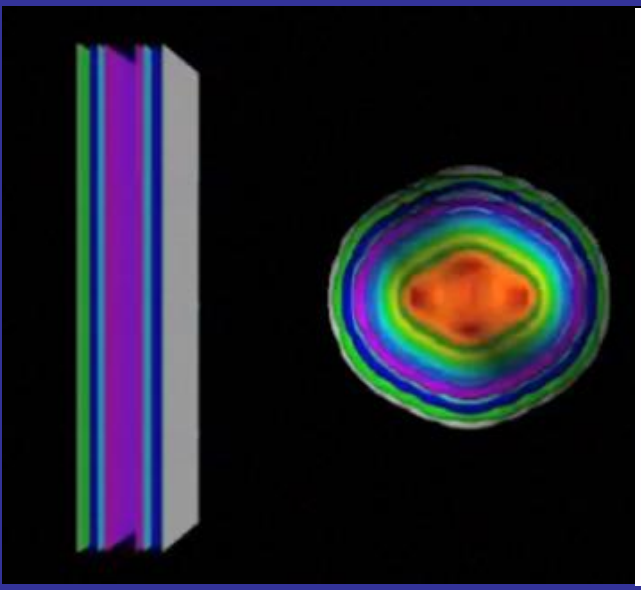
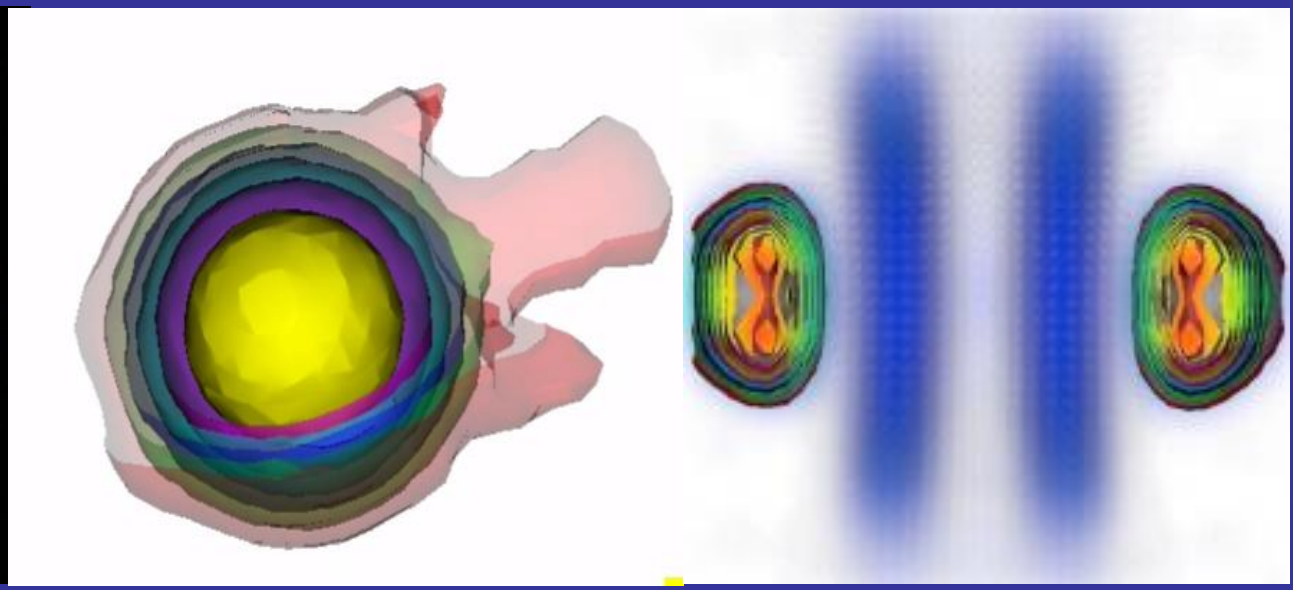
Nuclear Dynamics within Time Dependent Superfluid Local Density Approximation (TDSLDA)





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GOAL:

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

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: $\chi(\mathbf{r}) = \chi(\mathbf{r},\mathbf{r}')|_{r=r'}$

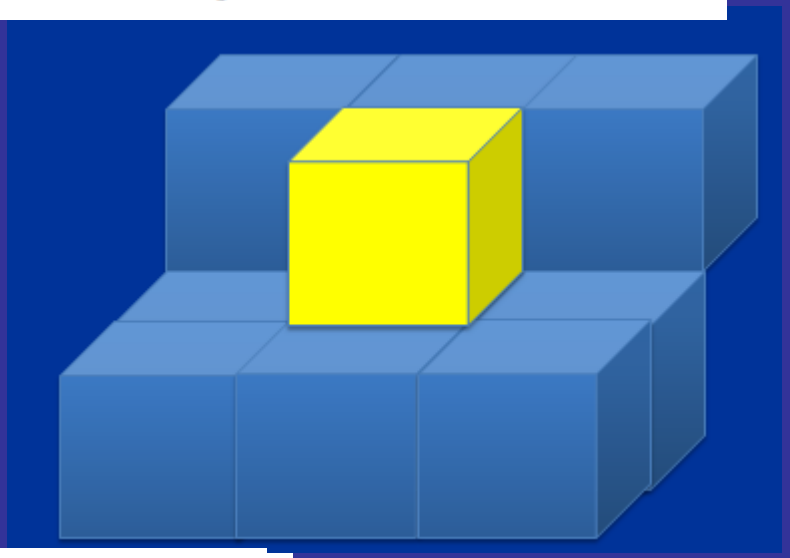
Treatment of the Coulomb potential

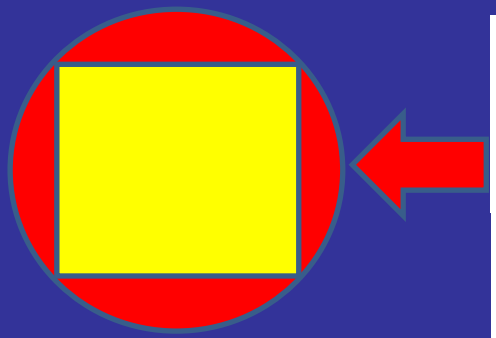
$$\nabla^2\Phi(\mathbf{r}) = 4\pi e^2\rho(\mathbf{r})$$

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

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

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:

$$27 \cdot N^3 LogN^3 < (3N)^3 Log(3N)^3$$

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:

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

- **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):

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

where

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

and pairing potential:

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

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.

