Real-Time Deterministic and Stochastic Dynamics of Fermionic Superfluids: Nuclei (and the Unitary Fermi Gas)

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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***
- **(Applications to Unitary Fermi Gas)**
- **Why we need to extend the eterministic TDSLDA to a Stochastic TDSLDA and why we need the exascale regime?**
- **How to implement Real-Time Path Integral for Interacting Many Fermion Systems**

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

JETP LETTERS VOLUME 68, NUMBER 3 10 AUGUST 1998

Towards a universal nuclear density functional

S. A. Fayans
Kurchatov Institute Russian Science Center, 123182 Moscow, Russia

The total energy density of a nuclear system is represented as

$$\varepsilon = \varepsilon_{\rm kin} + \varepsilon_v + \varepsilon_s + \varepsilon_{\rm Coul} + \varepsilon_{sl} + \varepsilon_{\rm anom}, \qquad (1)$$

where $\varepsilon_{\rm kin}$ is the kinetic energy term which, since we are constructing a Kohn–Sham type functional, is taken with the free operator $t = p^2/2m$, i.e., with the effective mass $m^* = m$; all the other terms are discussed below.

The volume term in (1) is chosen to be in the form

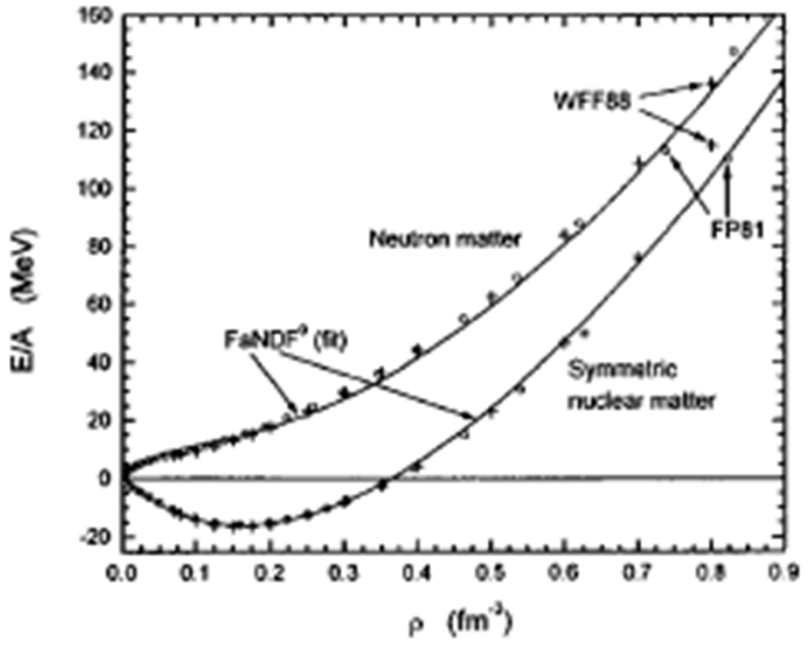
$$\varepsilon_v = \frac{2}{3}\epsilon_F^0 \rho_0 \left[a_+^v \frac{1 - h_{1+}^v x_+^\sigma}{1 + h_{2+}^v x_+^\sigma} x_+^2 + a_-^v \frac{1 - h_{1-}^v x_+}{1 + h_{2-}^v x_+} x_-^2 \right].$$

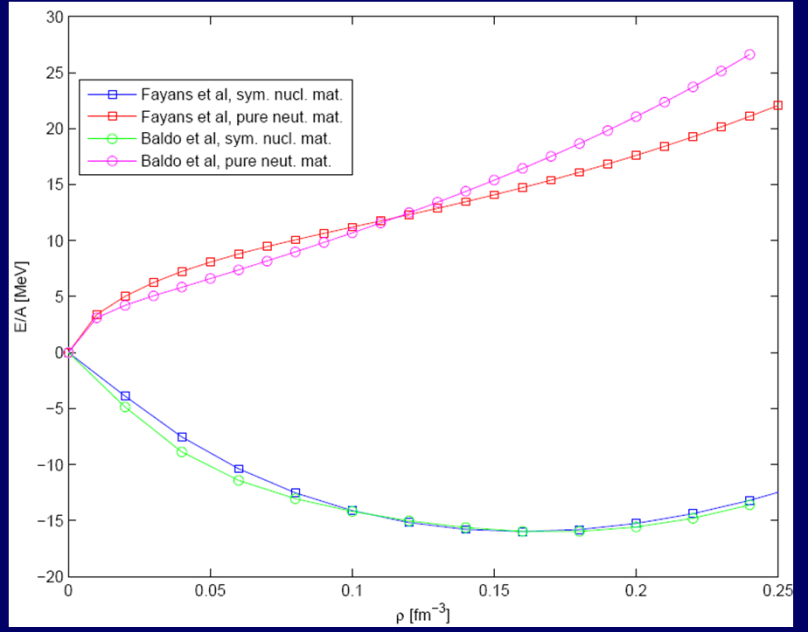
Here and in the following $x_\pm = (\rho_n \pm \rho_p)/2\rho_0$, $\rho_{n(p)}$ is the neutron ($2\rho_0$ is the equilibrium density of symmetric nuclear matter wit

The surface part in Eq. (1) is meant to describe the finite-range and nonlocal in-medium effects which may presumably be incorporated phenomenologically within the EDF framework in a localized form by introducing a dependence on density gradients. It is taken as follows:

$$\varepsilon_s = \frac{2}{3}\epsilon_F^0 \rho_0 \frac{a_+^s r_0^2 (\nabla x_+)^2}{1 + h_+^s x_+^\sigma + h_\nabla^s r_0^2 (\nabla x_+)^2}, \qquad (3)$$

with $h_+^s = h_2^v$, , a_+^s and h_∇^s the two free parameters. Such a form is obtained by adding





Baldo, Schuck, and Vinas, arXiv:0706.0658

Let us summarize some of the ingredients of the SLDA in nuclei

Energy Density (ED) describing the normal system

ED contribution due to superfluid correlations

$$E_{gs} = \int d^3 r \left\{ \varepsilon_N [\rho_n(\vec{r}), \rho_p(\vec{r})] + \varepsilon_S [\rho_n(\vec{r}), \rho_p(\vec{r}), \nu_n(\vec{r}), \nu_p(\vec{r})] \right\}$$

$$\begin{cases} \varepsilon_N [\rho_n(\vec{r}), \rho_p(\vec{r})] = \varepsilon_N [\rho_p(\vec{r}), \rho_n(\vec{r})] \\ \varepsilon_S [\rho_n(\vec{r}), \rho_p(\vec{r}), \nu_n(\vec{r}), \nu_p(\vec{r})] = \varepsilon_S [\rho_p(\vec{r}), \rho_n(\vec{r}), \nu_p(\vec{r}), \nu_n(\vec{r})] \end{cases}$$

Isospin symmetry constraints
(Coulomb energy and other relatively small terms not shown here.)

$$\varepsilon_S \left[\rho_n, \rho_p, \nu_p, \nu_n \right] = g(\rho_p, \rho_n)[|\nu_p|^2 + |\nu_n|^2]$$

$$+ f(\rho_p, \rho_n)[|\nu_p|^2 - |\nu_n|^2] \quad \frac{\rho_p - \rho_n}{\rho_p + \rho_n}$$

where $g(\rho_p, \rho_n) = g(\rho_n, \rho_p)$

and $f(\rho_p, \rho_n) = f(\rho_n, \rho_p)$

Nuclear energy functionals

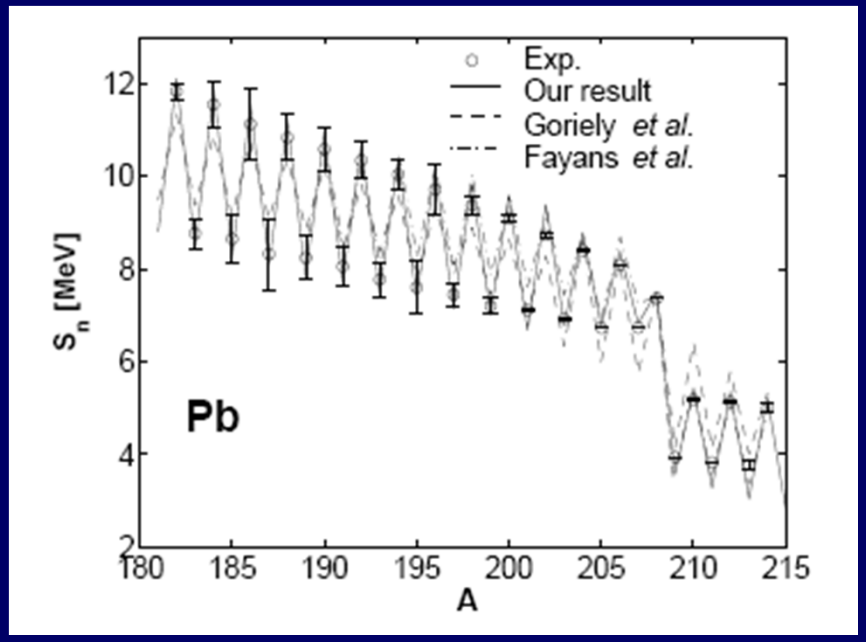
- Ab initio: DME (Negele, Vautherin, Furnstahl , Bogner, ...)
- Phenomenological functionals:

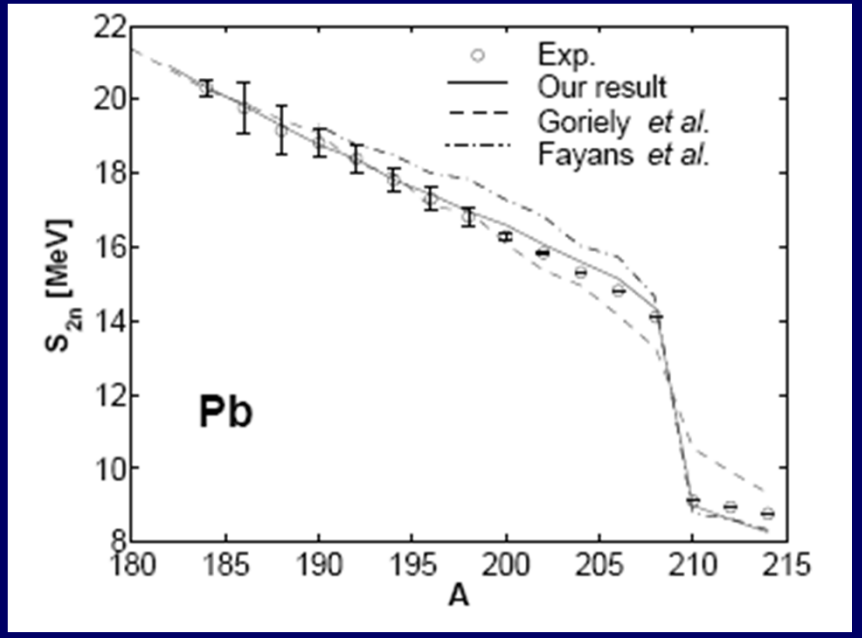
$$\mathcal{E}(\vec{r}) = \frac{1}{2M_n}\tau_n(\vec{r}) + \frac{1}{2M_p}\tau_p(\vec{r}) - \Delta(\vec{r})\nu_c(\vec{r})$$
$$+ \sum_{T=0,1} \Big(C_T^{\rho}\rho_T^2 + C_T^{\Delta}\rho_T\nabla^2\rho_T + C_{\gamma}\rho_0^{\gamma}\rho_T^2$$
$$+ C_T^{\tau}(\rho_T\tau_T - \vec{j}_T^2) + C_T^{\nabla J}(\rho_T\vec{\nabla}\cdot\vec{J} + \vec{s}_T\times\vec{j}_T)\Big)$$

