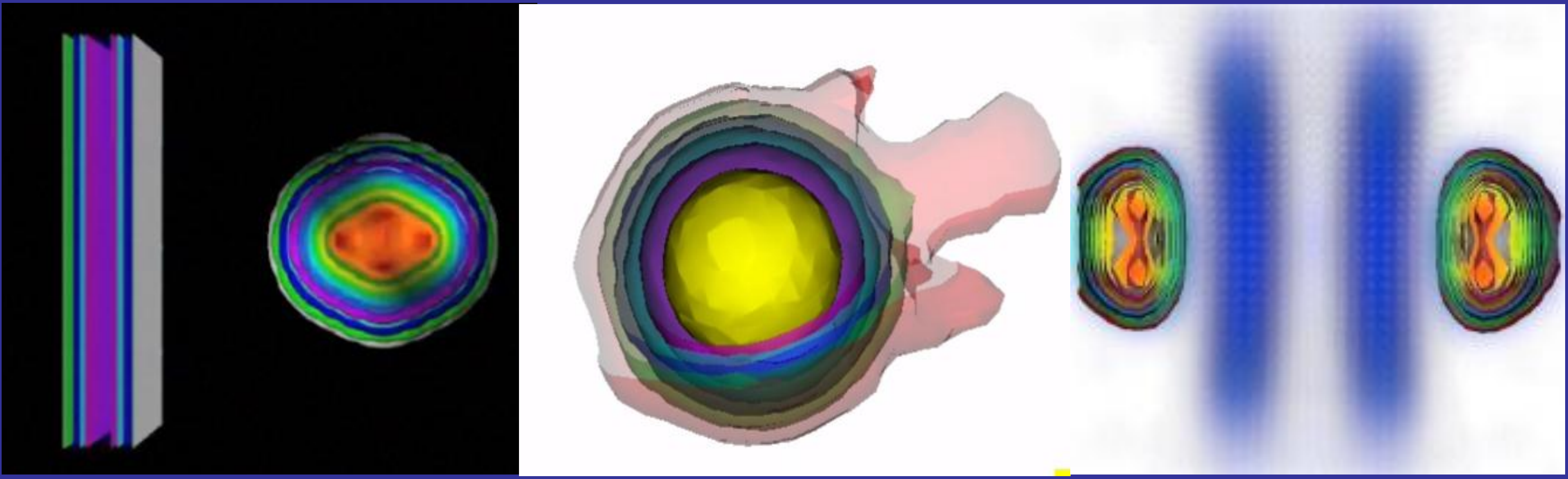
Nuclear Dynamics from Time Dependent Superfluid Local Density Approximation (TDSLDA)



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<u>GOAL:</u>

Description of nuclear dynamics far from equilibrium within the framework of TDDFT.

Nuclear Skyrme functional

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

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

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

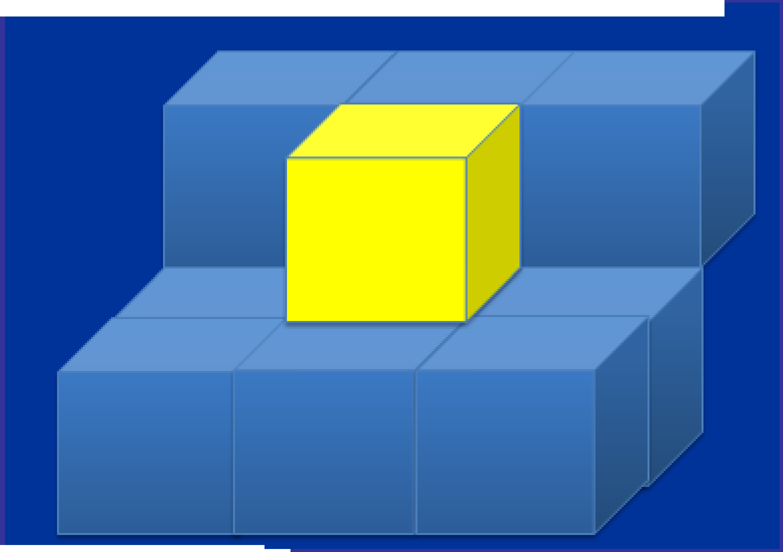
- density: $\rho(\mathbf{r}) = \rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
- spin density: $\vec{s}(\mathbf{r}) = \vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
- current: $\vec{j}(\mathbf{r}) = \frac{1}{2i}(\vec{\nabla} - \vec{\nabla}')\rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
- spin current (2nd rank tensor): $\mathbf{J}(\mathbf{r}) = \frac{1}{2i}(\vec{\nabla} - \vec{\nabla}')\otimes\vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
- 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: $\chi(\mathbf{r}) = \chi(\mathbf{r},\mathbf{r}')|_{r=r'}$

Treatment of the Coulomb potential

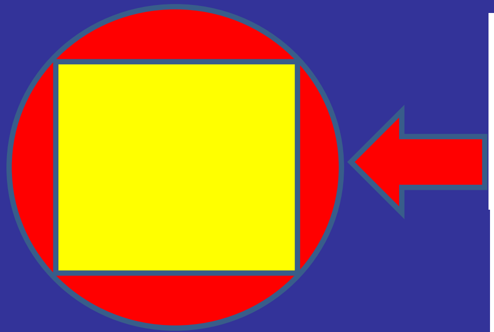
$$\nabla^2\Phi(\mathbf{r}) = 4\pi e^2\rho(\mathbf{r})$$

$$\Phi(\mathbf{r}) = \int d^3r' \frac{e^2\rho(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}$$

$$\Phi(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3}\frac{e^2\rho(\vec{k})}{k^2}\exp(i\vec{k}\cdot\mathbf{r}) = \frac{1}{27N_xN_yN_z}\sum_{\vec{k}\in L_xL_yL_z} e^2\rho(\vec{k})f(k)\exp(i\vec{k}\cdot\mathbf{r})$$



Defining an auxiliary potential *f(r)* on can get rid of spurious interaction with neighboring cells at the cost of performing FFT in 3 times larger box.



$$f(r) = 1/r \text{ for } r < \sqrt{L_x^2+L_y^2+L_z^2}$$
$$f(r) = 0 \text{ otherwise}$$

$$f(k) = 4\pi\frac{1-\cos(k\sqrt{L_x^2+L_y^2+L_z^2})}{k^2}$$

Castro, Rubio, Stott, arXive:0012024v1

However taking into account that FFT in a larger box means simply denser momentum space one can replace one FFT in 3 times larger box with 27 FFT's in the original box.

