Towards an implementation of a real-time path-integral for interacting fermions

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Outline:

- TDSLDA and its implementation in the petascale regime
- Applications to various nuclear processes:
  - *Spectral strength of collective excitations in nuclei*
  - *Coulomb excitation of nuclei with relativistic heavy-ions*
  - *Nuclear reactions – neutron scattering/capture*
  - *(Induced) nuclear fission*
- Why we need to extend the deterministic TDSLDA to a Stochastic TDSLDA and why we need the exascale regime?
- How to implement Real-Time Path Integral for Interacting Many Fermion Systems

Near and long term goals:

To describe *accurately* the time-dependent evolution of externally perturbed Fermi superfluid systems (cold atomic clouds, nuclei, neutron star crust, …)

We need a DFT extension to superfluid systems and time-dependent phenomena and subsequently we have to add quantum fluctuations and extend the theory to a stochastic incarnation

Why should one study fermionic superfluidity?

Superconductivity (which turned 100 years old on April 8th, 2011) and superfluidity in Fermi systems are manifestations of quantum coherence at a macroscopic level

- ✓ **Dilute atomic Fermi gases** $T_c \approx 10^{-9}$ eV
- ✓ **Liquid ^{3}He** $T_c \approx 10^{-7}$ eV
- ✓ **Metals, composite materials** $T_c \approx 10^{-3} - 10^{-2}$ eV
- ✓ **Nuclei, neutron stars** $T_c \approx 10^{5} - 10^{6}$ eV
- • **QCD color superconductivity** $T_c \approx 10^{7} - 10^{8}$ eV

units (1 eV ≈ 10^4 K)

Physical systems and processes:

- ✓ Collective states in nuclei
- ✓ Large amplitude collective motion (LACM)
- ✓ Excitation of nuclei with gamma rays and neutrons
- ✓ Coulomb excitation of nuclei with relativistic heavy-ions
- ✓ Nuclear fusion between colliding heavy-ions
- ✓ (Induced) nuclear fission
- ✓ Neutron star crust and dynamics of vortices and their pinning mechanism
- ✓ Dynamics of vortices, Anderson-Higgs Mode
- ✓ Vortex crossing and reconnection and the onset of quantum turbulence
- ✓ Dark solitons and shock waves in collision of fermionic superfluid atomic clouds

In order to treat this plethora of phenomena one needs to treat spatially inhomogeneous systems in real time!

- **Quantum Monte Carlo is feasible for small particle numbers only and has been implemented so far only (mostly) for static phenomena**

- **Density Functional Theory (large particle numbers)**

  One needs:

  1) to find an Energy Density Functional (EDF)
  2) to extend DFT to superfluid phenomena (SLDA)
  3) to extend SLDA to time-dependent phenomena (TDSLDA)

Kohn-Sham theorem

$$H = \sum_{i}^{N} T(i) + \sum_{i<j}^{N} U(ij) + \sum_{i<j<k}^{N} U(ijk) + \ldots + \sum_{i}^{N} V_{ext}(i)$$

$$H\Psi_0(1,2,\ldots N) = E_0\Psi_0(1,2,\ldots N)$$

$$n(\vec{r}) = \left\langle \Psi_0 \middle| \sum_{i}^{N} \delta(\vec{r} - \vec{r}_i) \middle| \Psi_0 \right\rangle$$

Injective map (one-to-one)

$$\Psi_0(1,2,\ldots N) \quad \Leftrightarrow \quad V_{ext}(\vec{r}) \quad \Leftrightarrow \quad n(\vec{r})$$

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

$$n(\vec{r}) = \sum_{i}^{N} \left| \varphi_i(\vec{r}) \right|^2 . \qquad \tau(\vec{r}) = \sum_{i}^{N} \left| \vec{\nabla} \varphi_i(\vec{r}) \right|^2$$

Universal functional of density independent of external potential

Time Dependent Phenomena

The time-dependent density functional theory is viewed in general as a reformulation of the exact quantum mechanical time evolution of a many-body system when only single-particle properties are considered.

TDDFT for normal systems:

A.K. Rajagopal and J. Callaway, Phys. Rev. B 7, 1912 (1973)

V. Peuckert, J. Phys. C 11, 4945 (1978)

E. Runge and E.K.U. Gross, Phys. Rev. Lett. 52, 997 (1984)

http://www.tddft.org

TDSLDA
(Time-Dependent Superfluid Local Density Aproximation)

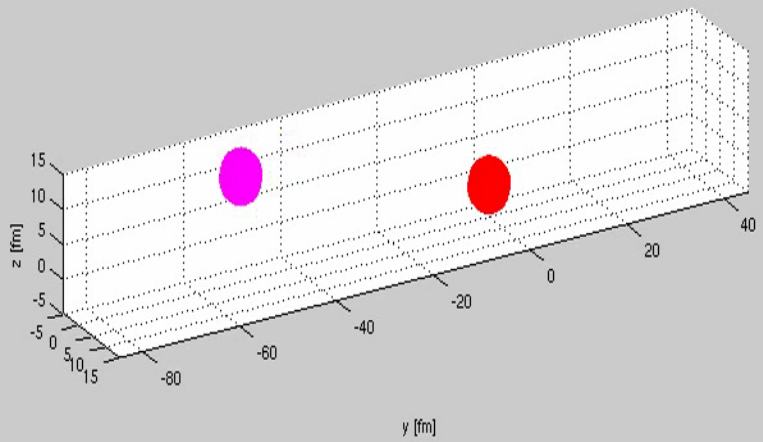
$$E(t)=\int d^3r\ \Big[\ \ \varepsilon(n(\vec{r},t),\tau(\vec{r},t),\nu(\vec{r},t),\vec{j}(\vec{r},t))+V_{ext}(\vec{r},t)n(\vec{r},t)+\ldots\Big]$$

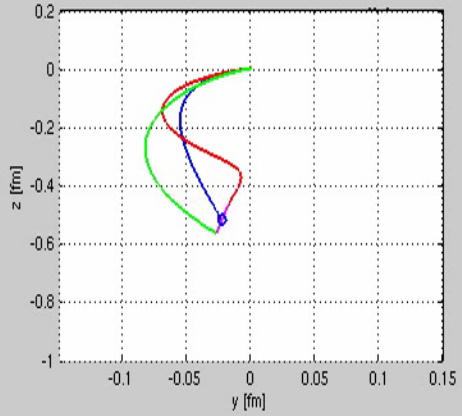
$$\begin{cases}[h(\vec{r},t)+V_{ext}(\vec{r},t)-\mu]\mathrm{u}_i(\vec{r},t)+[\Delta(\vec{r},t)+\Delta_{ext}(\vec{r},t)]\mathrm{v}_i(\vec{r},t)=i\hbar\dfrac{\partial \mathrm{u}_i(\vec{r},t)}{\partial t}\\ [\Delta^*(\vec{r},t)+\Delta^*_{ext}(\vec{r},t)]\mathrm{u}_i(\vec{r},t)-[h(\vec{r},t)+V_{ext}(\vec{r},t)-\mu]\mathrm{v}_i(\vec{r},t)=i\hbar\dfrac{\partial \mathrm{v}_i(\vec{r},t)}{\partial t}\end{cases}$$

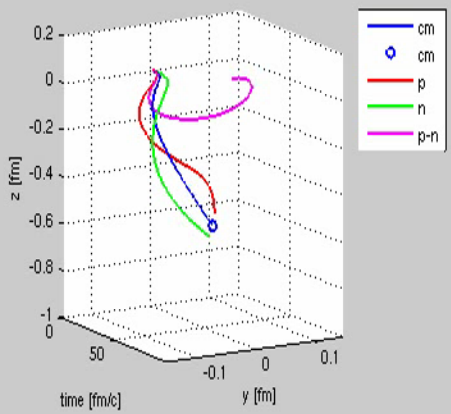
TDSLDA equations

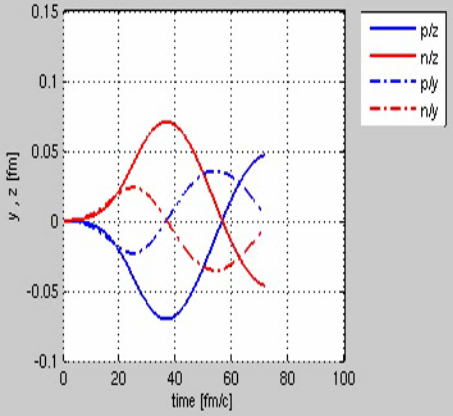
$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix} = \begin{pmatrix} \hat{h}_{\uparrow\uparrow}(\vec{r},t)-\mu & \hat{h}_{\uparrow\downarrow}(\vec{r},t) & 0 & \Delta(\vec{r},t) \\ \hat{h}_{\downarrow\uparrow}(\vec{r},t) & \hat{h}_{\downarrow\downarrow}(\vec{r},t)-\mu & -\Delta(\vec{r},t) & 0 \\ 0 & -\Delta^*(\vec{r},t) & -\hat{h}^*_{\uparrow\uparrow}(\vec{r},t)+\mu & -\hat{h}^*_{\uparrow\downarrow}(\vec{r},t) \\ \Delta^*(\vec{r},t) & 0 & -\hat{h}^*_{\downarrow\uparrow}(\vec{r},t) & -\hat{h}^*_{\downarrow\downarrow}(\vec{r},t)+\mu \end{pmatrix} \begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix}$$