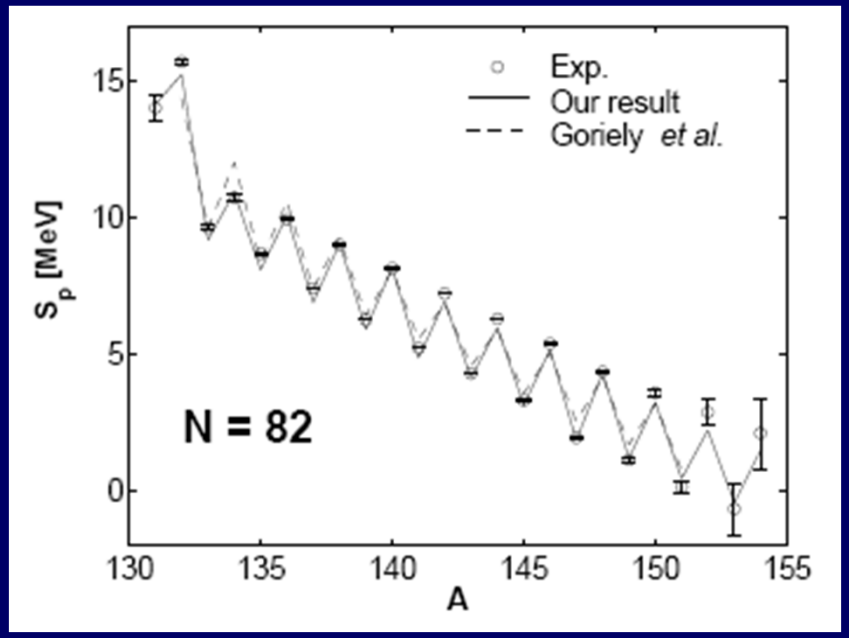
Galilean invariance

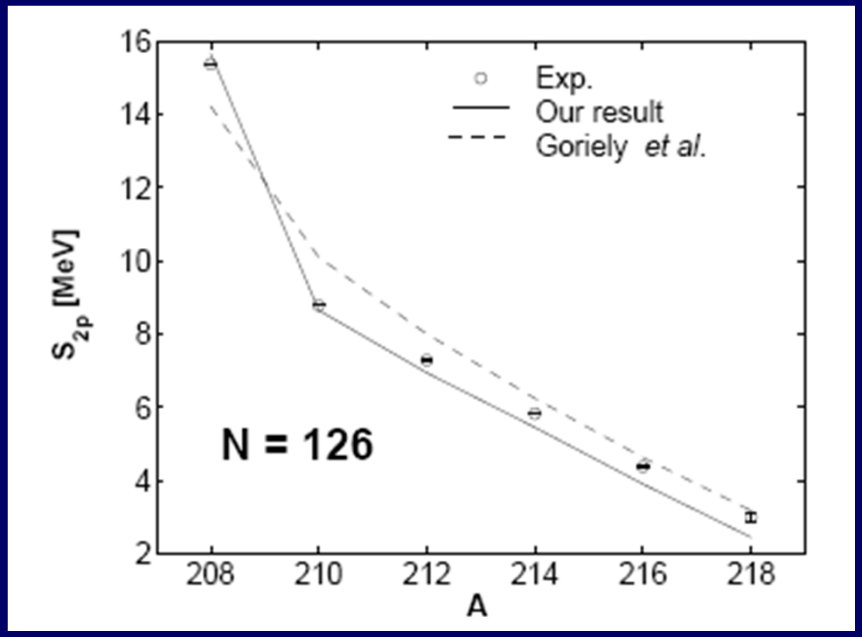
$$h(\vec{r}) = -\nabla\frac{\hbar^2}{2m(\vec{r})}\nabla + U(\vec{r}) + i\vec{\sigma}\cdot\vec{V}(\vec{r}) + i\vec{V}_1(\vec{r})\cdot\nabla + i\vec{W}(\vec{r})\cdot(\vec{\sigma}\times\nabla)$$

From a talk given by Ionel Stetcu recently at LANL









A single universal parameter for pairing!

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

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

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

For time-dependent phenomena one has to add currents!

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 with Galilean invariance**
- **Adams-Bashforth-Milne fifth order preditor-corrector-modifier integrator**
- **No symmetry restrictions**
- **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 implementated on JaguarPF, Franklin, Hopper, Hyak, Athena**
- **TDSLDA is about 1,000 times more complex than existing TDHF codes**
- **We used in 2010 and early 2011 about 75 million CPU hours on JaguarPF and Hopper alone, and over 217,000 cores on JaguarPF.**

TD formalism applications

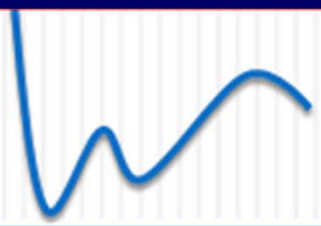
- Nuclear physics:
  - induced fission
  - heavy-ion collisions
  - neutron scattering/capture
  - pairing vibrations
  - electromagnetic response
- Neutron star crust: dynamics of vortices, vortex pinning mechanism
- Cold atoms physics, optical lattices

Limitations:

- only one-body observables can be described accurately
- the results depend on how good the functional is
- large computational resources necessary

Several slides from a talk given by Ionel Stetcu recently at LANL

RPA and linear response



RPA: small correlations on top of mean-field + excited states 1p-1h

$$|\psi_0\rangle = |HF\rangle + |2p-2h\rangle$$

$$|\nu\rangle \approx |1p-1h\rangle$$

$$\langle\nu|F|\psi_0\rangle = \sum_{ph}(F_{hp}X^{\nu}_{ph} + F_{ph}X^{\nu}_{ph})$$

$$\begin{pmatrix} A & B \\ B* & A* \end{pmatrix}\begin{pmatrix} X_\nu \\ Y_\nu \end{pmatrix} = E_\nu \begin{pmatrix} X_\nu \\ -Y_\nu \end{pmatrix}$$

- violates the Pauli principle mainly for non-collective states
- separates the spurious states associated w/ broken symmetry in mean field

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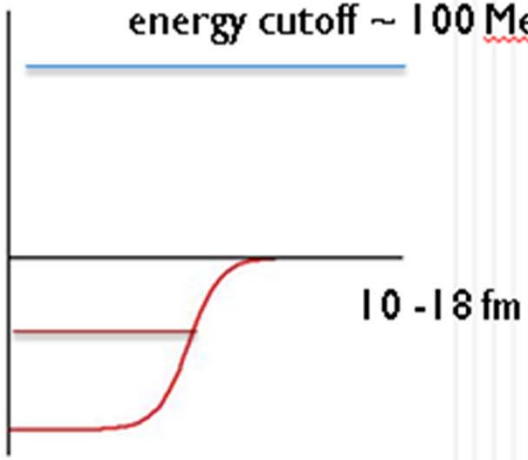
Linear response from TD-DFT: exclusively a model for excited states

$$i\hbar\dot{\rho} = [h[\rho] + f(t), \rho] \longrightarrow \left\{ \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - E \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \begin{pmatrix} \delta\rho^{ph} \\ \delta\rho^{hp} \end{pmatrix} = - \begin{pmatrix} f^{ph} \\ f^{hp} \end{pmatrix}$$

- Pauli principle preserved
- separates the spurious states associated w/ broken symmetries in mean field

Challenges for QRPA



HF: #s.p. states = # particles

HFB: #q.p. >> # particles
~ 2,500

QRPA: dimension ~ (# q.p.)^2 ~ 10^7

very difficult for today's computers:
- non-Hermitian matrix
- middle of the spectrum

Terasaki and Engel, PRC 82 (2010) 034326
QRPA w/ axial symmetry for ^{172}Yb
dimension ~ 160,000 (j-dependent)

in TDHFB: $$\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} \approx \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \exp(-iEt) + \begin{pmatrix} \delta u(t) \\ \delta v(t) \end{pmatrix}$$

# of evolved wfs. = # of q.p.
numerical advantage: can be easily parallelized

need latest generation computers to run

QRPA and TD

	QRPA	TD-SLDA
Dimensions	# qp. squared	# qp
Truncation	identification of spurious states difficult	N/A
Galilean invariance	(usually) not implemented	trivial (in functional)

Terasaki and Engel, PRC **82** (2010) 034326
QRPA w/ axial symmetry for ^{172}Yb
Energies of spurious states: 0.3 – 1.5 MeV

Terasaki, Engel, Bertsch, PRC **78** (2008) 044311

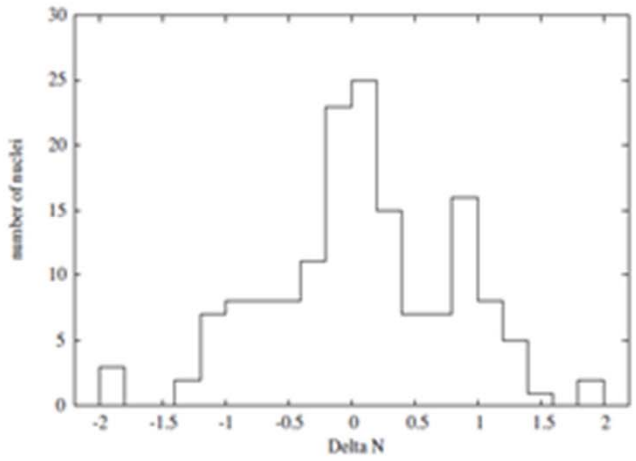


FIG. 1. Particle-hole character of the lowest 2^+ solutions. The histogram displays the quantity ΔN defined in Eq. (1) for 155 nuclei in the SLy4 data set (one of which we drop—see text). The values $-2, 0, +2$ correspond to excitations of hole-hole, particle-hole, and particle-particle character, respectively.