$$
\begin{aligned}
&\Phi(\mathbf{r}) = \\
= \quad & \frac{1}{27 N_x N_y N_z} \sum_{k,l,m=0}^{2} \left[\sum_{\vec{k} \in L^3} e^2 \rho_{klm}(\vec{k}) f\left(\vec{k} + \left(k\frac{2\pi}{3L_x}, l\frac{2\pi}{3L_y}, m\frac{2\pi}{3L_z} \right) \right) \exp(i\vec{k} \cdot \mathbf{r}) \right] \\
\times \quad & \exp\left(i \left(k\frac{2\pi}{3L_x} x + l\frac{2\pi}{3L_y} y + m\frac{2\pi}{3L_z} z \right) \right)
\end{aligned}
$$

where

$$
\rho_{klm}(\vec{k}) = \sum_{\mathbf{r} \in L^3} \rho(x,y,z) \exp\left(-i \left(k\frac{2\pi}{3L_x} x + l\frac{2\pi}{3L_y} y + m\frac{2\pi}{3L_z} z \right) \right) \exp(-i\vec{k} \cdot \mathbf{r})
$$

Gain in computational cost:

$$
\boxed{27 \cdot N^3 Log N^3 < (3N)^3 \, Log (3N)^3}
$$

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:

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

- **The system is placed on a large 3D spatial lattice.**
- **Derivatives are computed with FFTW**
- **Fully self-consistent treatment with fundamental symmetries respected (isospin, gauge, Galilean, rotation, translation)**
- **for TD high-accuracy and numerically stable Adams–Bashforth–Milne 5th order predictor-corrector-modifier algorithm with only 2 evaluations of the rhs per time step and with no matrix operations**
- **No symmetry restrictions**
- **Number of PDEs is of the order of the number of spatial lattice points**
- **Initial conditions for TDSLDA are generated from static SLDA code.**

In future: ground state may be generated through adiabatic switching and quantum friction (Bulgac et al. arXiv:1305.6891)

Single particle potential (Skyrme):

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

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

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.

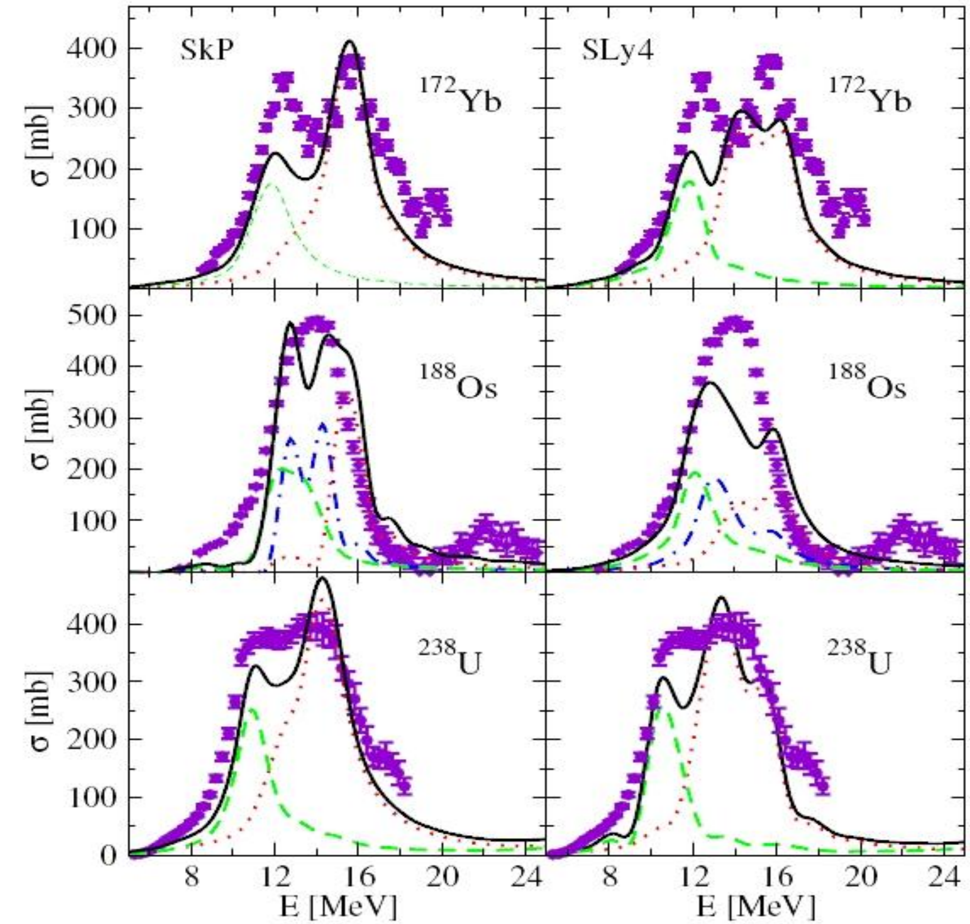
$$h_{\tau,\sigma\sigma}(\mathbf{r},t) \Rightarrow h_{\tau,\sigma\sigma}(\mathbf{r},t)+F_\tau(\mathbf{r})f(t) \qquad F_\tau(\mathbf{r}) = N_\tau \sin(\mathbf{k}\cdot\mathbf{r}_\tau)/|\mathbf{k}|$$