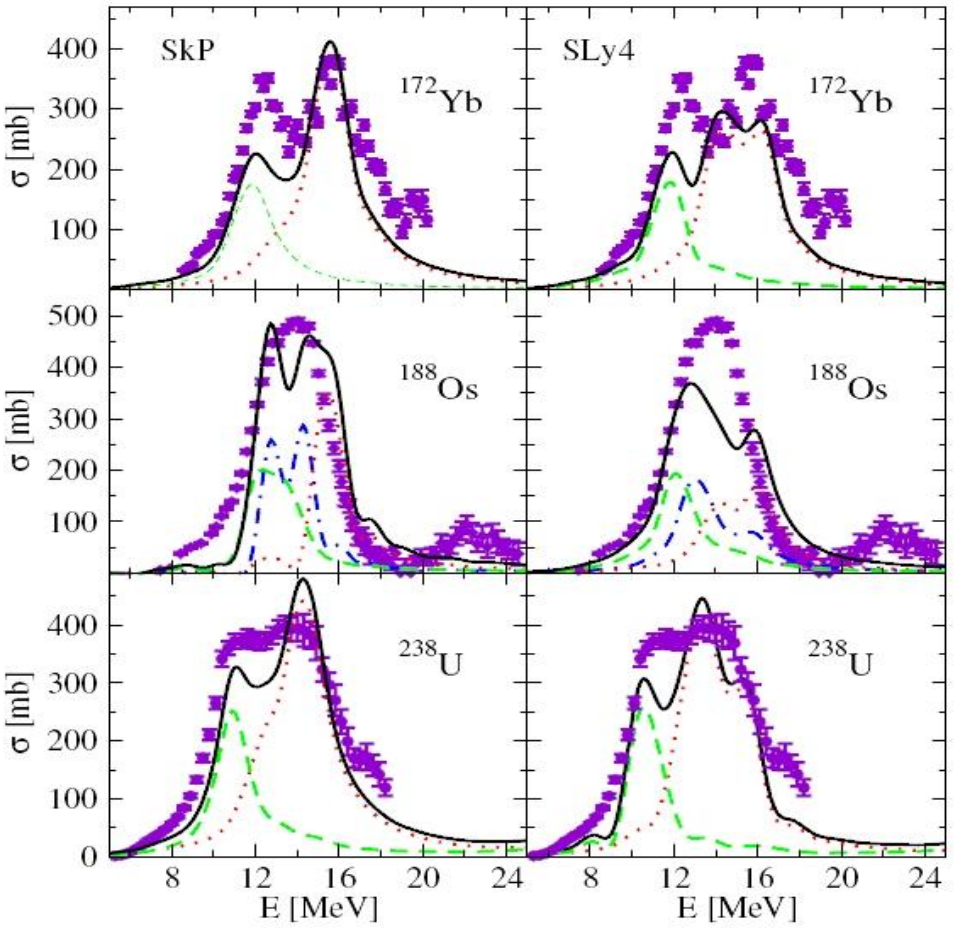
$$h_{\tau,\sigma\sigma}(\mathbf{r},t) \Rightarrow h_{\tau,\sigma\sigma}(\mathbf{r},t) + F_\tau(\mathbf{r}) f(t) \qquad F_\tau(\mathbf{r}) = N_\tau \sin(\mathbf{k}\cdot\mathbf{r}_\tau)/|\mathbf{k}|$$

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

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

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

(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

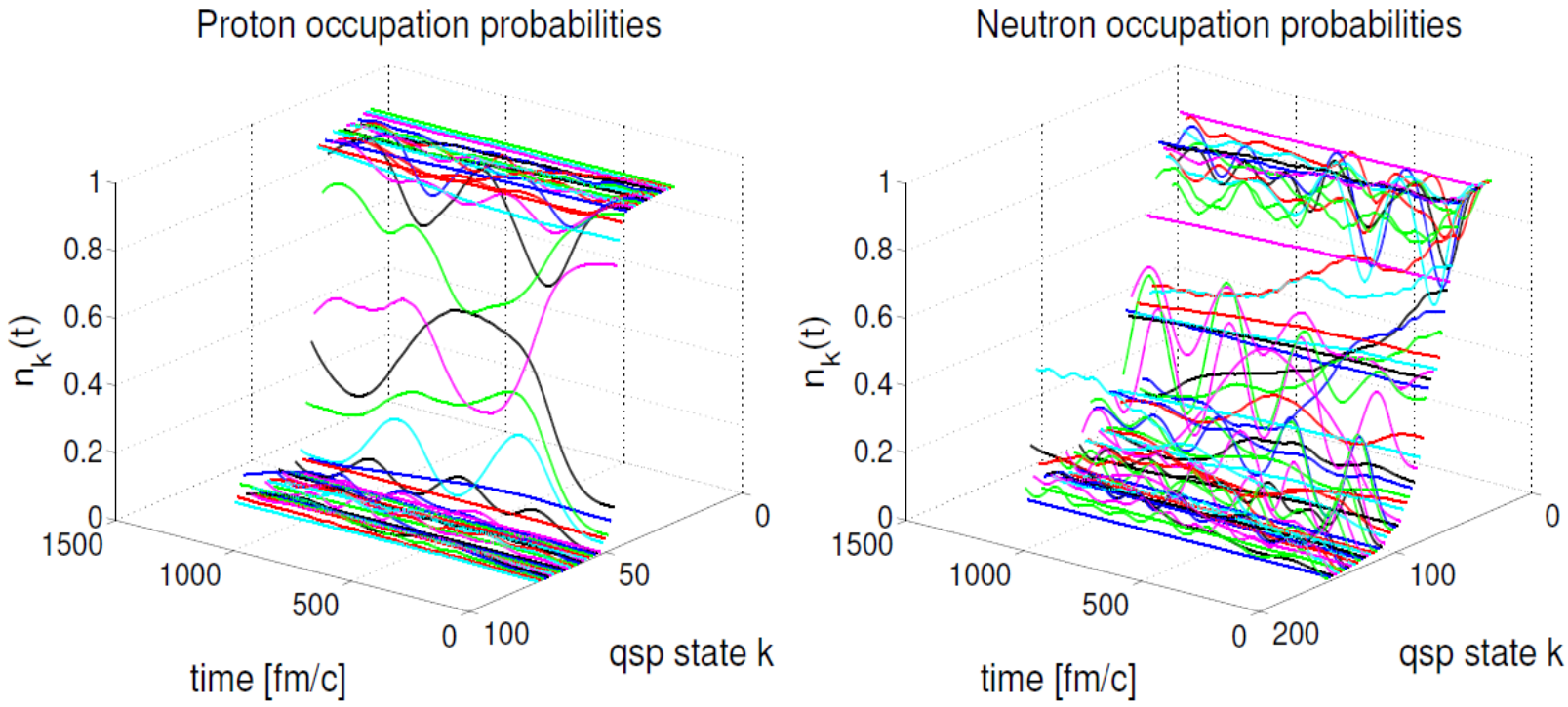


FIG. 1. (Color online) The time-dependent proton and neutron occupation probabilities of a a number of quasiparticle states around the Fermi level for ^{238}U calculated as described in the main text with SLy4.

Occupation probabilities vary significantly in time.

Pairing has to be treated fully selfconsistently!

Beyond linear regime:
Relativistic Coulomb excitation

Coupling to e.m. field:

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

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

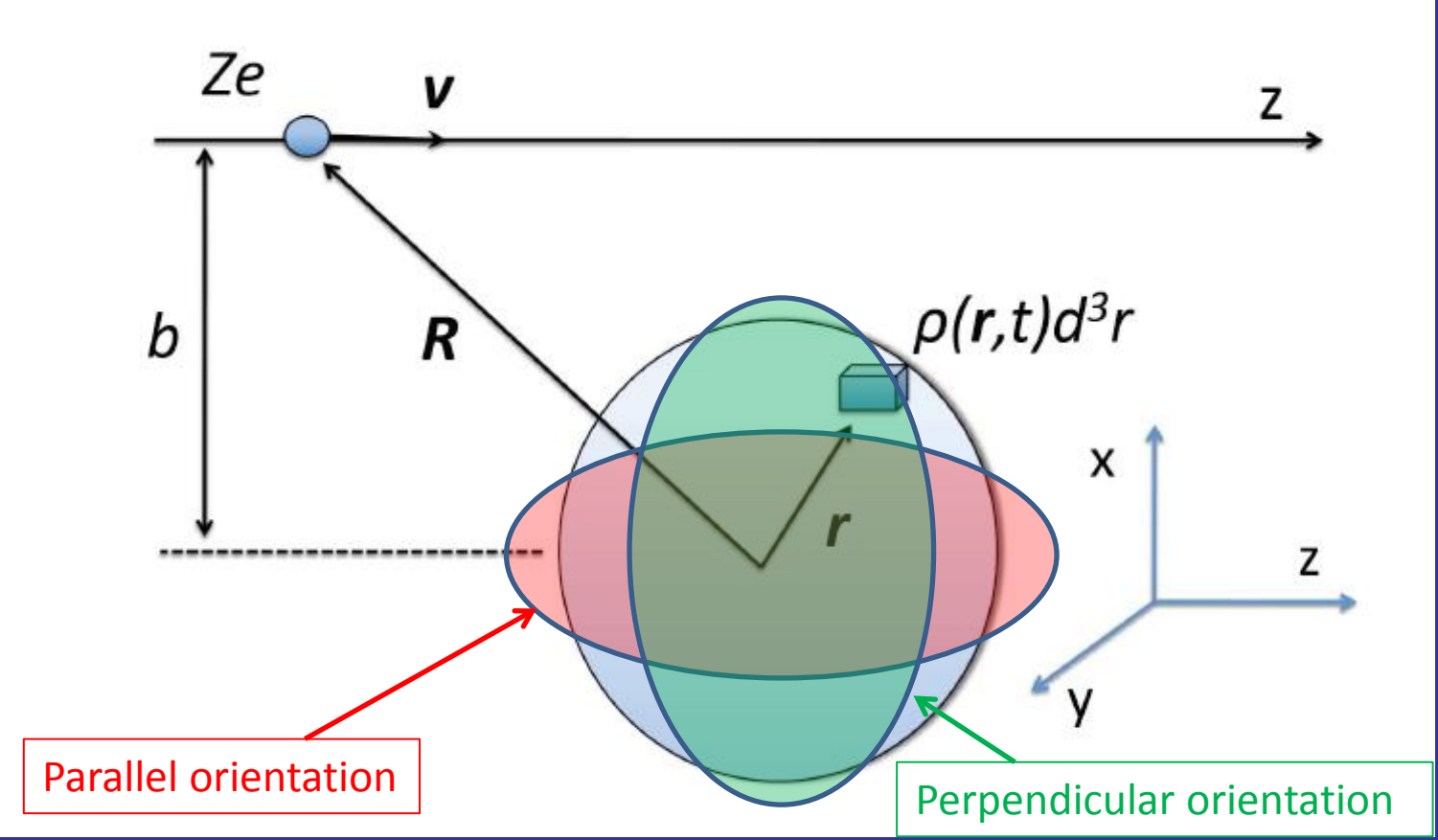
which implies that $\vec{\nabla}\psi\psi^* \to \vec{\nabla}\psi\psi^*$.

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

Relativistic Coulomb excitation

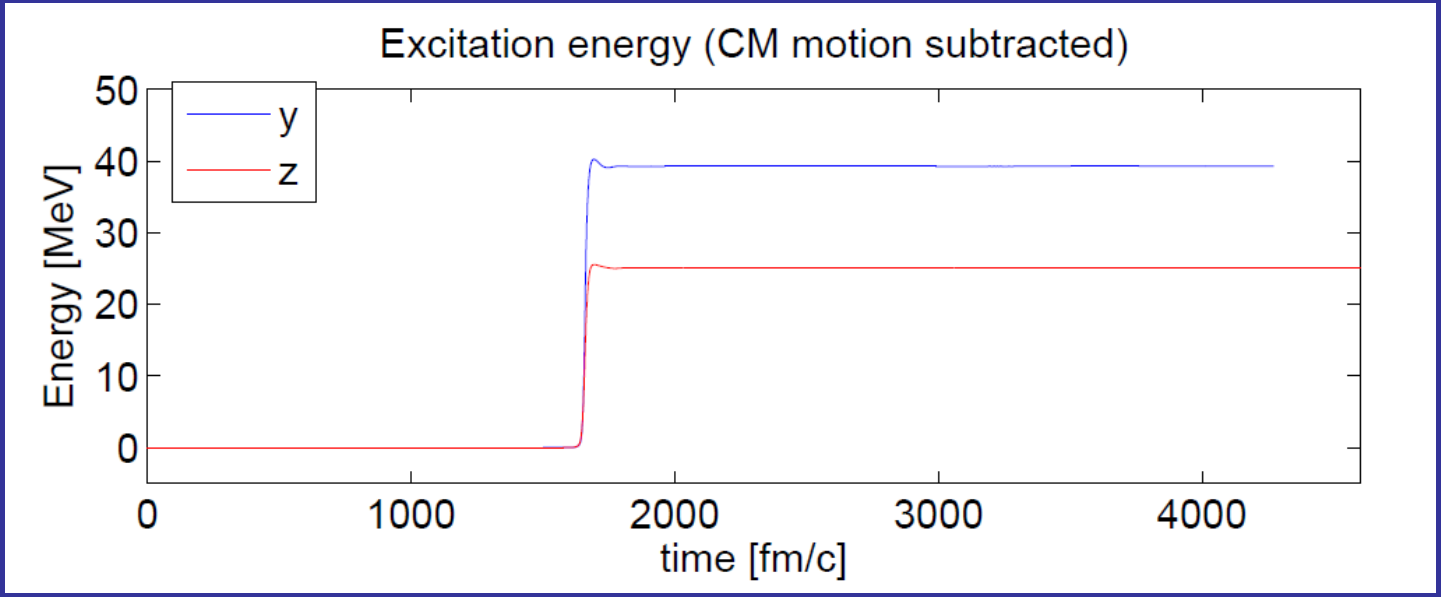
$$^{238}U + ^{238}U \rightarrow ^{238}U^{*} + \ldots \quad \text{at about 700 MeV/n}$$



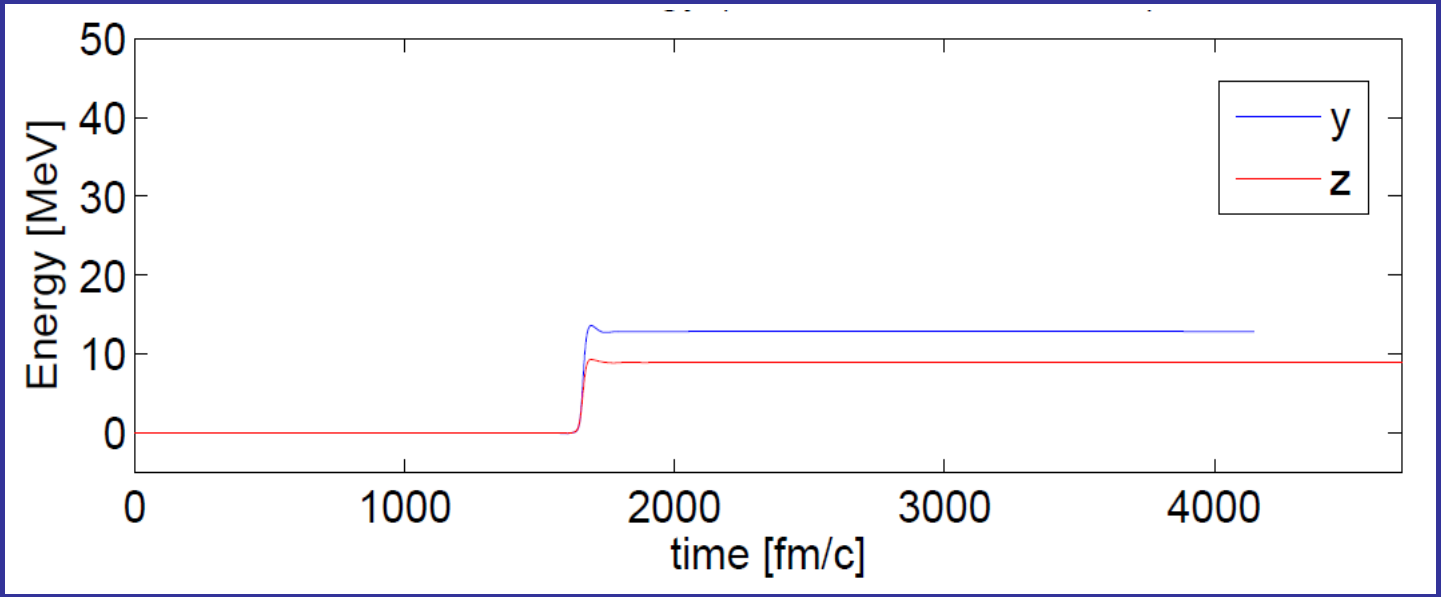
The coordinate transformation has been applied to keep CM in the center of the box at all times.

