# Exploring gamma strength through Time-dependent Hartree-Fock

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UNIVERSITY OF SURREY

## Overview

- Strength function
- The link to time-dependent Hartree–Fock
- The Sky3D code
- Examples:
    - Some GMR results in spherical nuclei
    - E1 strength / GDR / PDR
    - Pygmy in Se-76

# The strength function

## The link between the strength function and TDHF

Strength function for a one–body operator given by

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

Make Fourier representation of delta function

$$S(E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t \sum_{\nu} \left|\langle \nu|\hat{M}|0\rangle\right|^2 e^{i(E-E_\nu)t}.$$

Split integral over two parts, with infinitesimal convergence factors for contour integration:

$$S(E) = \frac{1}{2\pi}\sum_{\nu} \left|\langle \nu|\hat{M}|0\rangle\right|^2 \left(\int_{-\infty}^{0} \mathrm{d}t\, e^{i(E-E_\nu-i\delta)t} + \int_{0}^{\infty} \mathrm{d}t\, e^{i(E-E_\nu+i\delta)t}\right)$$

Perform integration to get:

$$S(E) = \frac{-i}{2\pi}\sum_{\nu} \left|\langle \nu|\hat{M}|0\rangle\right|^2 \left(\frac{1}{E-E_\nu-i\delta} - \frac{1}{E-E_\nu+i\delta}\right)$$

# The strength function

## The link between the strength function and TDHF

Can put the energy denominators inside matrix element:

$$S(E) = -\frac{i}{2\pi}\sum_{\nu}\langle 0|\hat{M}\left(\frac{1}{E-H-i\delta}-\frac{1}{E-H+i\delta}\right)|\nu\rangle\langle\nu|\hat{M}|0\rangle$$

Now can get rid of unit dyadic, leaving no explicit dependence on excited state

$$S(E) = \frac{i}{2\pi}\langle 0|\hat{M}\left(\frac{1}{H-E+i\delta}-\frac{1}{H-E-i\delta}\right)\hat{M}|0\rangle.$$

And use Dirac's formula to write this in a compact spectral representation as

$$S(E) \quad = \quad -\frac{1}{\pi}Im\langle 0|\hat{M}\frac{1}{H-E+i\delta}\hat{M}|0\rangle$$

Linear response theory gives this matrix element as equal to

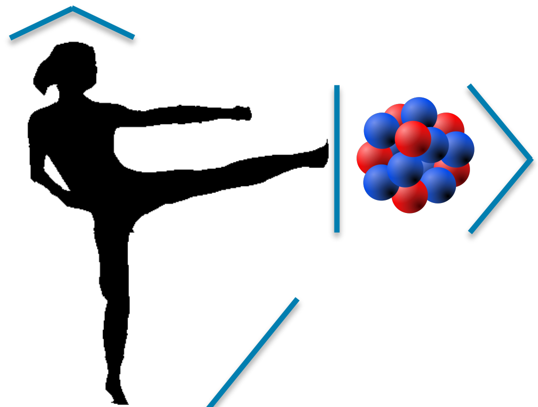
$$\int \mathrm{d}^3\mathrm{x}\, m(x)\frac{\delta\langle\rho(x,\omega)\rangle}{f(\omega)}$$

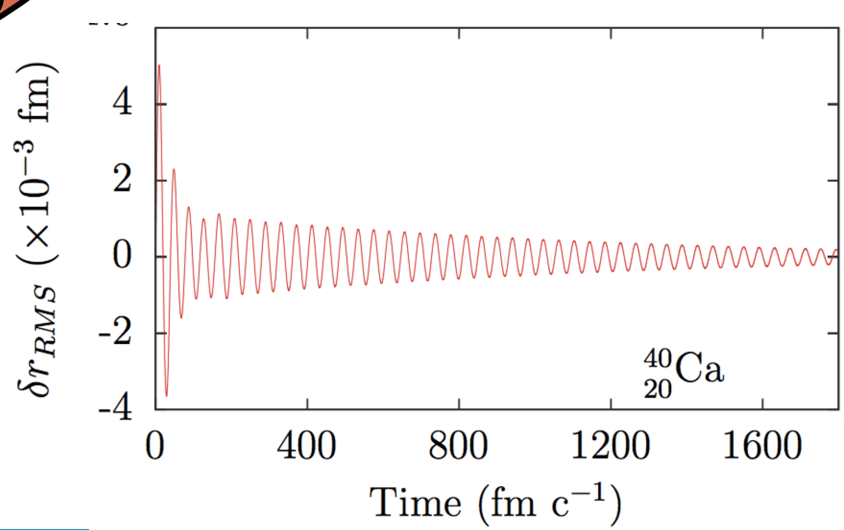
Fourier transform of time-dependent density fluctuations

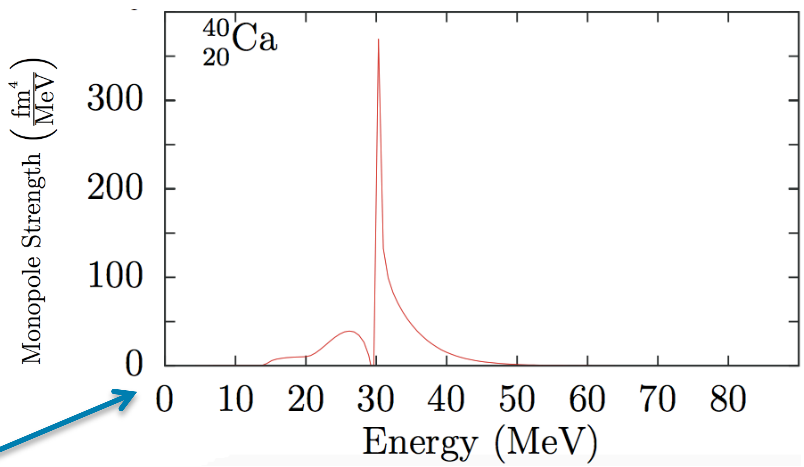
F-T of time profile of probing kick

# In practice for TDHF

(a very schematic guide)



# Sky3D code

An advertisment

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## The TDHF code Sky3D[☆]

