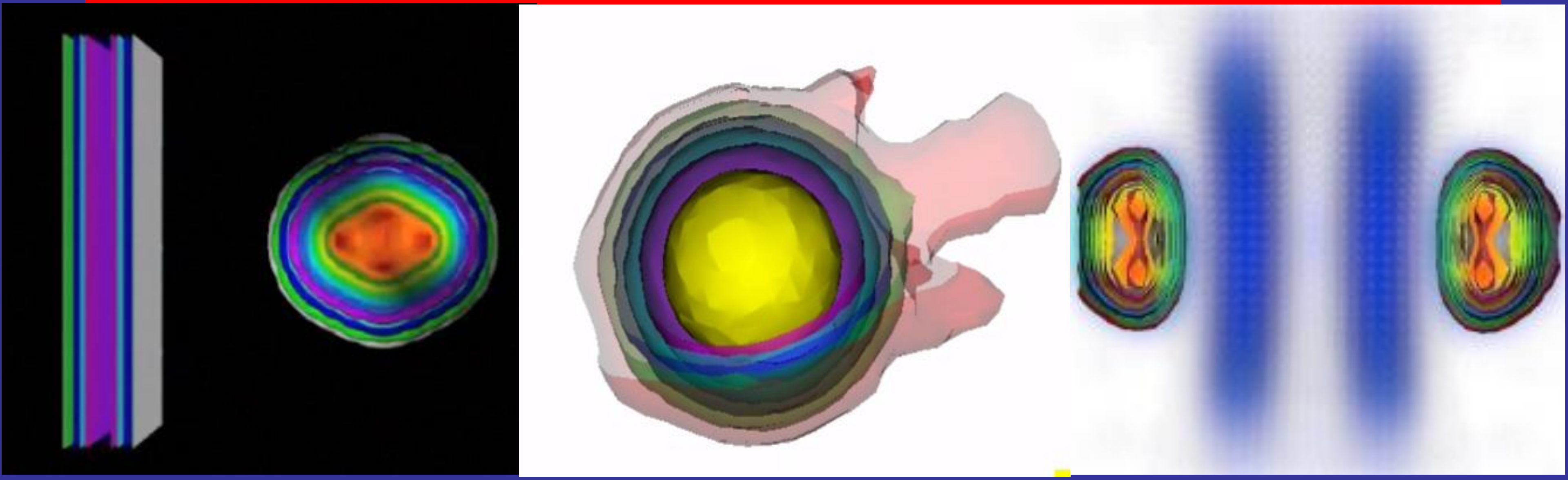
Nuclear Dynamics within Time Dependent Superfluid Local Density Approximation (TDSLDA)



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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 $\alpha(t)$

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.**

For nuclear systems one needs:
- to find an energy functional
- extend it to superfluid systems (SLDA)
- extend it to time dependent phenomena.

Superfluid Local Density Approximation:

$$E_{gs} = \int d^3r \varepsilon(n(\vec{r}), \tau(\vec{r}), \nu(\vec{r}))$$

$$n(\vec{r}) = 2\sum_k |\mathrm{v}_k(\vec{r})|^2, \quad \tau(\vec{r}) = 2\sum_k |\vec{\nabla}\mathrm{v}_k(\vec{r})|^2$$

$$\nu(\vec{r}) = \sum_k \mathrm{u}_k(\vec{r})\mathrm{v}_k^*(\vec{r})$$

pairing (anomalous) density

$$\begin{pmatrix} T + U(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^*(\vec{r}) & -(T + U(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} \mathrm{u}_k(\vec{r}) \\ \mathrm{v}_k(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} \mathrm{u}_k(\vec{r}) \\ \mathrm{v}_k(\vec{r}) \end{pmatrix}$$

Mean-field and pairing field are both local fields!
(for sake of simplicity spin degrees of freedom are not shown)

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:

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

- **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

Nuclear Skyrme functional

$$E = \int d^3r \mathcal{H}(\mathbf{r})$$

where

$$\begin{aligned}
\mathcal{H}(\mathbf{r}) &= C^\rho \rho^2 + C^s \vec{s}\cdot\vec{s} + C^{\Delta\rho}\rho\nabla^2\rho + C^{\Delta s}\vec{s}\cdot\nabla^2\vec{s} + C^\tau(\rho\tau - \vec{j}\cdot\vec{j}) + \\
&+ C^{sT}(\vec{s}\cdot\vec{T} - \mathbf{J}^2) + C^{\nabla J}(\rho\vec{\nabla}\cdot\vec{J} + \vec{s}\cdot(\vec{\nabla}\times\vec{j})) + C^{\nabla s}(\vec{\nabla}\cdot\vec{s})^2 + C^\gamma\rho^\gamma - \Delta\chi^*
\end{aligned}$$

where

$$\begin{aligned}
J_i &= \sum_{k,l} \epsilon_{ikl}\mathbf{J}_{kl} \\
\mathbf{J}^2 &= \sum_{k,l} \mathbf{J}_{kl}^2
\end{aligned}$$

- density: $\rho(\mathbf{r}) = \rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
- spin density: $\vec{s}(\mathbf{r}) = \vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
- current: $\vec{j}(\mathbf{r}) = \frac{1}{2i}(\vec{\nabla} - \vec{\nabla}')\rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
- spin current (2nd rank tensor): $\mathbf{J}(\mathbf{r}) = \frac{1}{2i}(\vec{\nabla} - \vec{\nabla}')\otimes\vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
- kinetic energy density: $\tau(\mathbf{r}) = \vec{\nabla}\cdot\vec{\nabla}'\rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
- spin kinetic energy density: $\vec{T}(\mathbf{r}) = \vec{\nabla}\cdot\vec{\nabla}'\vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
- anomalous (pairing) density: $\chi(\mathbf{r}) = \chi(\mathbf{r},\mathbf{r}')|_{r=r'}$

Linear response regime:
GDR of deformed nuclei

Box size: 32.5fm (mesh size: 1.25fm)
Energy deposited into a nucleus: 45-50MeV
Adiabatic switching of external perturbation: C*exp[-(t-10)^2/2]
Time window for Fourier transform: 1600 fm/c
Time step: 0.12fm/c -> relative accuracy: 10^(-7)