- The system is placed on a 3D spatial lattice
- Derivatives are computed with FFTW
- Fully self-consistent treatment
- Adams-Bashforth-Milne fifth order preditor-corrector-modifier integrator
- No symmetry restrictions, Galilean invariance
- Number of PDEs is of the order of the number of spatial lattice points
  - from $O(10^4)$ to $O(10^6)$
- Initial state is the ground state of the SLDA (formally like HFB/BdG)
- The code was implemented on JaguarPF, Franklin, Hopper, Hyak, Athena
- TDSLDA is about 1,000-2,000 times more complex than any existing TDHF codes









Geometry of the collision of a relativistic heavy-ion with a nucleus

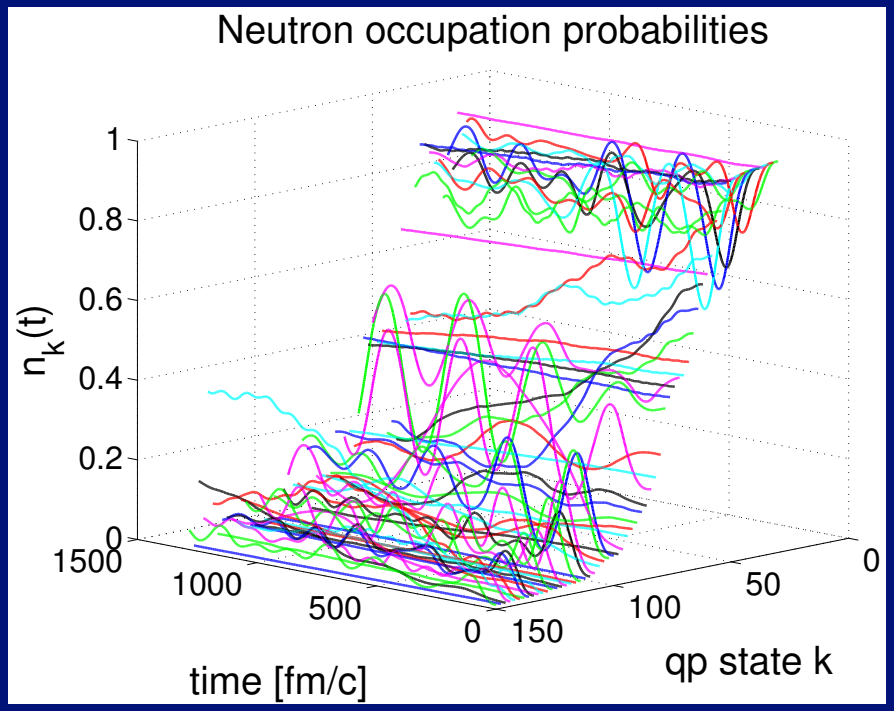
I. Stetcu *et al.*

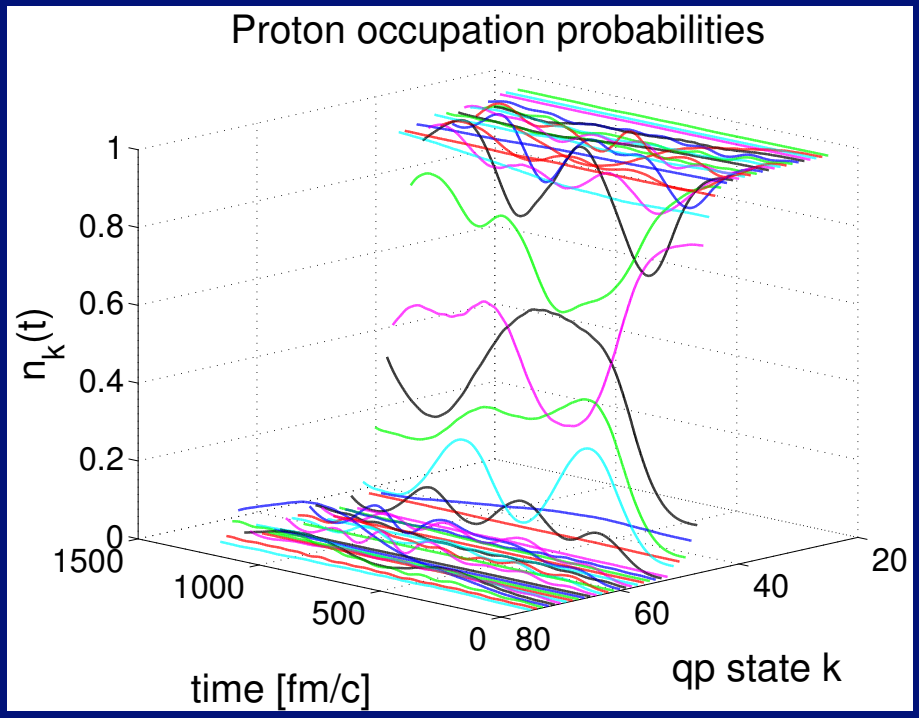
Movie

GDR Coulomb excitation with a relativistic heavy-ion computed in TDSLDA

Movie

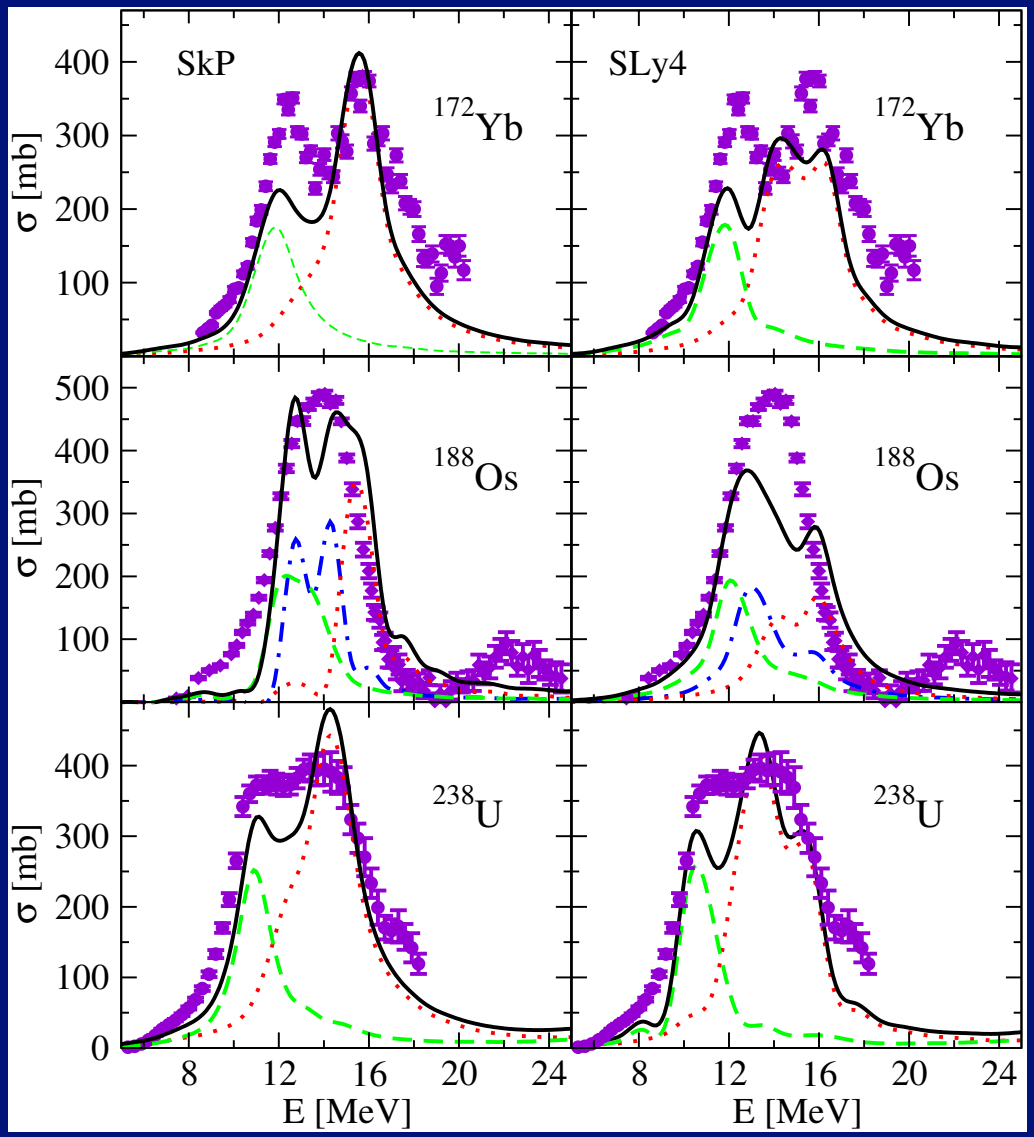
I. Stetcu *et al.*





Time dependent occupation probabilities when exciting isoscalar GDR with a short pulse in ^{238}U within TDSLDA using SLy4