CrossMark

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- Paper itself is open access
- Detailed subsidiary manual
- Code from CPC program library (or directly from me)

# Sky3d code

An advertisment

- Modern style Fortran (95/2003)
- Parallelized with OpenMP & MPI
- Very standard conforming – compiles anywhere (so far)

Sky3D-Code — bash — 80×27

bash

```
[~/codes/sky3d/Sky3D-Code] hare $ make
gfortran -O3  -c params.f90
gfortran -O3  -c forces.f90
gfortran -O3  -c grids.f90
gfortran -O3  -c fourier.f90
gfortran -O3  -c trivial.f90
gfortran -O3  -c levels.f90
gfortran -O3  -c densities.f90
gfortran -O3  -c sequential.f90
gfortran -O3  -c moment.f90
gfortran -O3  -c coulomb.f90
gfortran -O3  -c meanfield.f90
gfortran -O3  -c inout.f90
gfortran -O3  -c twobody.f90
gfortran -O3  -c fragments.f90
gfortran -O3  -c pairs.f90
gfortran -O3  -c energies.f90
gfortran -O3  -c static.f90
gfortran -O3  -c external.f90
gfortran -O3  -c dynamic.f90
gfortran -O3  -c user.f90
gfortran -O3  -c main3d.f90
gfortran -O3 -o sky3d.seq  params.o grids.o levels.o fourier.o forces.o sequenti
al.o inout.o coulomb.o trivial.o densities.o fragments.o twobody.o energies.o st
atic.o meanfield.o dynamic.o pairs.o moment.o main3d.o user.o external.o -lfftw3
 -llapack
[~/codes/sky3d/Sky3D-Code] hare $
```

Emacs@hare.local

New File | Open | Open Directory | Close | Save | Undo | Cut | Copy | Paste | Search

```fortran
MODULE Forces
  USE Params, ONLY: db,scratch,wflag, hbc, e2, pi
  IMPLICIT NONE
  SAVE
  ! Record defining pairing
  TYPE Pairing
     REAL(db) :: v0prot,v0neut,rho0pr
  END TYPE Pairing
  ! Record defining Skyrme force
  TYPE Force
     CHARACTER(8) :: name
     INTEGER :: ex,zpe
     REAL(db) :: h2m(2)
     REAL(db) :: t0,t1,t2,t3,t4
     REAL(db) :: x0,x1,x2,x3,b4p
     REAL(db) :: power
     TYPE(Pairing) :: vdi  ! volume-delta
     TYPE(Pairing) :: dddi ! density-dependent delta
  END TYPE Force
  ! include predefined forces
  INCLUDE 'forces.data'
  ! now the structure used in the run itself
  INTEGER :: ipair
  TYPE(Force) :: f          ! force actually used
  TYPE(Pairing) :: p        !pairing parameters actually used
  ! charge and mass number in static case for pairing
  REAL(db) :: h2ma ! average h2m over p and n, used in some places
  REAL(db) :: nucleon_mass
  ! derived "b" and Slater coefficients
  REAL(db) :: b0,b0p,b1,b1p,b2,b2p,b3,b3p,b4,b4p,slate
CONTAINS
  SUBROUTINE read_force
    CHARACTER(8) :: name,pairing
```

# Continuum-TDHF

(an aside)

PHYSICAL REVIEW E **89**, 033312 (2014)

**Extension of the continuum time-dependent Hartree-Fock method to proton states**

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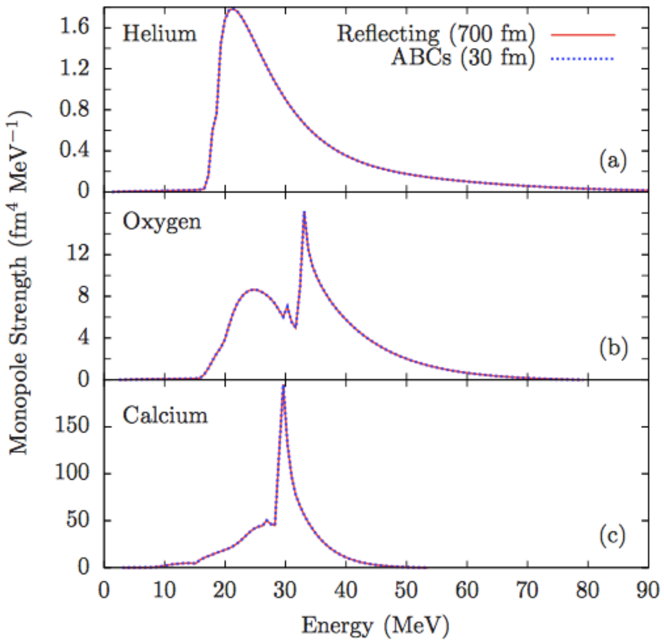
K. Xu[‡]
*Mathematical Institute, University of Oxford, Oxford, Oxfordshire OX1 3LB, United Kingdom*
(Received 19 June 2013; published 31 March 2014)




