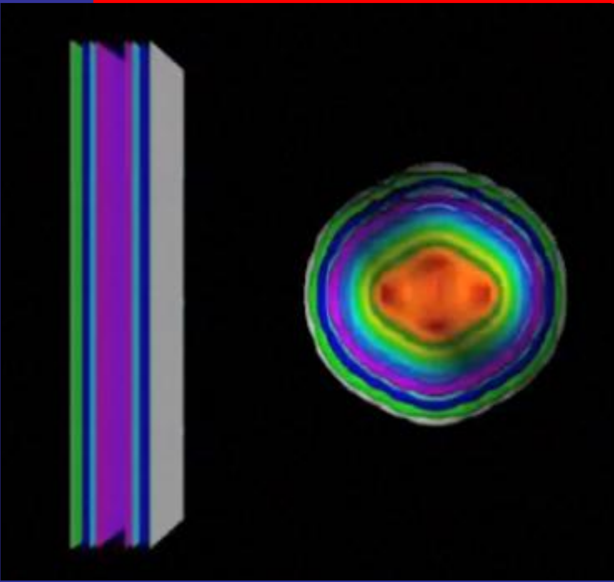
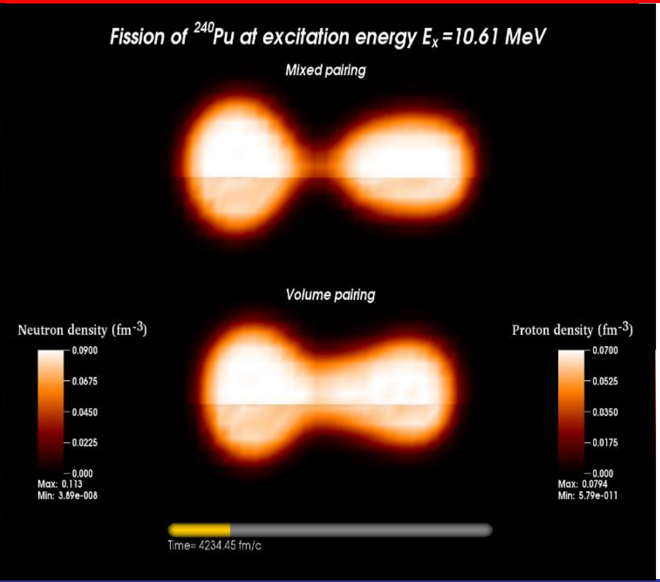
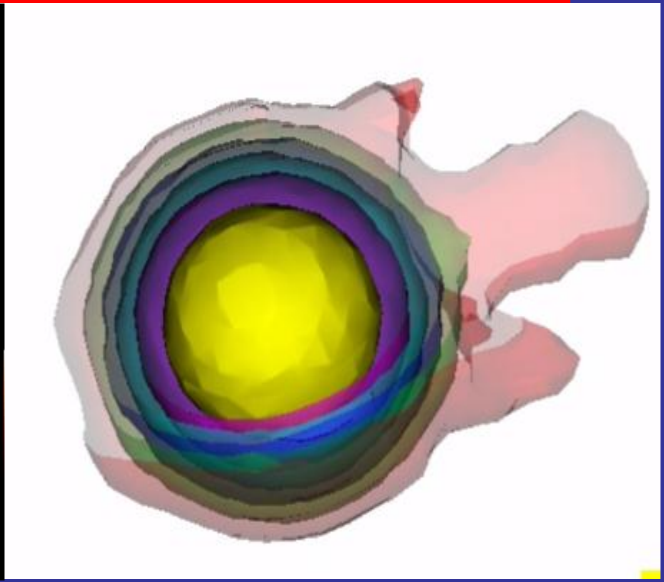
Nuclear Fission and Fusion within Superfluid TDDFT







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<u>Applications to nuclei, neutron stars and cold atomic gases:</u>
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Michael M. Forbes (Washington State University)

GOAL:

Description of nuclear dynamics far from equilibrium within the framework of Time Dependent Density Functional Theory (TDDFT).