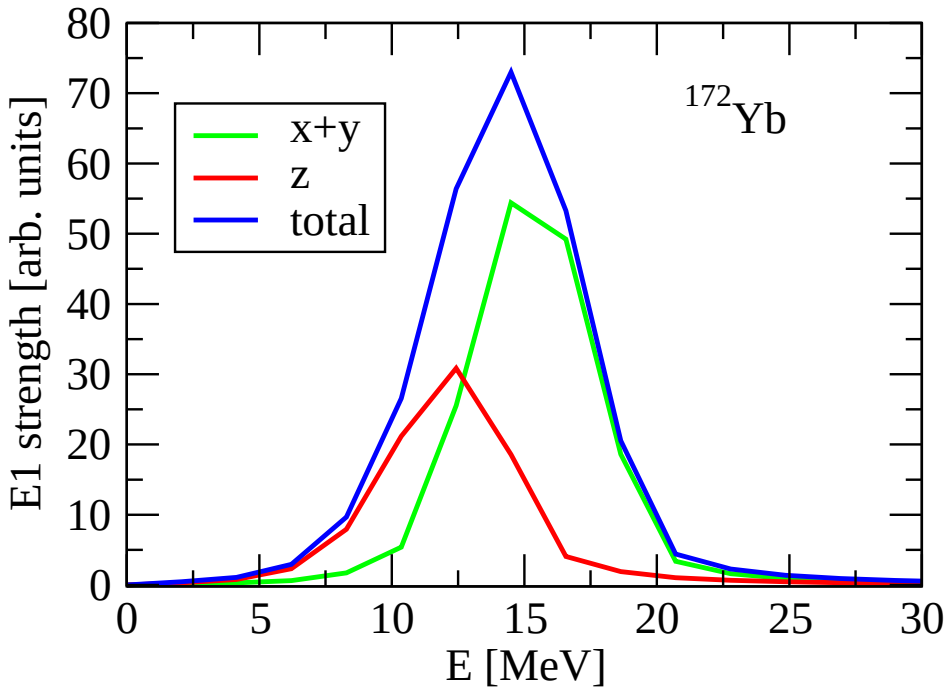
Formalism

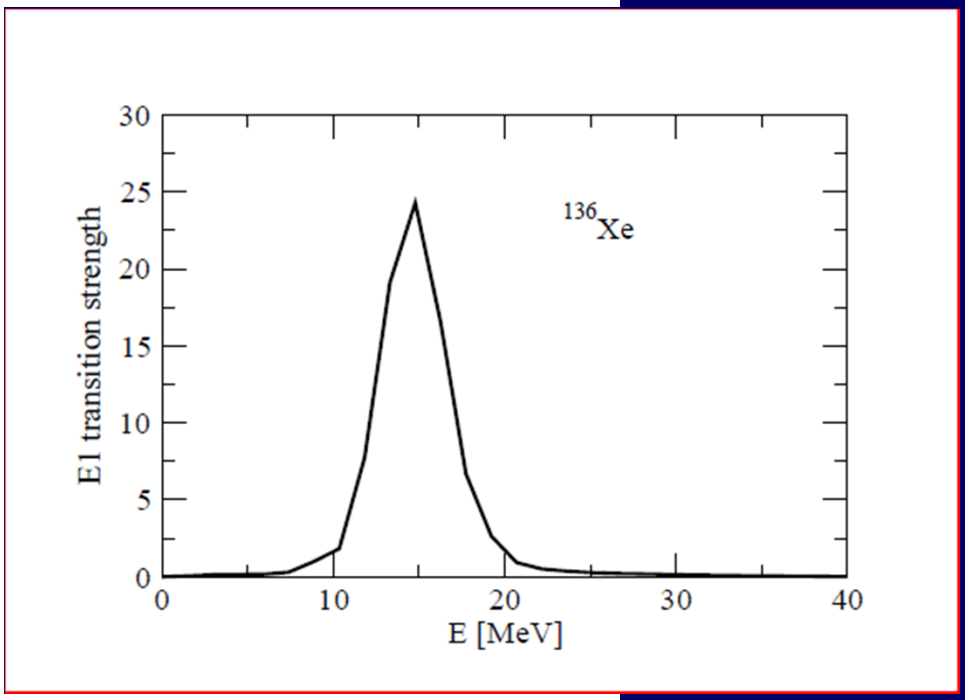
$$H_0\Psi(\vec{r}_1,\cdots,\vec{r}_A) = E_0\Psi(\vec{r}_1,\cdots,\vec{r}_A)$$

$$V_{ext}(\vec{r},t) = O(\vec{r})f(t)$$

$$\tilde{O}(\omega) = \int d^3r\, O^*(\vec{r})\,\delta\rho(\vec{r},\omega)$$

$$S(\omega) = \sum_n \langle\Psi_0|O|\Psi_n\rangle|^2\delta(\omega-\omega_n) = -\frac{1}{\pi}\Im\left(\frac{\tilde{O}(\omega)}{\tilde{f}(\omega)}\right)$$