- Laplace transformation technique
- So far limited to spherical symmetry

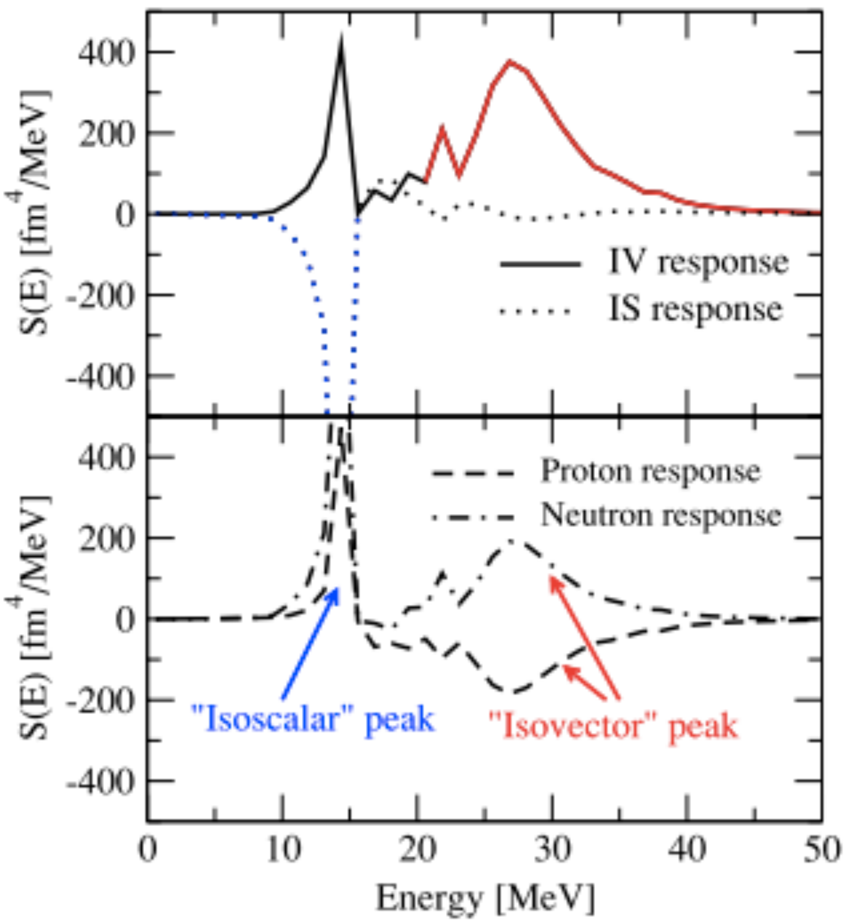
$$Q(R,t) = \int_0^t G_{\kappa,\mu}(R,\tau) \left.\frac{\partial Q(r,t-\tau)}{\partial r}\right|_{r=R} d\tau,$$

where

$$\hat{G}_{\kappa,\mu}(R,s) = \frac{1}{b\sqrt{s}} \left.\left( \frac{W_{\kappa,\mu}(br\sqrt{s})}{\frac{\partial W_{\kappa,\mu}(br\sqrt{s})}{\partial r}} \right)\right|_{r=R}.$$

# A few selected results

Mixed strength functions




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

F and F-bar different operators – can learn about individual matrix elements

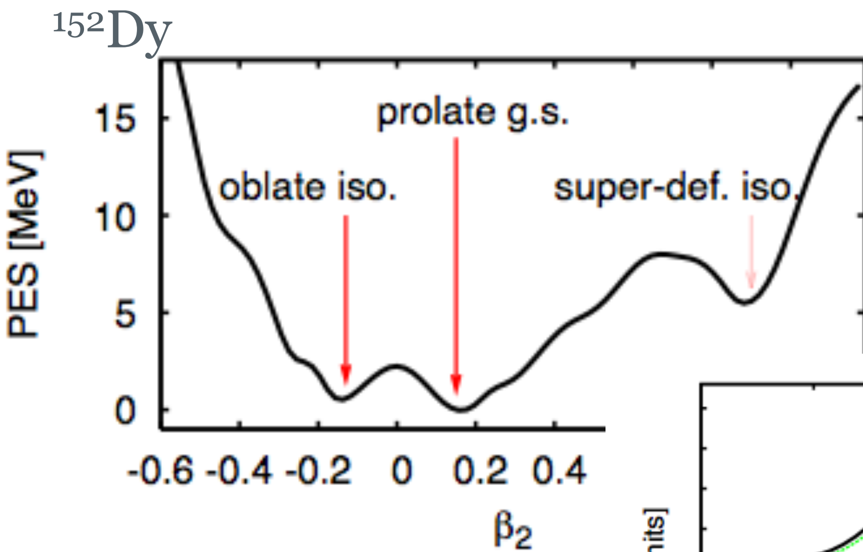
Identify normal modes

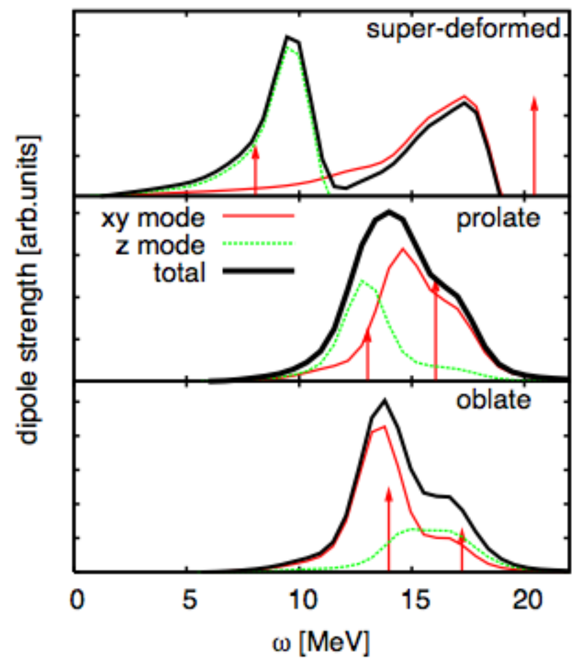
Calculations is $^{208}$Pb monopole resonances with SkO Skyrme force