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

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

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

(gamma,n) reaction through the excitation of GDR



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

Evolution of occupation probabilities

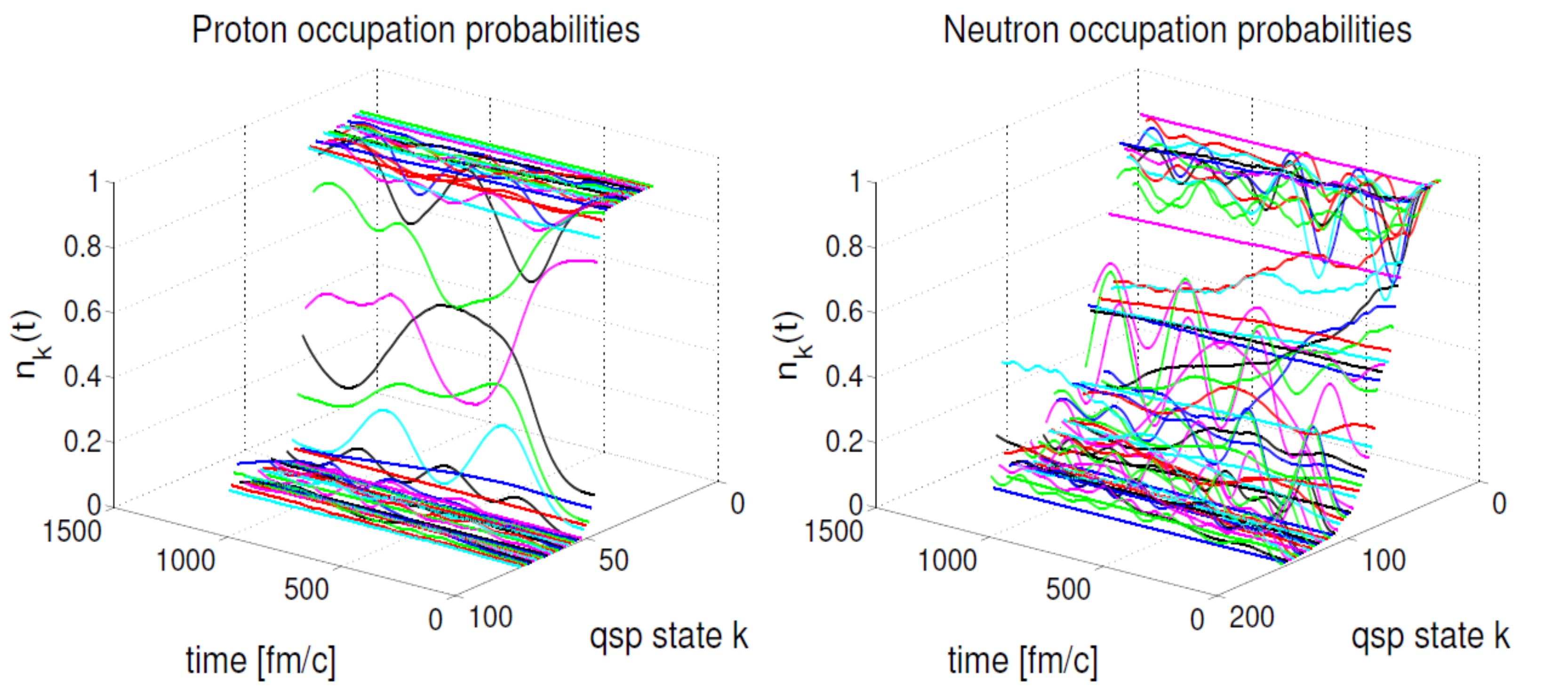


FIG. 1. (Color online) The time-dependent proton and neutron occupation probabilities of a a number of quasiparticle states around the Fermi level for ^{238}U calculated as described in the main text with SLy4.

Occupation probabilities vary significantly in time.

Pairing has to be treated fully selfconsistently!

Beyond linear regime:
Relativistic Coulomb excitation

Coupling to e.m. field:

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

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

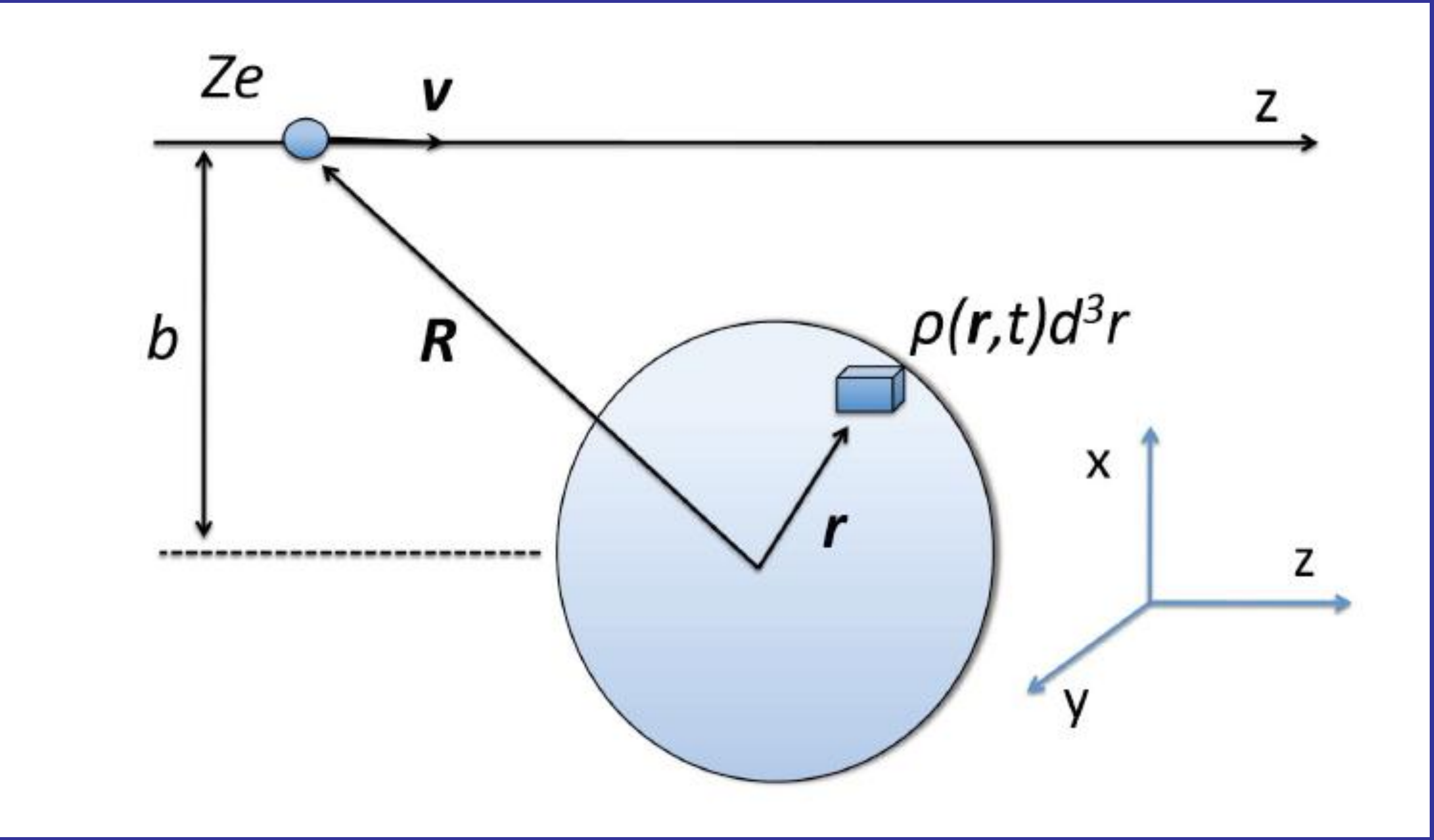
which implies that $\vec{\nabla}\psi\psi^* \to \vec{\nabla}\psi\psi^*$.