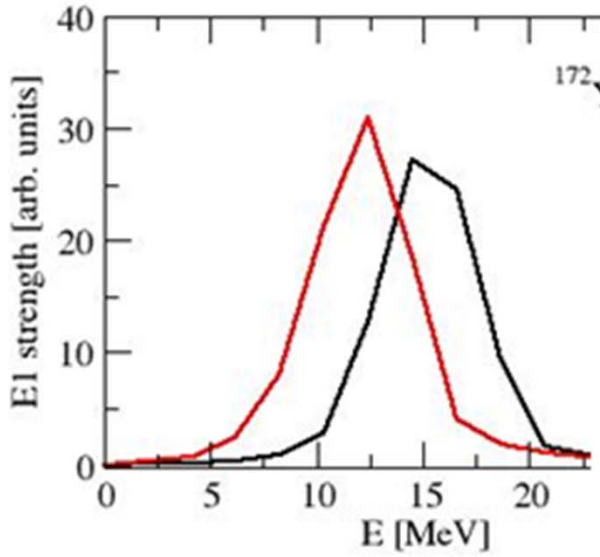


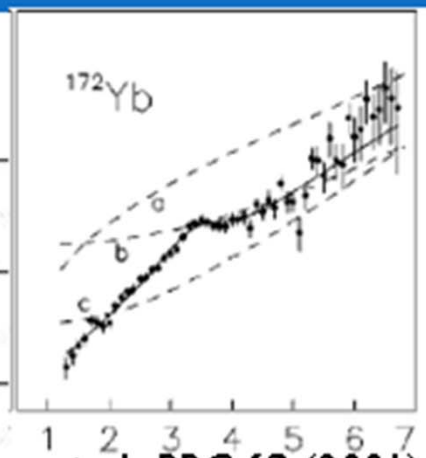


Isovector dipole strength computed in TDSLDA

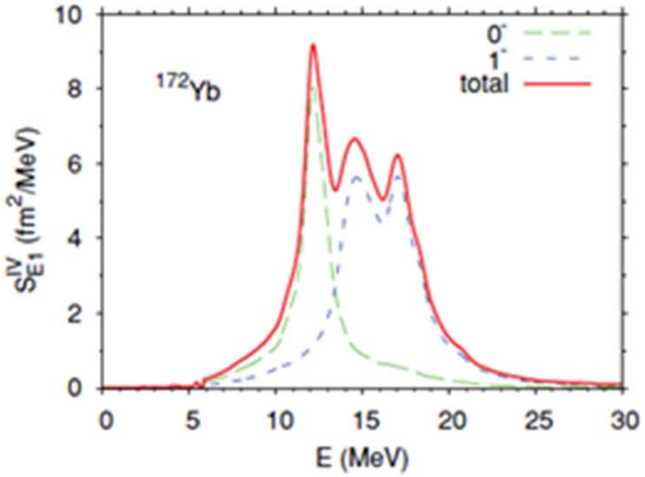
I. Stetcu *et al.*

^{172}Yb dipole giant resonance



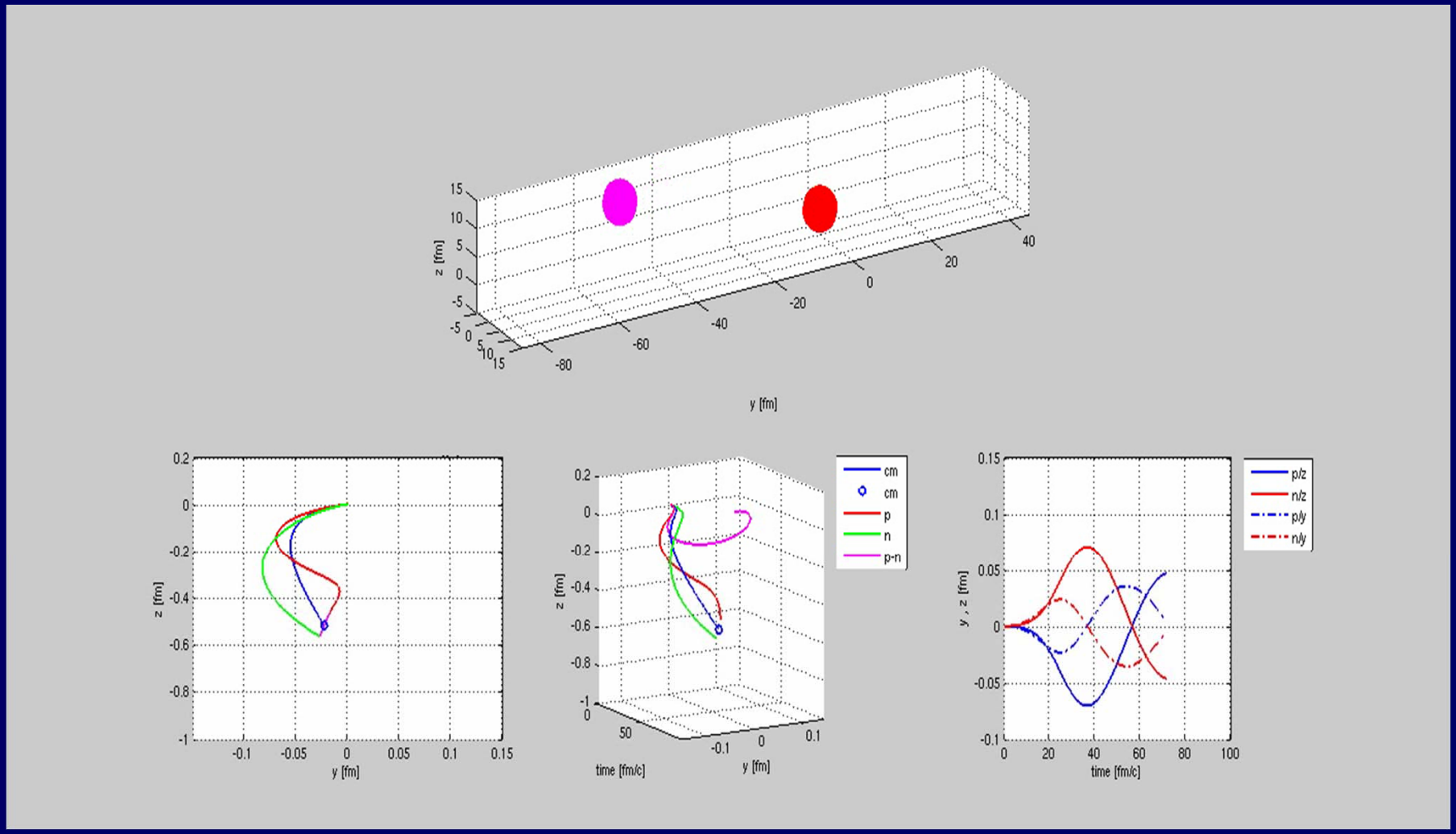


Voinov et. al., PRC **63** (2001) 044313



Phenomenological position: $80\,A^{-1/3 \div -1/6} \sim 15$ MeV

Terasaki, Engel, PRC **82** (2010) 03426



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

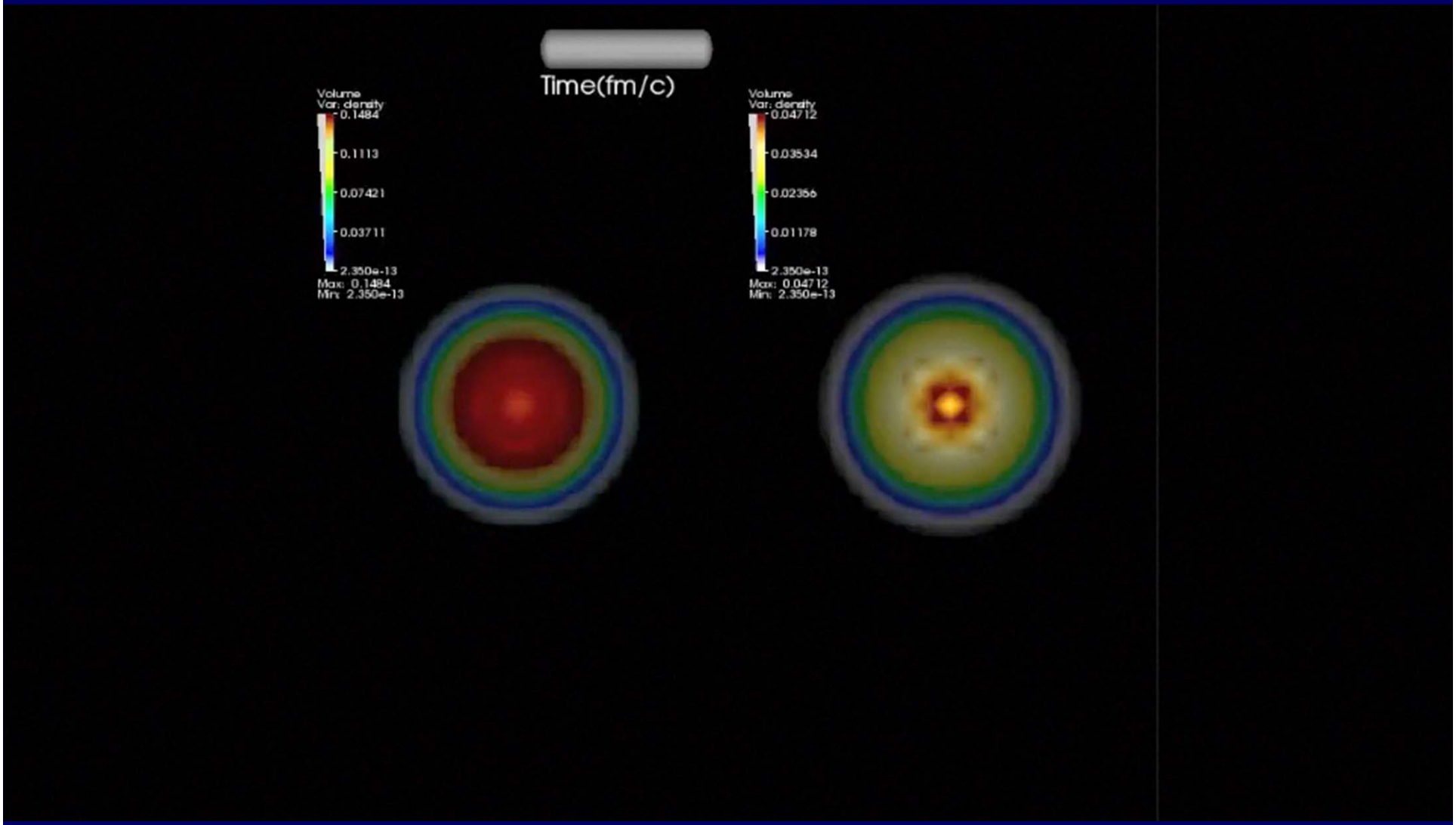
I. Stetcu *et al.*

Movie

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

Movie

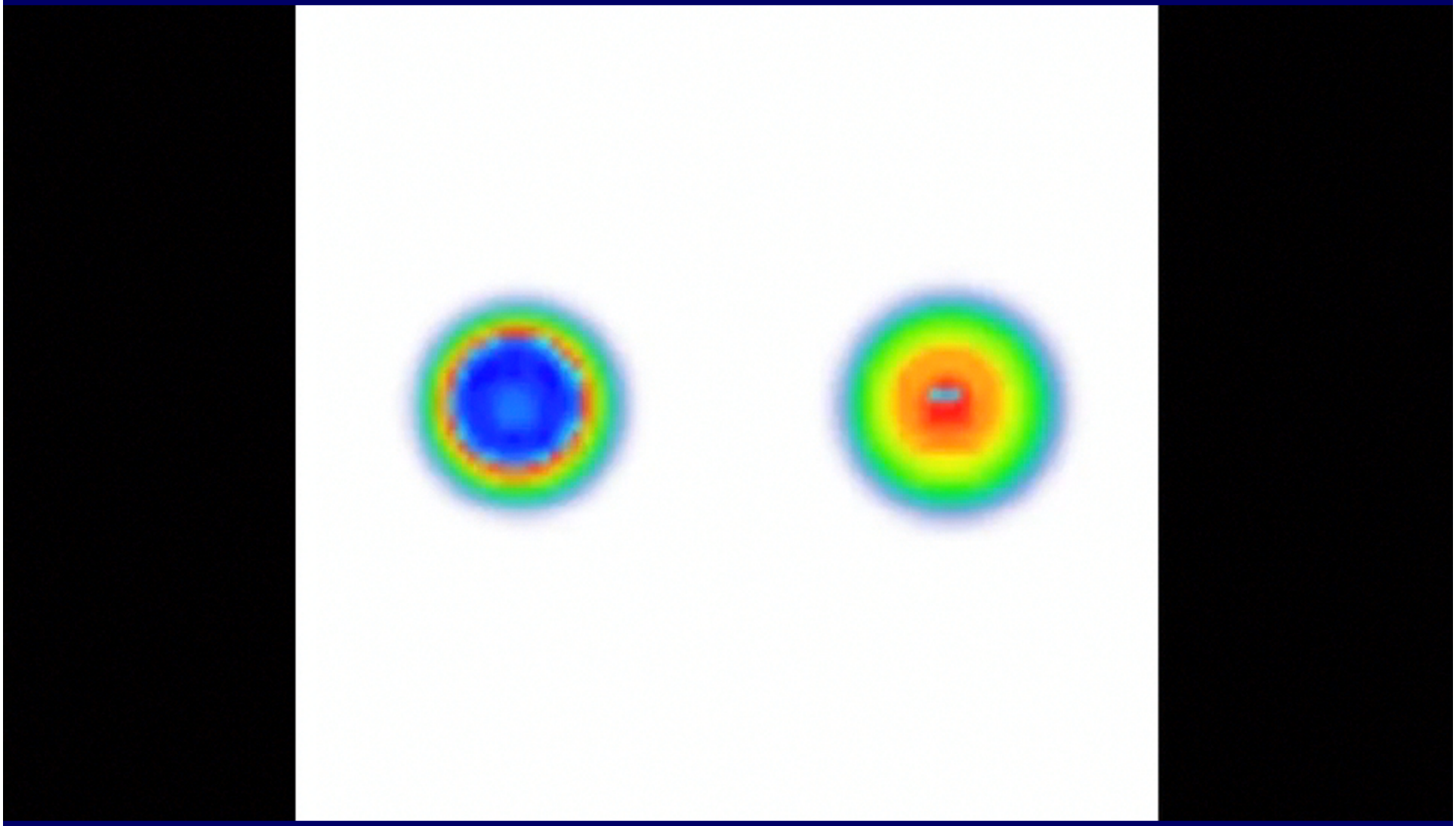
I. Stetcu *et al.*



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

Movie

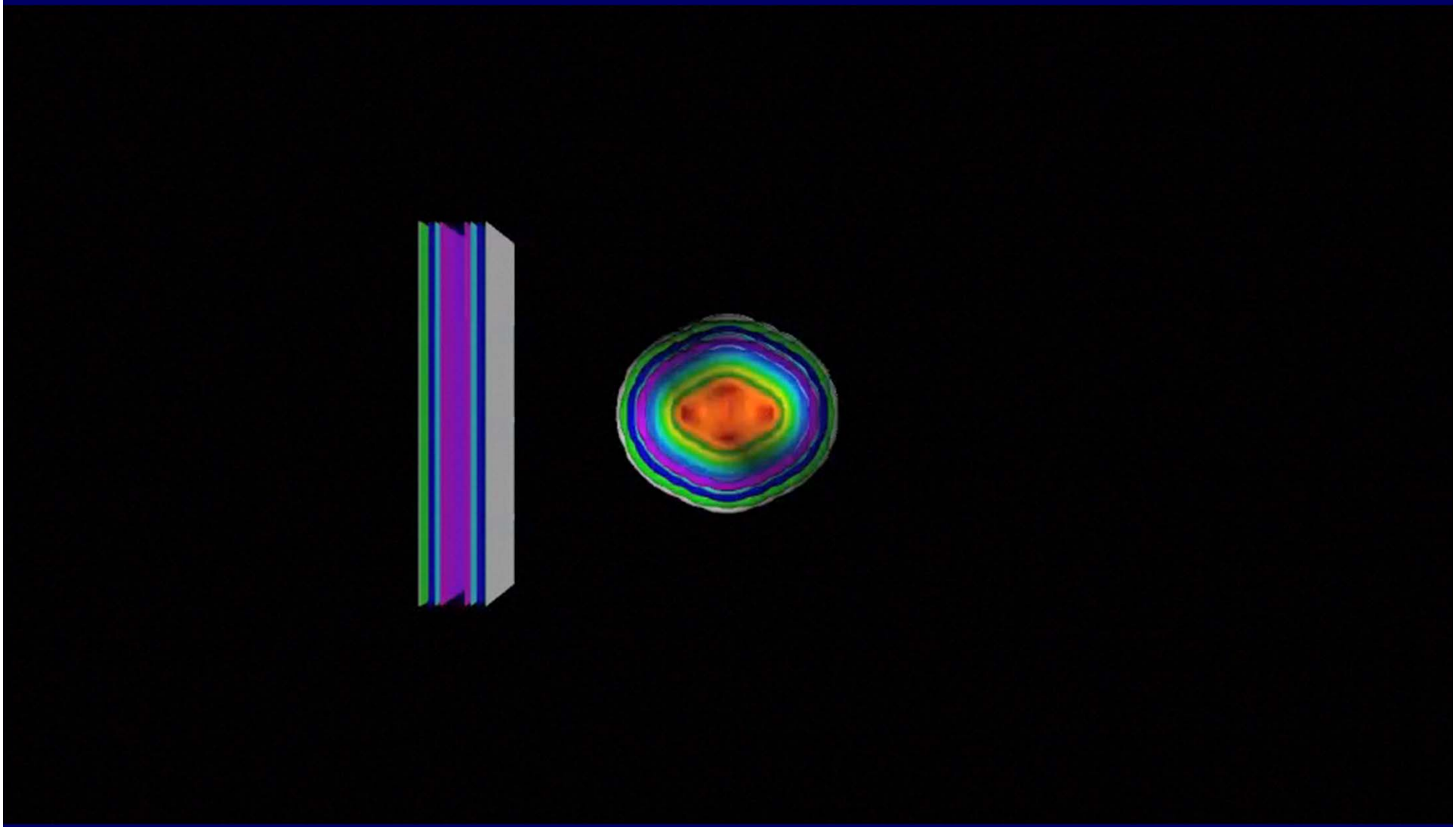
I. Stetcu *et al.*



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

Movie

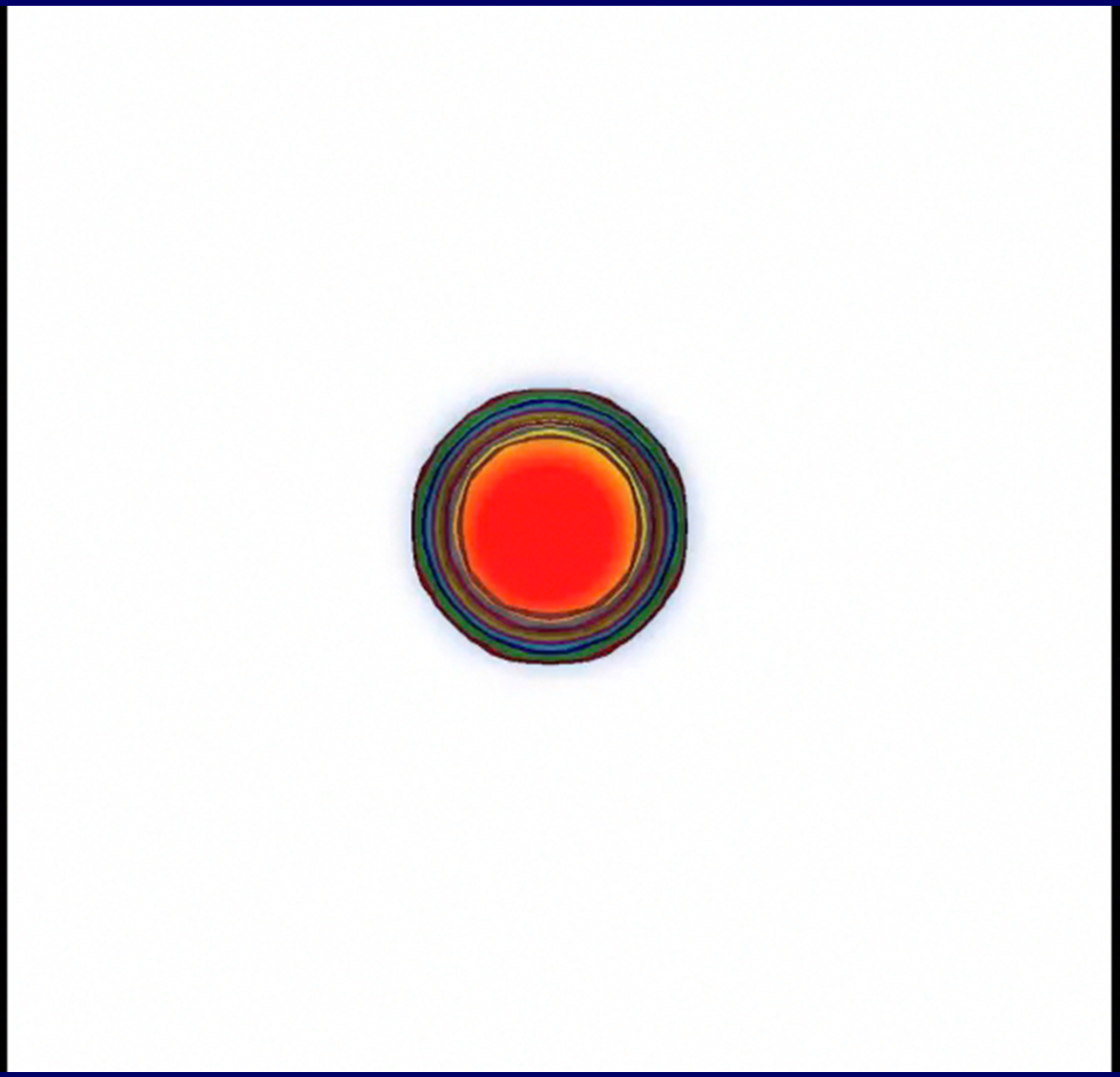
I. Stetcu *et al.*



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