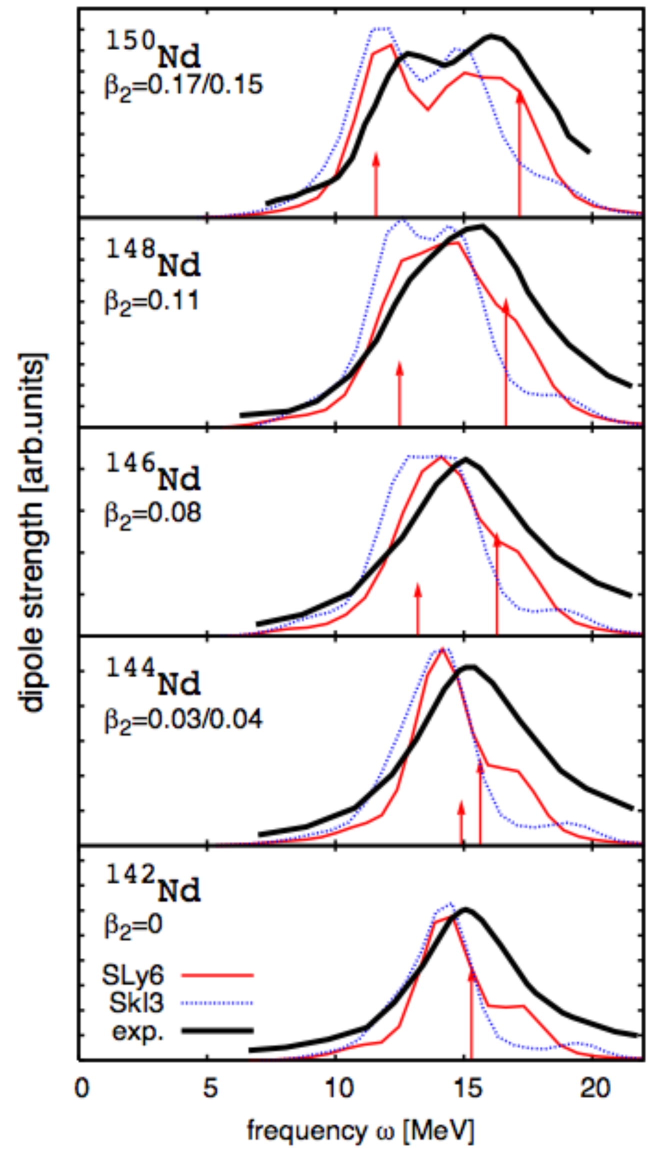
D. Almehed and P. D. Stevenson, J. Phys. G 31, S1819 (2005)

# E1 strength

Deformation splitting // GDR on excited states



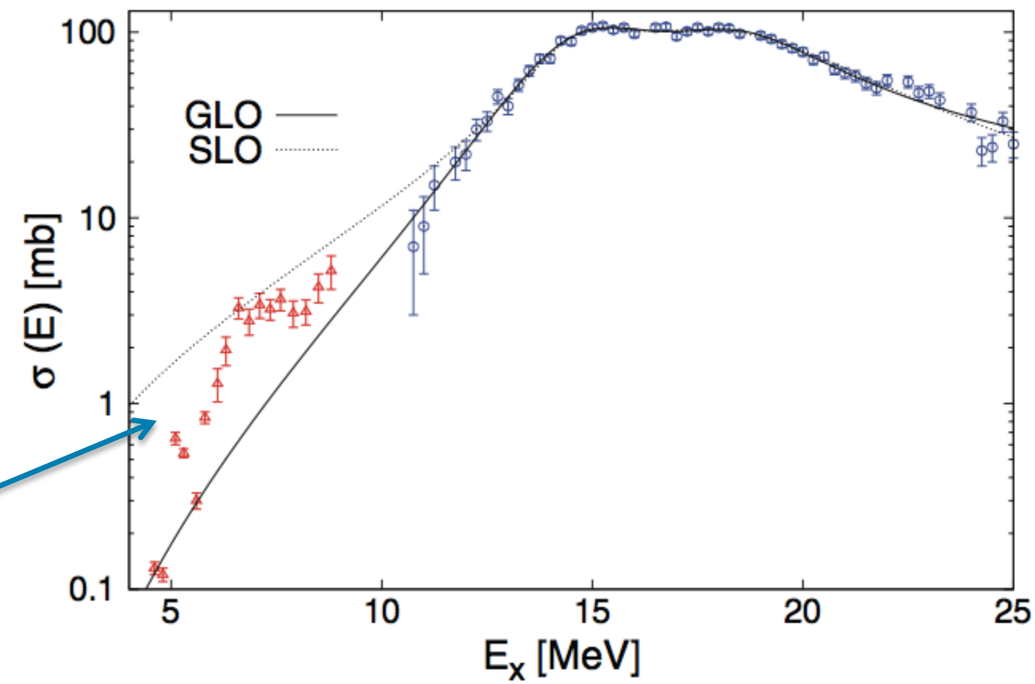




“numerical” width given by end time of simulation ~2MeV in this case

# $^{76}$Se @ HIγS

## NRF Technique

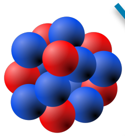

Red triangles: P. M. Goddard, N. Cooper, V. Werner, G. Rusev, P. D. Stevenson. A. Rios, C. Bernards, A. Chakraborty, B. P. Crider, J. Glorius, R. S. Ilieva, J. H. Kelley, E. Kwan, E. E. Peters, N. Pietrella, R. Raut, C. Romig, D. Savran, L. Schnorrenberger, M. K. Smith, K. Sonnabend, A. P. Tonchev, W. Tornow and S. W. Yates, Phys. Rev. C 88, 064308 (2013)

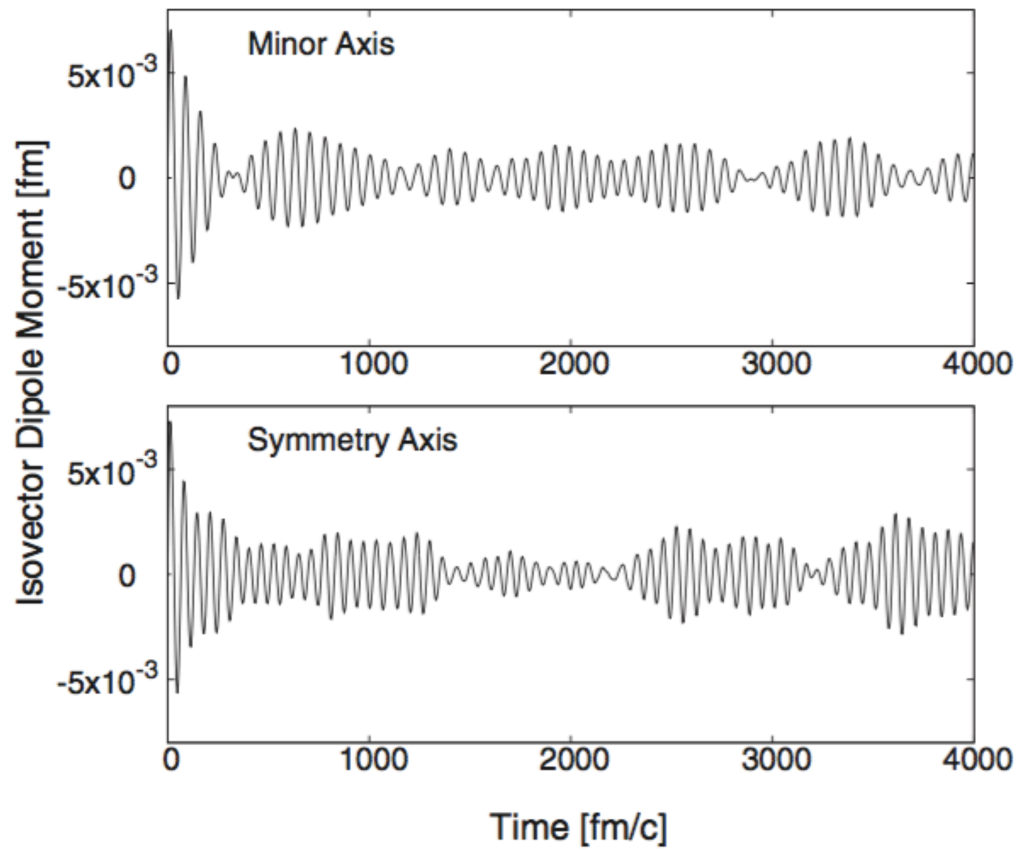
Above threshold data: P. Carlos, H. Beil, R. Bergre, J. Fagot, A Leprêtre, A. Veyssière and G. Solodukhov, Nucl. Phys. A **258**, 365 (1976)