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: $\vec{T}_A(\mathbf{r}) = \left(\vec{\nabla} - i\frac{e}{\hbar c}\vec{A}\right) \cdot \left(\vec{\nabla}' + i\frac{e}{\hbar c}\vec{A}\right)\vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
  $= \vec{T}(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}^T\cdot\mathbf{J}(\mathbf{r}) + \frac{e^2}{\hbar^2 c^2}|\vec{A}|^2\vec{s}(\mathbf{r}) = \vec{T}(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}^T\cdot\mathbf{J}_A(\mathbf{r}) - \frac{e^2}{\hbar^2 c^2}|\vec{A}|^2\vec{s}(\mathbf{r})$

Relativistic Coulomb excitation

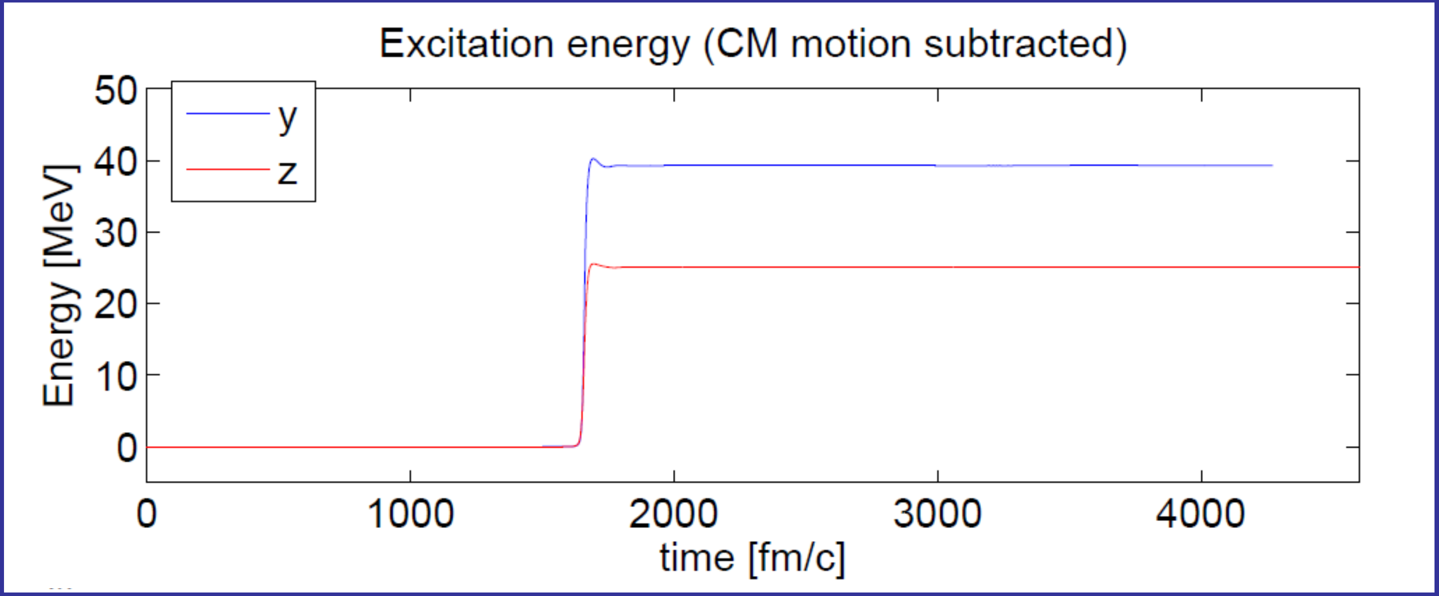
$$^{238}U + ^{238}U \rightarrow ^{238}U^{*} + \ldots \text{ at about 700 MeV/n}$$



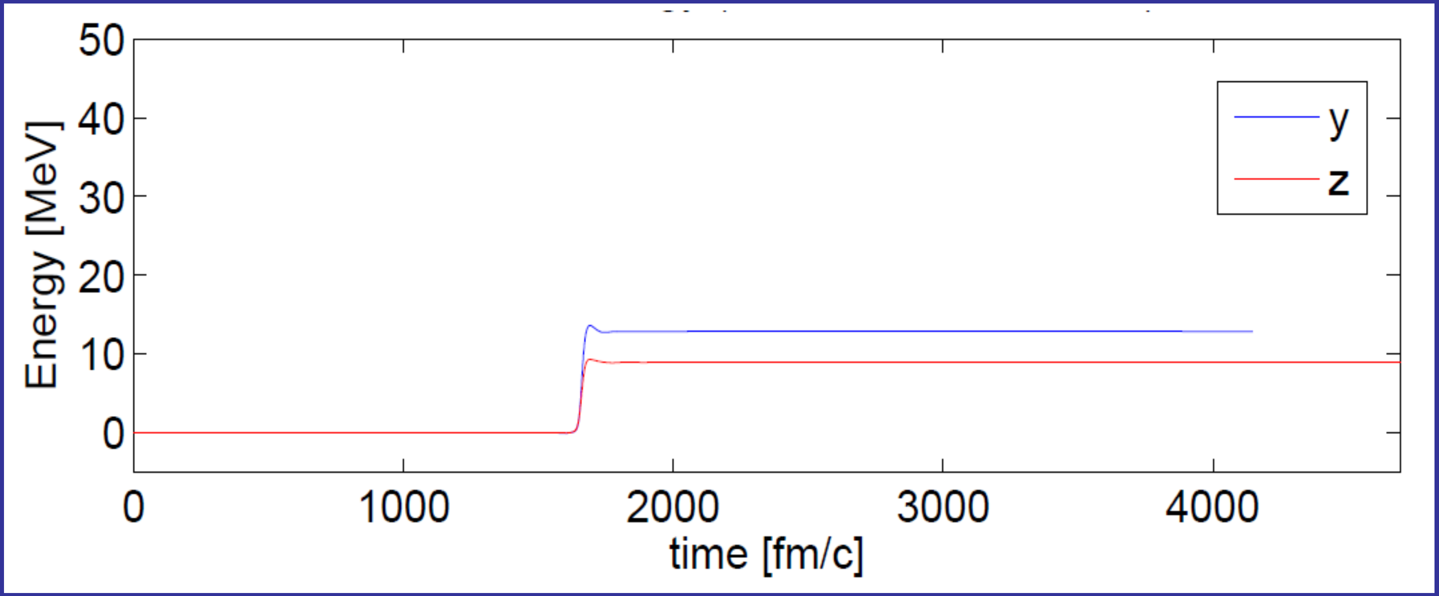
The coordinate transformation has been applied to keep CM in the center of the box at all times.

