Time-dependent approach to nuclear response in the continuum

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Institute for Nuclear Theory, Nov. 28, 2005

Workshop on “Nuclear Structure near the limits of stability”

Time-dependent approach to quantum mechanical problems

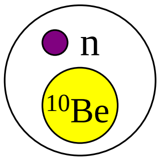
- Time representation vs Energy representation
- Boundary Condition
- Electronic TDDFT
  - Optical response (linear response)
- Nuclear TDDFT (TDHF)
  - Giant resonances
- Summary

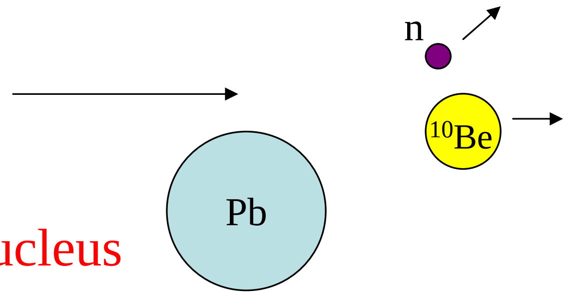
Time Domain	Energy Domain
Basic equations • Time-dep. Schroedinger eq. • Time-dep. Kohn-Sham eq. • $d\mathbf{x}/dt = A\mathbf{x}$	**Basic equations** • Time-indep. Schroedinger eq. • Static Kohn-Sham eq. • $A\mathbf{x}=a\mathbf{x}$ (Eigenvalue problem) • $A\mathbf{x}=b$ (Linear equation)
Energy resolution $\Delta E \sim \hbar/T$ All energies	**Energy resolution** $\Delta E \sim 0$ A single energy point
Boundary Condition • Approximate boundary condition • Easy for complex systems	**Boundary condition** • Exact scattering boundary condition is possible • Difficult for complex systems

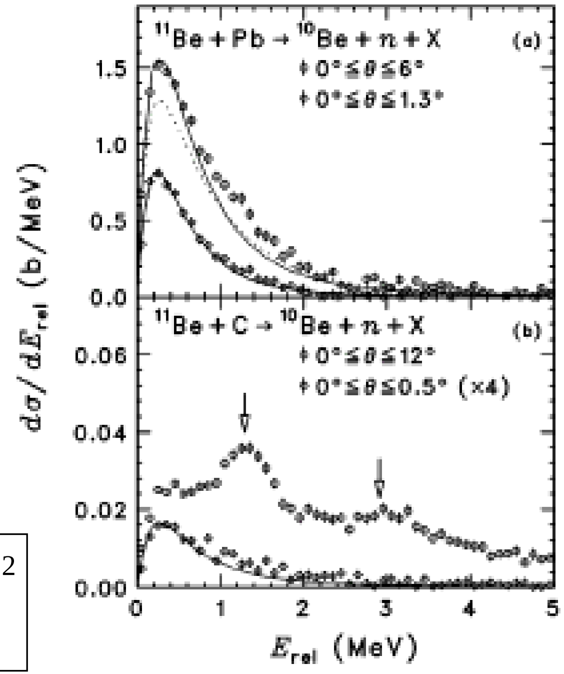
Response Function

Coulomb breakup

Strong low-energy E1 peak







N. Fukuda, et.al,
Phys. Rev. C60(2004)054606

^{11}Be: Halo Nucleus

^{11}Be = ^{10}Be + n

Electric Dipole Strength Distribution

$$\frac{dB(E1,E)}{dE} = \sum_{lm'} \int dE' \delta(E-E') \left| \left\langle \phi_{E,l=1,m} \middle| M_{1m} \middle| \phi_0 \right\rangle \right|^2$$