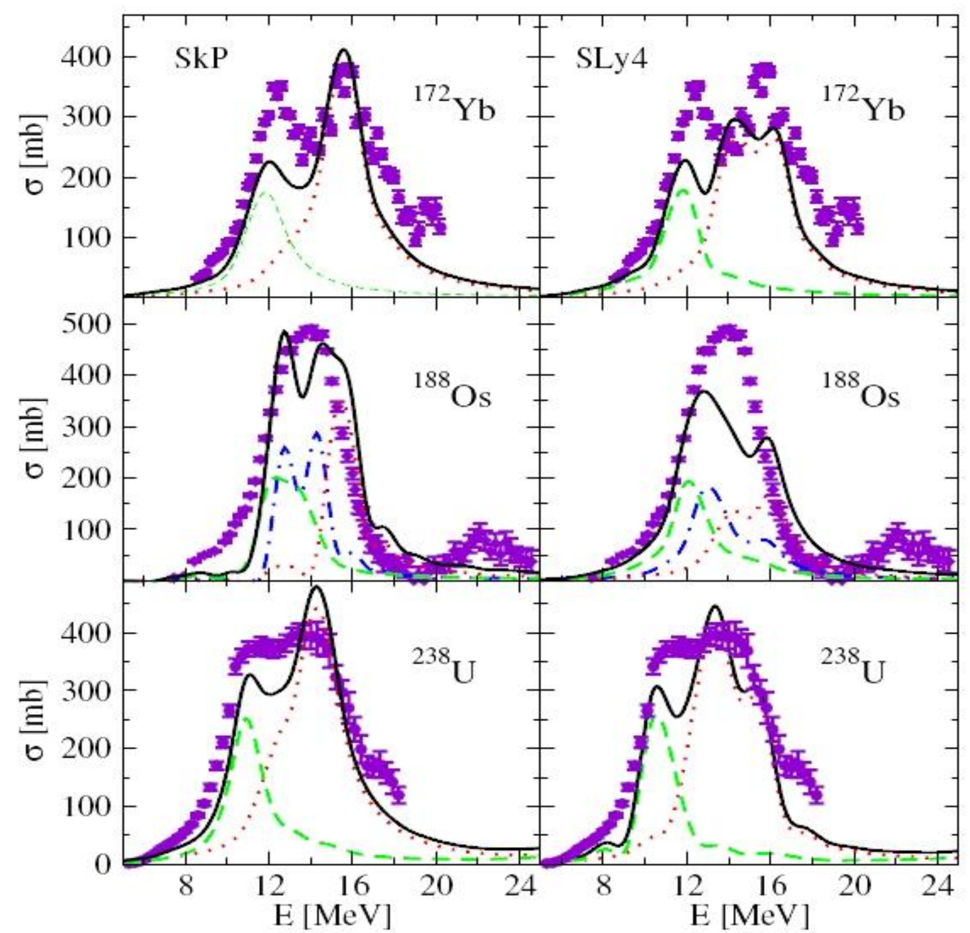
Photoabsorption cross section for heavy, deformed nuclei.

$$h_{\tau,\sigma\sigma}(\mathbf{r},t) \Rightarrow h_{\tau,\sigma\sigma}(\mathbf{r},t) + F_\tau(\mathbf{r}) f(t) \quad F_\tau(\mathbf{r}) = N_\tau \sin(\mathbf{k}\cdot\mathbf{r}_\tau)/|\mathbf{k}|,$$

$$S(E) = \sum_\nu |\langle \nu|\hat{F}|0\rangle|^2 \delta(E - E_\nu)$$

$$S(\omega) = \mathrm{Im}\{\delta F(\omega)/[\pi f(\omega)]\}$$

$$\delta F(t) = \langle \hat{F}\rangle_t - \langle \hat{F}\rangle_0 = \int d^3 r \delta\rho(\mathbf{r},t) F(\mathbf{r}) \quad f(t) = C \exp[-(t-10)^2/2]$$

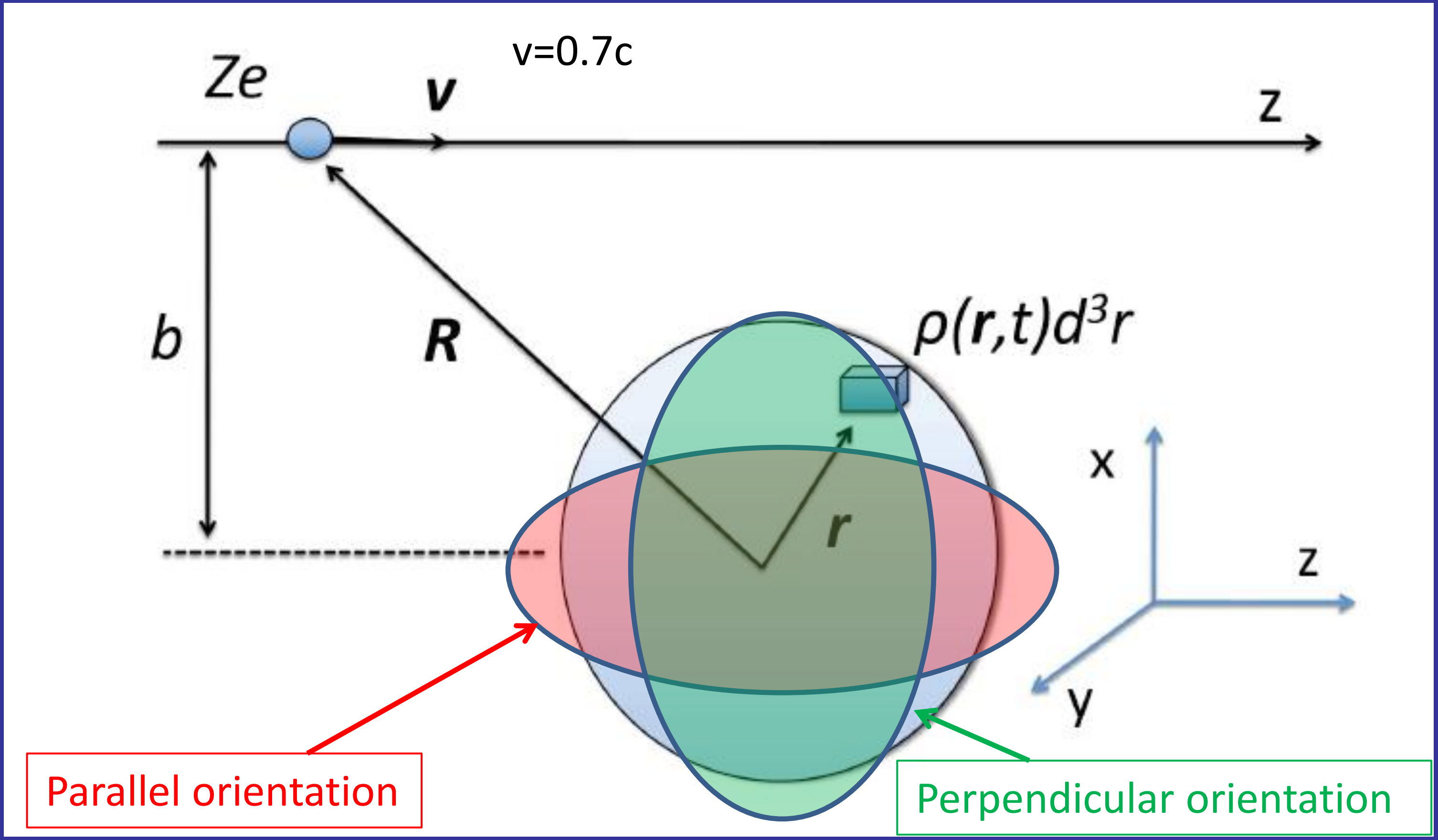


I.Stetcu, A.Bulgac, P. Magierski, K.J. Roche, Phys. Rev. C84 051309 (2011)

Beyond linear regime:
Relativistic Coulomb excitation

Relativistic Coulomb excitation

$$^{238}U + {}^{238}U \rightarrow {}^{238}U^{*} + \ldots$$



- Projectile is treated classically (its de Broglie wavelength is of the order of 0.01 fm)
- Extreme forward scattering: no deflection of the projectile
- Since we want to excite high energy modes (i.e. couple of tens of MeV) the projectile has to be relativistic:

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

Coupling to e.m. field:

$$\vec{E} = -\vec{\nabla}\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$
$$\vec{B} = \vec{\nabla} \times \vec{A}$$

$$\vec{\nabla}\psi \to \vec{\nabla}_A\psi = \left(\vec{\nabla} - i\frac{e}{\hbar c}\vec{A}\right)\psi$$
$$\vec{\nabla}\psi^* \to \vec{\nabla}_{-A}\psi^* = \left(\vec{\nabla} + i\frac{e}{\hbar c}\vec{A}\right)\psi^*$$
$$i\hbar\frac{\partial}{\partial t}\psi \to \left(i\hbar\frac{\partial}{\partial t} - e\phi\right)\psi$$

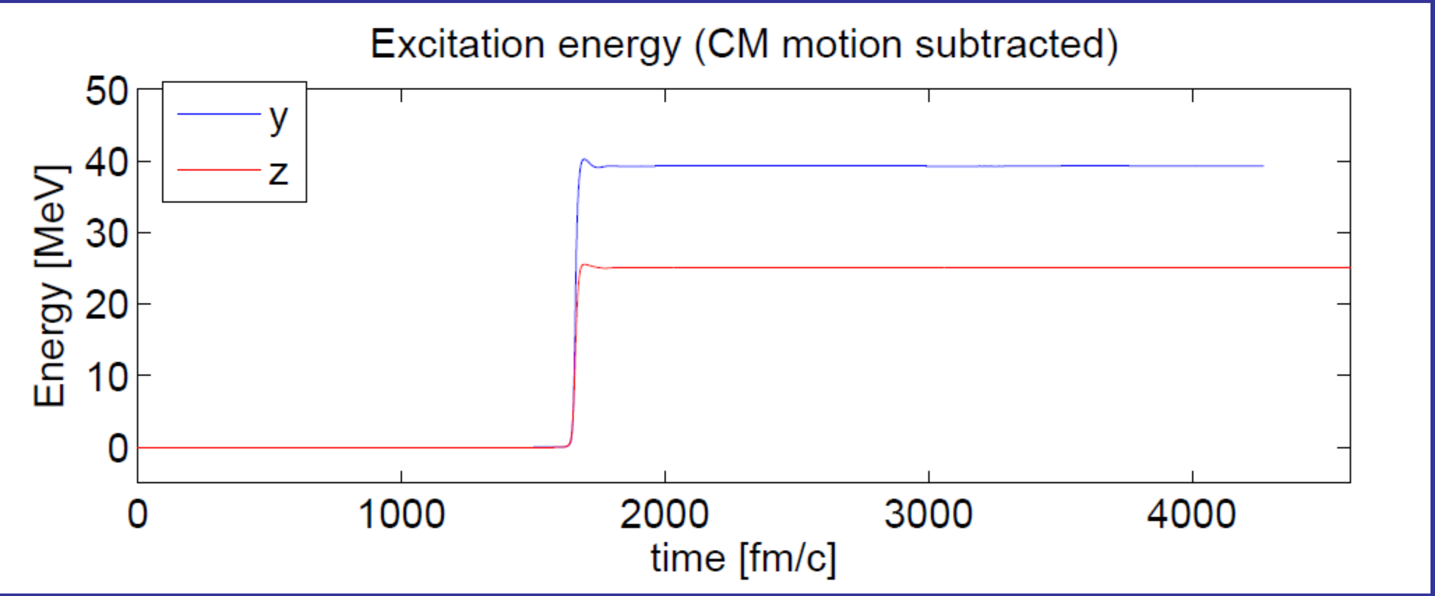
which implies that $\vec{\nabla}\psi\psi^* \to \vec{\nabla}\psi\psi^*$.

Consequently the densities change according to:

- density: $\rho_A(\mathbf{r}) = \rho_A(\mathbf{r})$
- spin density: $\vec{s}_A(\mathbf{r}) = \vec{s}(\mathbf{r})$
- current: $\vec{j}_A(\mathbf{r}) = \vec{j}(\mathbf{r}) - \frac{e}{\hbar c}\vec{A}\rho(\mathbf{r})$
- spin current (2nd rank tensor): $\mathbf{J}_A(\mathbf{r}) = \mathbf{J}(\mathbf{r}) - \frac{e}{\hbar c}\vec{A} \otimes \vec{s}(\mathbf{r})$
- spin current (vector): $\vec{J}_A(\mathbf{r}) = \vec{J}(\mathbf{r}) - \frac{e}{\hbar c}\vec{A} \times \vec{s}(\mathbf{r})$
- kinetic energy density: $\tau_A(\mathbf{r}) = \left(\vec{\nabla} - i\frac{e}{\hbar c}\vec{A}\right)\cdot\left(\vec{\nabla}' + i\frac{e}{\hbar c}\vec{A}\right)\rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
  $= \tau(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}\cdot\vec{j}(\mathbf{r}) + \frac{e^2}{\hbar^2 c^2}|\vec{A}|^2\rho(\mathbf{r}) = \tau(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}\cdot\vec{j}_A(\mathbf{r}) - \frac{e^2}{\hbar^2 c^2}|\vec{A}|^2\rho(\mathbf{r})$
- spin kinetic energy density: $\vec{T}_A(\mathbf{r}) = \left(\vec{\nabla} - i\frac{e}{\hbar c}\vec{A}\right)\cdot\left(\vec{\nabla}' + i\frac{e}{\hbar c}\vec{A}\right)\vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
  $= \vec{T}(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}^T\cdot\mathbf{J}(\mathbf{r}) + \frac{e^2}{\hbar^2 c^2}|\vec{A}|^2\vec{s}(\mathbf{r}) = \vec{T}(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}^T\cdot\mathbf{J}_A(\mathbf{r}) - \frac{e^2}{\hbar^2 c^2}|\vec{A}|^2\vec{s}(\mathbf{r})$

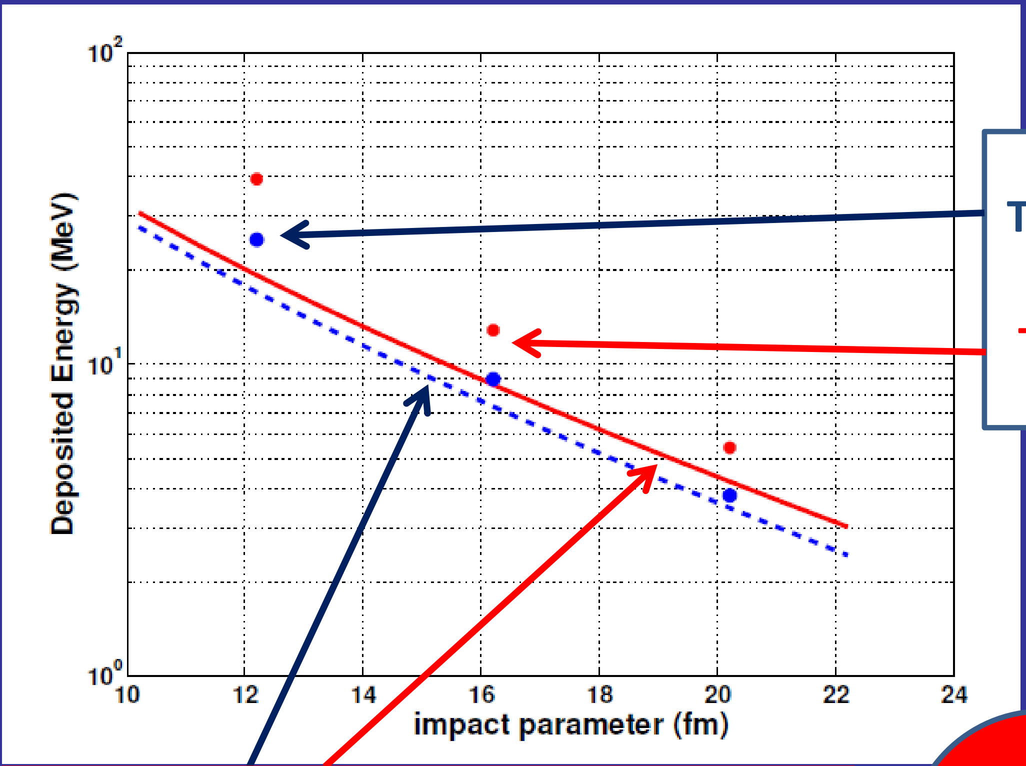
Energy deposited for two nuclear orientations (y – perpendicular, z – parallel)