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

Impact parameter b=12.2fm

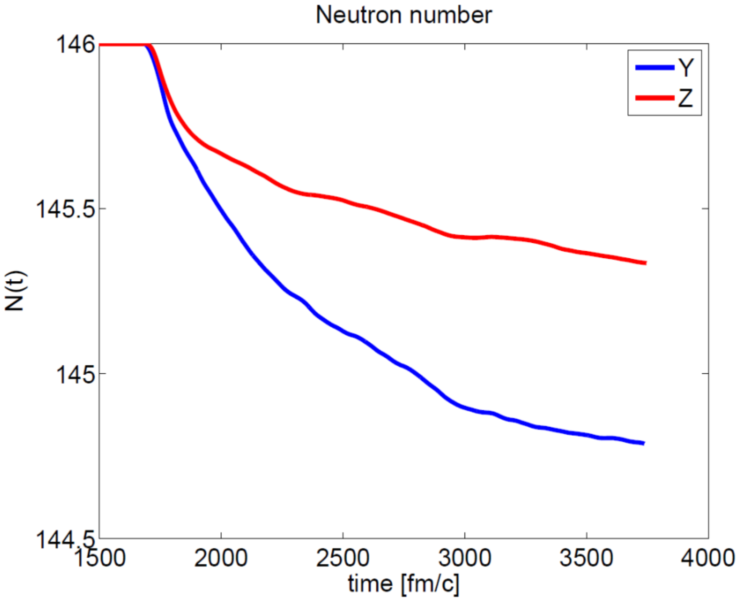


Impact parameter b=16.2fm

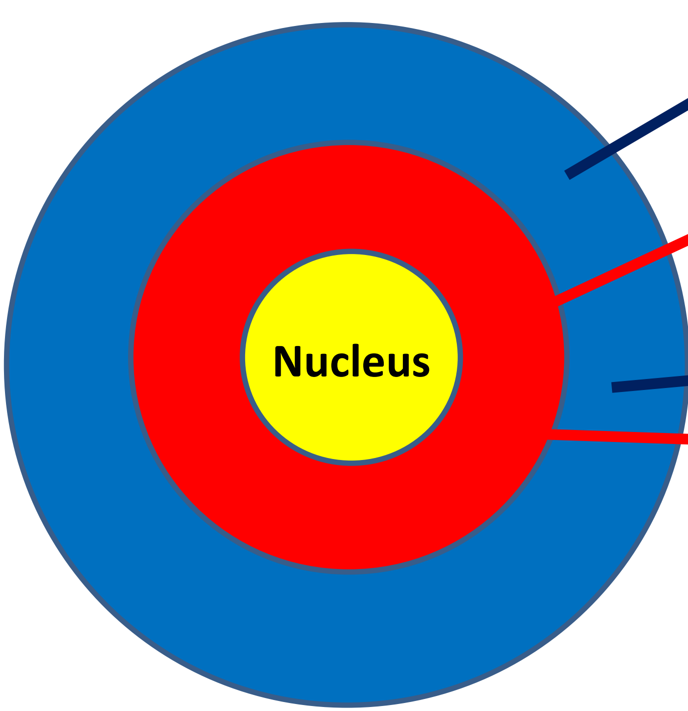


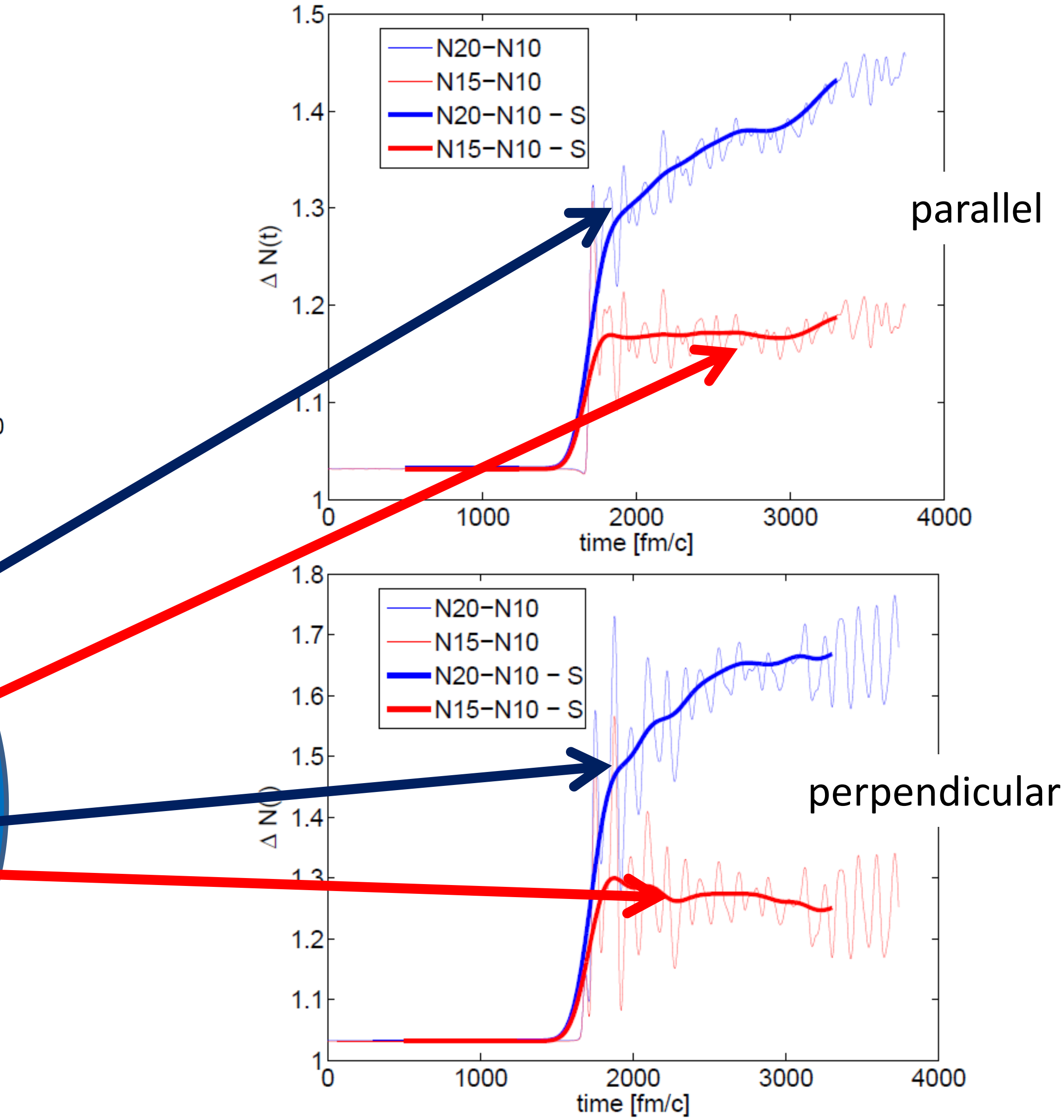
Neutron emission

Impact parameter b=12.2fm



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

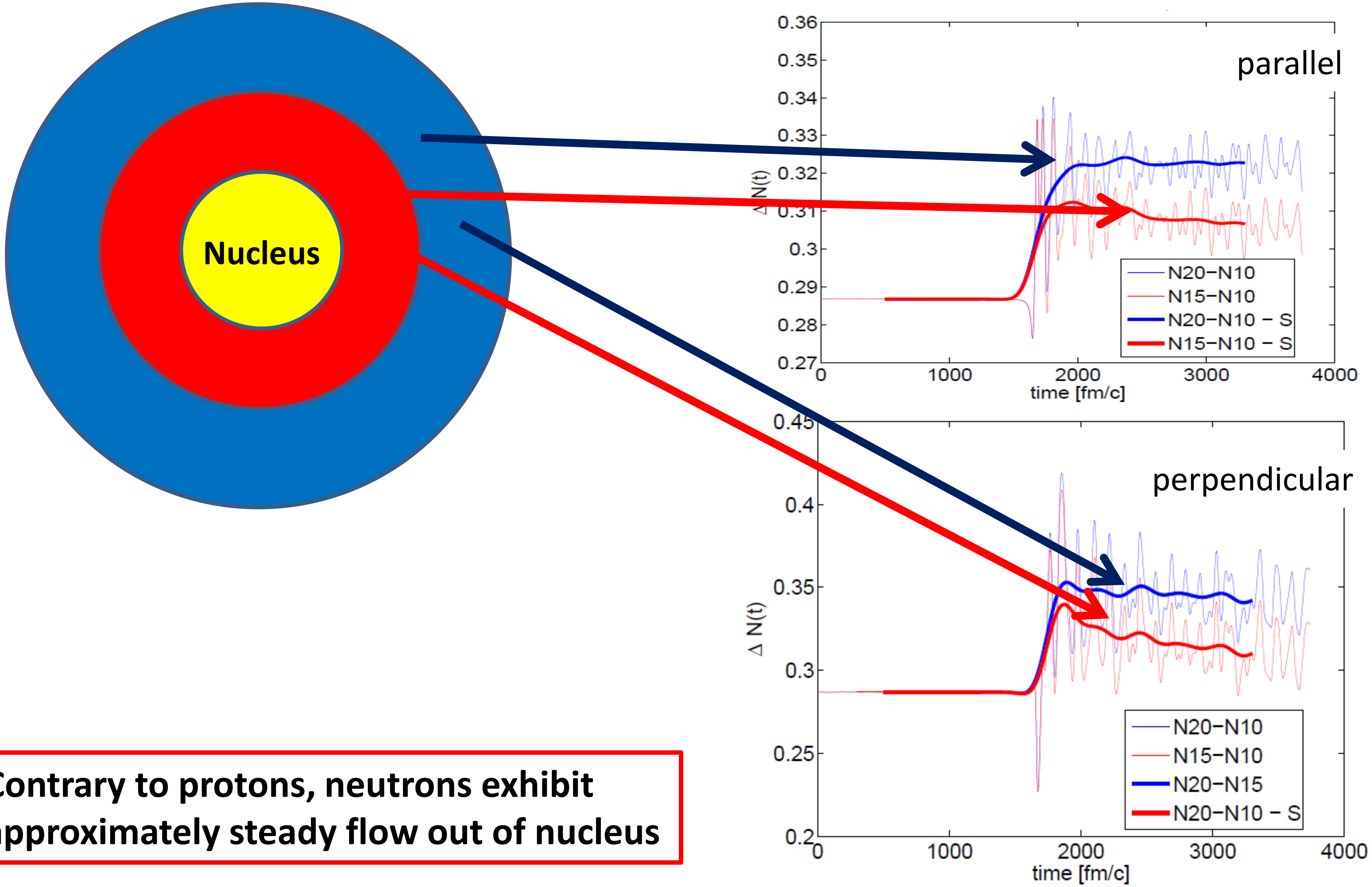




Protons