$\phi_0(\vec{r})$ Initial bound state of ^{11}Be = ^{10}Be + n

$\phi_{E,lm}(\vec{r})$ Final continuum (breakup) states of ^{11}Be = ^{10}Be + n

We can rewrite E1 strength function as

$$\frac{dB(E1,E)}{dE} = \sum_{lm'} \int dE' \delta(E-E') \left| \left\langle \phi_{E,l=1,m} \middle| M_{1m} \middle| \phi_0 \right\rangle \right|^2$$

$$= \left\langle \phi_0 \middle| M_{1m}^{+} \delta(E-H) M_{1m} \middle| \phi_0 \right\rangle$$

$$= -\frac{1}{\pi} \mathrm{Im} \left\langle \phi_0 \middle| M_{1m}^{+} \frac{1}{E+i\varepsilon-H} M_{1m} \middle| \phi_0 \right\rangle$$

$$\frac{dB(E1,E)}{dE} = -\frac{1}{\pi} \mathrm{Im} \sum_m \frac{1}{i\hbar} \int_0^\infty dt e^{iEt/\hbar} \left\langle \phi_0 \middle| M_{1m}^{+} e^{-iHt/\hbar} M_{1m} \middle| \phi_0 \right\rangle$$

$$= \frac{1}{\pi\hbar} \mathrm{Re} \int_0^\infty dt e^{iEt/\hbar} \int \sum_m \psi_{1m}^{*}(\mathbf{r},0) \psi_{1m}(\mathbf{r},t) d\mathbf{r}$$

Time propagation

$$\psi(\vec{r}, t=0) = M_{1m} \phi_0(\vec{r})$$

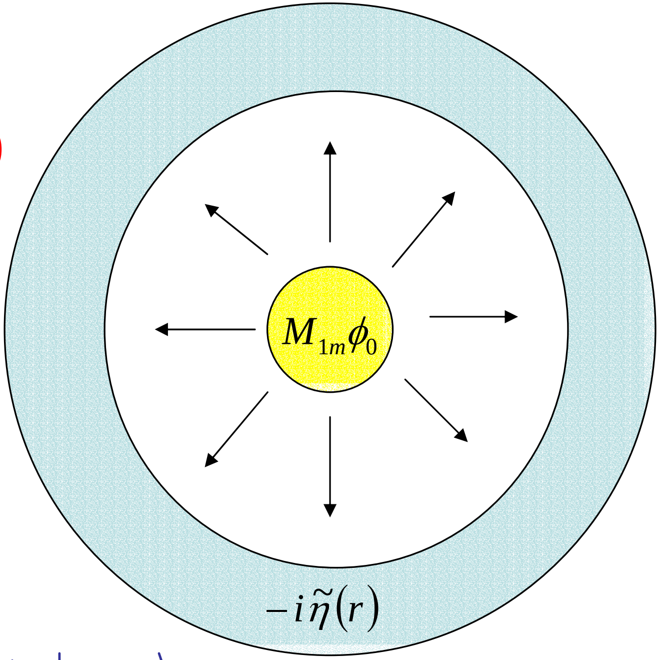
$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r},t) = H \psi(\vec{r},t)$$

Boundary Condition

Absorbing boundary condition (ABC)

Absorb all outgoing waves outside the interacting region

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = \left(H - i\tilde{\eta}(r)\right)\psi(\vec{r},t)$$



How is this justified?

$$\langle \mathbf{k}'|S|\mathbf{k}\rangle = \delta(\mathbf{k}'-\mathbf{k}) + 2\pi i\delta(E'-E)\langle \mathbf{k}'|V|\phi^{(+)}\rangle$$