Very little about the Unitary Fermi Gas (UFG):

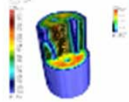
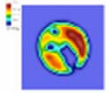
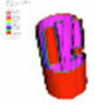
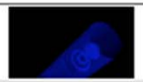
(arXiv:1011.5999, in press in Xxxxxxx)

- Qualitatively similar to dilute neutron matter (Bertsch - Many Body Challenge, 1999)
- A number of new phenomena were observed: Higgs modes, superfluid to normal transition under the action of external quantum stirrers, generation of quantized vortices, supercritical superfluid flow, crossing and reconnection of vortex lines (quantum turbulence), excitation of vortex rings, …
- Excitation of dark solitons and shock waves in the collision of unitary Fermi gas clouds
- One can study a large variety of time-dependent phenomena when basically any parameters are varied as function of time and space

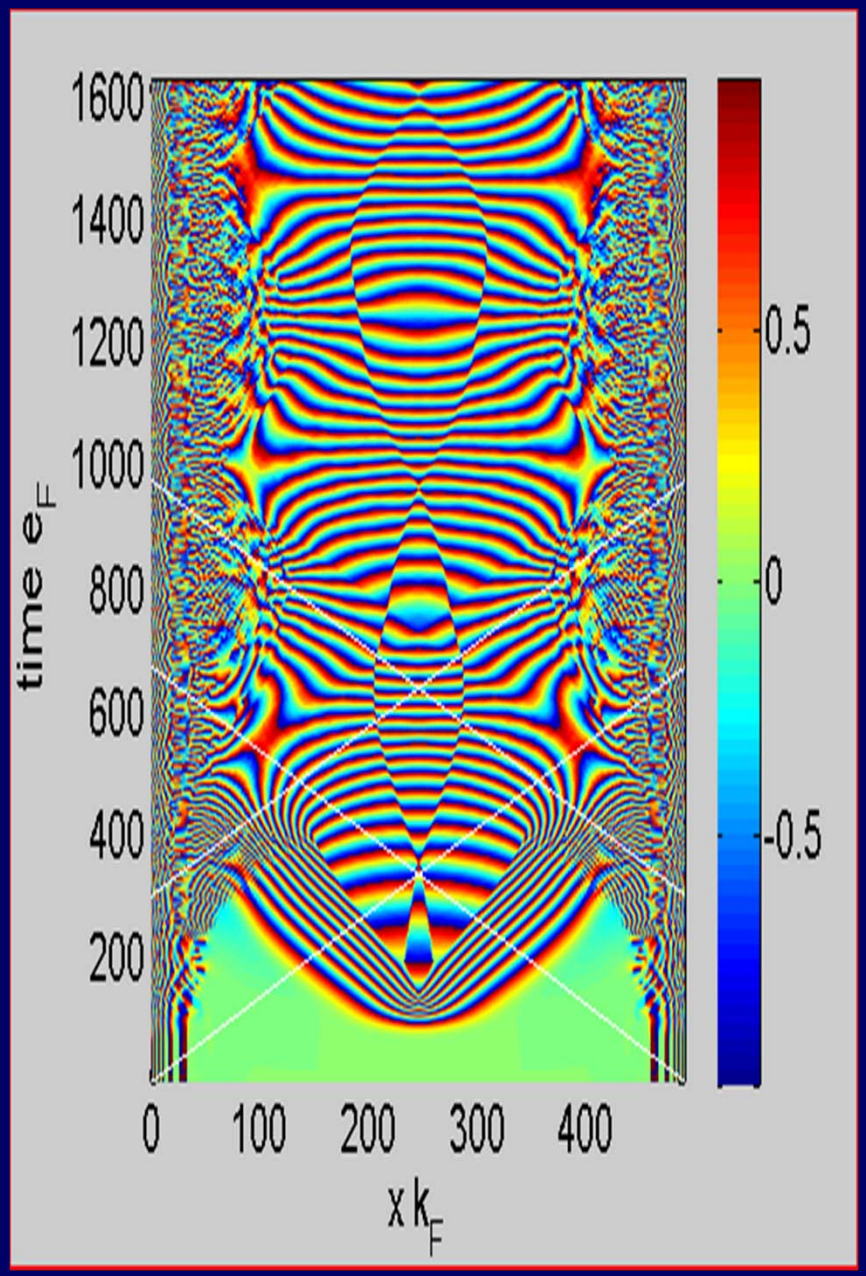
The Superfluid Local Density Approximation Applied to Unitary Fermi Gases -Supplementary Material