Why DFT?

We need to describe the time evolution of (externally perturbed) spatially inhomogeneous, superfluid Fermi system and in particular such phenomena as:

- **Nuclear large amplitude collective motion (induced fission)**
- **Coulomb excitation with realtivistic heavy ions**
- **Excitation of nuclei with gamma rays and neutrons**
- **Nuclear reactions, fusion between colliding heavy ions**
- **Nuclear dynamics in the neutron star crust, dynamics of vortices and their pinning mechanism.**
- **And plenty of phenomena in superfluid clouds of atomic gases: atomic clouds collisions, vortex reconnections, quantum turbulence, domain wall solitons , etc.**

Runge Gross mapping

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle, \quad \left|\psi_0\right\rangle = \left|\psi(t_0)\right\rangle$$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0$$

$$\left.\begin{matrix}\rho(\vec{r},t) \\ \left|\psi(t_0)\right\rangle\end{matrix}\right\} \leftrightarrow e^{i\alpha(t)}\left|\psi(t)\right\rangle$$

Up to an arbitrary function α(t)

and consequently the functional exists:

$$F[\psi_0,\rho] = \int_{t_0}^{t_1}\left\langle\psi[\rho]\right|\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)\left|\psi[\rho]\right\rangle dt$$

E. Runge, E.K.U Gross, PRL 52, 997 (1984)

B.-X. Xu, A.K. Rajagopal, PRA 31, 2682 (1985)

G. Vignale, PRA77, 062511 (2008)

Kohn-Sham approach

Suppose we are given the density of an interacting system.
There exists a unique noninteracting system with the same density.

Interacting system

$$i\hbar \frac{\partial}{\partial t}\left|\psi(t)\right\rangle = (\hat{T} + \hat{V}(t) + \hat{W})\left|\psi(t)\right\rangle$$

Noninteracting system

$$i\hbar \frac{\partial}{\partial t}\left|\varphi(t)\right\rangle = (\hat{T} + \hat{V}_{KS}(t))\left|\varphi(t)\right\rangle$$

$$\rho(\vec{r},t) = \left\langle \psi(t)\right|\hat{\rho}(\vec{r})\left|\psi(t)\right\rangle = \left\langle \varphi(t)\right|\hat{\rho}(\vec{r})\left|\varphi(t)\right\rangle$$

Hence the DFT approach is essentially exact.

However as always there is a price to pay:

- **Kohn-Sham potential in principle depends on the past (memory).**
  Very little is known about the memory term and usually it is disregarded (adiabatic TDDFT).
- **Only one body observables can be reliably evaluated within standard DFT.**

Formalism for Time Dependent Phenomena: TDSLDA

Local density approximation (no memory terms – adiabatic TDDFT)

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow,\uparrow}(\mathbf{r},t) & h_{\uparrow,\downarrow}(\mathbf{r},t) & 0 & \Delta(\mathbf{r},t) \\ h_{\downarrow,\uparrow}(\mathbf{r},t) & h_{\downarrow,\downarrow}(\mathbf{r},t) & -\Delta(\mathbf{r},t) & 0 \\ 0 & -\Delta^*(\mathbf{r},t) & -h^*_{\uparrow,\uparrow}(\mathbf{r},t) & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & 0 & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) & -h^*_{\downarrow,\downarrow}(\mathbf{r},t) \end{pmatrix}\begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix}$$

Density functional contains normal densities, anomalous density (pairing) and currents:

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

- **The system is placed on a large 3D spatial lattice.**
- **No symmetry restrictions**
- **Number of PDEs is of the order of the number of spatial lattice points**

Current capabilities of the code:

- **volumes of the order of (L = 80^3) capable of simulating time evolution of 42000 neutrons at saturation density (possible application: neutron stars)**
- **capable of simulating up to times of the order of 10^{-19} s (a few million time steps)**
- **CPU vs GPU on Titan ≈ 15 speed-up (likely an additional factor of 4 possible)**