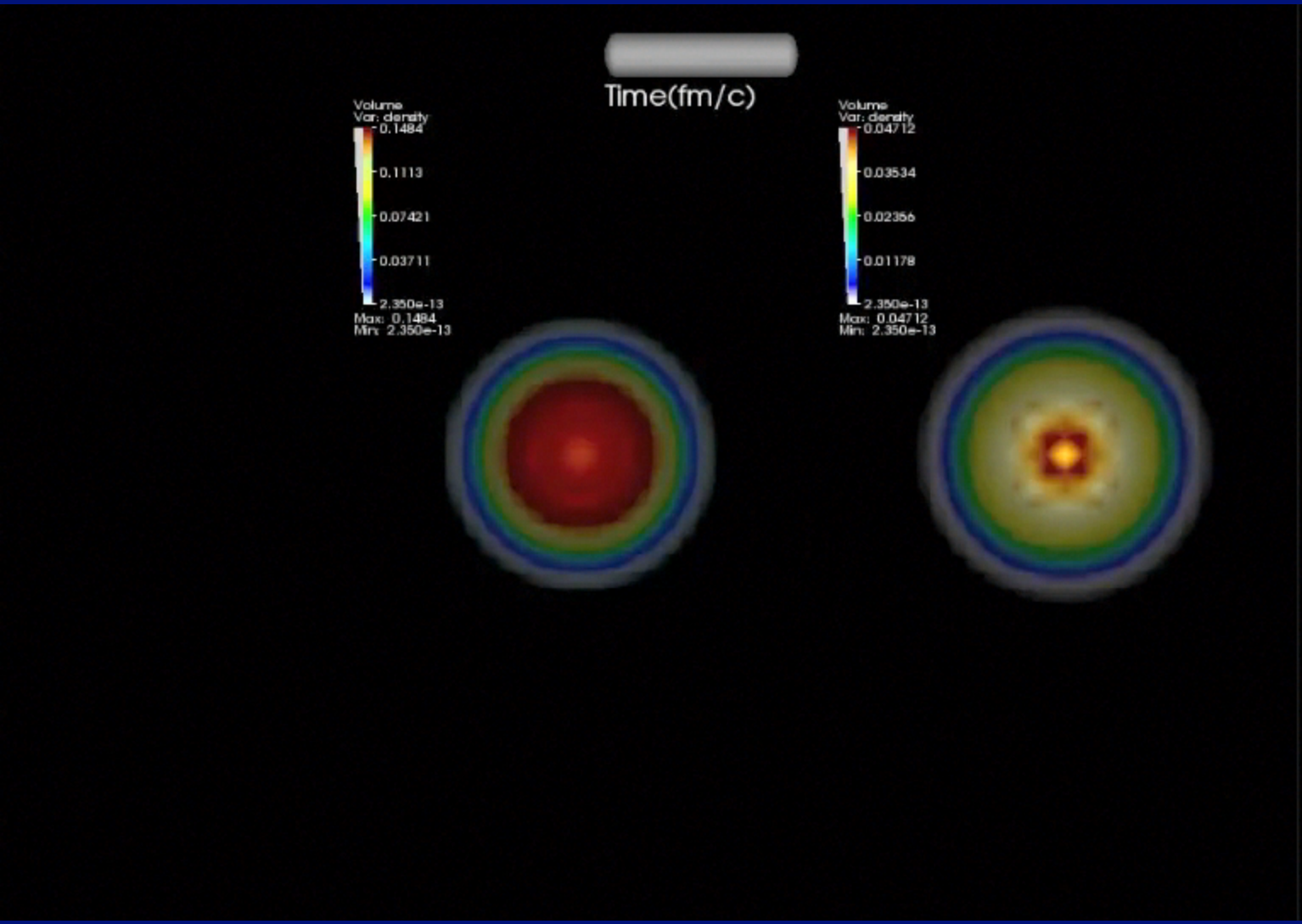
Isovector giant dipole resonance from the 3D time-dependent density functional theory for superfluid nuclei, Stetcu, Bulgac, Magierski, and Roche, Phys. Rev. C **84**, 051309 (2011)



Full unrestricted TDSLDA vs experiment

Isovector giant dipole resonance from the 3D time-dependent density functional theory for superfluid nuclei

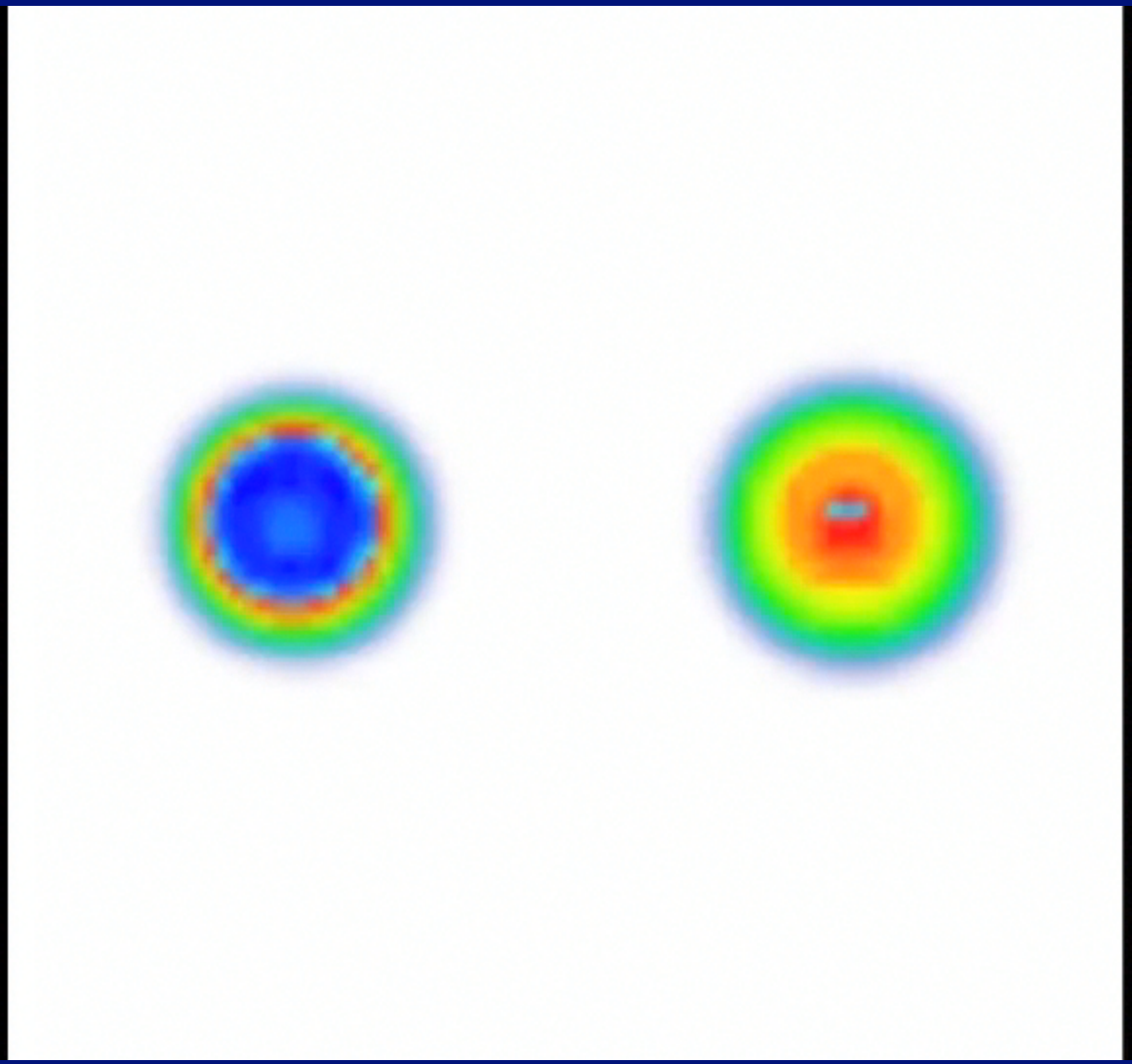
Stetcu, Bulgac, Magierski, and Roche, Phys. Rev. C **84**, 051309 (2011)