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

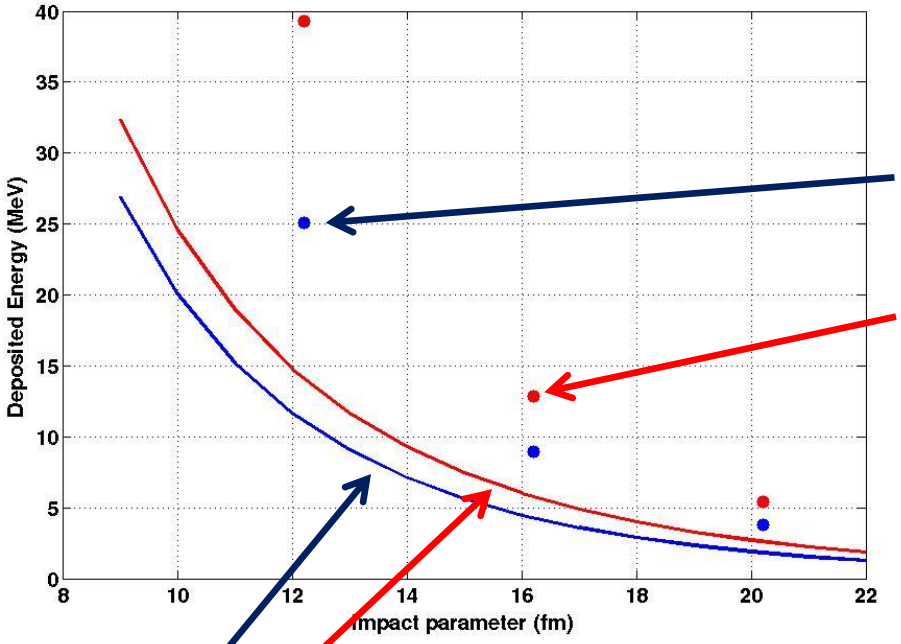
Impact parameter b=12.2fm



Impact parameter b=16.2fm



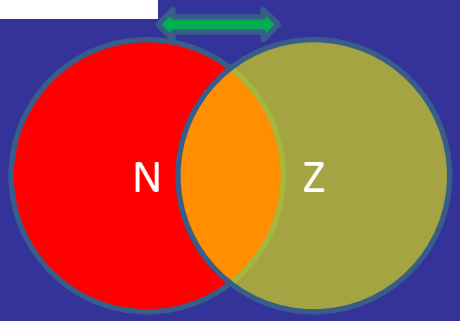
Energy transferred to the target nucleus in the form of internal excitations



TDSLDA – parallel orientation

TDSLDA – perpendicular orientation

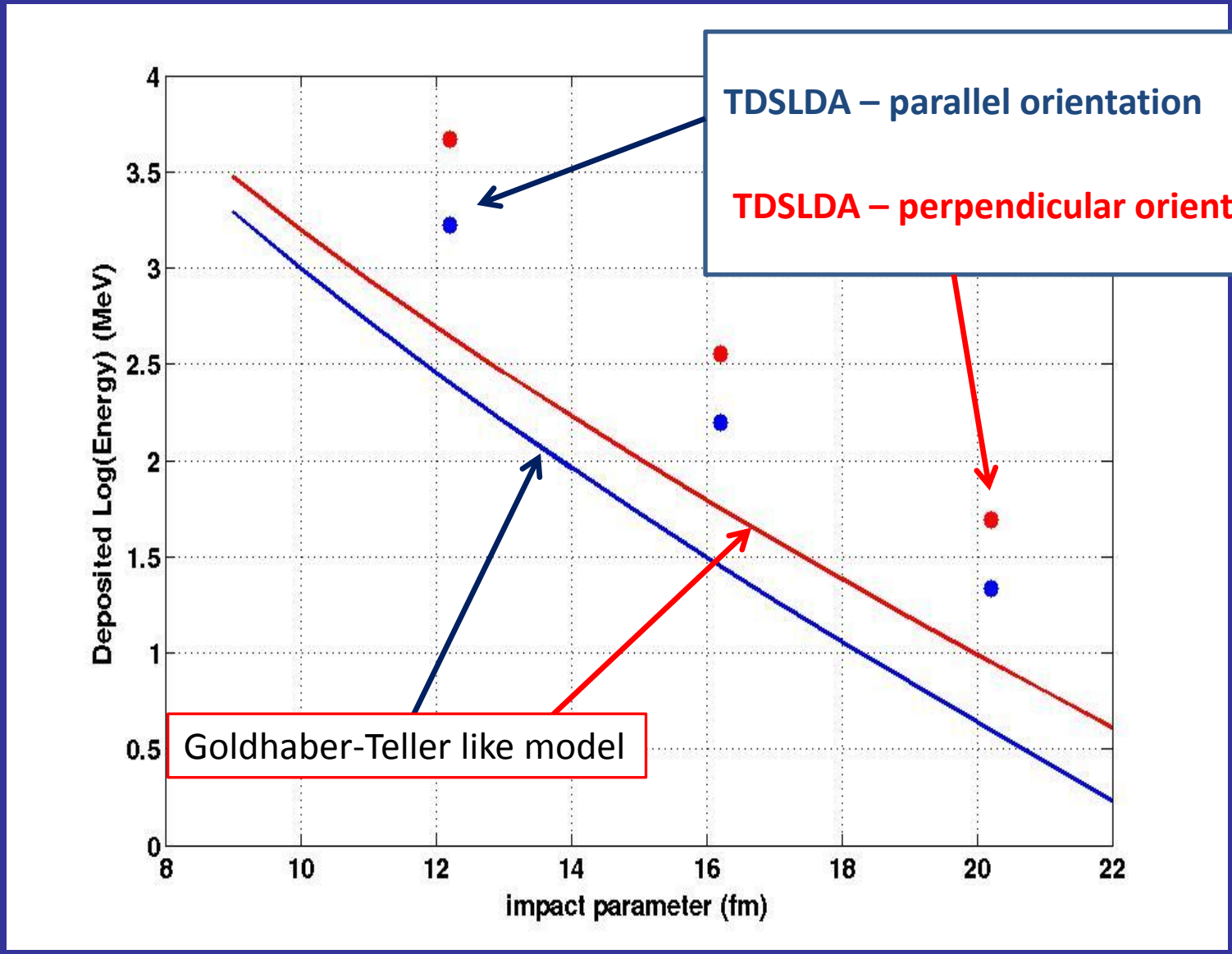
Goldhaber-Teller like model:
proton and neutron density distributions oscillating against each other



