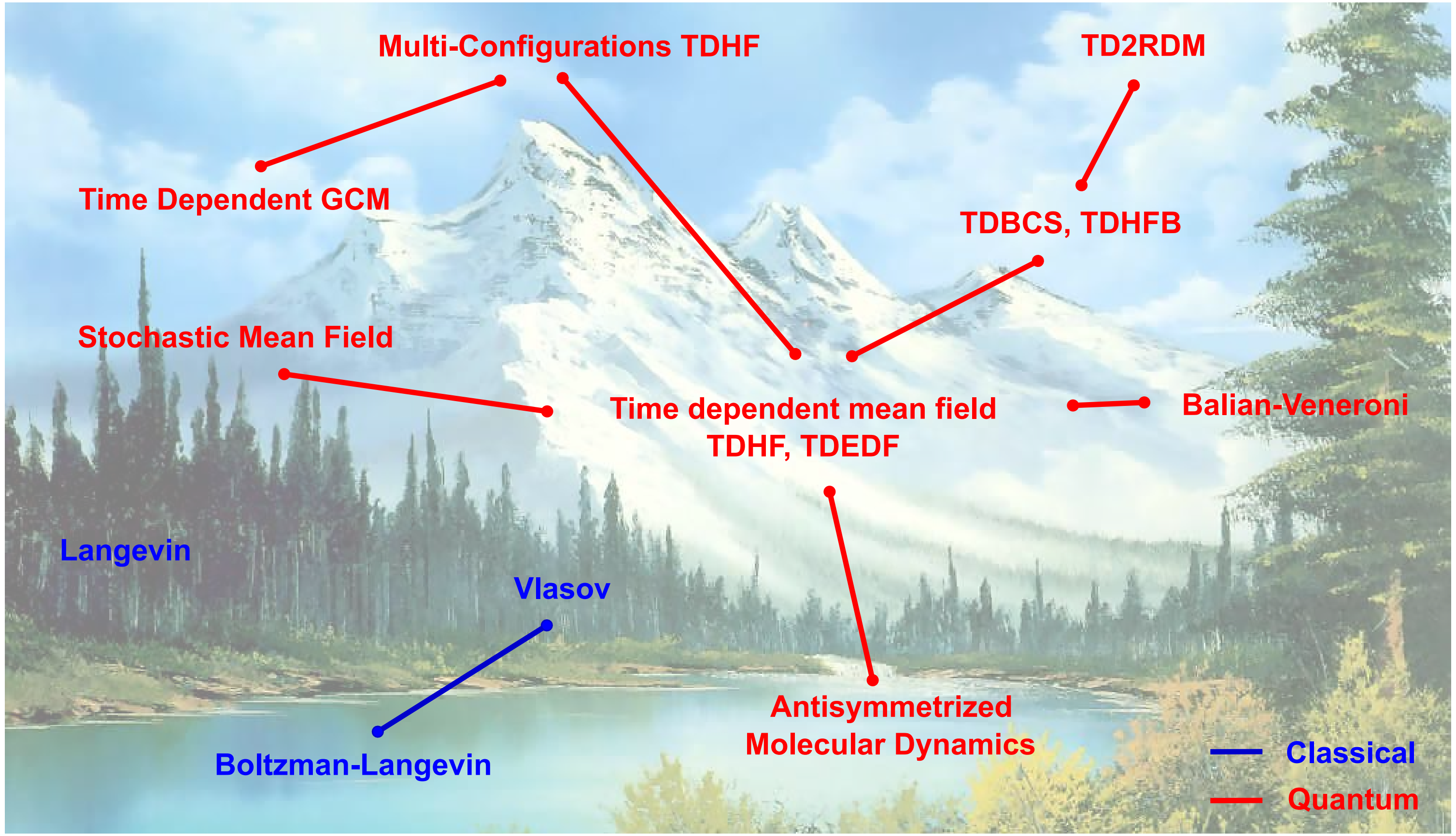
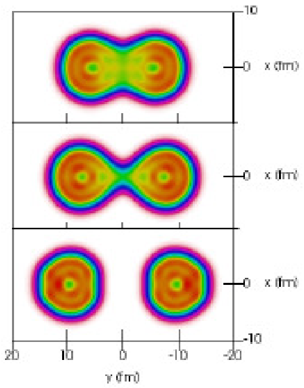
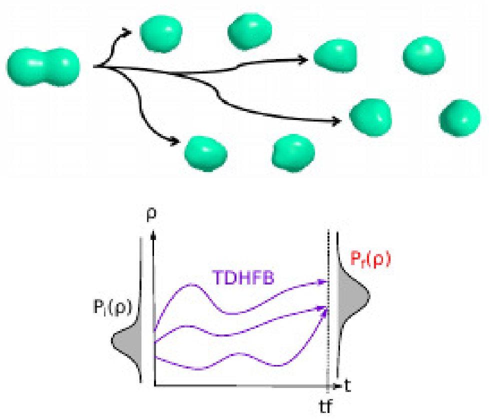
A landscape of theoretical methods