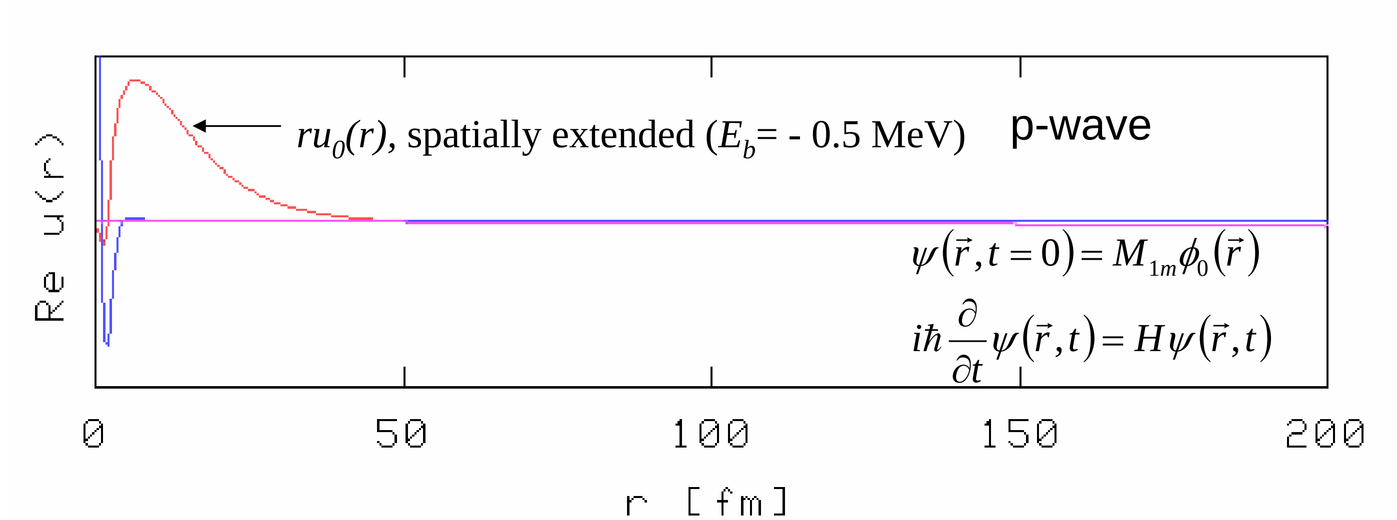
$$\frac{dB(E1,E)}{dE} = \frac{1}{\pi\hbar}\mathrm{Re}\int_0^\infty dt\, e^{iEt/\hbar}\sum_m \boxed{\langle \psi_{1m}(0)|}\psi_{1m}(t)\rangle$$

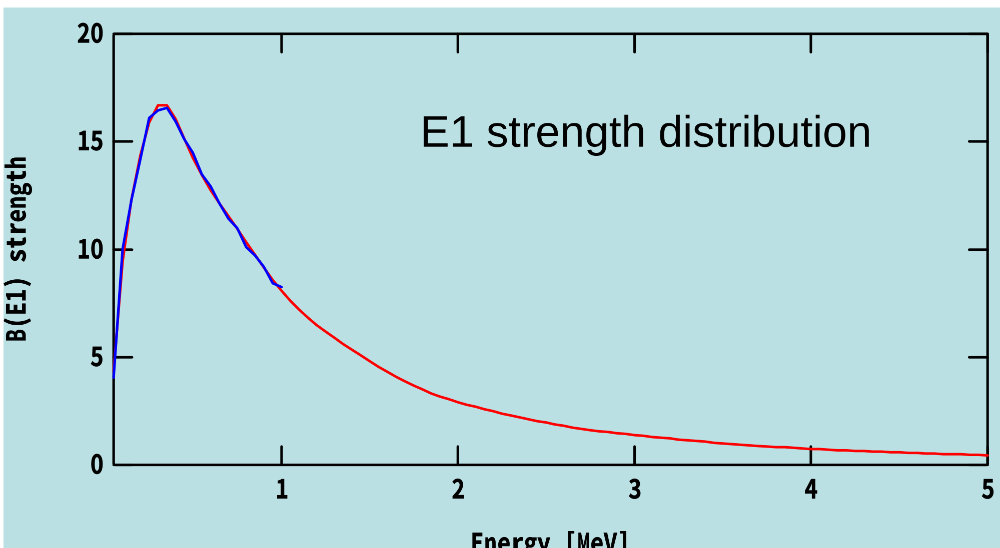
Localized w.f.

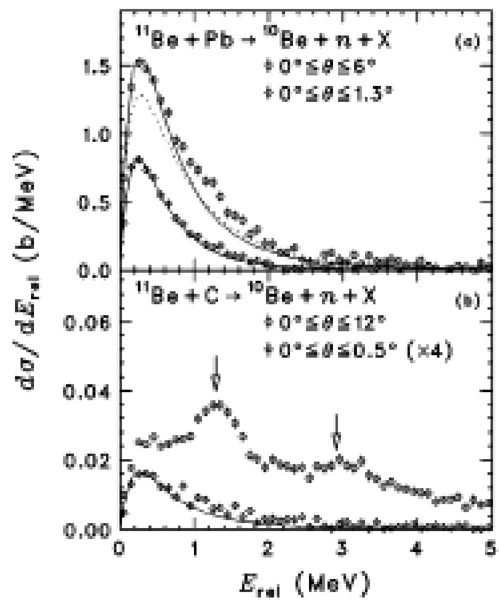
Finite time period up to *T*

Time evolution can stop when all the outgoing waves are absorbed.