Eg. for 137062 two component wave functions:

CPU version (4096 nodes x 16 PEs) - 27.90 sec for 10 time steps

GPU version (4096 PEs + 4096GPU) - 1.84 sec for 10 time step

Single particle potential (Skyrme):

$$h(\mathbf{r}) = -\vec{\nabla}\cdot\Big(B(\mathbf{r})+\vec{\sigma}\cdot\vec{C}(\mathbf{r})\Big)\vec{\nabla}+U(\mathbf{r})+\frac{1}{2i}\Big[\vec{W}(\mathbf{r})\cdot(\vec{\nabla}\times\vec{\sigma})+\vec{\nabla}\cdot(\vec{\sigma}\times\vec{W}(\mathbf{r}))\Big]$$
$$+\vec{U}_{\sigma}(\mathbf{r})\cdot\vec{\sigma}+\frac{1}{i}\Big(\vec{\nabla}\cdot\vec{U}_{\Delta}(\mathbf{r})+\vec{U}_{\Delta}(\mathbf{r})\cdot\vec{\nabla}\Big)$$

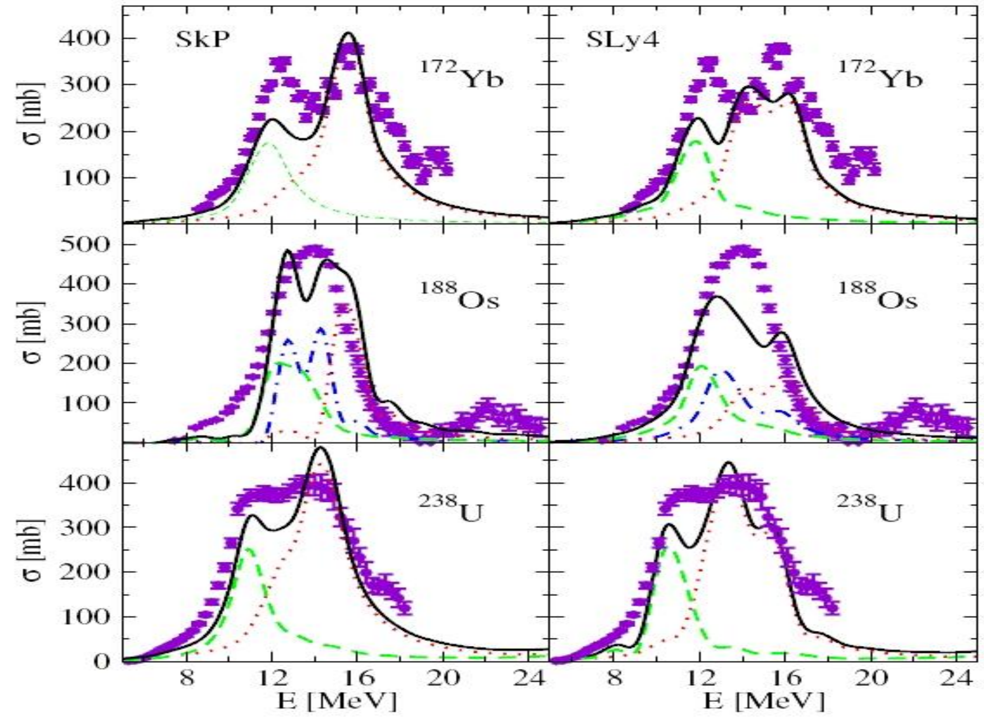
where

$$\begin{aligned}
B(\mathbf{r}) &= \frac{\hbar^2}{2m}+C^{\tau}\rho \\
\vec{C}(\mathbf{r}) &= C^{sT}\vec{s} \\
U(\mathbf{r}) &= 2C^{\rho}\rho+2C^{\Delta\rho}\nabla^2\rho+C^{\tau}\tau+C^{\nabla J}\vec{\nabla}\cdot\vec{J}+C^{\gamma}(\gamma+2)\rho^{\gamma+1} \\
\vec{W}(\mathbf{r}) &= -C^{\nabla J}\vec{\nabla}\rho \\
\vec{U}_{\sigma}(\mathbf{r}) &= 2C^{s}\vec{s}+2C^{\Delta s}\nabla^2\vec{s}+C^{sT}\vec{T}+C^{\nabla J}\vec{\nabla}\times\vec{j} \\
\vec{U}_{\Delta}(\mathbf{r}) &= C^{j}\vec{j}+\frac{1}{2}C^{\nabla j}\vec{\nabla}\times\vec{s}
\end{aligned}$$

and pairing potential:

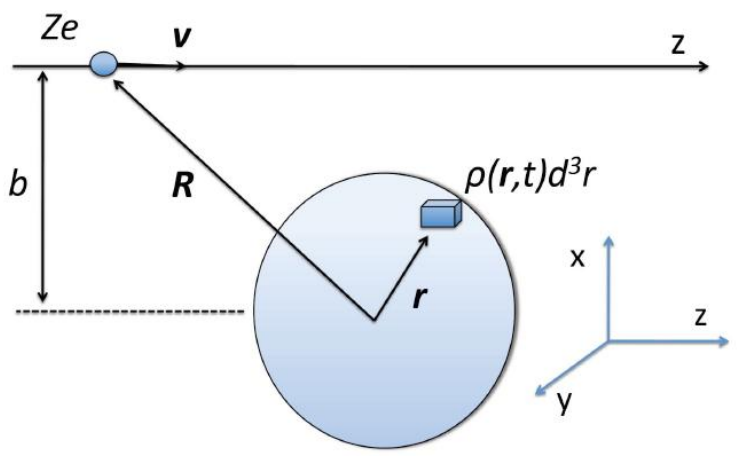
$$\Delta(\mathbf{r},t) = -g_{eff}(\mathbf{r})\chi(\mathbf{r},t)$$