Coulomb excitation of GDR with a relativistic heavy-ion computed in TDSLDA

Movie

I. Stetcu *et al.*



Coulomb excitation of GDR with relativistic heavy-ions computed in TDSLDA

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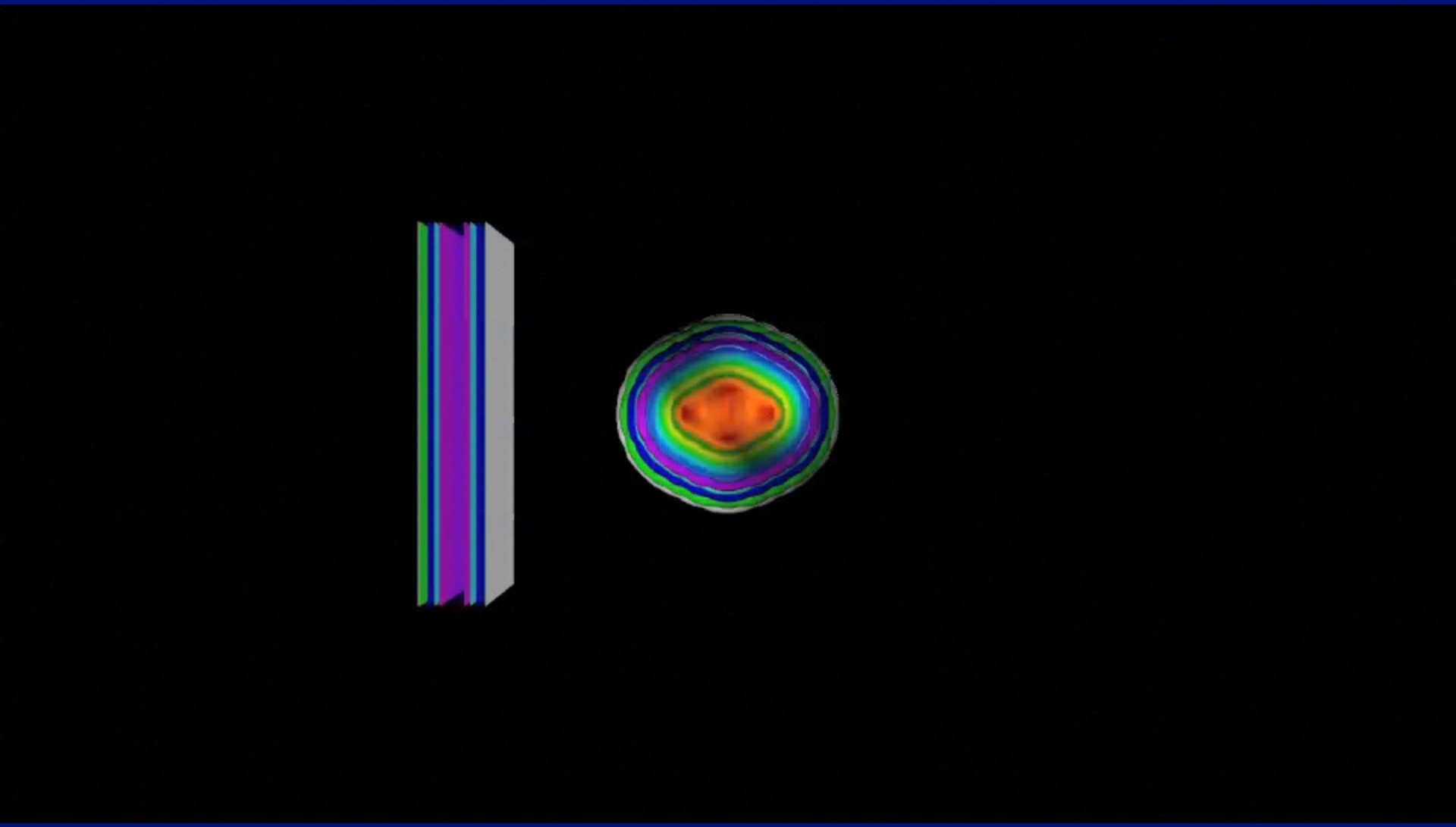
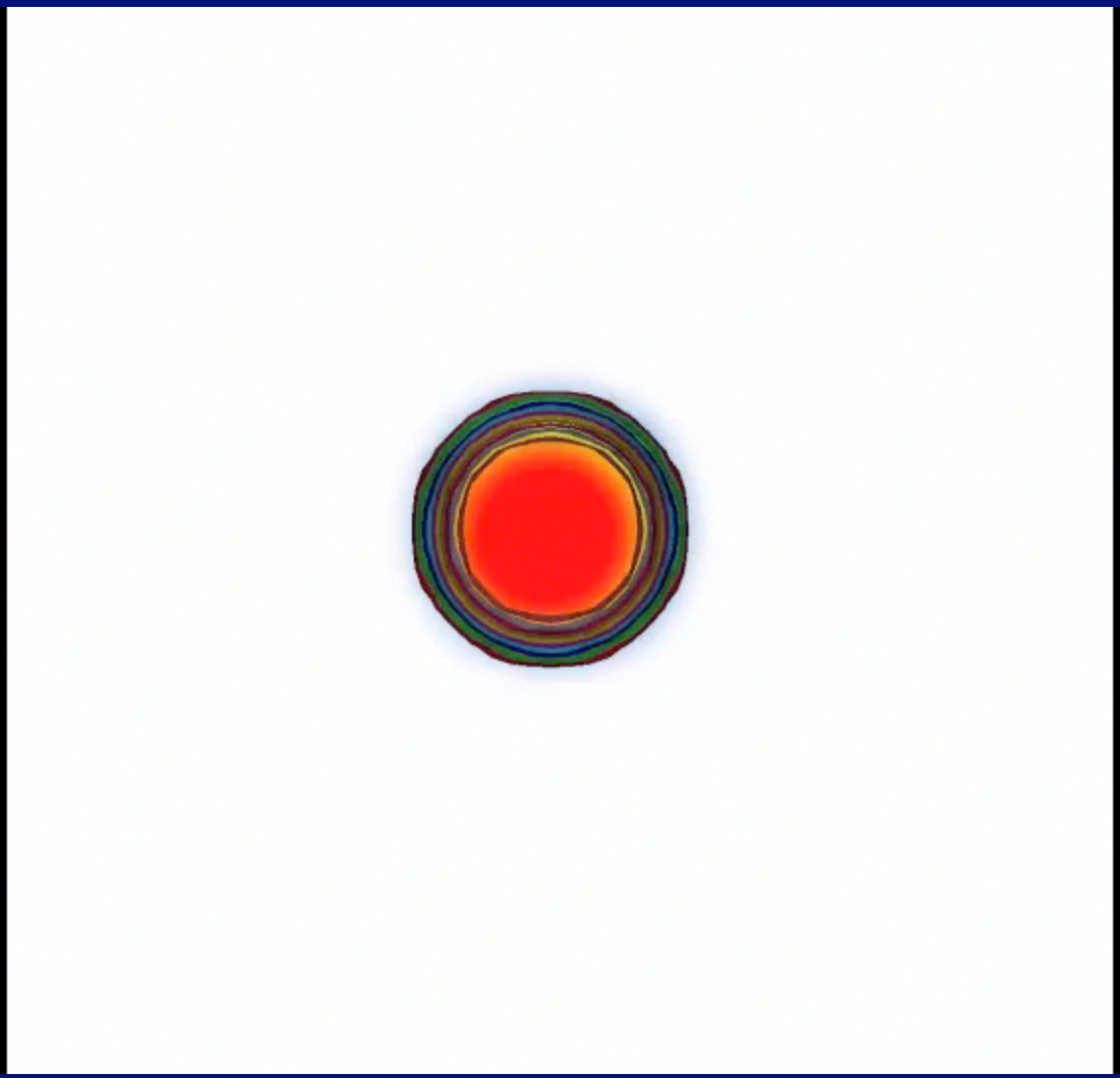


Neutron scattering of ^{238}U computed in TDSLDA

I. Stetcu *et al.*

Movie



Real-time induced fission of ^{280}Cf computed in TDSLDA

I. Stetcu *et al.*

Movie

Present theoretical approaches and phenomenology for Large Amplitude Collective Motion (LACM) and fission studies:

- **Pure phenomenogical stochastic dynamics :**
  - **Langevin/Kramers equations**
  - **Stochastic/Langevin TDHF**

- **Adiabatic Time-Dependent Hartree-Fock-Bogoliubov (ATDHFB) theory**
  - **The basic assumption is that LACM/nuclear fission can be described with a many-body wave function with the GCM- structure:**

$$\int \prod_{i=1}^{n} dq_i \Phi_{\text{Coll.}}(q_1,\ldots,q_n)\Psi_{\text{Slater det.}}(x_1,\ldots,x_A,\{q_1,\ldots,q_n\})$$

- **Microscopic-macroscopic <u>model</u>**
  - **not based on *ab intio* input**
  - **no self-consistency**
  - **physical intuition drives the definition of relevant degrees of freedom**

3D-Langevin Eq.

$$M\frac{dv}{dt} = -\beta v + F(t) \qquad \left\langle F_i(t)F_j(t')\right\rangle = D^2\delta_{ij}\delta(t-t')$$

$$D^2 = 2\beta T$$

$$m\frac{d^2q}{dt^2} = -\frac{\partial V}{\partial q} - \beta m\frac{dq}{dt} + \sqrt{\beta T}\, f(t)$$

Inertia Tensor

Friction Tensor

q_1 = deformation

q_2 = neck size

q_3 = mass asymmetry

Karpov, Nadtochy et al. Phys.Rev. C63, 2001

Extended, … Stochastic TDHF approaches

Wong and Tang, Phys. Rev. Lett. 40, 1070 (1978)
Ayik, Z. Phys. A 298, 83 (1980)
...
Ayik Phys. Lett. B658, 174 (2008)

$$i\mathrm{h}\frac{\partial \psi_k(x,t)}{\partial t} = h[\rho(x,y,t)]\psi_k(x,t)$$

$$\rho(x,y,t) = \sum_{kl} \psi_k^*(x,t)\, n_{kl}(t) \psi_l(x,t)$$

$$\langle n_{kl}(t)\rangle = \delta_{kl} n_k$$

$$\langle \delta n_{kl}(t)\delta n_{ij}(t)\rangle = \frac{1}{2}\delta_{kj}\delta_{li}\left[n_i(1-n_j)+n_j(1-n_i)\right]$$