# TDHF in $^{76}$Se

1. Applying a regular E1 dipole kick

$$\hat{\mathbf{D}} = \frac{N}{A}\sum_{p=1}^{Z}\mathbf{r}_p - \frac{Z}{A}\sum_{n=1}^{N}\mathbf{r}_n,$$

$e^{i\mathbf{k}\cdot\hat{\mathbf{D}}}$ |  ⟩

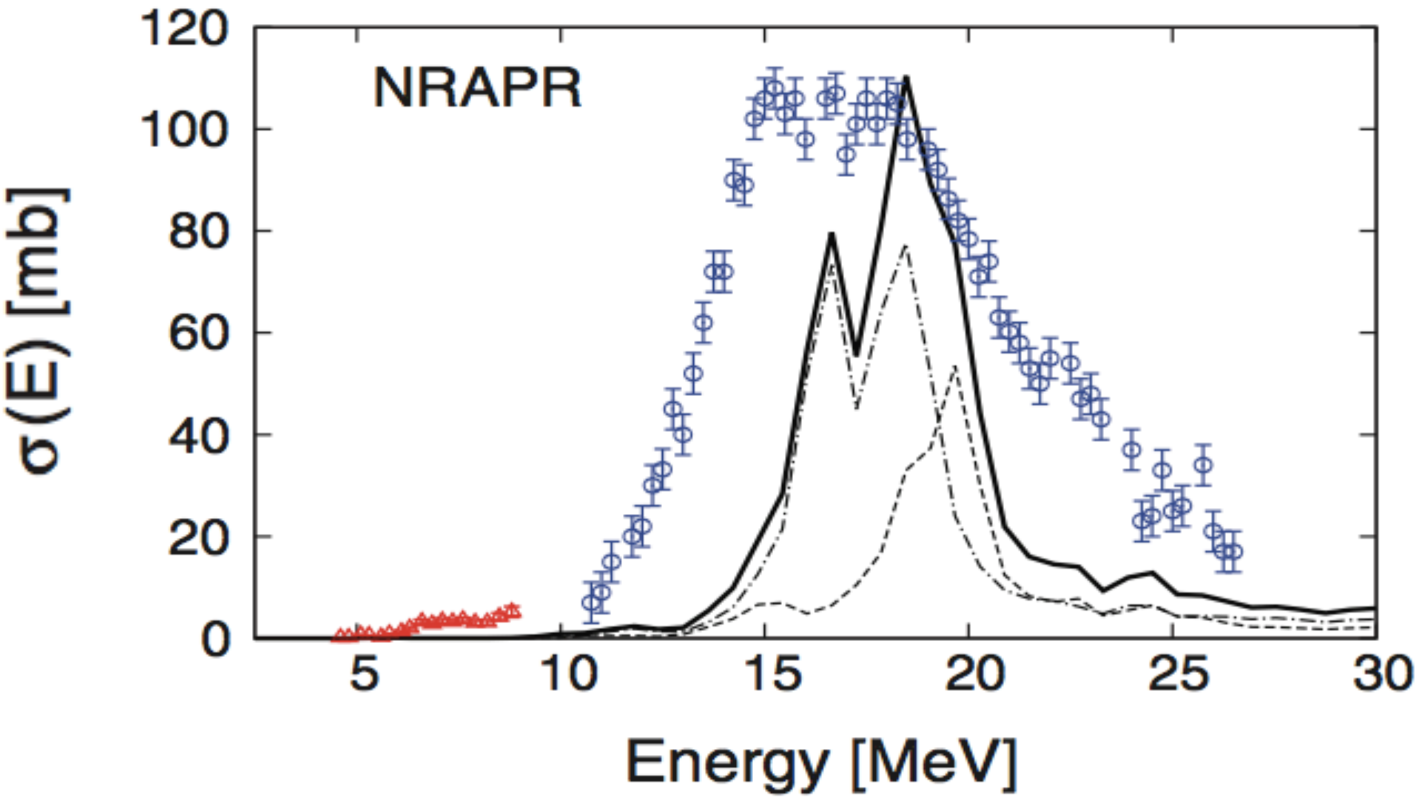



We used Skyrme forces that passed stringent tests for IS and IV nuclear matter properties – M. Dutra, O. Lourenço, J. S. Sá. Martins, A. Delfino, J. R. Stone and P. D. Stevenson, *Phys. Rev.* **C 85**, 035201 (2012)

Time-dependent response to dipole kick. Skyrme force NRAPR from A. Steiner, M. Prakash, J. Lattimer and P. Ellis, Phys. Rep. **411**, 325 (2005)