Impact parameter b=12.2fm



$b(fm)$	E_{int} (MeV)	E_{int}/E	$E_{\gamma}^{int}(MeV)$	$E_{\gamma}^{int}/E_{\gamma}$	E_{GT}
12.2 $\|\|$	25.11	0.588	0.5	0.941	17.05
16.2 $\|\|$	8.966	0.470	0.217	0.939	7.33
20.2 $\|\|$	3.798	0.367	0.106	0.934	3.47
12.2 $\perp$	39.29	0.668	0.911	0.960	19.33
16.2 $\perp$	12.87	0.547	0.411	0.963	8.6
20.2 $\perp$	5.413	0.444	0.199	0.961	4.21

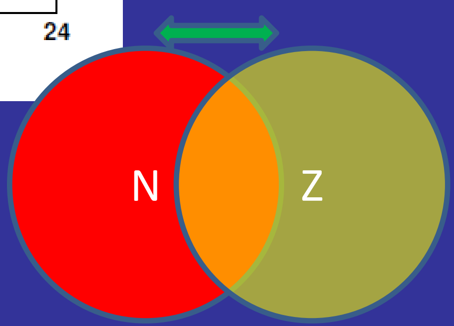
Energy transferred to the target nucleus in the form of internal excitations



TDSLDA – parallel orientation

TDSLDA – perpendicular orientation

Goldhaber-Teller like model:
proton and neutron density distributions oscillating against each other



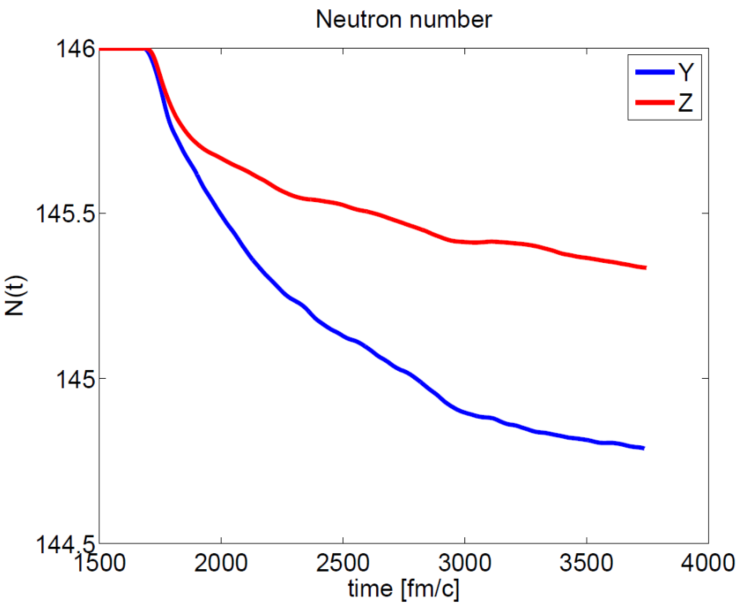
Two characteristic frequencies

$$\hbar\omega_1 = 10 MeV$$
$$\hbar\omega_2 = 12 MeV$$

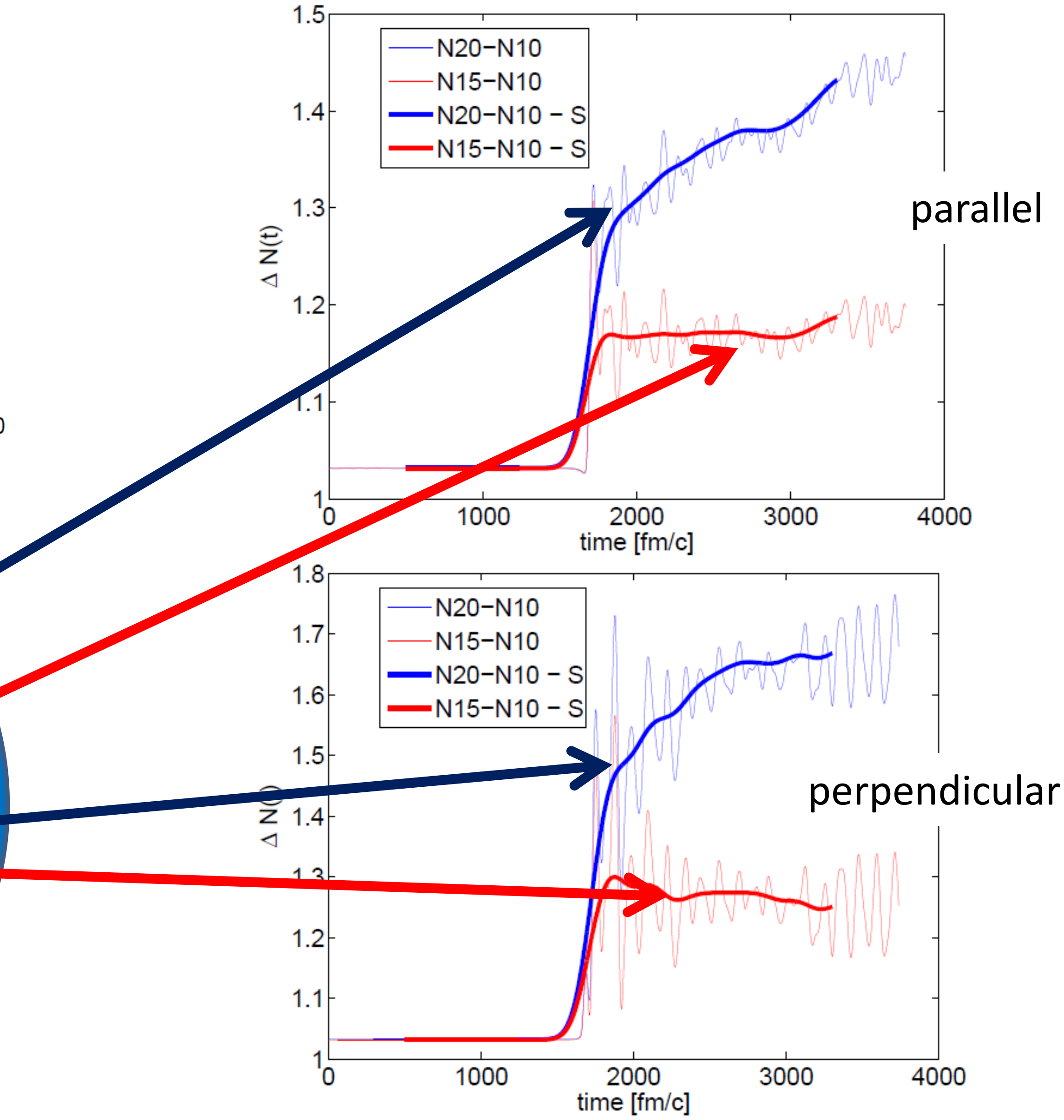
Part of the energy is transferred to other degrees of freedom than pure dipole moment oscillations.