Impact parameter b=12.2fm

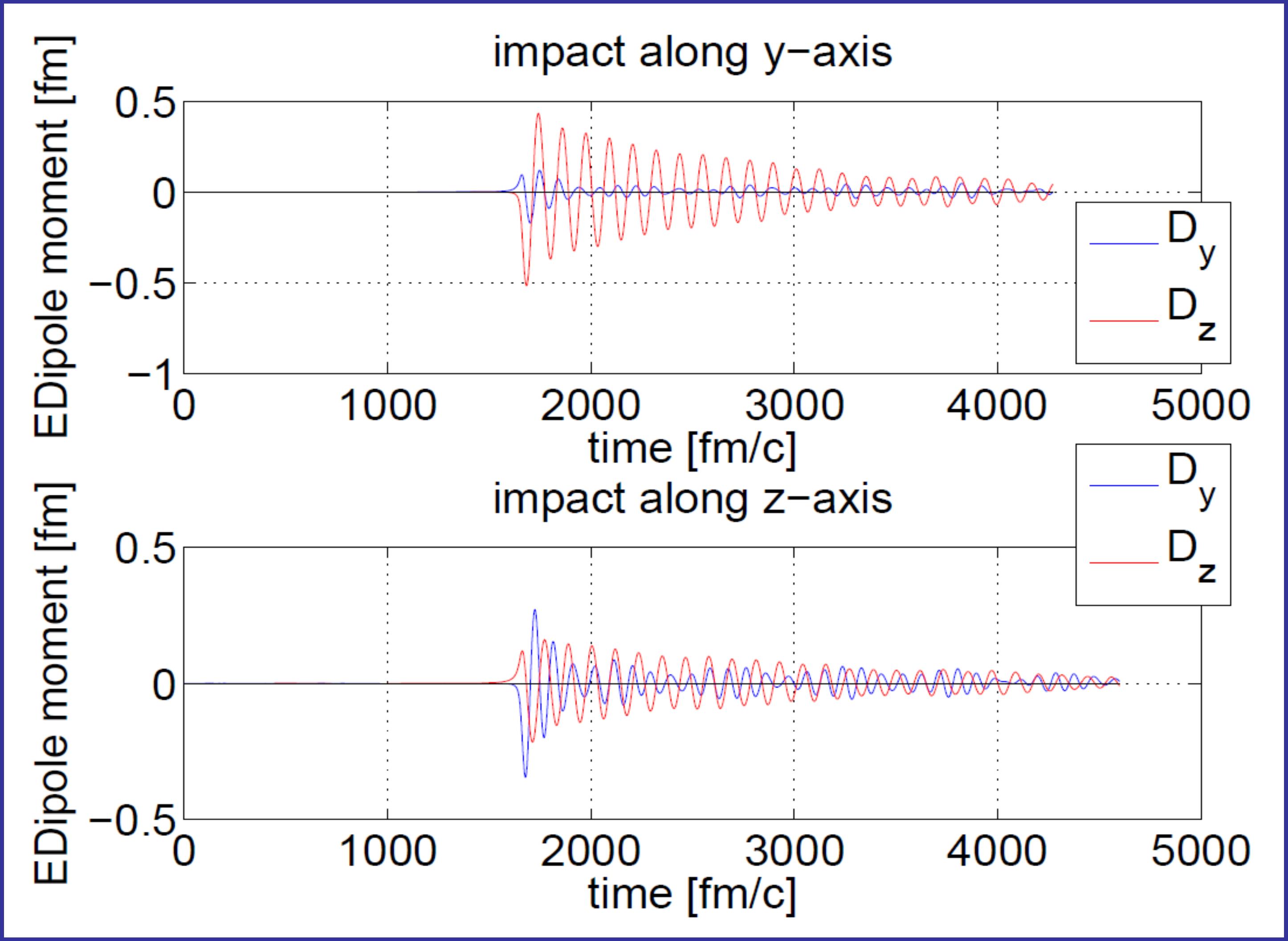
Number of protons in two shells surrounding nucleus:



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

Electromagnetic radiation from excited nucleus

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

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

From TDSLDA

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