# Response in 76Se

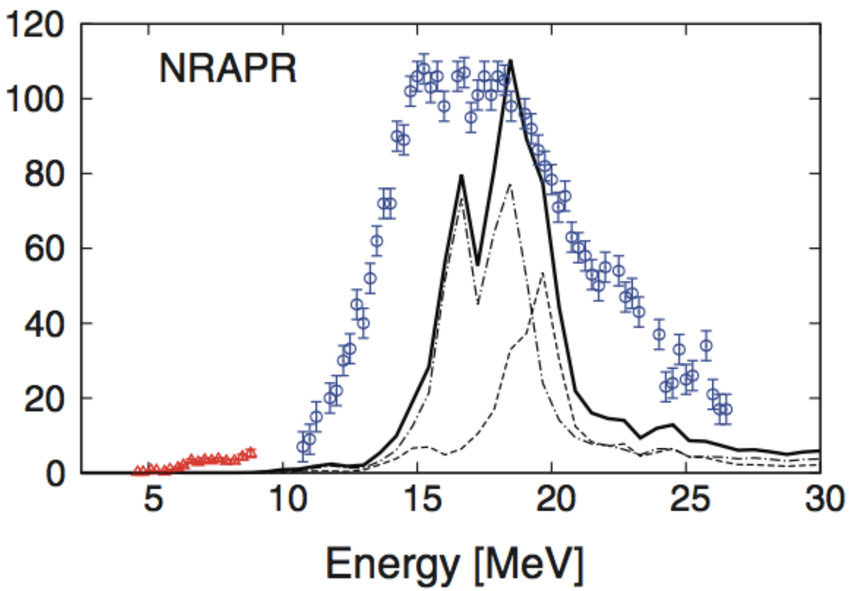
Using NRAPR Skyrme interaction

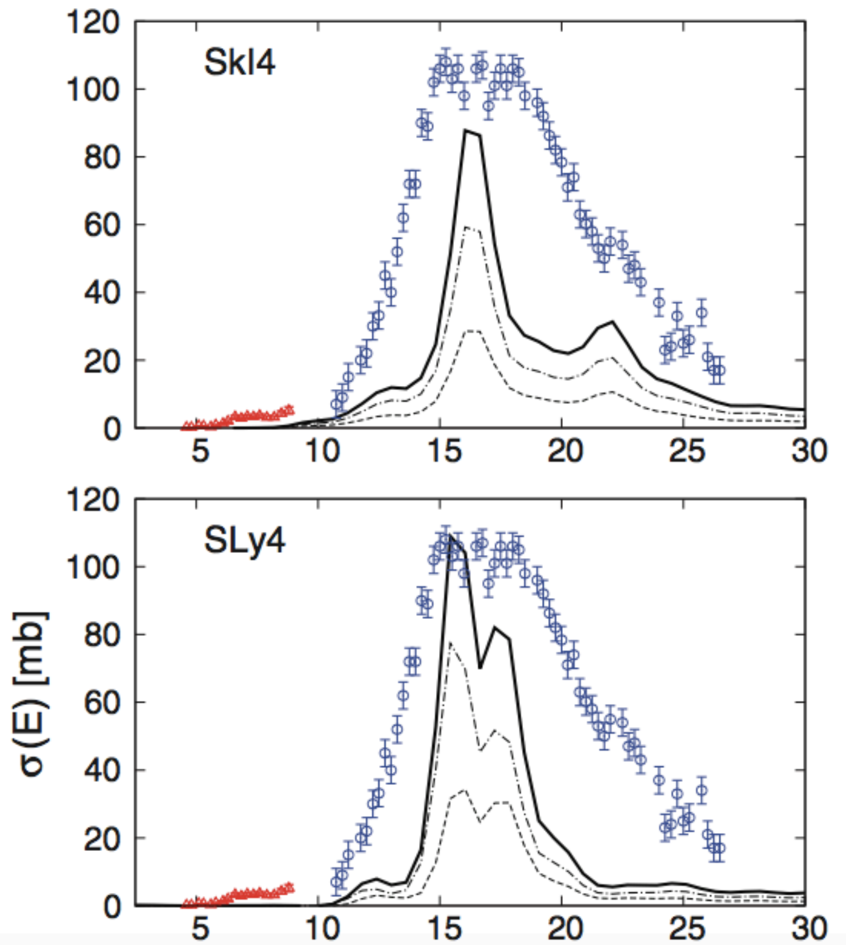


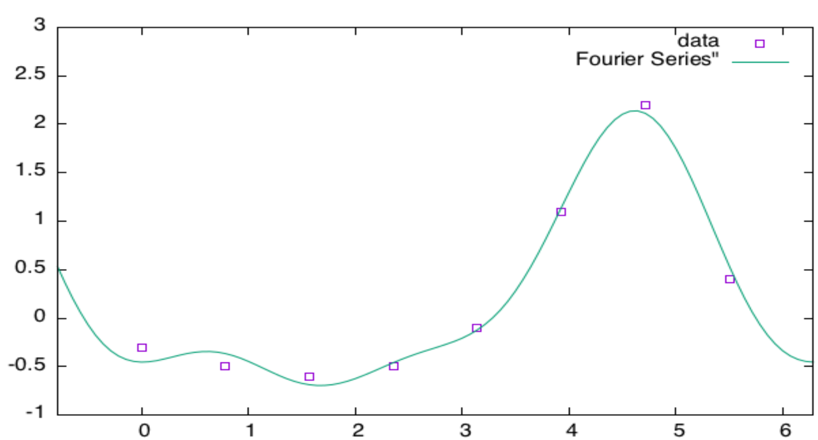

- Missing spreading width (of course)
- structure from K–splitting and single particle effects