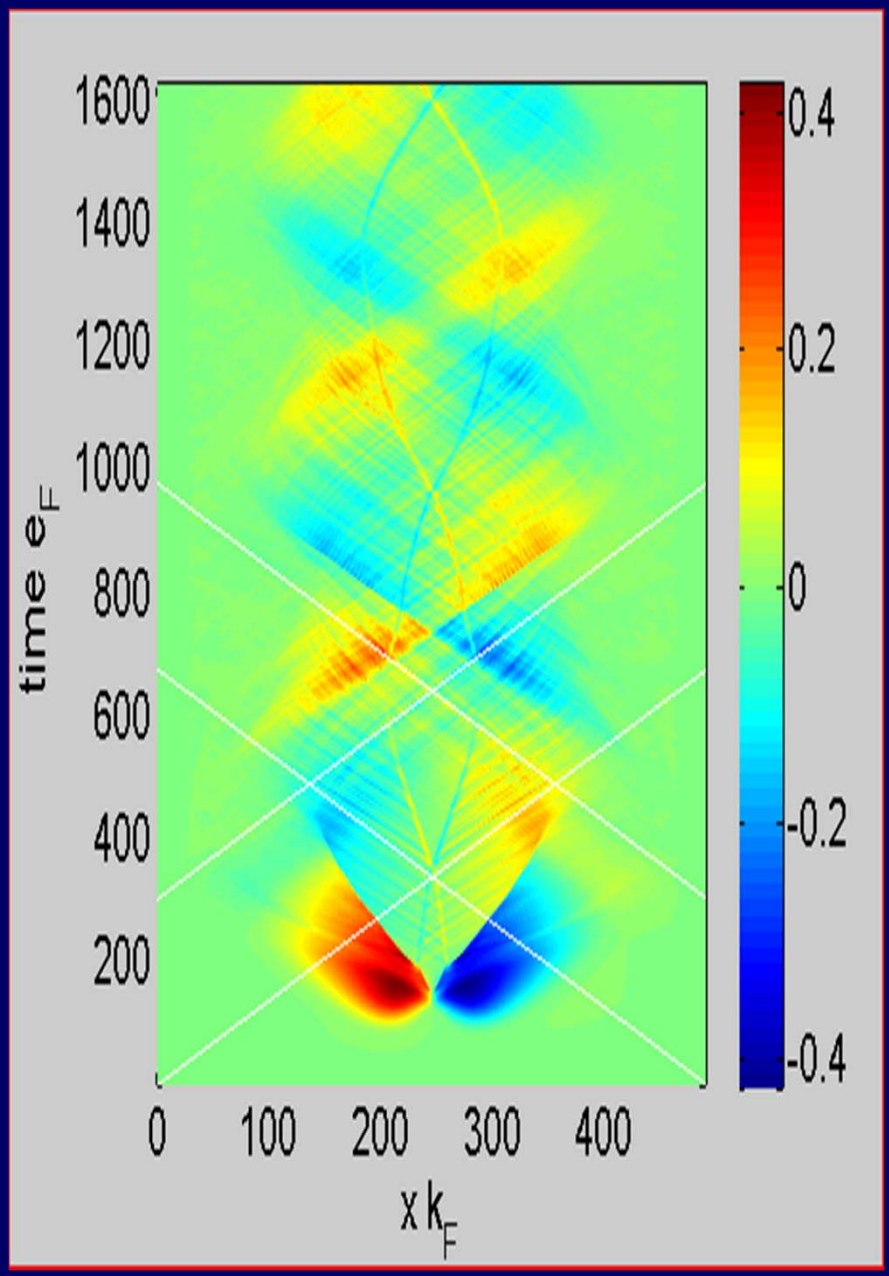
All simulations can be found here: http://www.phys.washington.edu/groups/qmbnt/UFG. The simulations can be categorized by the excitations: ball and rod, centered ball, centered small ball, centered big ball, centered supersonic ball, off-centered ball, and twisted stirrer. The following table matches simulations with numerical experiments. In several studies, we present multiple perspectives of the event as well as different plotting schemes to reveal different features of the dynamics.

3D Simulations

Excitation	Link	Description
Ball and Rod		
	nt-ball-rod-dns.m4v	density volume plot of magnitude of pairing field; front facing with quarter segment slice; 5m28s duration (20.9 MB)
	nt-ball-rod-dns-pln.m4v	density volume plot of magnitude of pairing field; 2D slice; 5m28s duration (9.8MB)
	nt-ball-rod-thin-angl.m4v	density contour plot of magnitude of pairing field focused on vortices ; angled front-facing with quarter segment slice; 5m28s duration (12.8MB)
Centered Ball		
	nt-ball-c.m4v	density contour plot of magnitude of pairing field focused on vortices; full geometry ; 3m29s

The website will become accessible again on June 9th, 2011





Dark solitons (domain walls) and shock waves in the collision of two UFG clouds

Present theoretical approaches and phenomenology for 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:**

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

- **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

Talk of E. Vardaci at FISSION 2009

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)

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

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

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

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

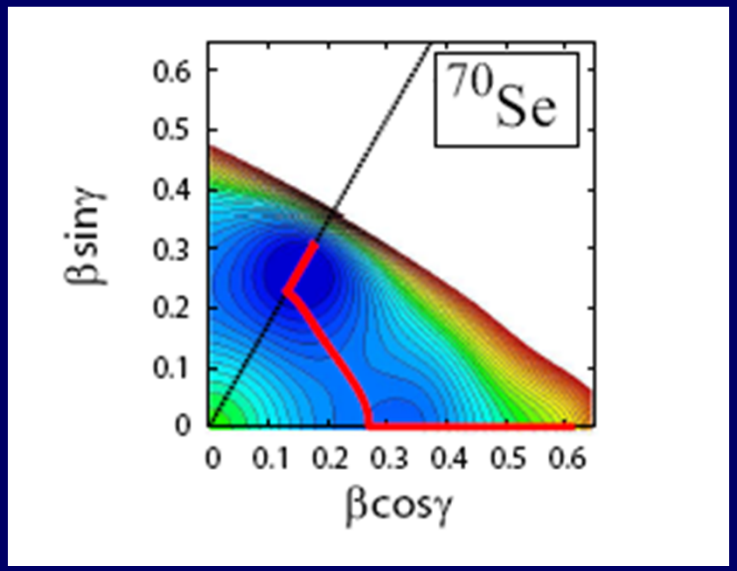
Gaussian random numbers defined a prescribed temperature in a Fermi-Dirac distribution

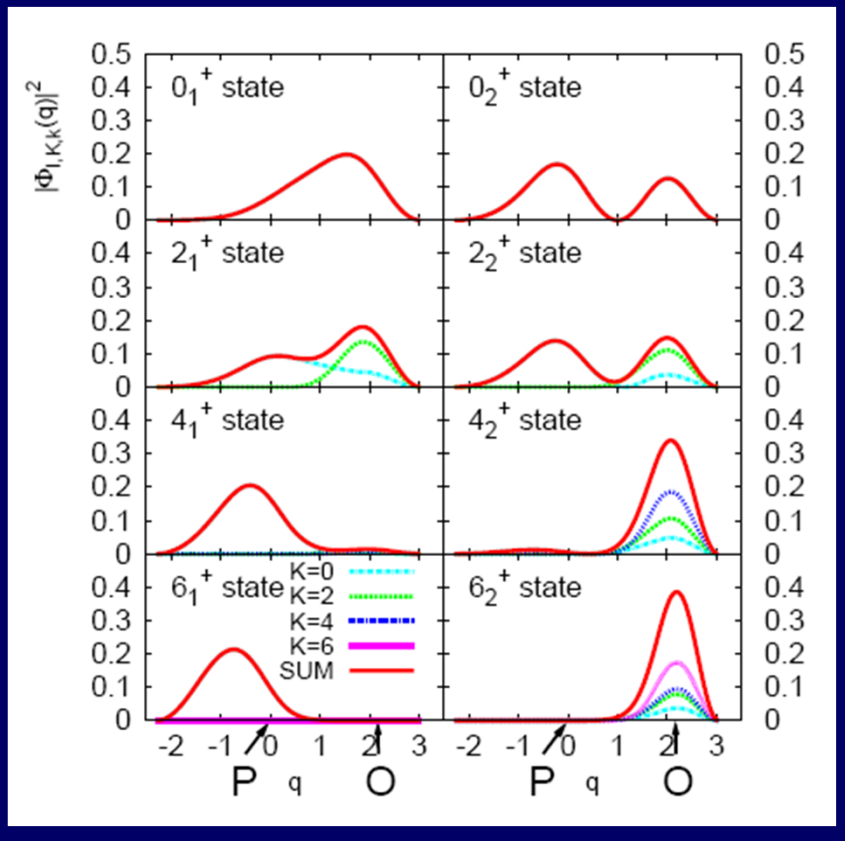
Subsequently these equations are *projected* on a collective subspace and a Langevin equation is introduced for the collective DoF

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.