Linear response regime:
GDR of deformed nuclei



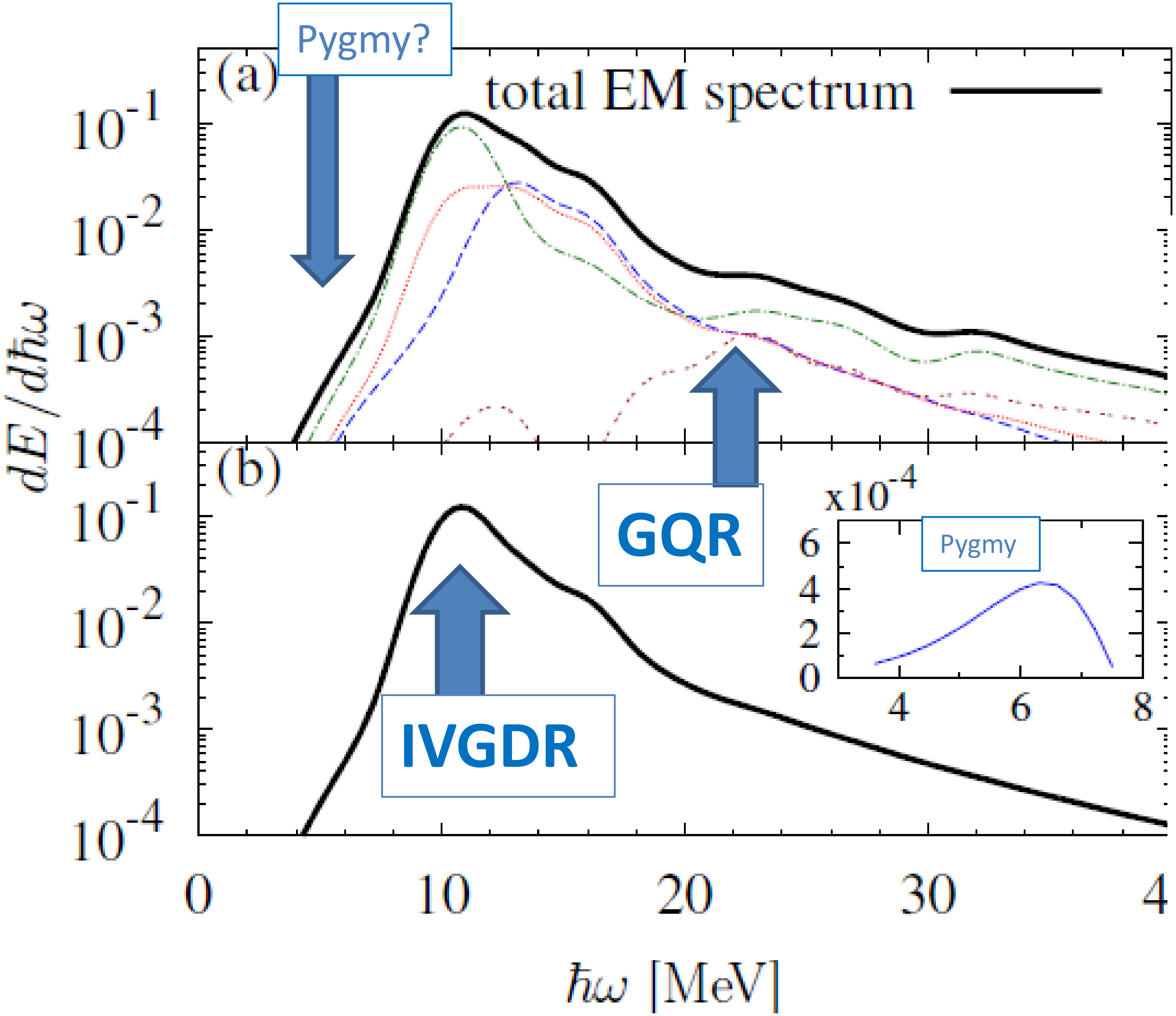
I.Stetcu, A.Bulgac, P. Magierski, K.J. Roche, Phys. Rev. C84 051309 (2011)

Beyond linear regime:
Relativistic Coulomb excitation

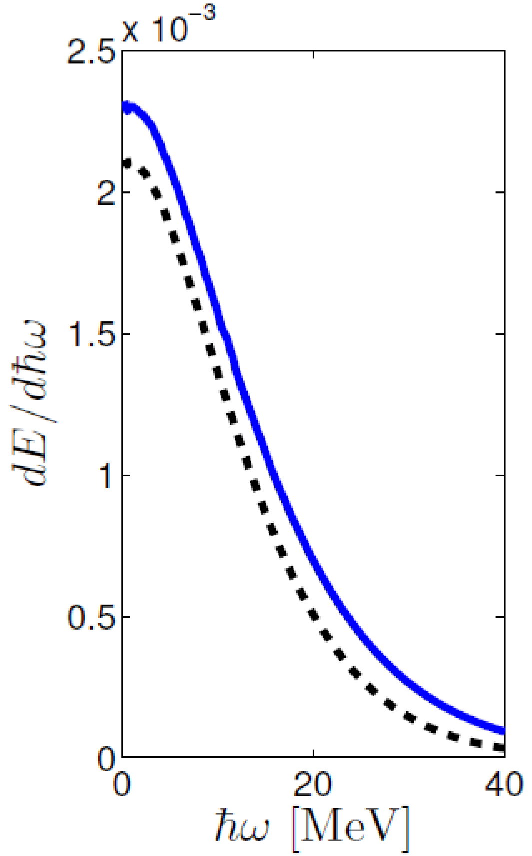


$$\hbar\omega \approx \hbar/\tau_{coll} = \frac{\gamma v}{b} \approx 12MeV \;\; ; \;\; \gamma = \frac{1}{\sqrt{1-\left(v/c\right)^2}}$$