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

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

Angular distribution of radiated power

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

Angular distribution and ferquency distribution of emitted radiation

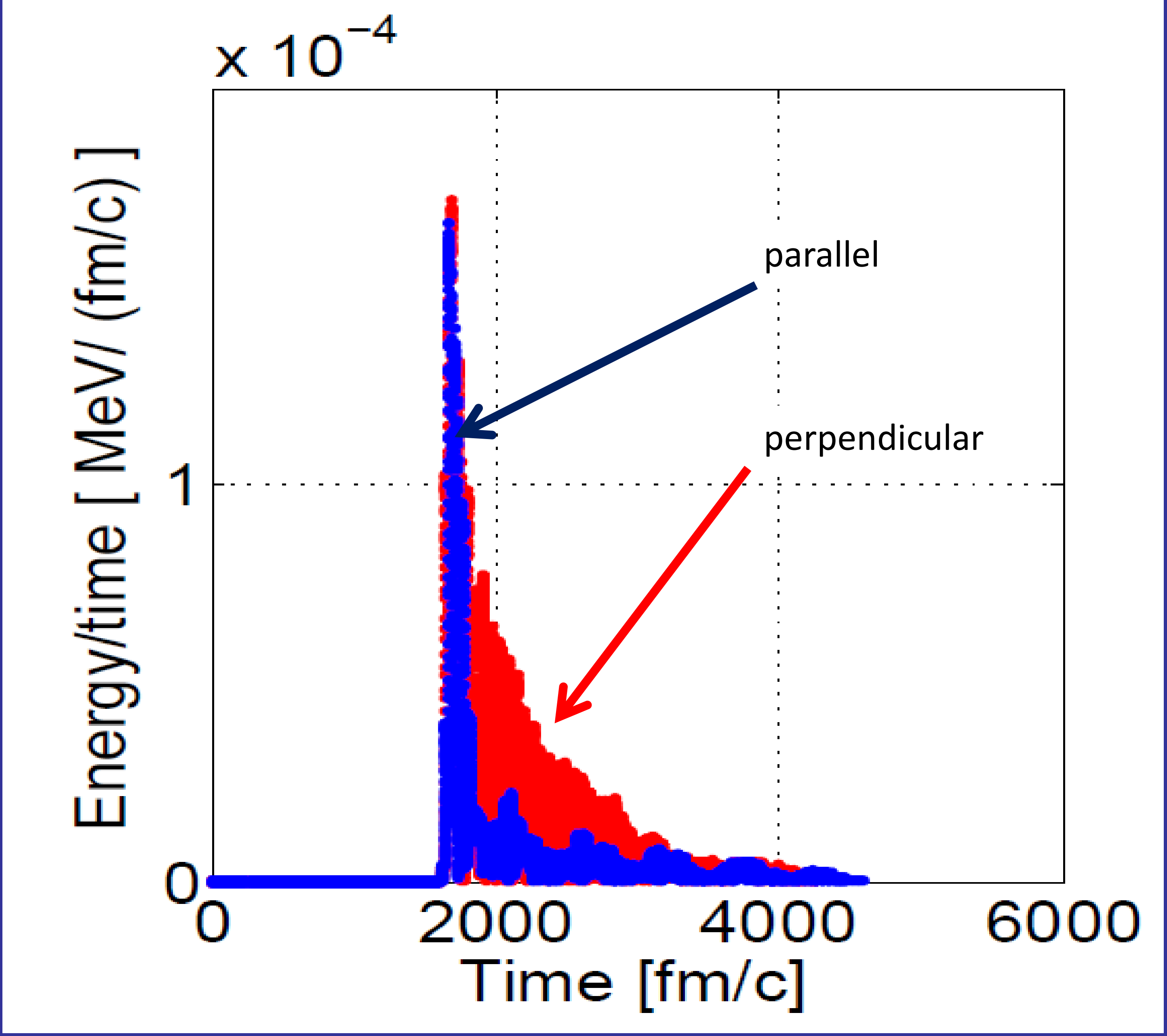
In practice it is better to perform multipole expansion:

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

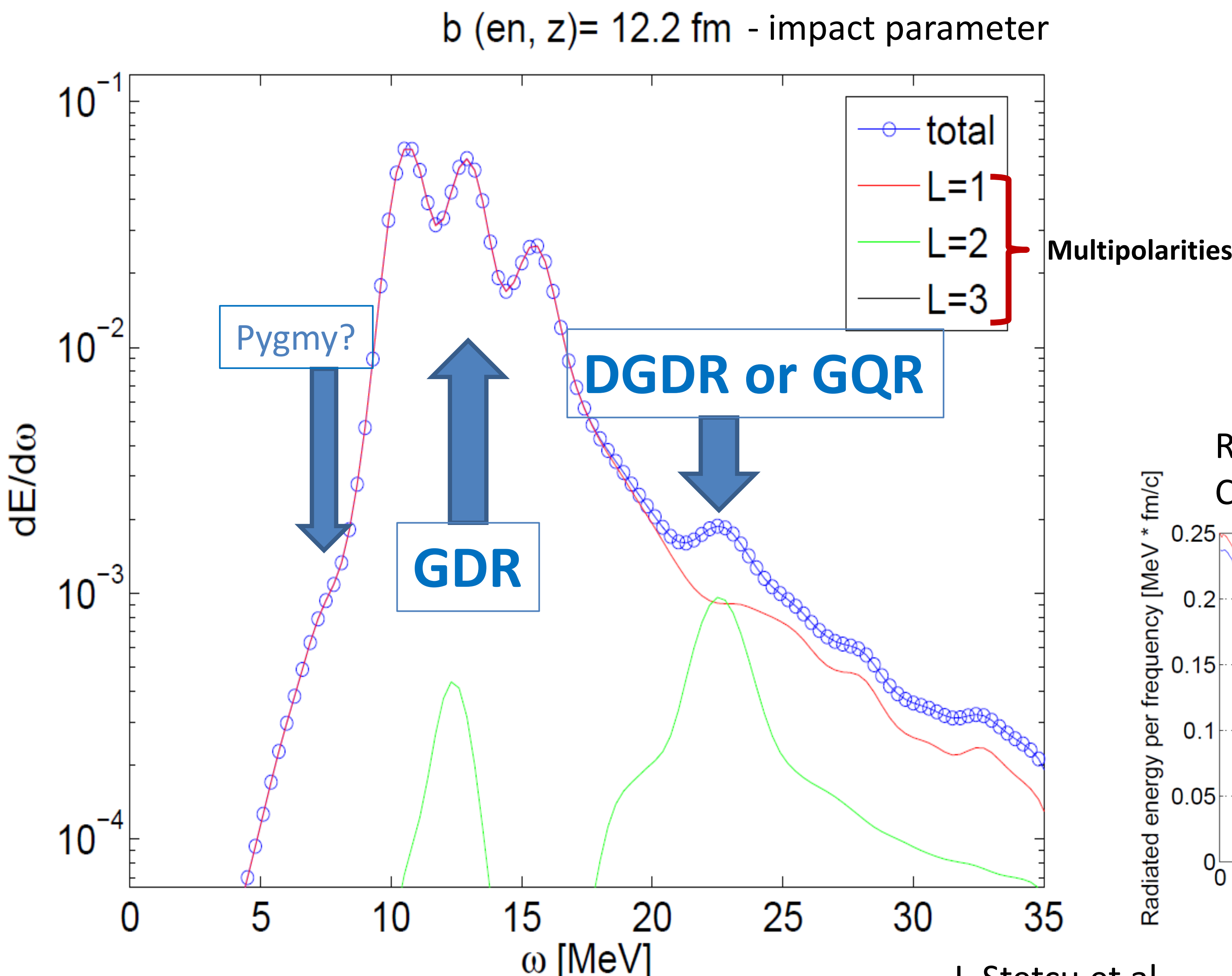
$$\vec{b}_{lm}(k,t) = \int d^3r\vec{b}(\mathrm{r},t)j_l(kr)Y^*_{lm}(\hat{r})$$

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

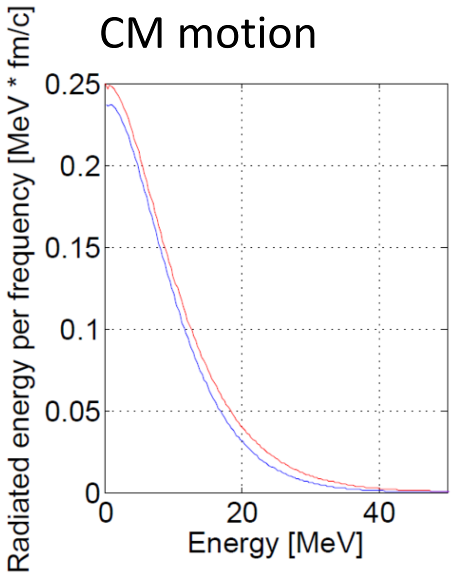
Electromagnetic radiation rate due to the internal motion



Electromagnetic radiation due to the internal nuclear motion



Radiation due to CM motion



I. Stetcu et al.

Summary

- ***TDSLDA is a flexible tool to study nuclear dynamics.***
- ***Pairing field is treated on the same footing like single particle potentais (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

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 steps