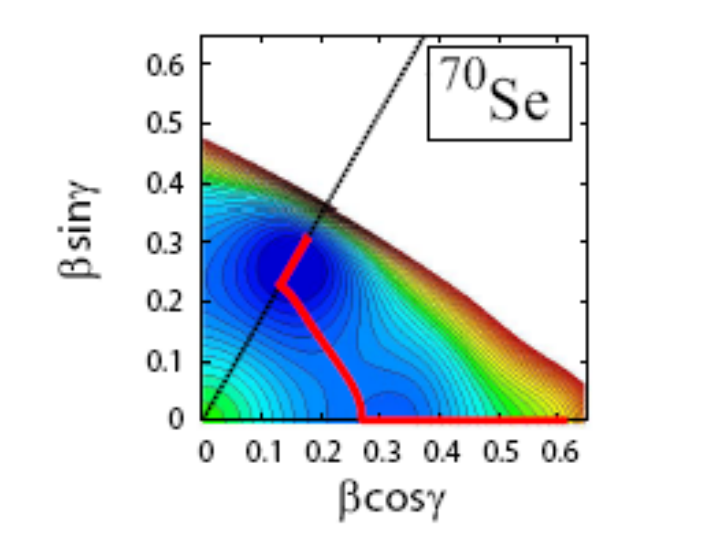
Gaussian random numbers defined by a prescribed temperature in a Fermi-Dirac distribution

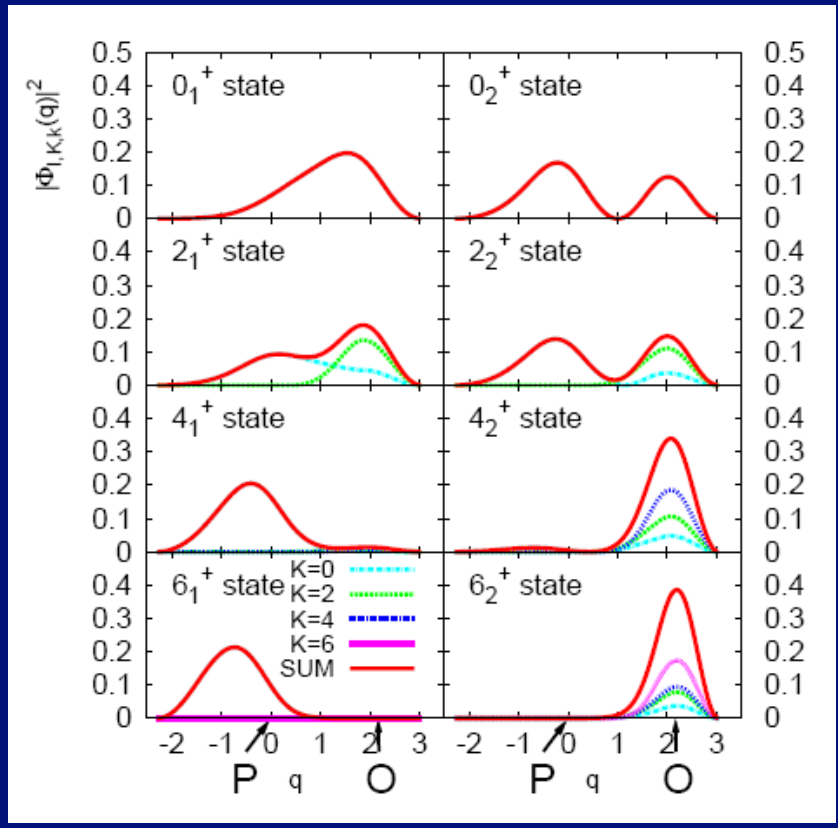
Subsequently these equations are *projected* on a collective subspace and a Langevin equation is introduced for the collective DoF

While ATDHFB approximation has a great number of positive aspects, it comes with a long series of great deficiencies:

- The determination of the number of relevant degrees of freedom is as a rule determined by the practioner using intuition/prejudice or prevailing attitudes.

There are knows methods on how to mechanize this process and eliminate arbitrariness, but they are extremely difficult to implement in practice.



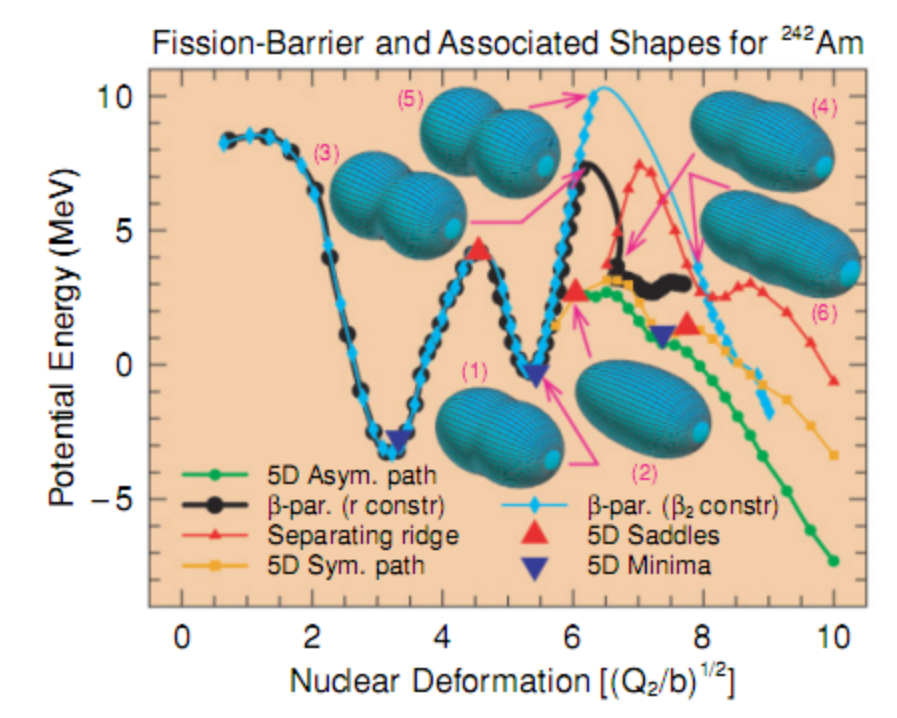


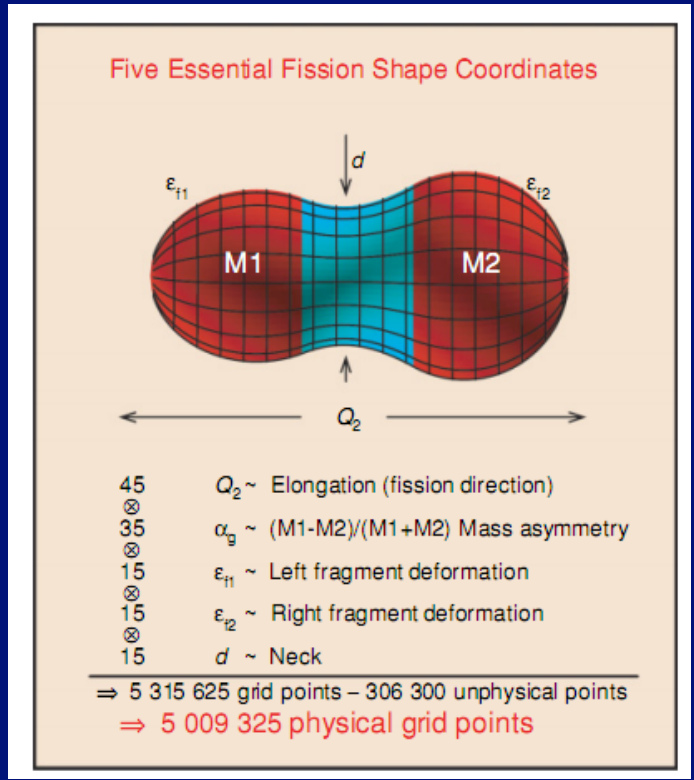
Hinohara, Nakatsukasa, Matsuo, and Matsuyanagi, Phys. Rev. C 80, 014305 (2009)

• **Computing the potential energy surface alone for only 2-3 collective degrees of freedom is equivalent to computing the entire nuclear mass table.**

P. Moller and collaborators need more than 5,000,000 shapes in a five dimensional space.

Is this the right and the entire complete set of collective coordinates?





P.Moller *et al.* Phys. Rev. C 79, 064304 (2009)

$$\int \prod_{i=1}^{n} dq_i \Phi_{\text{Coll.}}(q_1,\ldots,q_n)\Psi_{\text{Slater det.}}(x_1,\ldots,x_A,\{q_1,\ldots,q_n\})$$

- **In order to determine the collective part of the wave function one needs to solve the Hill-Wheeler integral equation in the corresponding *n*-dimensional space.**

This is routinely (but not always) performed by invoking a further approximation (Gaussian Overlap Approximation) the accuracy of which is difficult to assess and one generates a Schrödinger equation in collective coordinates.