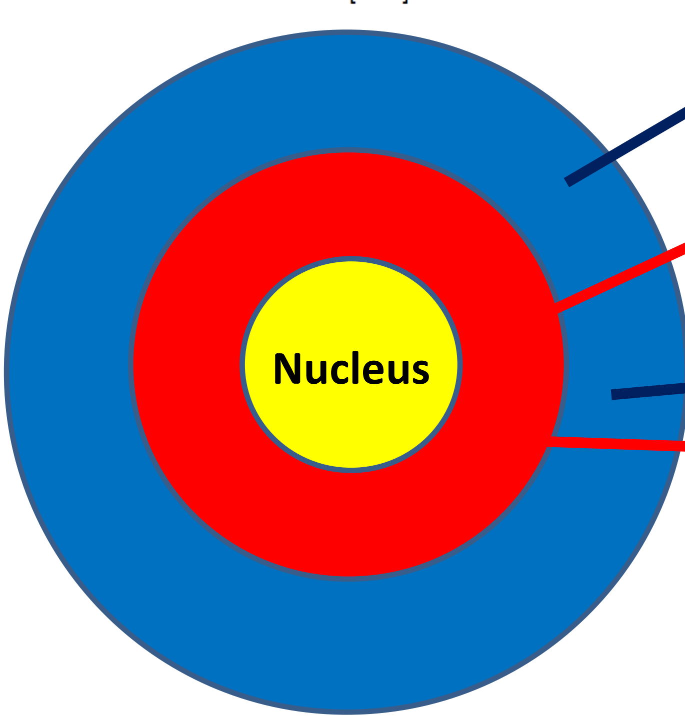
Neutron emission

Impact parameter b=12.2fm



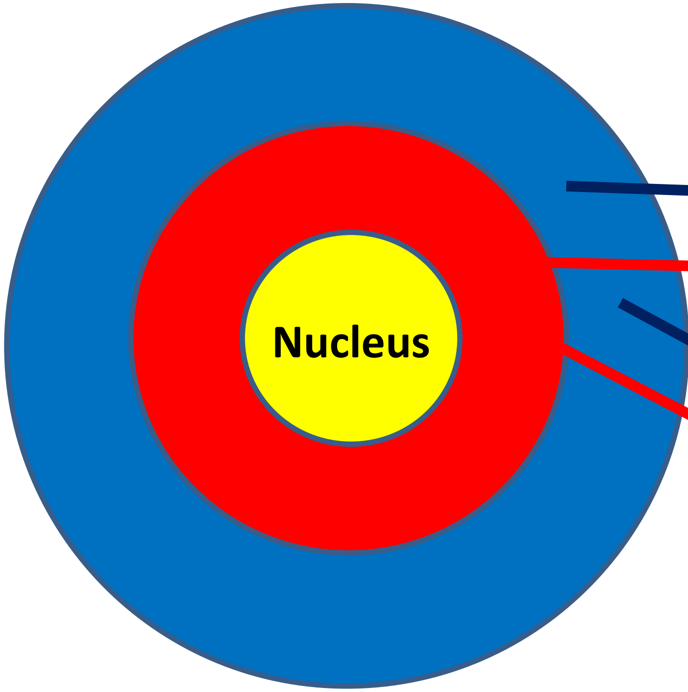
Number of neutrons in two shells surrounding nucleus for two nuclear orientations with respect to incoming projectile:



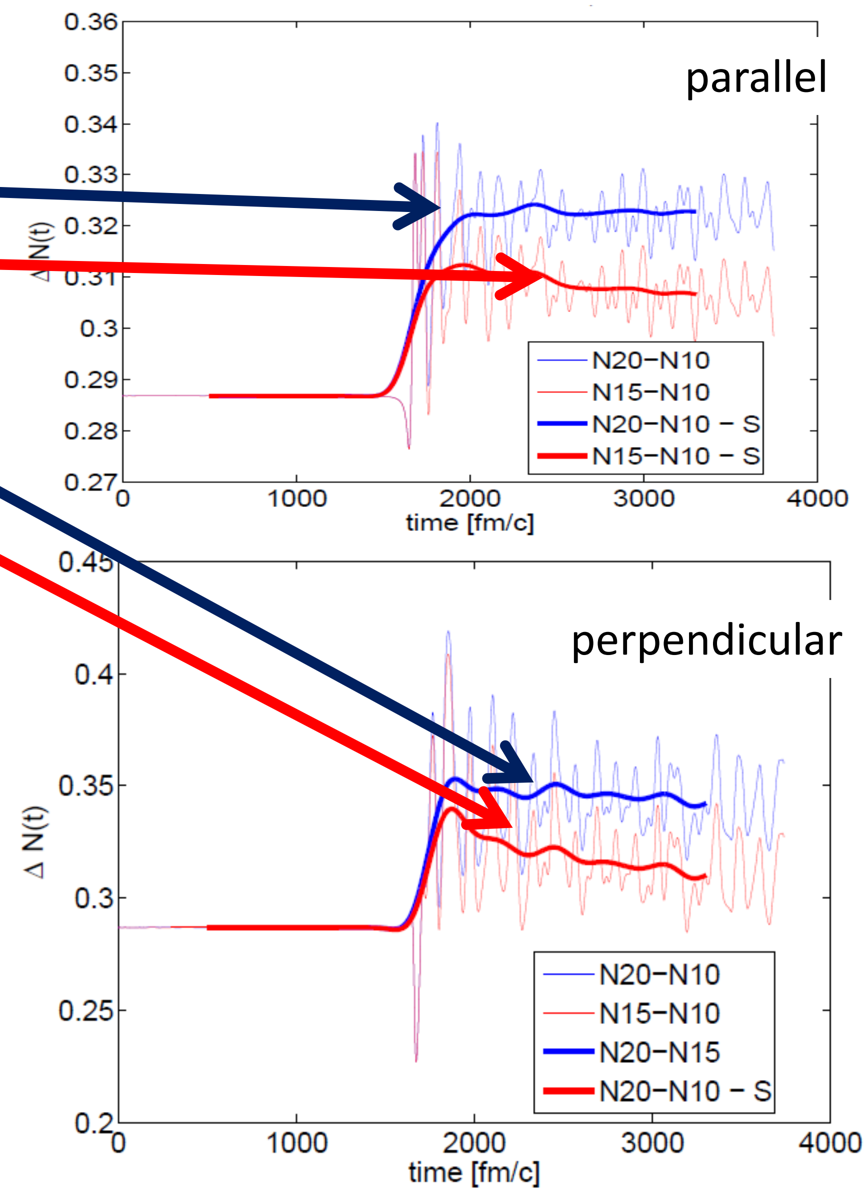


Protons

Impact parameter b=12.2fm



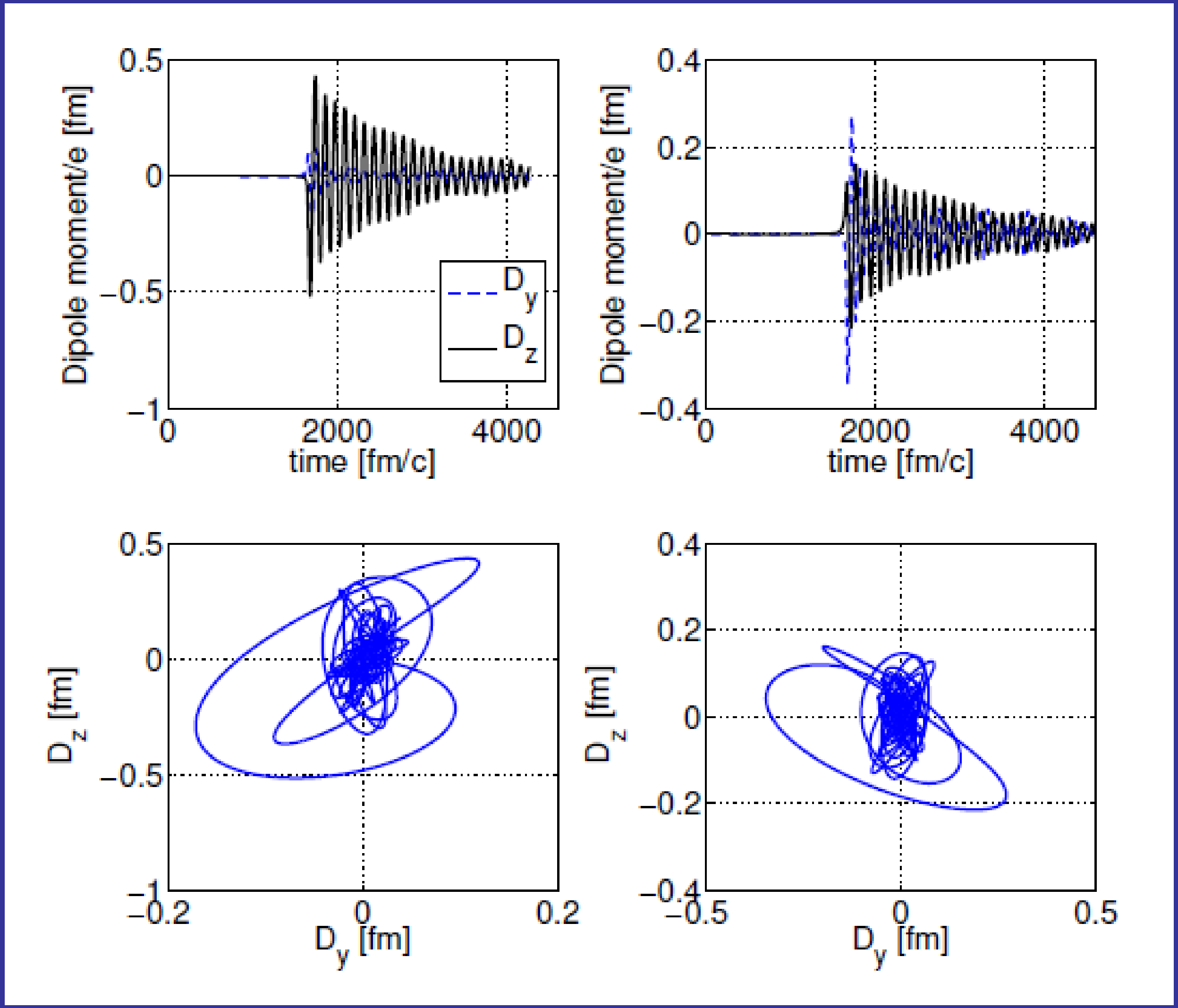
Number of protons in two shells surrounding nucleus:



Contrary to protons, neutrons exhibit approximately steady flow out of nucleus

Internal nuclear excitations

Electric dipole moment (along two axes: y, z) as a function of time

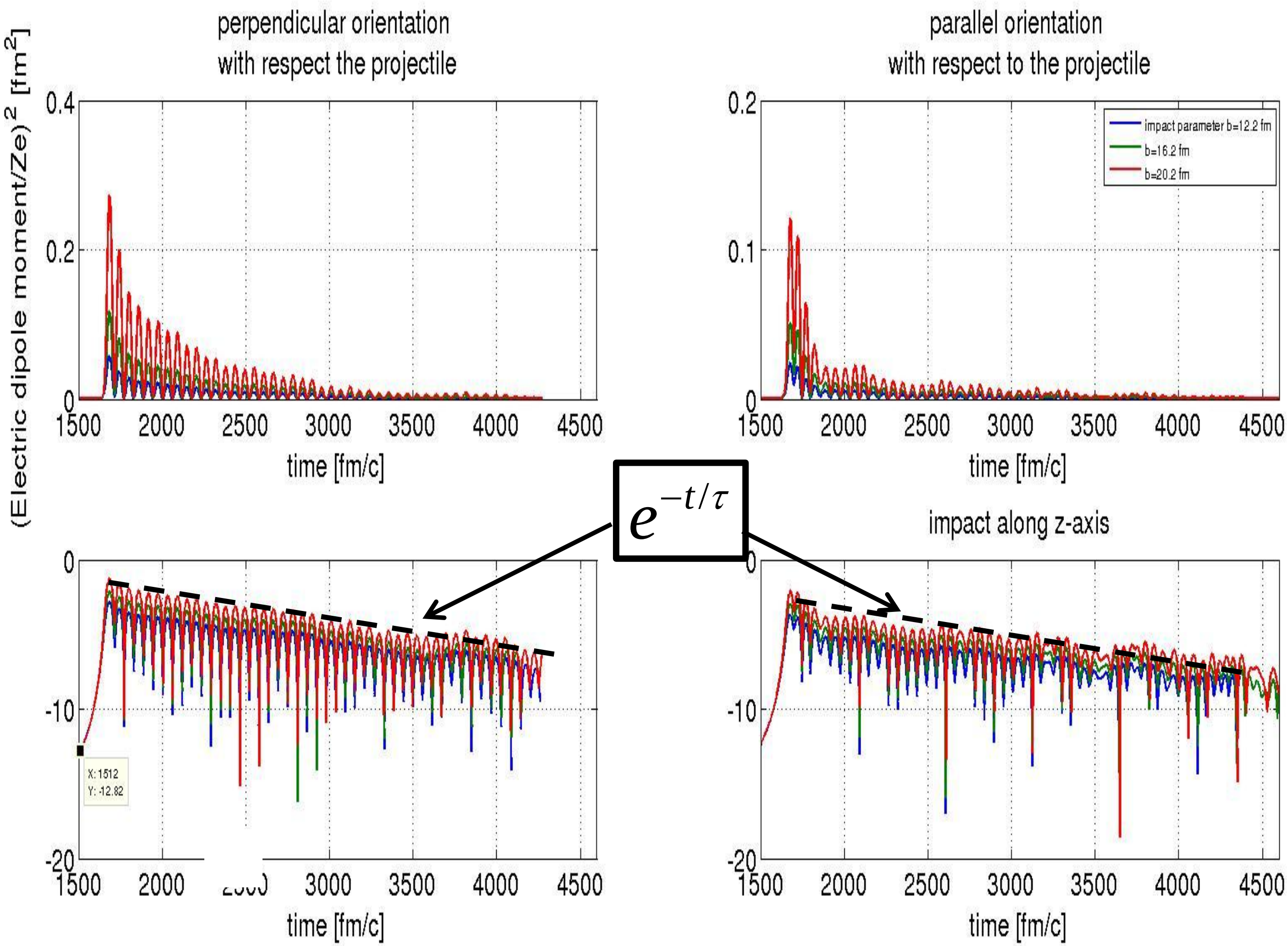


Oscillations are damped due to the one-body dissipation mechanism

One body dissipation

Let us assume that the collective energy of dipole oscillation is proportional the square of the amplitude of electric dipole moment:

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



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

Electromagnetic radiation from excited nucleus

$$\rho(\mathbf{r},t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\rho(\mathbf{r},\omega)\exp(-i\omega t)$$

$$\vec{j}(\mathbf{r},t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \vec{j}(\mathbf{r},\omega)\exp(-i\omega t)$$

From TDSLDA

$$\vec{B}(\mathbf{r},\omega) = \frac{ie}{c}\frac{\exp(ikr)}{r}\int d^3r'\vec{k}\times\vec{j}(\mathbf{r}',\omega)\exp(-i\vec{k}\cdot\mathbf{r}') = \frac{ie}{c}\frac{\exp(ikr)}{r}\vec{k}\times\vec{j}(\vec{k},\omega)$$

$$\vec{E}(\mathbf{r},\omega) = \frac{ie}{c}\frac{\exp(ikr)}{r}\frac{\mathbf{r}}{r}\times\int d^3r'(\vec{j}(\mathbf{r}',\omega)\times\vec{k})\exp(-i\vec{k}\cdot\mathbf{r}') = \frac{ie}{c}\frac{\exp(ikr)}{r}\frac{\mathbf{r}}{r}\times\left(\vec{j}(\vec{k},\omega)\times\vec{k}\right)$$

$$\frac{dP}{d\Omega}(t) = \frac{e^2}{4\pi c}\left|\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(\vec{k}\times\vec{j}(\vec{k},\omega))\exp(-i\omega(t-r/c))\right|^2$$

Angular distribution of radiated power

$$\frac{dE}{d\Omega d\omega}(\omega) = \frac{e^2}{4\pi^2 c}\left|\vec{k}\times\vec{j}(\vec{k},\omega)\right|^2 = \frac{e^2}{4\pi^2 c}\left|\int d^3r\left(\nabla\times\vec{j}(\mathbf{r},\omega)\right)\exp(-i\vec{k}\cdot\mathbf{r})\right|^2$$

Angular distribution and ferquency distribution of emitted radiation

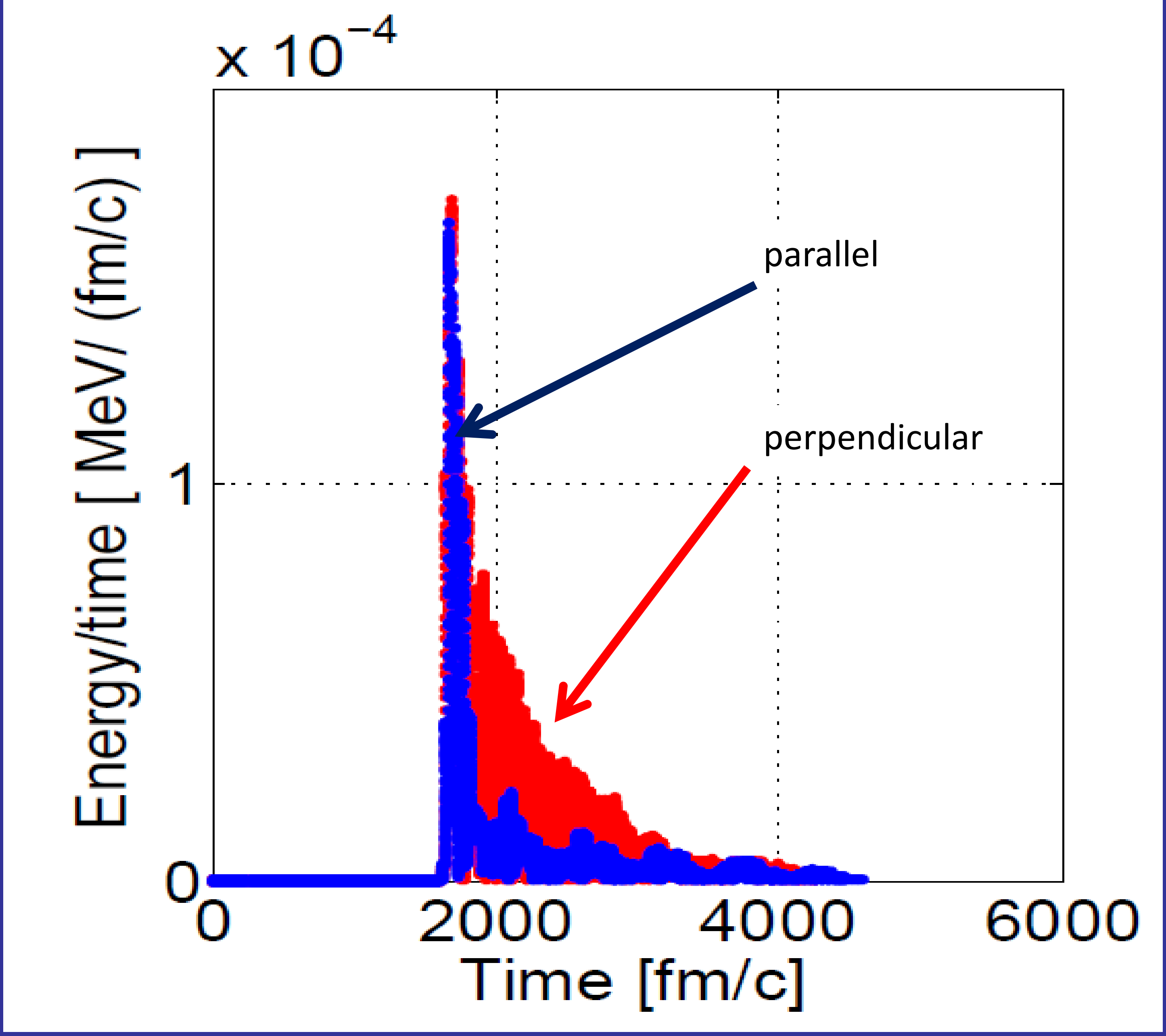
In practice it is better to perform multipole expansion:

$$\boxed{\begin{aligned}\frac{dE}{d\omega} &= \frac{4e^2}{c}\sum_{l,m}|\vec{b}_{lm}(k,\omega)|^2\\ P(t+r/c) &= \int\frac{dP}{d\Omega}(t+r/c)d\Omega = \frac{e^2}{\pi c}\sum_{l,m}\left|\int_{-\infty}^{\infty}\vec{b}_{lm}(k,\omega)\exp(-i\omega t)d\omega\right|^2\end{aligned}}$$

$$\vec{b}_{lm}(k,t) = \int d^3r\vec{b}(\mathbf{r},t)j_l(kr)Y^*_{lm}(\hat{r})$$

$$\vec{b}_{lm}(k,\omega) = \int_{-\infty}^{\infty}\vec{b}_{lm}(k,t)\exp(i\omega t)dt$$