Electromagnetic radiation due to the internal nuclear motion



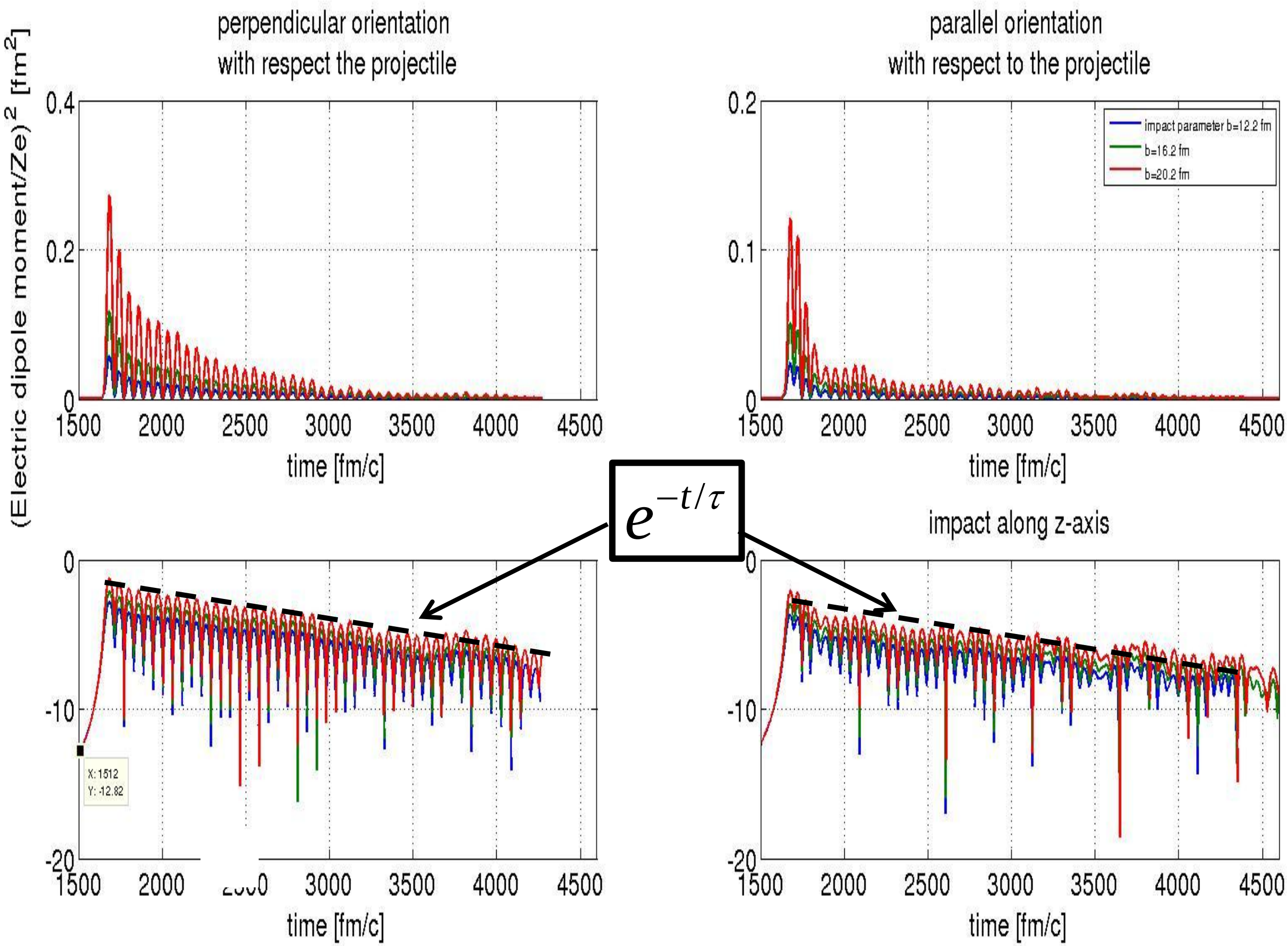
Bremsstrahlung at b=12.2fm



I. Stetcu, C. Bertulani, A. Bulgac, P. Magierski, K.J. Roche
Phys. Rev. Lett. 114, 012701 (2015)

One body dissipation can be properly within this formalism

Damping of GDR (excited in coulex reaction) due to one-body dissipation mechanism:



$$E_{coll}(t) \propto e^{-t/\tau}; \quad \tau \approx 500\ fm/c \Rightarrow \Gamma_{\downarrow} \approx 0.4 MeV$$

$$E_{coll}(t) \propto \left[D_{\max}(t)\right]^2$$

Description of the fission process within TDSLDA

What is doable, what is probable and what is not possible in this approach?

Time scale for nuclear processes that can be described within TDSLDA: 10^(-19) sec.

Fission time scales:

- From ground state to saddle point: <10^(-15) sec.
  Maybe: depending on the excitation energy

- From saddle to scission: 10^(-20) - 10^(-21) sec.
  Doable!

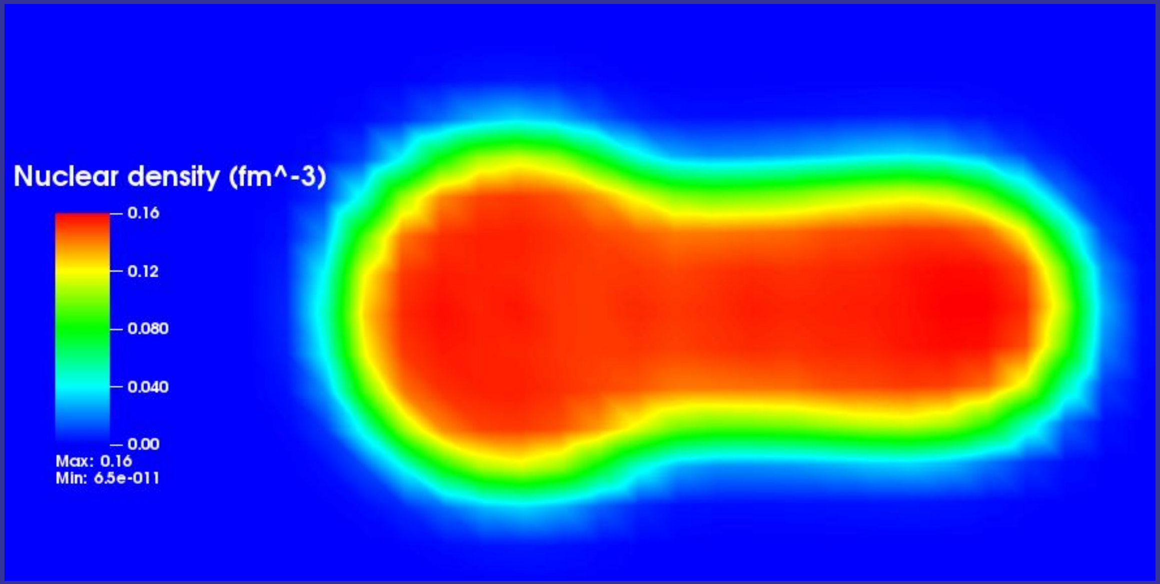
- Emission of scission neutrons:
  Doable!

- Prompt neutrons: 10^(-18)-10^(-14) sec.
  Unlikely

- Prompt gammas: >10^(-14) sec.
  Out of question

Complexity of fission dynamics

Initial configuration of ^{240}Pu is prepared beyond the barrier at quadrupole deformation *Q=165b* and excitation energy *E=10.61 MeV*:



Fragment masses:

During the process , the exchange of about 2 neutrons and 3 protons occur between fragments before splitting.

Interestingly the fragment masses seem to be relatively stiff with respect to variations of the initial conditions.