Two characteristic frequencies

$$\hbar\omega_1 = 12 MeV$$
$$\hbar\omega_2 = 16 MeV$$

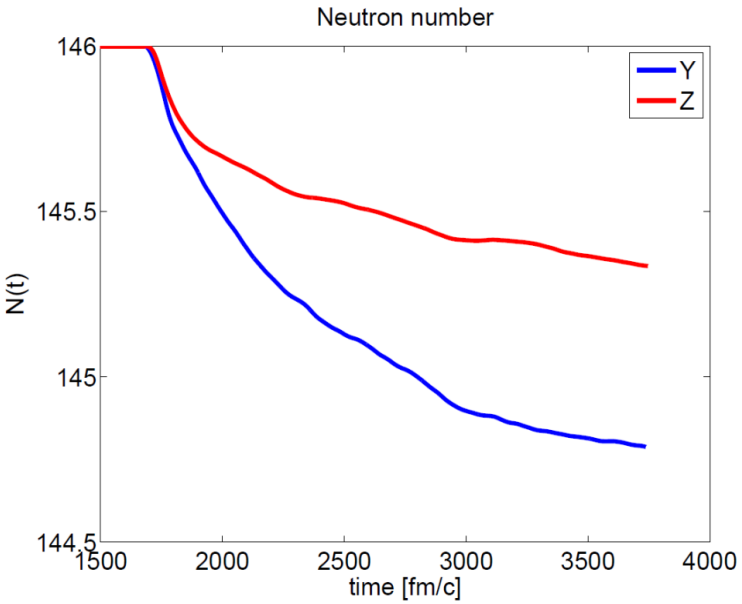
Part of the energy is transferred to other degrees of freedom than pure dipole moment oscillations.



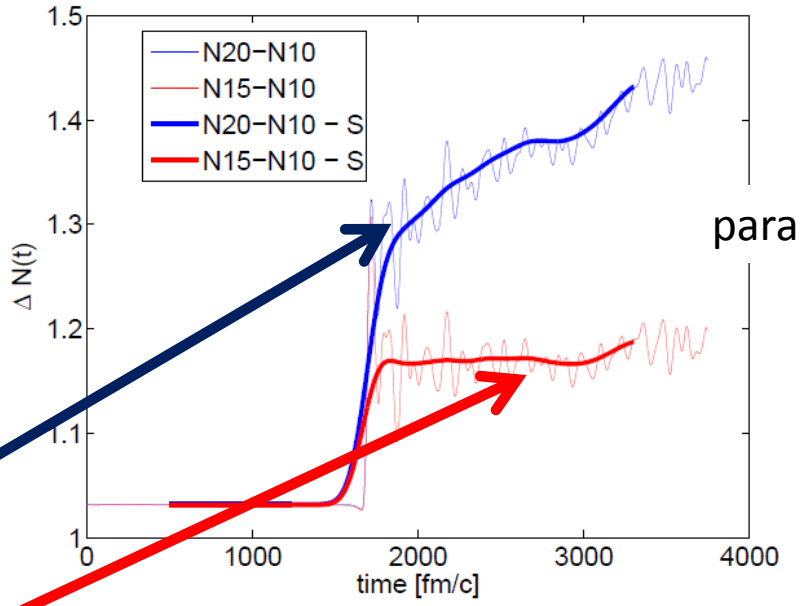
To get the same slope in GT model as in the corresponding TDSLDA results the frequencies of GDR should lie in the interval (10,18) MeV

Neutron emission

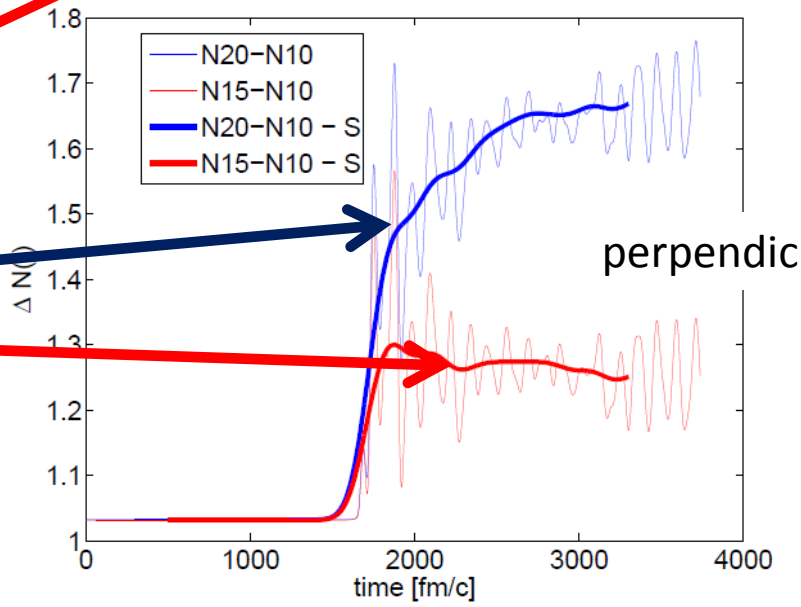
Impact parameter b=12.2fm



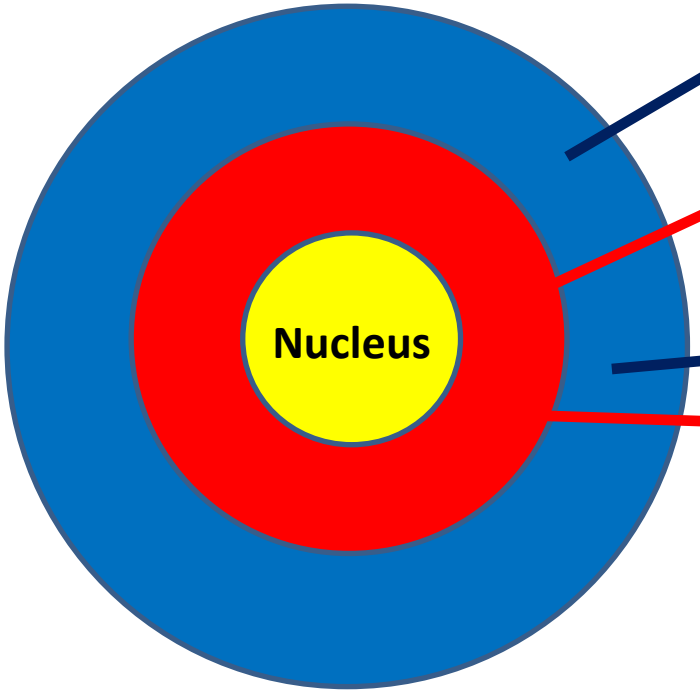
Number of neutrons in two shells surrounding nucleus for two nuclear orientations with respect to incoming projectile:



parallel

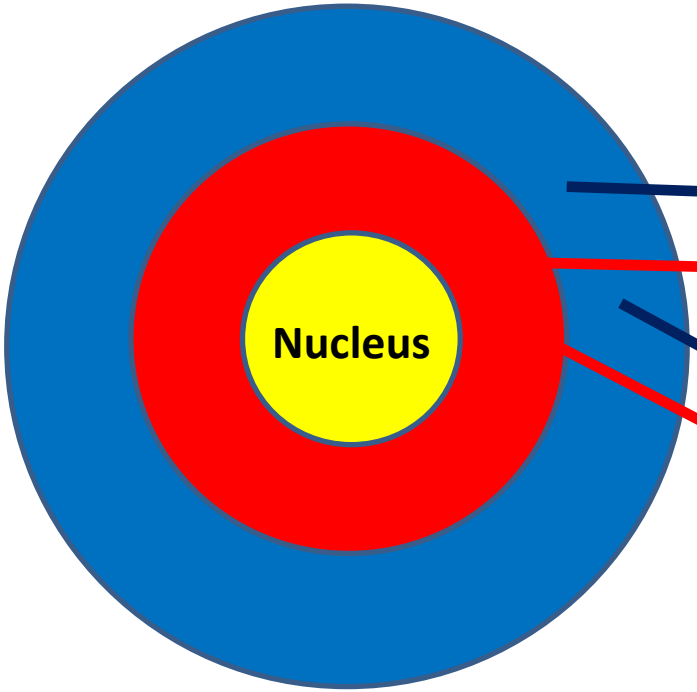


perpendicular

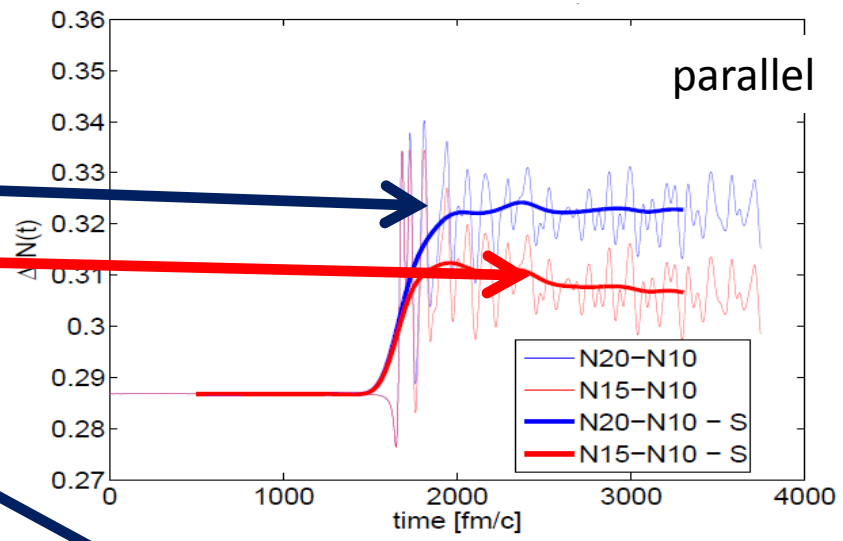


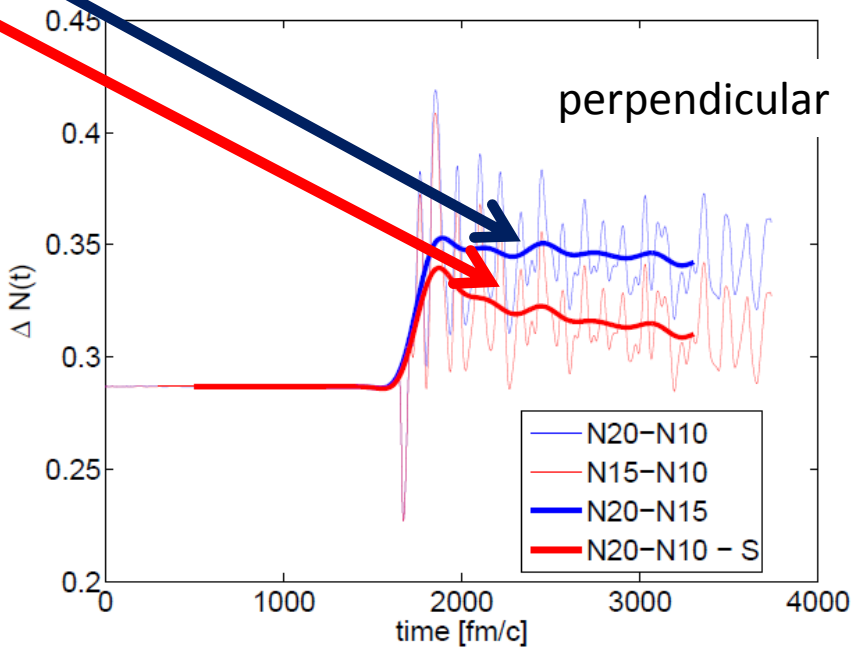
Protons

Impact parameter b=12.2fm



Number of protons in two shells surrounding nucleus:

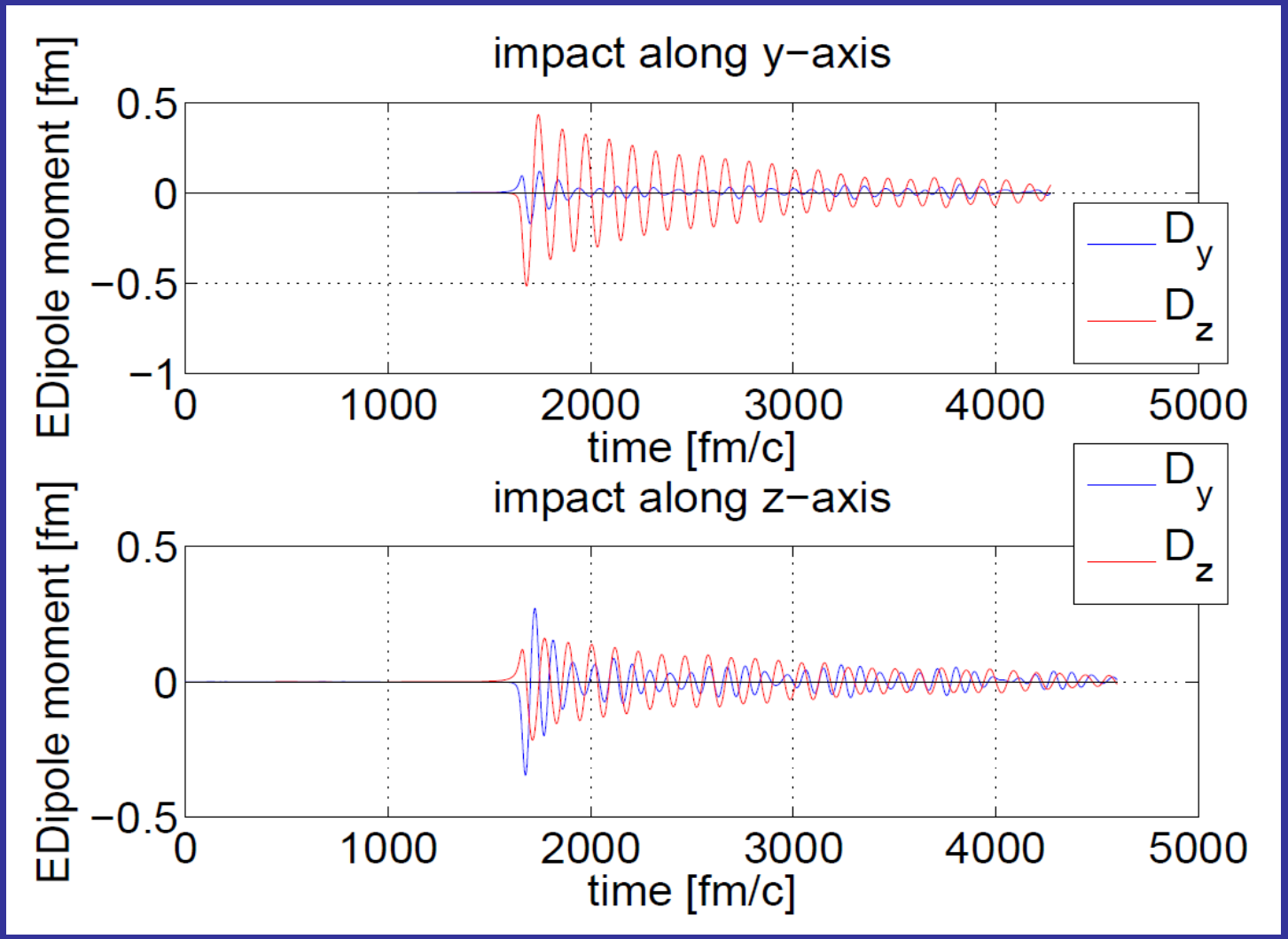




Contrary to protons, neutrons exhibit approximately steady flow out of nucleus

Internal nuclear excitations

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

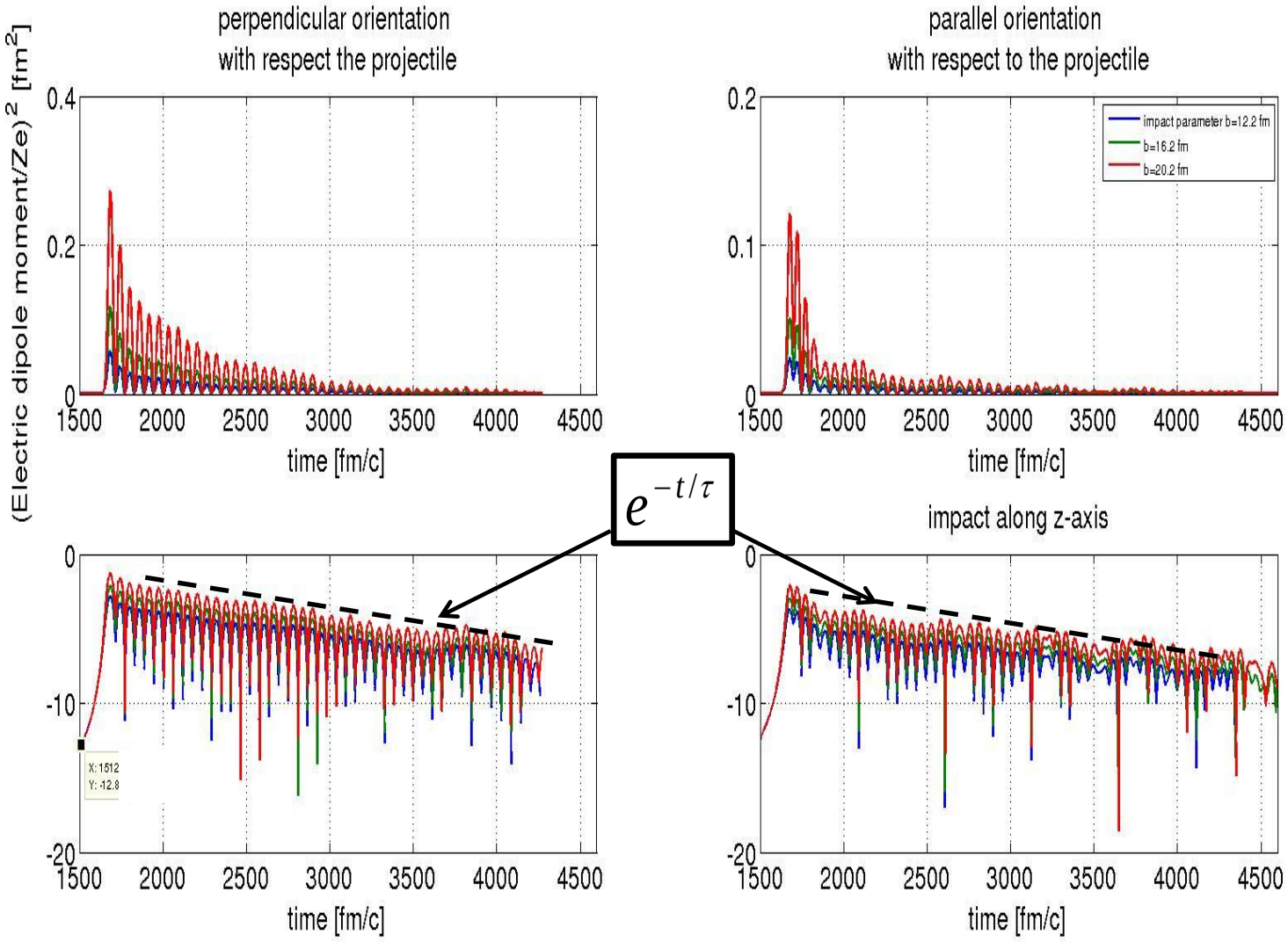


Oscillations are damped due to the one-body dissipation mechanism

One body dissipation

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

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



The rate of the dissipation weakly depends on the amplitude and approximately behaves like:

$$E_{coll}(t) \propto e^{-t/\tau}; \quad \tau \approx 500\, fm/c$$

From the wall formula (assuming classically chaotic single particle motion) :

$$\frac{d\langle v^n \rangle}{dt} = \frac{n(n+2)}{4}\langle v^{n-1} \rangle \frac{1}{V}\int \dot{n}^2 d\sigma$$

- Relation between velocity moments from F-P eq.

$$\langle v^n \rangle_0 = \frac{3}{n+3} v_F^n$$

$$\frac{\Delta E}{E_0} = \frac{\langle E \rangle - \langle E \rangle_0}{\langle E \rangle_0} = \frac{3}{4}\tilde{\beta}\eta\left[\omega t - \frac{1}{2}\sin(2\omega t)\right] + O(\eta^2)$$

- Wall formula

$\eta = \frac{\tilde{\beta}\omega R_0}{v_F}$ - Adiabaticity parameter for GDR: $\eta \approx 0.3$

$\tilde{\beta}$ - Deformation parameter

Note that wall formula does not predict exponential damping and it scales with the square of the oscillation amplitude.

Estimation of τ gives $250\, fm/c < \tau_{wall} < 500\, fm/c$

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:

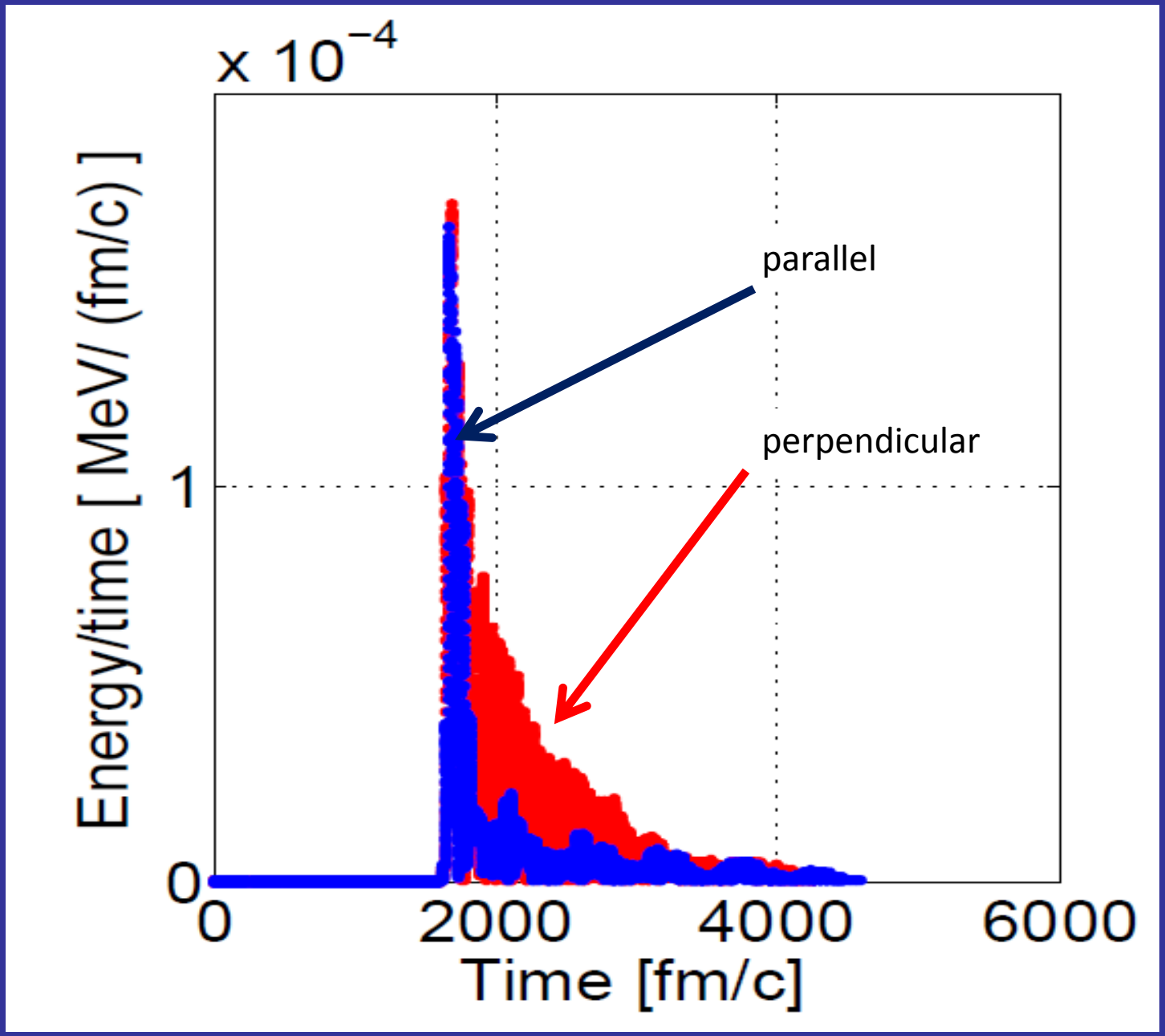
$$\frac{dE}{d\omega} = \frac{4e^2}{c}\sum_{l,m}|\vec{b}_{lm}(k,\omega)|^2$$

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

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

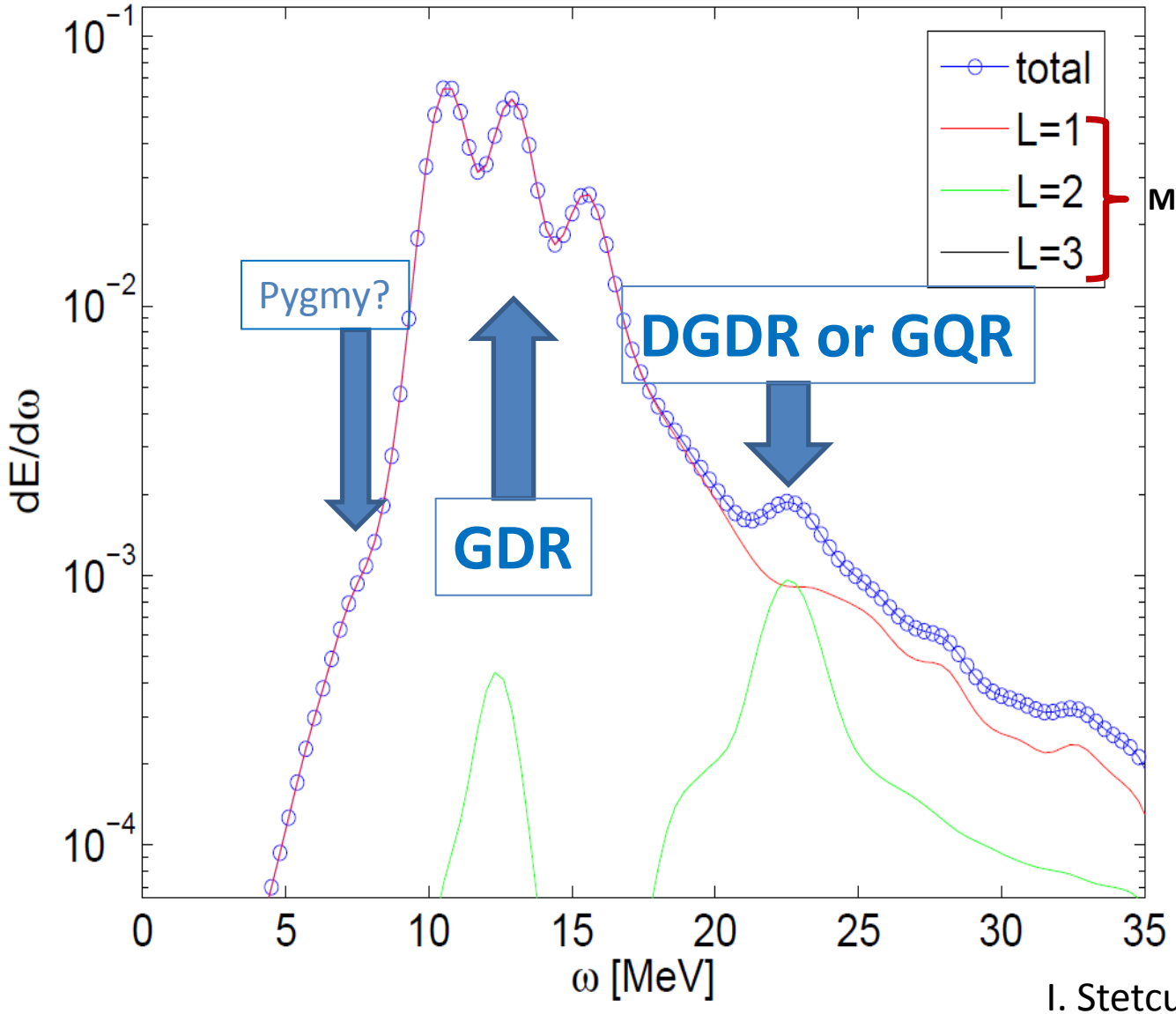
$$\vec{b}_{lm}(k,\omega) = \int_{-\infty}^{\infty}\vec{b}_{lm}(k,t)\exp(i\omega t)dt$$

Electromagnetic radiation rate due to the internal motion

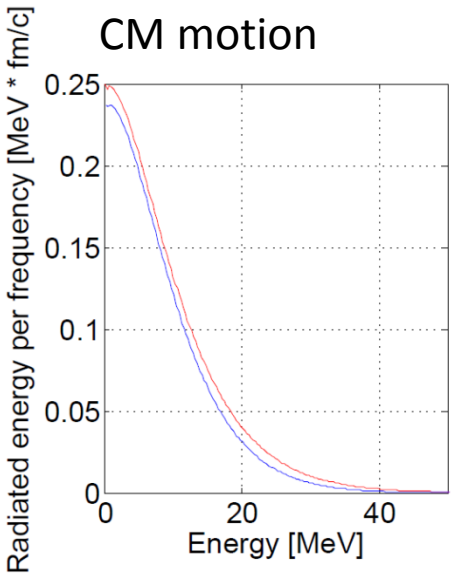


Electromagnetic radiation due to the internal nuclear motion

b (en, z)= 12.2 fm - impact parameter



Radiation due to CM motion



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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