$$\int_0^\infty dt \Rightarrow \int_0^T dt$$


Re u(r)
$ru_0(r)$, spatially extended (E_b= - 0.5 MeV)
p-wave
$\psi(\vec{r},t=0)=M_{1m}\phi_0(\vec{r})$
$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)=H\psi(\vec{r},t)$
0
50
100
150
200
r [fm]


E1 strength distribution
B(E1) strength
20
15
10
5
0
1
2
3
4
5
Energy [MeV]


^{11}Be + Pb → ^{10}Be + n + X
(a)
0° ≤ θ ≤ 6°
0° ≤ θ ≤ 1.3°
^{11}Be + C → ^{10}Be + n + X
(b)
0° ≤ θ ≤ 12°
0° ≤ θ ≤ 0.5° (×4)
$d\sigma/dE_{rel}$ (b/MeV)
E_{rel} (MeV)

Time-Dependent Density Functional Theory (TDDFT)

In nuclear theory, the concept is very similar to

TDHF with effective interactions.

Electronic TDDFT vs Nuclear TDHF

Density Functional Theory
- Hohenberg, Kohn (1964)
- Kohn, Sham (1965)

  Existence of density functional

  Free particles in a KS potential

Time-dependent DFT
- Runge, Gross (1985)

  Existence of density functional to reproduce the time evolution of interacting many-particle systems

TDDFT in real space & real time
- Yabana, Bertsch (1996)
- Nakatukasa, Yabana (2001)

  Continuum boundary condition

Brueckner HF → Skyrme HF
- Negele (1972) DME
- Vautherin, Brink (1972)

  Density functional to reproduce mass, radius, deformation of nuclear ground states

TDHF in real space & real time
- Bonche, Koonin, Negele (1976)
- Flocard, Koonin, Weiss (1978)

  Heavy ion reactions, fusion prob.

- Nakatsukasa, Yabana (2005)