Electromagnetic radiation rate due to the internal motion



Electromagnetic radiation due to the internal nuclear motion

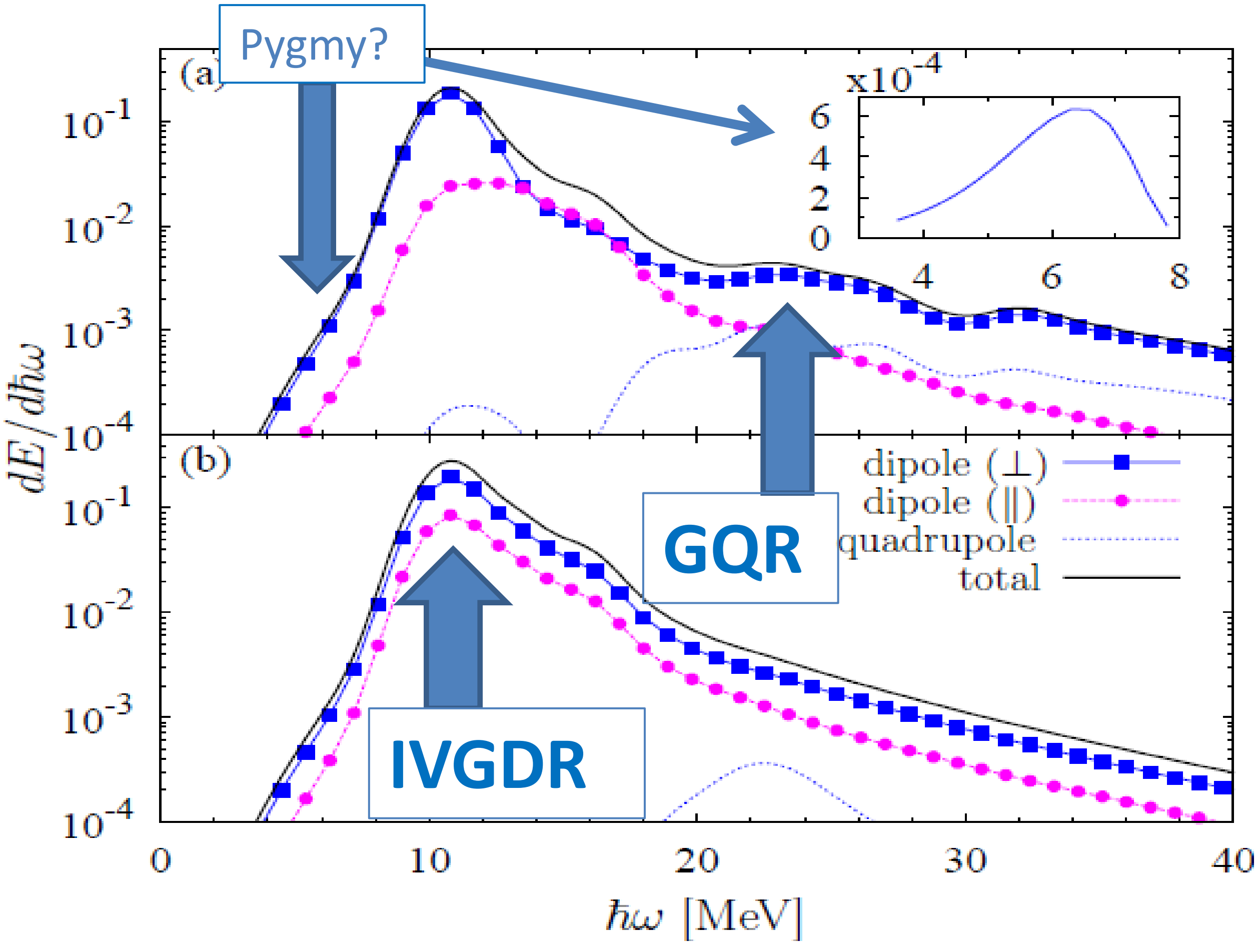
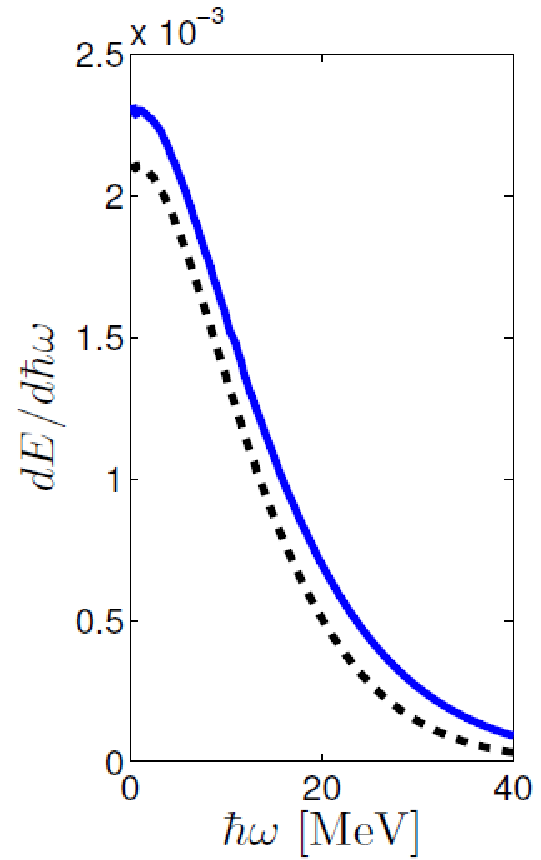


FIG. 2. (color online) The energy spectrum of emitted EM at the impact parameter $b = 12.2$ fm. We show the dipole contributions for both orientations, and the total quadrupole contribution. The lower panel shows the radiation emitted from the target nucleus excited when only the dipole component of the projectile electromagnetic field is used.

Bremsstrahlung at b=12.2fm



I. Stetcu et al. arXive:[1403.2671]

Summary

- ***TDSLDA is a flexible tool to study nuclear dynamics.***
- ***Pairing field is treated on the same footing like single particle potentials (no frozen occupation number approximation).***
- ***Nuclear excitation modes (beyond linear response!) can be identified from e.m. radiation.***
- ***Various nonequilibrium nuclear processes can be studied:***

  - Nuclear large amplitude collective motion (LACM)
  - (induced) nuclear fission
  - Excitation of nuclei with gamma rays and neutrons
  - Coulomb excitation of nuclei with relativistic heavy-ions
  - Nuclear reactions, fusion between colliding heavy-ions
  - Neutron star crust and dynamics of vortices and their pinning mechanism