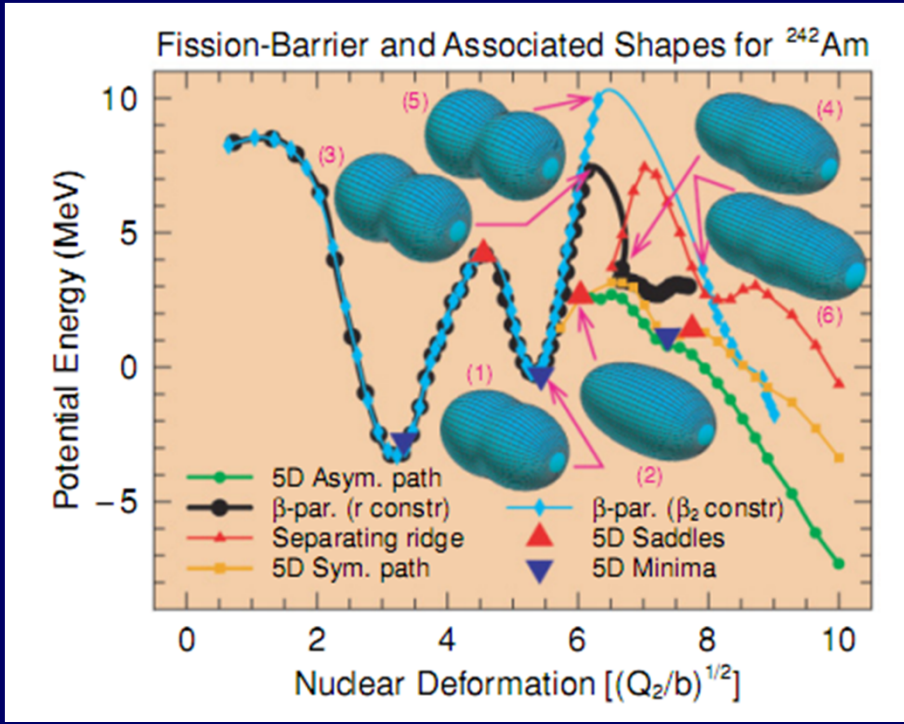


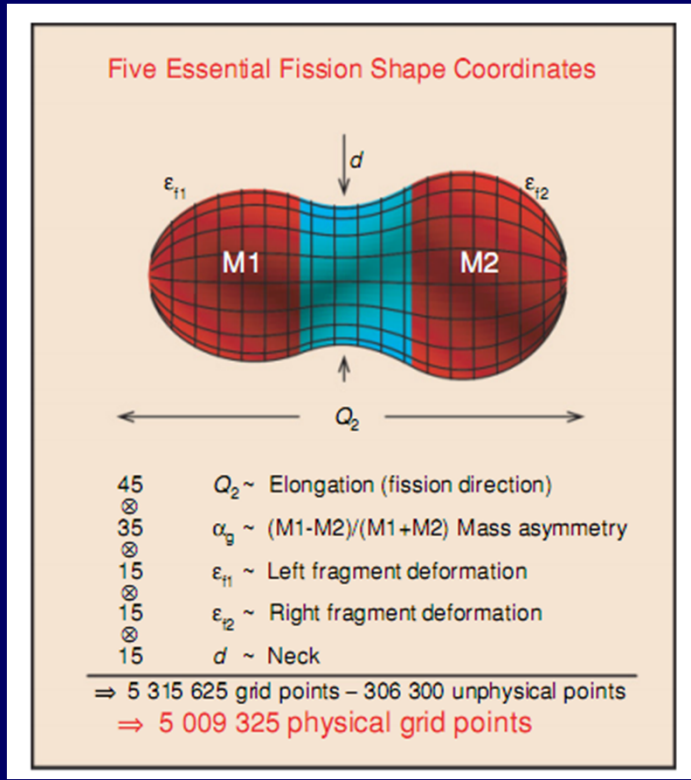
Hinohara, Nakatsukasa, Matsuo, and Matsuyanagi, Phys. Rev. C 80, 014305 (2009)

• **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)

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

• 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.

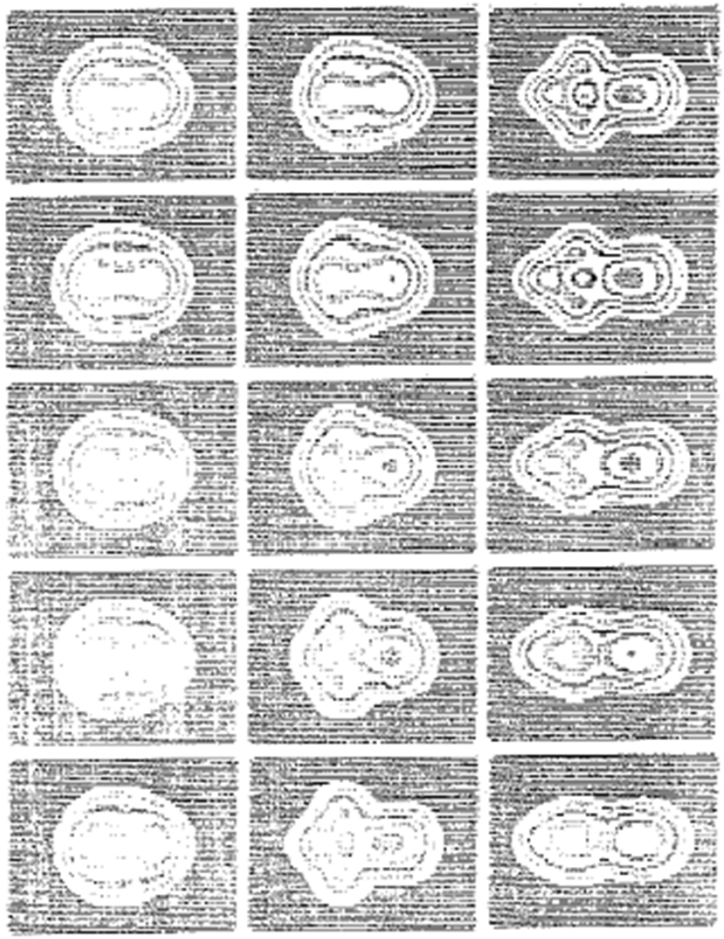
• The inertial tensor is usually hard to evaluate and often approximate methods are used.

•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



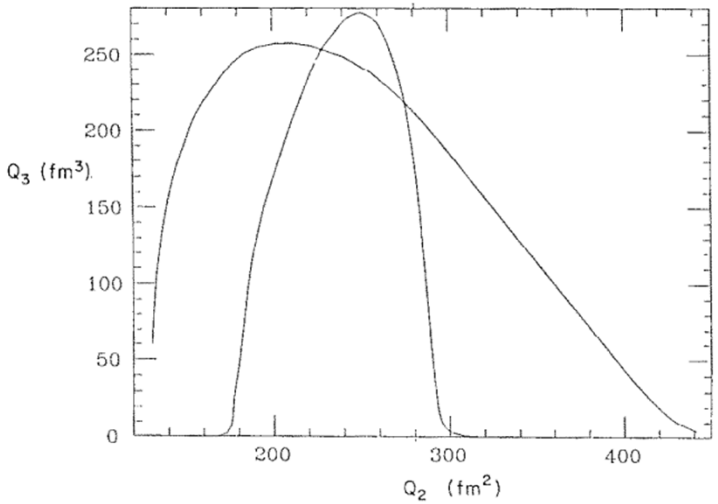


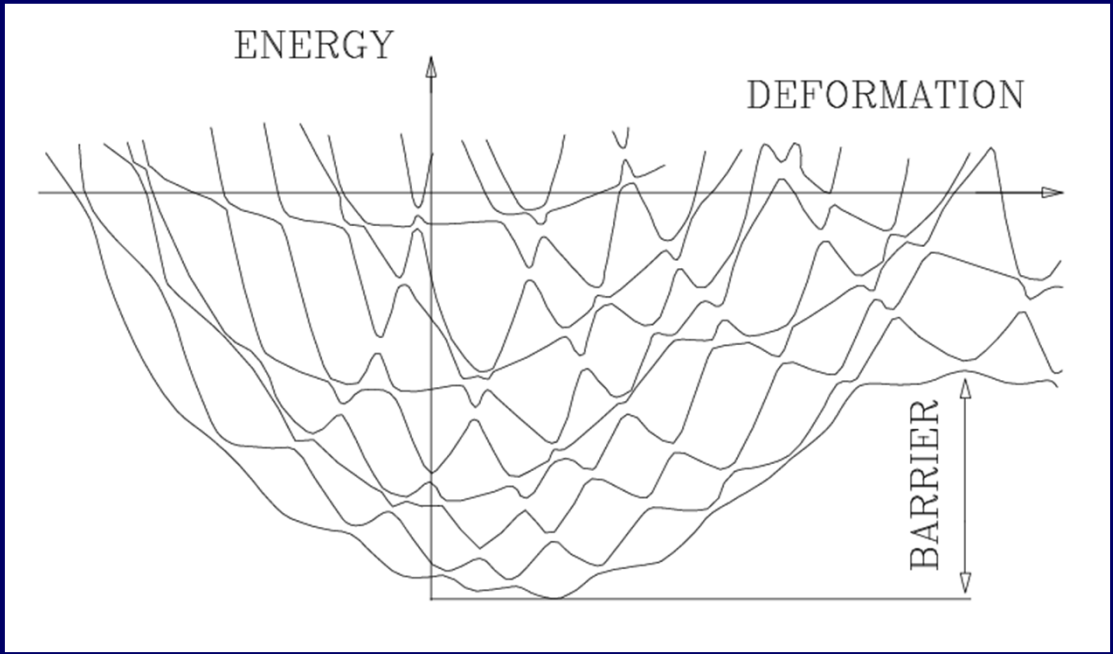
Fig. 8: Collective motion path for the fission of ^{23}S in constrained mean-field theory (dashed line) and in imaginary-time mean-field theory (solid line).

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 best 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)

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

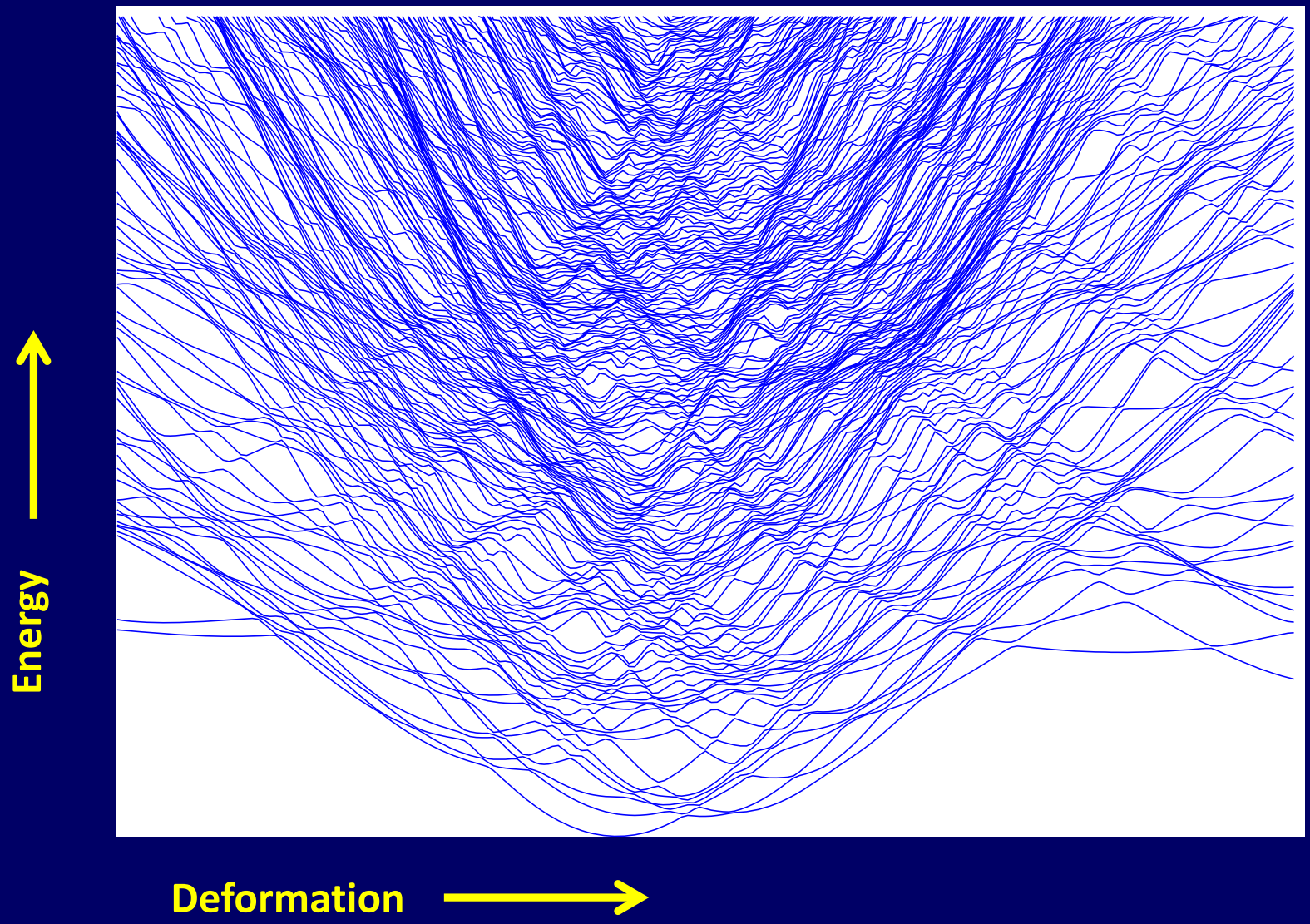
$$\sigma(t_1,\varepsilon) = \exp\left(i\varepsilon\hat{Q}\right)\rho(t_1)\exp\left(-i\varepsilon\hat{Q}\right)$$