- **ATDHFB theory is based on the assumption that an expansion in velocities is accurate up to second order terms. However there are clear examples where this is wrong.**

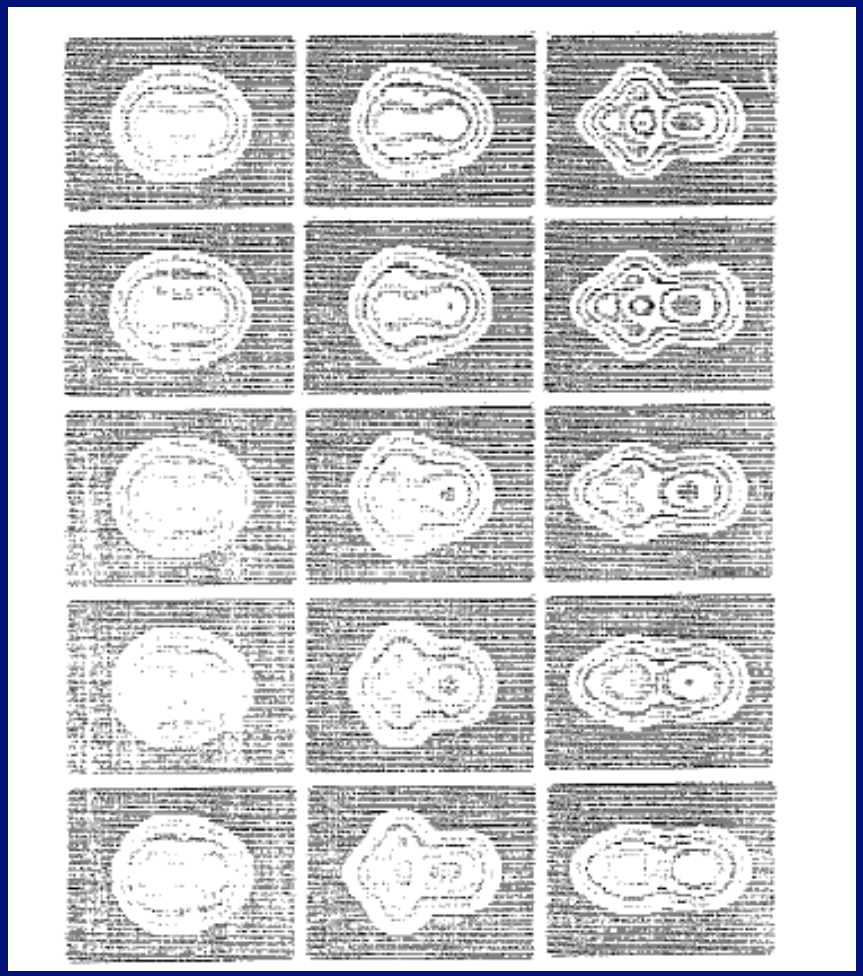
- **The inertial tensor is usually hard to evaluate and often approximate methods are used.**

•It is obvious that a significantly larger number of degrees of freedom are necessary to describe LACM and fission in particular.

One would like to have as well: charge asymmetry, shapes of the fragments, excitation energy of the fragments, quantum numbers, …

The ATHFB approach becomes clearly unmanageable, even for computers envisioned in the next decade, and the veracity of the approximation is questionable .

``Spontaneous fission“ of ^{32}S



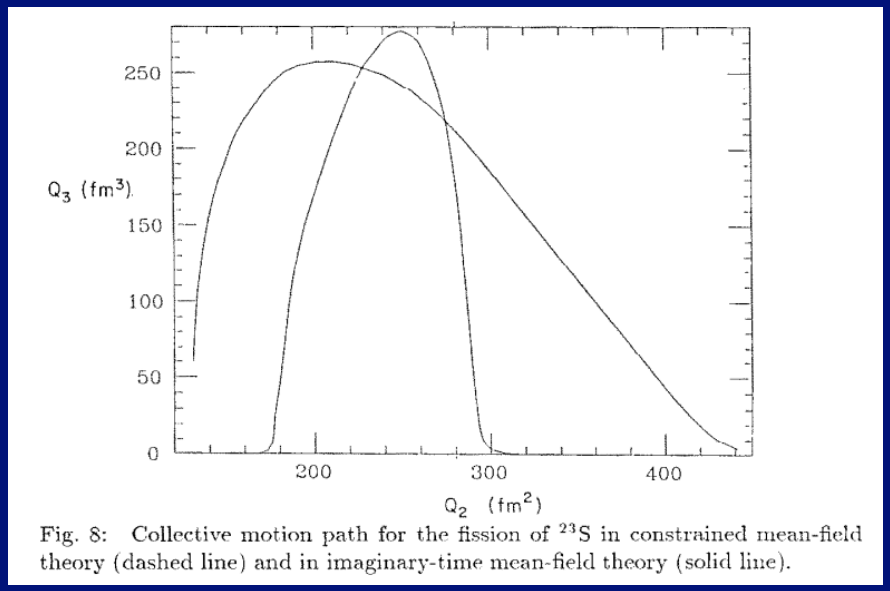


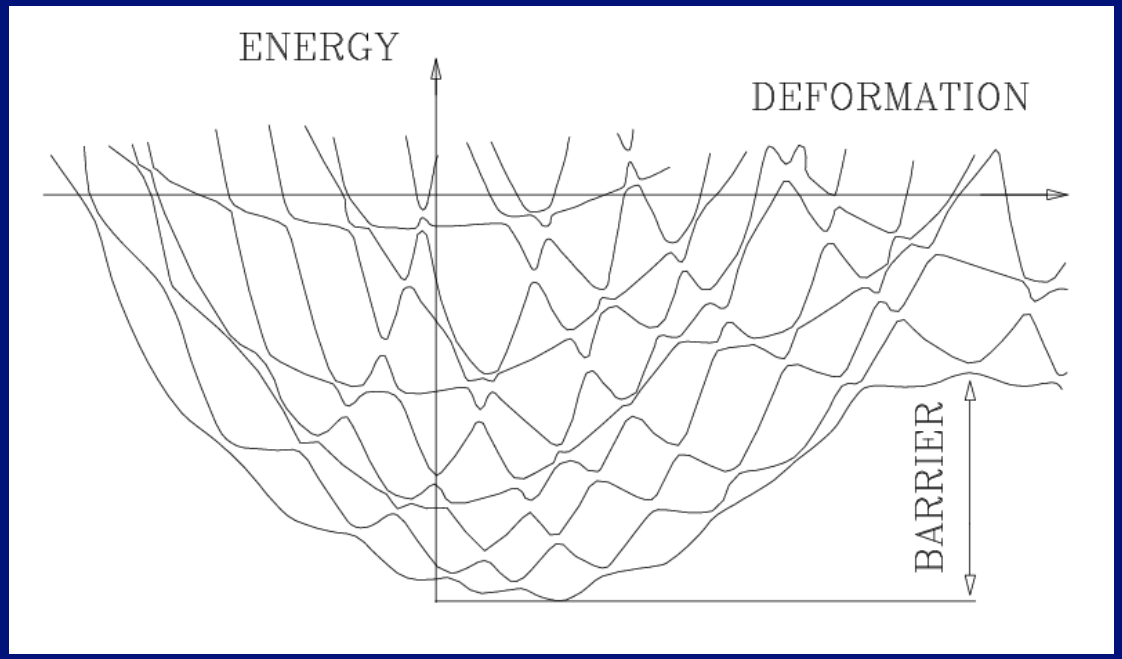
Fig. 8: Collective motion path for the fission of ^{23}S in constrained mean-field theory (dashed line) and in imaginary-time mean-field theory (solid line).

Even though the initial and final states have axial symmetry, along the fission path this symmetry is broken in order to rearrange occupation probabilities and avoid a diabolical point/level crossing, where a Dirac monopole resides.

J.W. Negele, Nucl. Phys. A 502, 371c (1989)
An unpublished calculation due to R. Wolff, G. Puddu and J.W. Negele

- **8 occupied orbitals evolved in 3D and imaginary time on a mesh 20^3x1000**
- **no isospin dof, no pairing, simplified nuclear EDF**

Generic adiabatic large amplitude potential energy SURFACES



(I ``borrowed'' this figure from a paper a long time ago and I do not remember where from.)

- In LACM adiabaticity/isentropic or isothermal behavior is not a guaranteed
- The most efficient mechanism for transitions at level crossing is due to pairing
- Level crossings are a great source of : entropy production (dissipation), dynamical symmetry breaking , non-abelian gauge fields (Dirac monopoles reside at level crossings)

Evolution operator of an interacting many-body system

(after a Trotter expansion and a Hubbard-Stratonovich transformation)

$$\exp\left[-iH(t_f - t_i)\right] \propto \int \prod_n \prod_{ab} d\sigma_{ab}(n) \exp\left[i \frac{\Delta t}{2} \sum_{abcd} \sigma_{ab}(n) V_{abcd} \sigma_{cd}(n) \right] \times$$

$$\exp\left[i\Delta t \sum_{ab} \left(T_{ab} + \sum_{cd} V_{abcd} \sigma_{cd}(n) \right) \alpha_a^\dagger \alpha_b \right]$$

This representation is not unique!

The one-body evolution operator is arbitrary!!!

Kerman, Levit, and Troudet, Ann. Phys. 148, 443 (1983)

$$\exp\left[-iH(t_f - t_i)\right] \propto \int \prod_n \prod_{ab} d\sigma_{ab}(n) \exp\left[i \frac{\Delta t}{2} \sum_{abcd} \sigma_{ab}(n) V_{abcd} \sigma_{cd}(n) \right] \times$$

$$\exp\left[i\Delta t \sum_{ab} \left(T_{ab} + \sum_{cd} V_{abcd} \sigma_{cd}(n) \right) \alpha_a^\dagger \alpha_b \right]$$

What is the <u>best</u> one-body propagator?

Stationary phase approximation leads to some form of Time-Dependent Meanfield

However, there is a bright spot if one is interested in one-body densities alone

Time-Dependent Density Functional Theory (TDDFT) asserts that there exists an exact description, which formally looks like Time-Dependent Selfconsistent Meanfield.

A.K. Rajagopal and J. Callaway, Phys. Rev. B 7, 1912 (1973)
V. Peuckert, J. Phys. C 11, 4945 (1978)
E. Runge and E.K.U. Gross, Phys. Rev. Lett. 52, 997 (1984)

http://www.tddft.org

There is a problem however!