# Dependence on Skyrme parameterisation

## NRAPR vs SkI4 vs SLy4

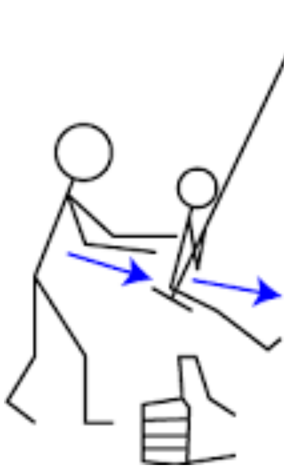


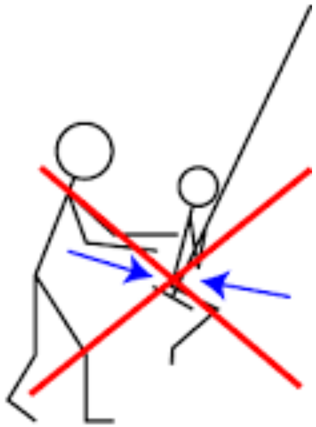



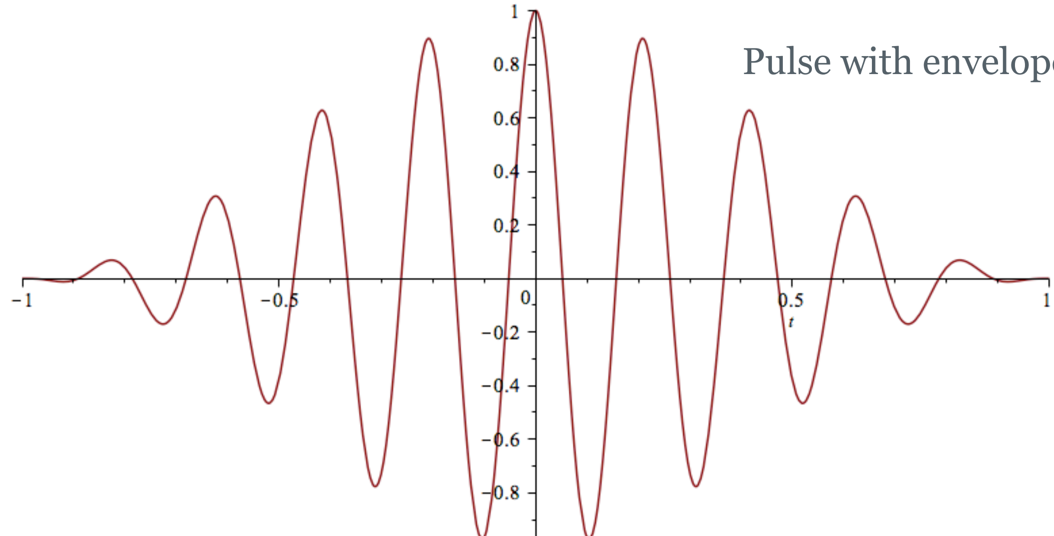
# Forcing the nucleus

## Driving with a narrowband pulse



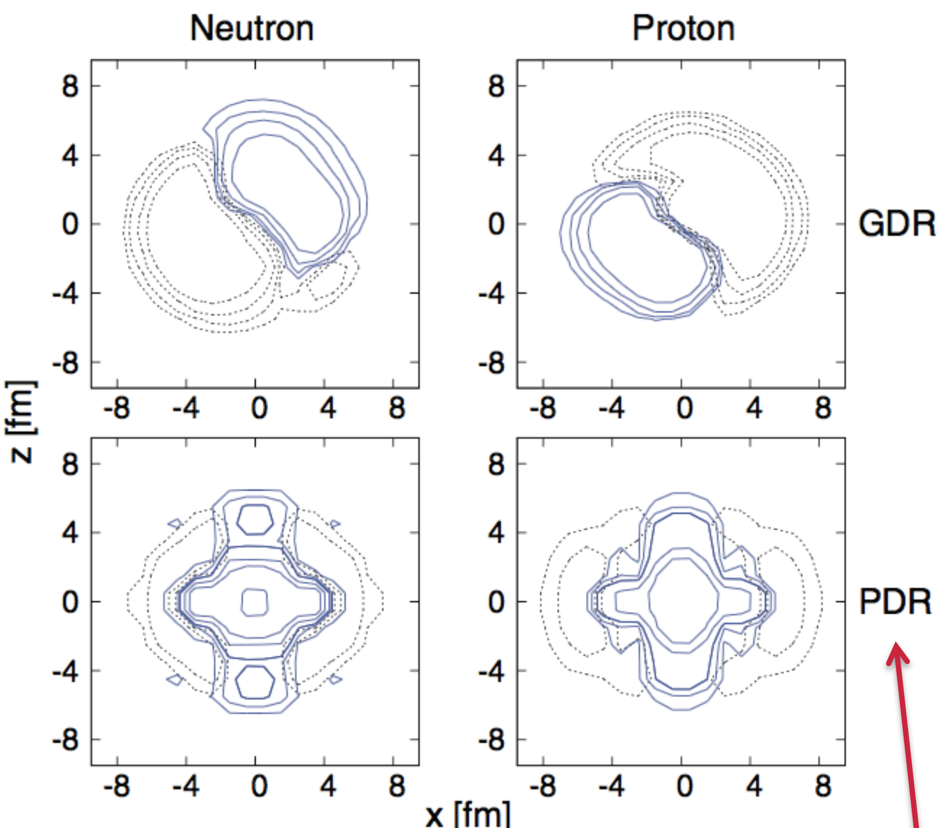


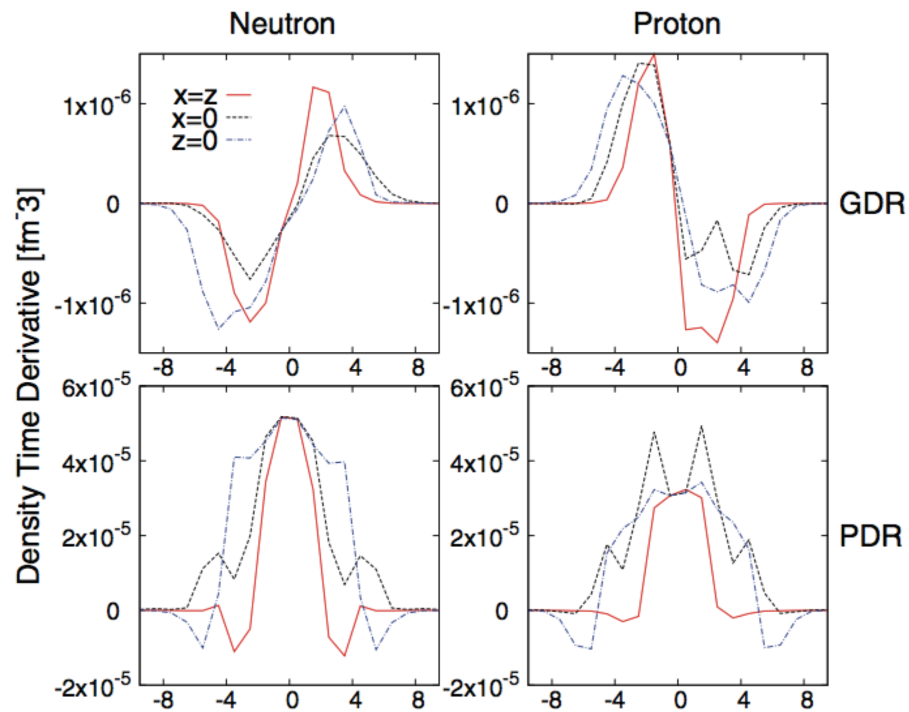
Pulse with envelope

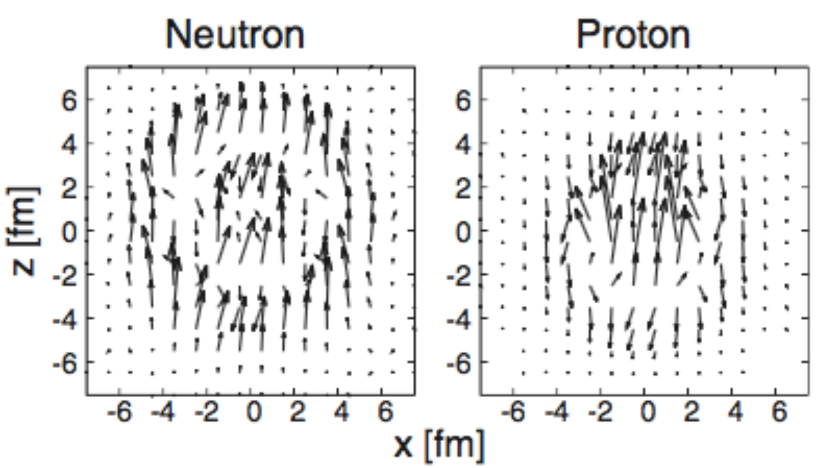



$$i\hbar\frac{\partial\rho}{\partial t} = [(\hat{h}_{\mathrm{HF}}[\rho] + f(t))\,,\ \rho],$$

# Driven density derivatives




ω=5 MeV/ħ

# Surface kick

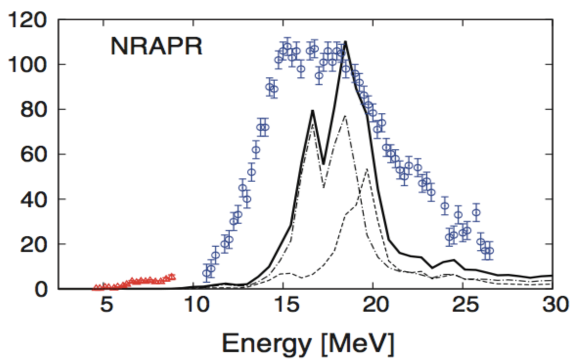
Apply selective dipole boost:

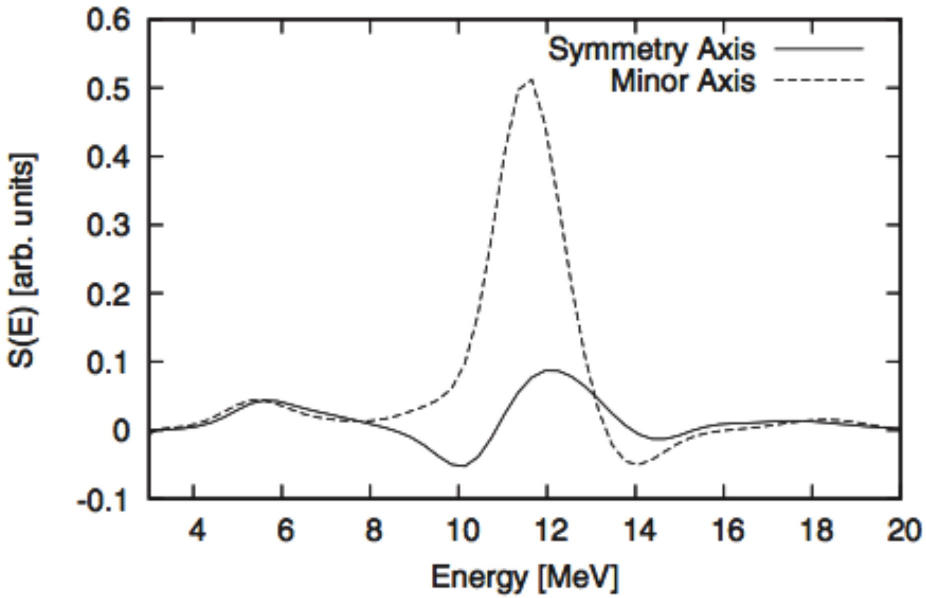
$$\hat{\mathbf{D}}' = \frac{A - \sum v^2}{A} \sum_{i=1}^{\eta} \mathbf{r}_{\text{skin}} - \frac{\sum v^2}{A} \sum_{j=1}^{\zeta} \mathbf{r}_{\text{core}},$$

Sum runs over defined set of core orbitals (the complement of the other sum)

Sum runs over defined set of skin orbitals – corresponding roughly to 1g9/2 neutron orbital (though we have a deformed ground state so correspondence is not exact)

-- Strong response around 10–13 MeV
-- also spherical bump around 5 MeV
-- GDR region unexcited



# Other things

Can initialize TDHF code as collision & study resulting resonance

32S + 48Ti @ 66MeV CM

… or look at time-evolution of fission fragments, or initialise t=0 configuration as a cluster state, or …

👏TDHF is a powerful and general method. With some imagination can explore wide range of nuclear response (of a one-body nature)

# Slutten

Thank you:

P. M. Goddard, University of Surrey

J. A. Maruhn, University of Frankfurt