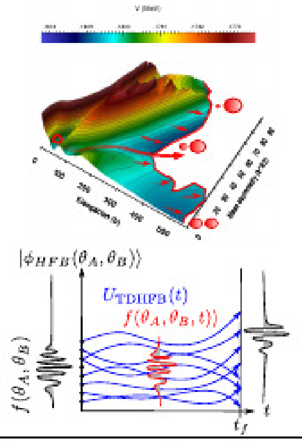


- Balian-Veneroni: variance of one-body observables
- TD-2RDM: evolution of the 2-body density matrix
- MC-TDHF: mix of TDHF and TDGCM

Overall comparison







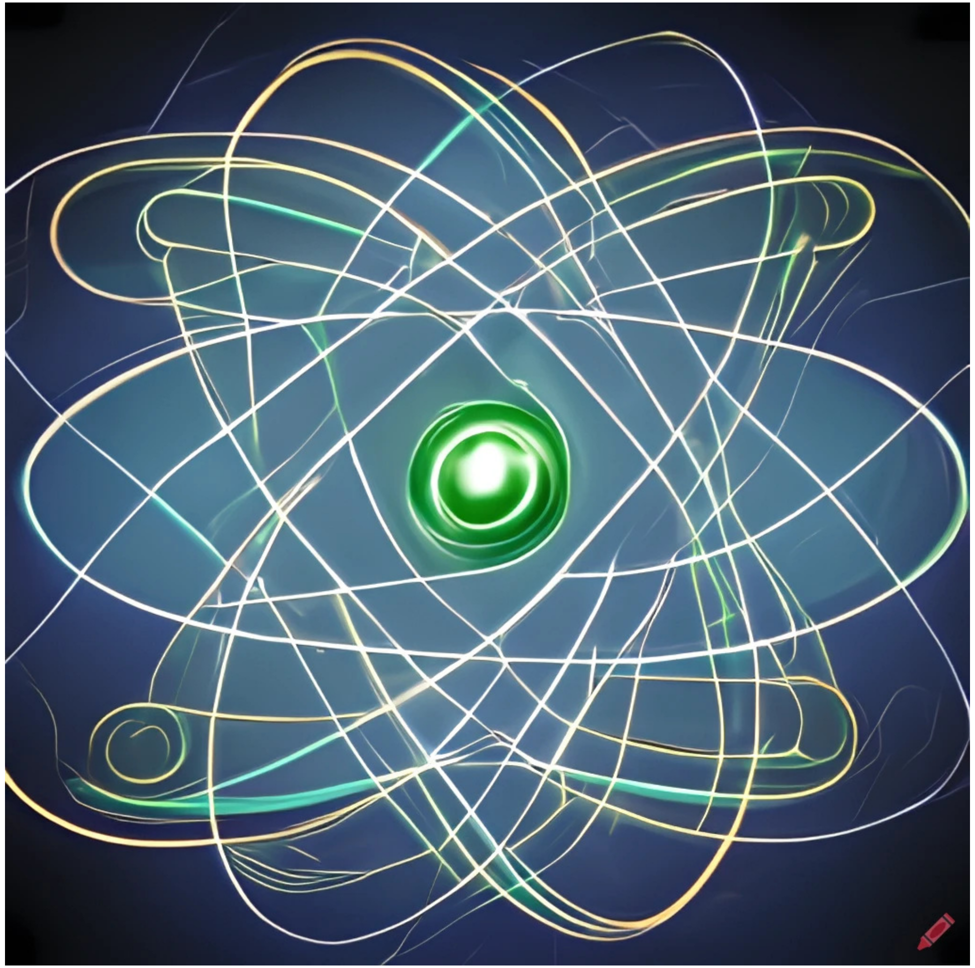
Single reference	Semi-classical ensemble	Multi-configuration
• Diabatic dynamics • Misses collective fluctuations • Breaks symmetries • No collective tunnelling	• More collective fluctuations (standard deviation of 1-body observables) • Low cost, parallel algorithms • Misses quantum interferences	• Quantum fluctuations, probability distribution • Difficulty to get both fluctuations and diabatic motion • High cost, parallel algorithms in some cases • Issue with EDF kernels

We **count on you** to develop the ultimate approach !

Bonus

Some open source codes for nuclear dynamics

- **Sky3D-1.1**
  B. Schuetrumpf *et al.*, CPC 229 (2018):
  The reference Skyrme TDHF+BCS open source code
- **LISE**
  S. Jin *et al.*, CPC 269 (2020):
  A Skyrme full TDHFB package
- **FELIX-2.0**
  D. Regnier *et al*, CPC 225 (2018):
  A time dependent Schrödinger equation solver for TDGCM+GOA purposes



CRAIYON: 'Atomic nucleus in the quantum realm'

Thank you for your attention !