Nobody knows how the true Time-Dependent Density Functional looks like.

But we know that it exists.

DFT has another serious restriction.
One cannot extract any information about two-body observables.

For example, if we were to study the fission of a nucleus, we will in principle determine the average masses of the daughters, but we will have no information about the width of the mass distribution.

There is a relatively simple solution in time-dependent meanfield theory due to Balian and Veneroni (late 1980's and early 1990's)

$$\rho(t_0) \overset{TDHF}{\Rightarrow} \rho(t_1)$$

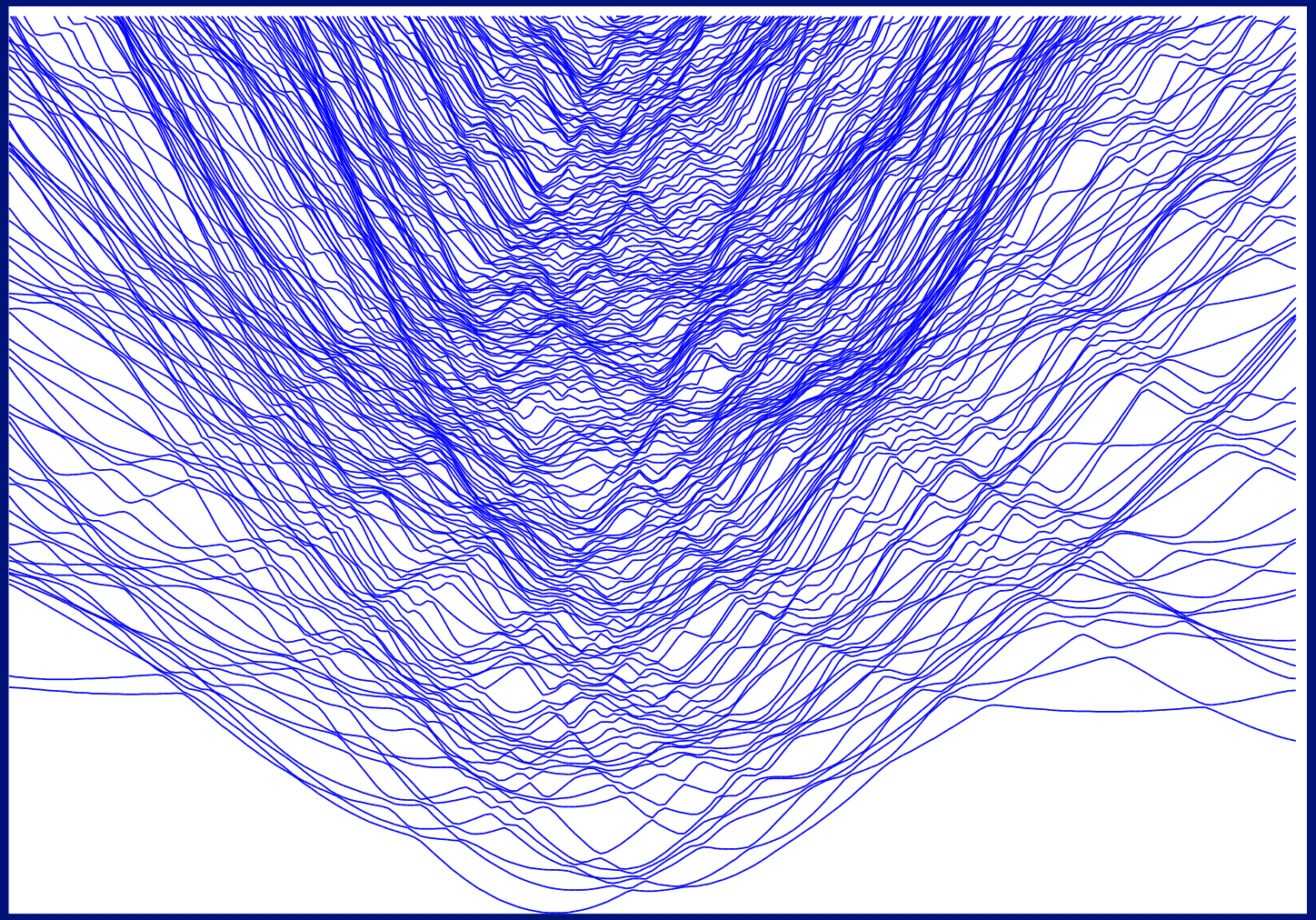
$$\sigma(t_1,\varepsilon) = \exp\left(i\varepsilon\hat{Q}\right)\rho(t_1)\exp\left(-i\varepsilon\hat{Q}\right)$$

$$\sigma(t_0,\varepsilon) \overset{TDHF}{\Leftarrow} \sigma(t_1,\varepsilon)$$

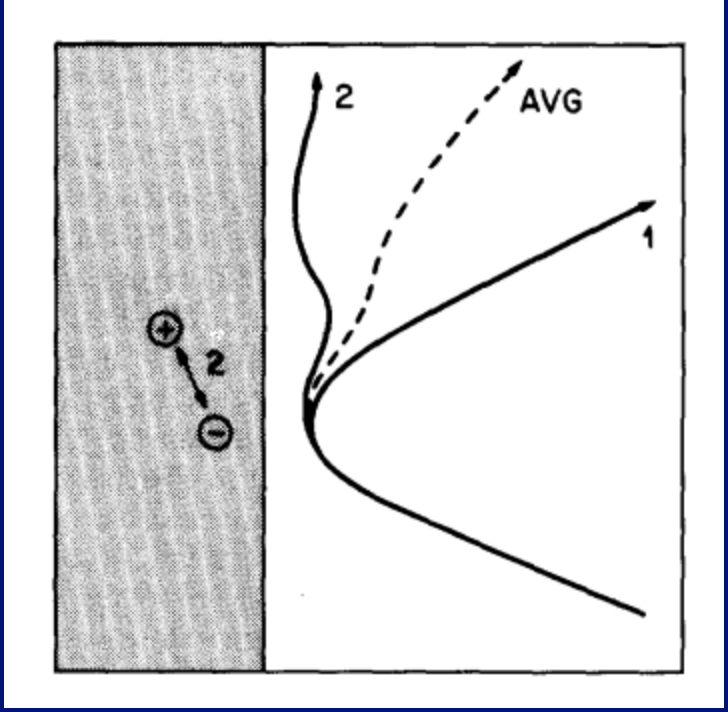
$$\left(\Delta Q_{BV}\right)^2\Big|_{t_1} = \lim_{\varepsilon\to 0}\frac{1}{2\varepsilon^2}\mathrm{Tr}\left[\rho(t_0)-\sigma(t_0,\varepsilon)\right]$$

This method allows in principle the evaluation of both averages and widths.

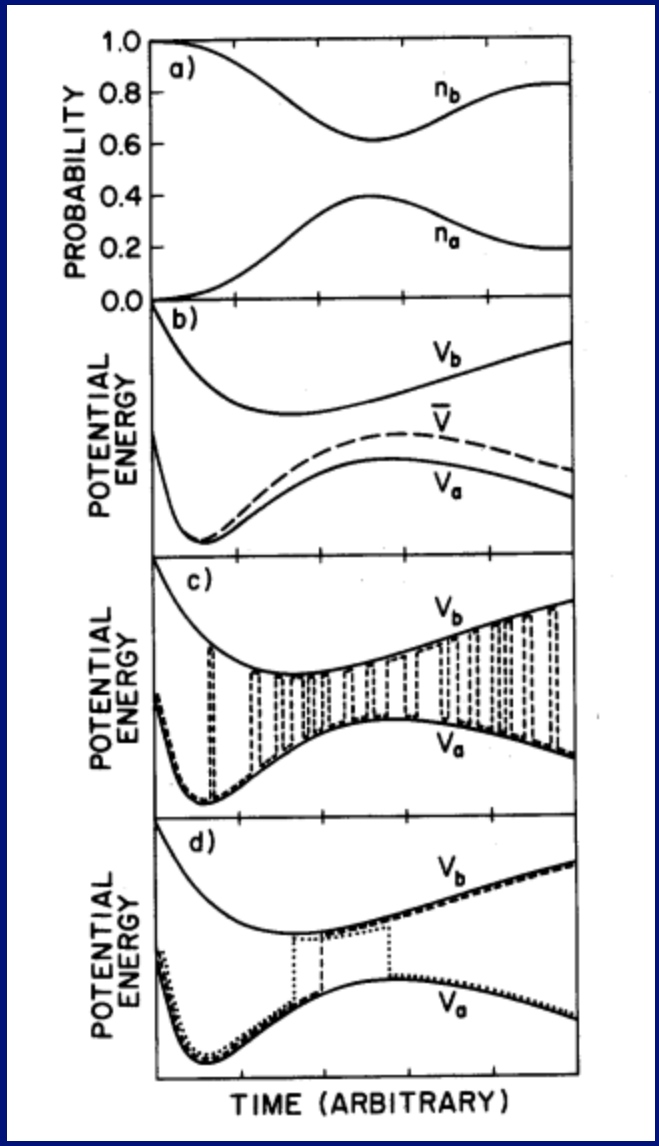
The main problem however is that we have to consider the generic situation with multiple potential energy surfaces.