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

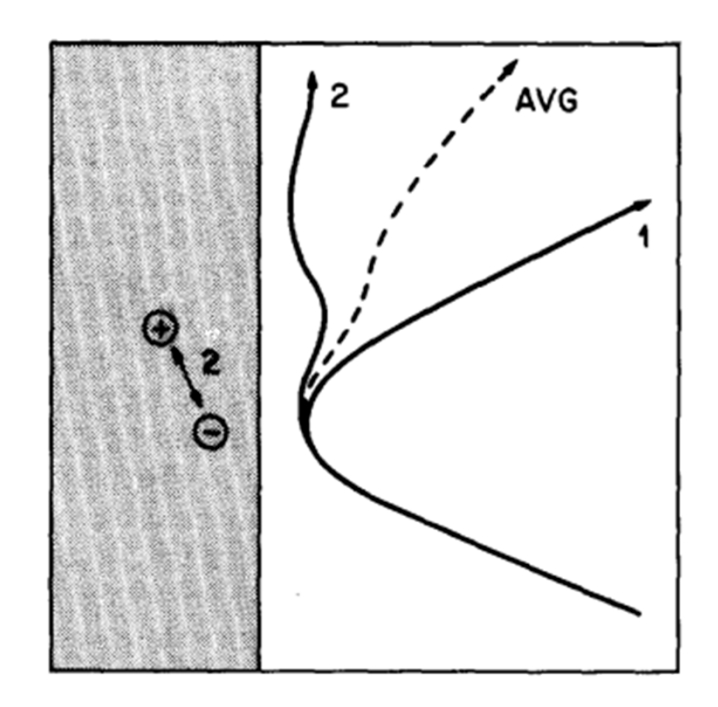
$$\left(\Delta Q_{BV}\right)^2\Big|_{t_1} = \lim_{\varepsilon\to 0}\frac{1}{2\varepsilon^2}\mathrm{Tr}\left[\rho(t_0)-\sigma(t_0,\varepsilon)\right]$$

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

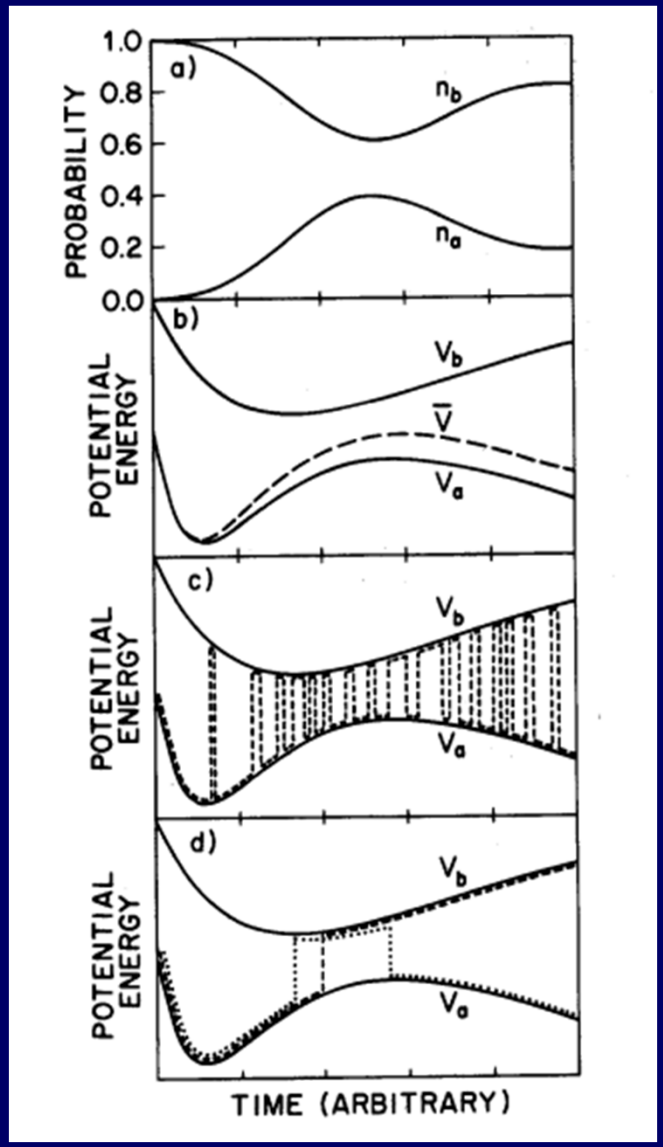
The main problem however is that we have to consider the generic situation with multiple potential energy surfaces.



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

We place several fermions on a square lattice

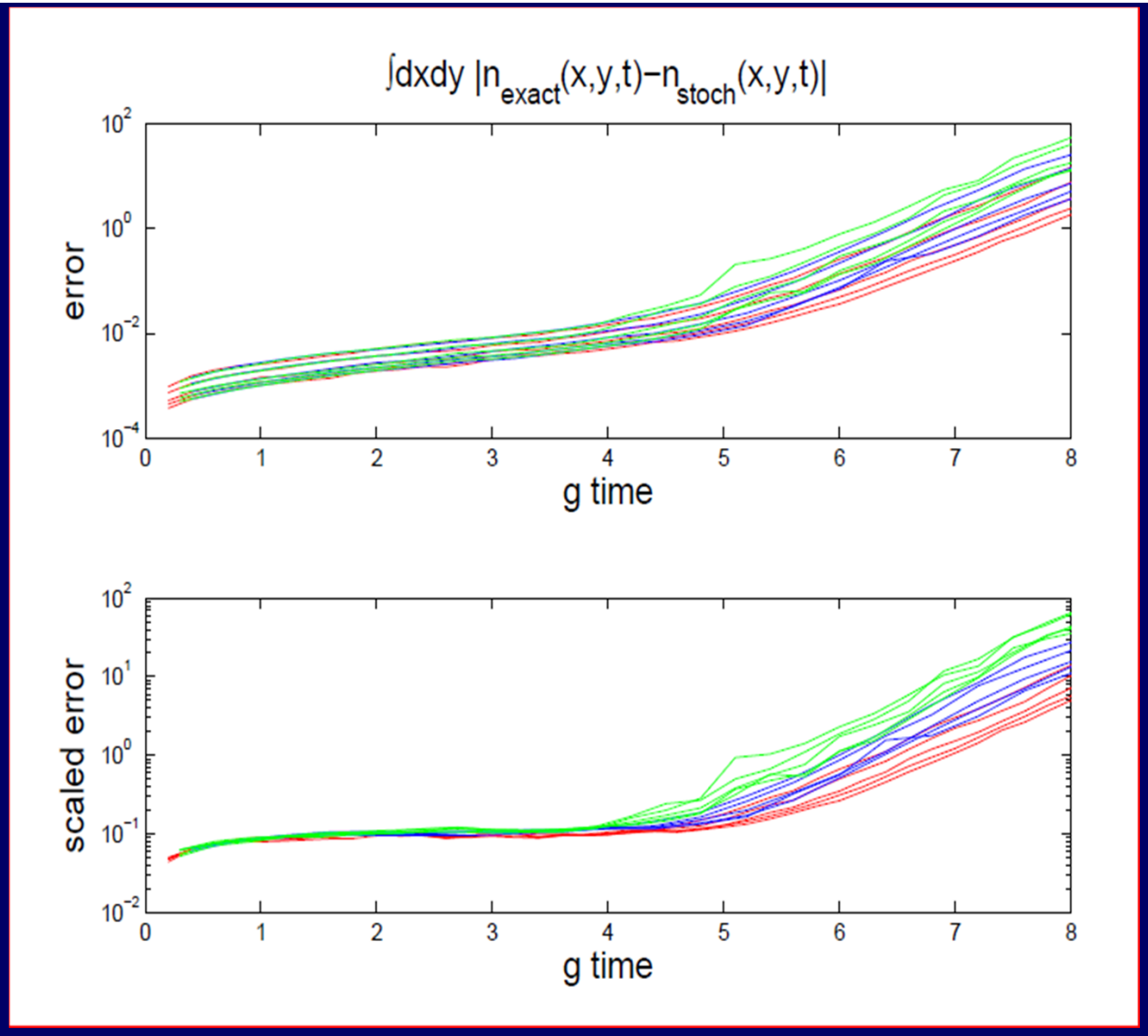
$$H = \sum_{\vec{k},\sigma} \frac{\vec{k}^2}{2} \alpha^{\dagger}_{\vec{k},\sigma} \alpha_{\vec{k},\sigma} + g \sum_{\vec{r}} \alpha^{\dagger}_{\vec{r},\uparrow} \alpha^{\dagger}_{\vec{r},\downarrow} \alpha_{\vec{r},\downarrow} \alpha_{\vec{r},\uparrow}$$

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

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

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

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



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 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**

For the sake of discussion let us see what we could in principle be able to calculate?

- **We do not need to determine any collective coordinates, potential energy surfaces, inertia tensor, non-abelian gauge fields, etc. as the system will find naturally the right collective manifold**

- **We will not need to assume either isentropic, isothermal, … meanfield solutions. Instead the temperature and entropy of the collective subsystem will evolve according to the rules of QM. This will be the most natural framework to describe dissipation in collective nuclear motion.**

- **We should be able to compute directly the mass, charge distributions and the excitation energy distributions of each fragment**

- **We should be able to follow in real time a real experimental situation, such as induced fission or fusion**

All this is naturally not limited to nuclear physics alone, this is a general approach to solve a large class of many-body problems numerically exactly, with quantifying errors, within the next decade … or sooner.