Preliminary results of TDSLDA:

Fragment masses:

Heavy fragment: N≈82, Z≈52, A ≈ 134

Light fragment: N≈64, Z≈42, A ≈ 106

Experiment for 240Pu(n,f) at E_n =1.5-15 MeV:

Average mass for heavy fragment: A ≈ 140

Average mass for light fragment: A ≈ 100

Max. charge yields: Z=40 and Z=54

H. Thierens et al. Phys. Rev. C 23, 2104 (1981).
C. Wagemans, et al. Phys. Rev. C 30, 218 (1984).
M.B. Chadwick et al, Nucl. Data Sheets 107, 2931 (2006).

Pairing dynamics

Volume pairing vs mixed pairing

$$\begin{cases} [h(\vec{r})-\mu]\mathrm{u}_i(\vec{r})+\Delta(\vec{r})\mathrm{v}_i(\vec{r})=E_i\mathrm{u}_i(\vec{r}) \\ \Delta^*(\vec{r})\mathrm{u}_i(\vec{r})-[h(\vec{r})-\mu]\mathrm{v}_i(\vec{r})=E_i\mathrm{v}_i(\vec{r}) \end{cases} \qquad \begin{cases} h(\vec{r})=-\vec{\nabla}\dfrac{\hbar^2}{2m(\vec{r})}\vec{\nabla}+U(\vec{r}) \\ \Delta(\vec{r})=-g_{\mathrm{eff}}(\vec{r})\nu_c(\vec{r}) \end{cases}$$

$$\boxed{\frac{1}{g_{eff}(\vec{r})}=\frac{1}{g[n(\vec{r})]}-\frac{m(\vec{r})k_c(\vec{r})}{2\pi^2\hbar^2}\left\{1-\frac{k_F(\vec{r})}{2k_c(\vec{r})}\ln\frac{k_c(\vec{r})+k_F(\vec{r})}{k_c(\vec{r})-k_F(\vec{r})}\right\}}$$

$$\rho_c(\vec{r})=2\sum_{E_i\geq 0}^{E_c}\left|\mathrm{v}_i(\vec{r})\right|^2, \qquad \nu_c(\vec{r})=\sum_{E_i\geq 0}^{E_c}\mathrm{v}_i^*(\vec{r})\mathrm{u}_i(\vec{r})$$

$$E_c+\mu=\frac{\hbar^2k_c^2(\vec{r})}{2m(\vec{r})}+U(\vec{r}), \qquad \mu=\frac{\hbar^2k_F^2(\vec{r})}{2m(\vec{r})}+U(\vec{r})$$

Bulgac, Yu, Phys. Rev. Lett. 88 (2002) 042504
Bulgac, Phys. Rev. C65 (2002) 051305

$$g[n(r)]=-250MeV\cdot fm^3 - Volume\ pairing$$

$$g[n(r)]=V\left(1-\frac{n(r)}{n_c}\right) - Mixed\ half\ volume - half\ surface\ pairing$$

$$V=-370MeV\cdot fm^3; n_c=0.32fm^{-3}$$

Pairing concentrated at nuclear surface leads to shorter fission times.

Consequently the TKE is larger and the excitation energies of the fragments are smaller.

Volume pairing gives to high excitation energies of the fragments:
E(heavy fragment) ≈ 11.8MeV
E(light fragment) ≈ 29.8MeV
And TKE ≈ 170MeV

Mixed pairing leads to lower excitation energies which will give rise only to about 2 neutron emission (Exp. about 3 neutron emission)
TKE increases to about 184.3 MeV (Exp. 177.28 MeV)

Summary

- *TDSLDA is a flexible tool to study nuclear dynamics.*

- *In order to use TDSLDA one needs accurate initial conditions. Various methods are used at the moment and a promissing method is tested (talk of Gabriel Wlazłowski on Thursday)*

- *Approaches based on an adiabatic approximation seem to be not correct, at least for the description of dynamics beyond the saddle point.*
- *Fission process is extremely sensitive to pairing and its character (volume, surface, mixed). Fission times and TKE/E_{exc} ratio may vary substantially (see poster of Janina Grineviciute).*

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