John C. Tully suggested the following recipe for condensed matter and chemistry applications
J. Chem. Phys. 93, 1061 (1990)



$$\psi(\vec{r},\vec{R},t)=\sum_i c_i(\vec{R},t)\varphi_i\left(\vec{r}\,\middle|\,\vec{R}\right)$$



The questions is:

Can one even ``dream'' of implementing the real-time path integral for strongly interacting fermions?

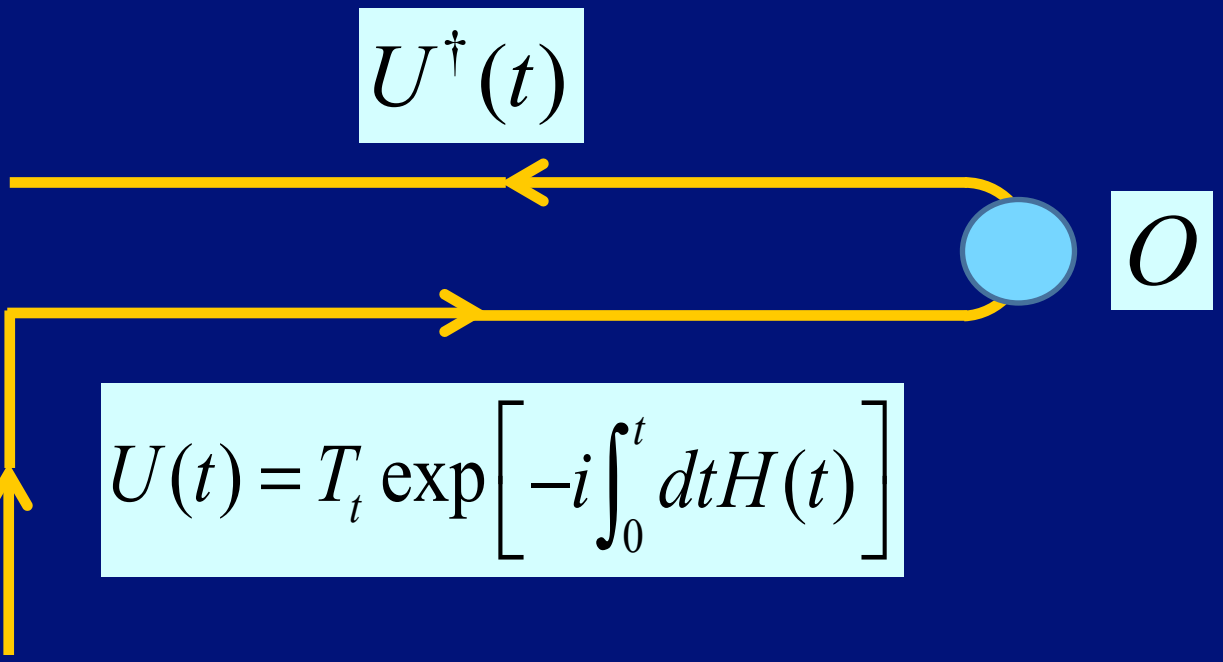
Does such formalism even have any mathematical meaning?

$$\exp\left[-iH(t_f - t_i)\right] \propto \int \prod_n \prod_{ab} d\sigma_{ab}(n) \exp\left[i \frac{\Delta t}{2} \sum_{abcd} \sigma_{ab}(n) V_{abcd} \sigma_{cd}(n) \right] \times$$
$$\exp\left[i\Delta t \sum_{ab} \left(T_{ab} + \sum_{cd} V_{abcd} \sigma_{cd}(n) \right) \alpha_a^\dagger \alpha_b \right]$$

<u>This looks much worse that the infamous fermion sign problem!!!</u>

There is a little bit of ``light of the end of the tunnel" and a numerical implementation of real-time path integral for interacting many-fermion appears feasible.

What we need is a bit more complicated, to simulate dynamics along the Schwinger complex time-ordered contour



$$H(t) = H_0 + V_{ext}(t), \qquad t>0$$

$$i\mathrm{h}\frac{\partial \rho(t)}{\partial t} = [H(t), \rho(t)], \qquad \rho(0)=\rho_0$$

$$O(t) = \mathrm{Tr}[O\rho(t)] = \mathrm{Tr}\left[\rho_0 U^{\dagger}(t) O U(t)\right]$$

Here is how this can be done and has already been implemented numerically on Hyak-UW (MRI-NSF funded cluster, Intel chips, 1120 cores, 3Gb RAM/core)

We place several fermions on a square lattice

$$H = \sum_{\vec{k},\sigma} \frac{\vec{k}^2}{2} \alpha^{\dagger}_{\vec{k},\sigma} \alpha_{\vec{k},\sigma} + g \sum_{\vec{r}} \alpha^{\dagger}_{\vec{r},\uparrow} \alpha^{\dagger}_{\vec{r},\downarrow} \alpha_{\vec{r},\downarrow} \alpha_{\vec{r},\uparrow}$$

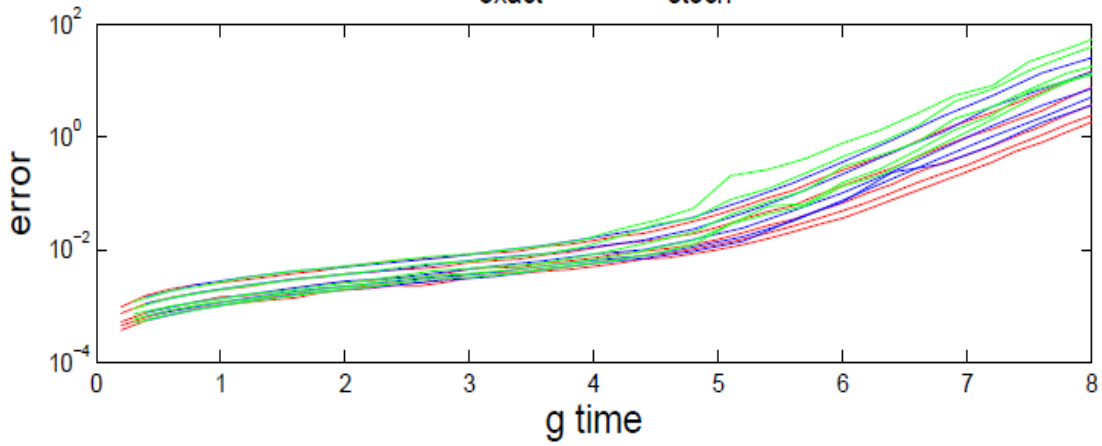
NB The coordinate and momentum creation/annihilation operators are linked by the usual unitary transformations.

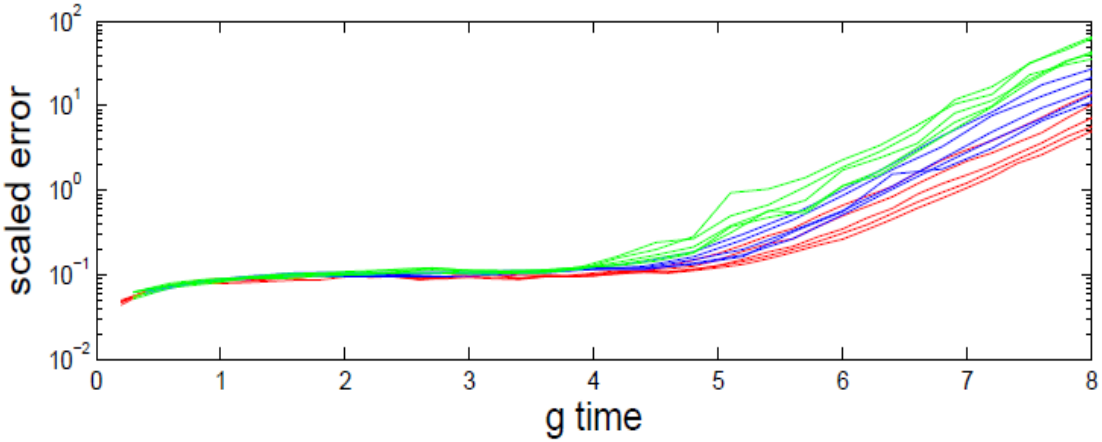
We evolve an initial many-fermion wave function using independent real-time path integral representations of the propagators for the bra (backward in time) and ket (forward in time) many-body wave functions:

$$\exp\left[-iH(t_f - t_i)\right] \propto \int \prod_n \prod_{ab} d\sigma_{ab}(n) \exp\left[i \frac{\Delta t}{2} \sum_{abcd} \sigma_{ab}(n) V_{abcd} \sigma_{cd}(n) \right] \times$$

$$\exp\left[i\Delta t \sum_{ab} \left(T_{ab} + \sum_{cd} V_{abcd} \sigma_{cd}(n) \right) \alpha^{\dagger}_a \alpha_b \right]$$

We used both discrete and continuous HS transformations, and simulated up to 6 fermions.





Results for two fermions, for g=1 (red), 2 (blue), and 3 (green), and a 16x16 lattice
Sample sizes for the propagator M= 2,500, 5,000, 10,000 and 20,000.
Lower plot shows that error scales as theoretically expected

$$\propto \exp(gt/2)/\sqrt{M}\,.$$

Theoretical analysis and further numerical simulations for systems with up to six fermions so far show that for N interacting fermions the simulation error behaves as

$$\propto \exp(Ngt/2)/\sqrt{M}.$$

NB The error is independent of:

- the dimensionality of the space
- the spatial volume/size of lattice
- a relatively small number of samples is needed for a decent accuracy