  Nuclear response in the continuum

TDHF(TDDFT) calculation in 3D real space

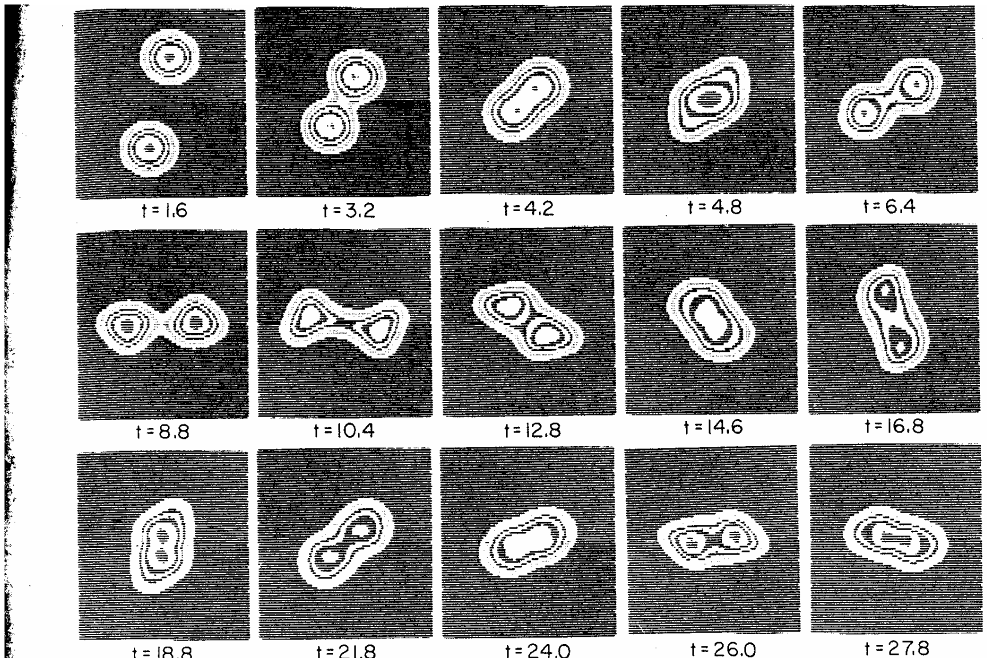


FIG. 2. Contour lines of the density integrated over the coordinate normal to the scattering plane for an $^{16}O + ^{16}O$ collision at $E_{lab} = 105$ MeV and incident angular momentum $L = 13\hbar$. The times t are given in units of 10^{-22} sec.

H. Flocard, S.E. Koonin, M.S. Weiss, Phys. Rev. 17(1978)1682.

Real-space TDDFT calculations

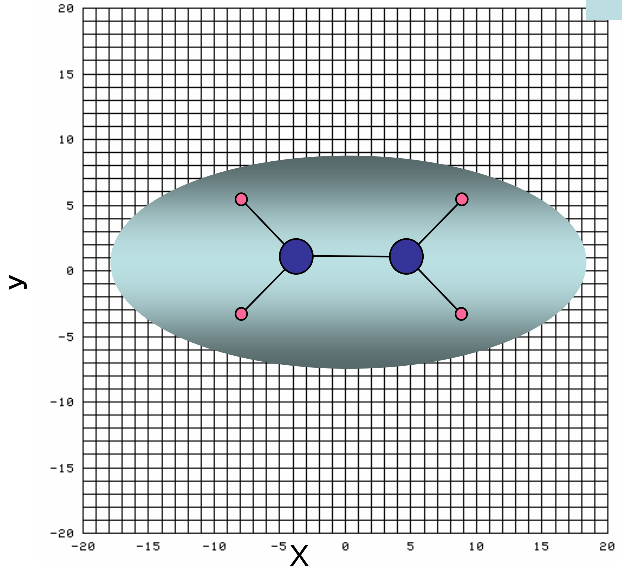
Time-Dependent Kohn-Sham equation

$$-i\tilde{\eta}(r)$$

$$i\frac{\partial}{\partial t}\psi_i(\mathbf{r},t) = \left(-\frac{1}{2m}\nabla^2 + V_{\text{ion}}(\mathbf{r}) + V_{\text{H}}[\rho(\mathbf{r},t)] + \mu_{\text{xc}}[\rho(\mathbf{r},t)] + V_{\text{ext}}(\mathbf{r},t)\right)\psi_i(\mathbf{r},t)$$

3D space is discretized in lattice

Each Kohn-Sham orbital: $\varphi_i(\mathbf{r},t) = \{\varphi_i(\mathbf{r}_k,t_n)\}_{k=1,\cdots Mr}^{n=1,\cdots Mt}, \quad i=1,\cdots,N$



N : Number of particles

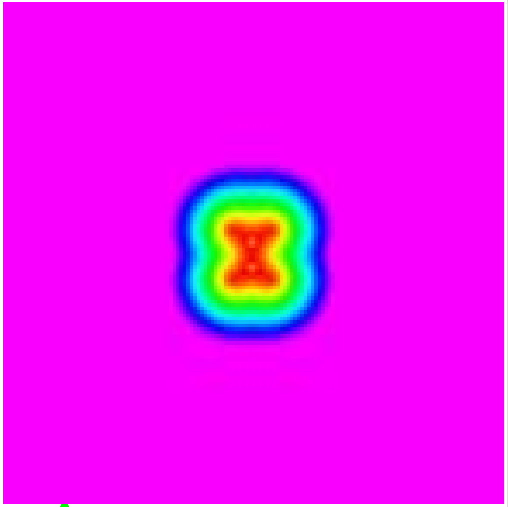
Mr : Number of mesh points

Mt : Number of time slices

K. Yabana, G.F. Bertsch, Phys. Rev. B54, 4484 (1996).

T. Nakatsukasa, K. Yabana, J. Chem. Phys. 114, 2550 (2001).

Real-time dynamics of electrons in photoabsorption of molecules

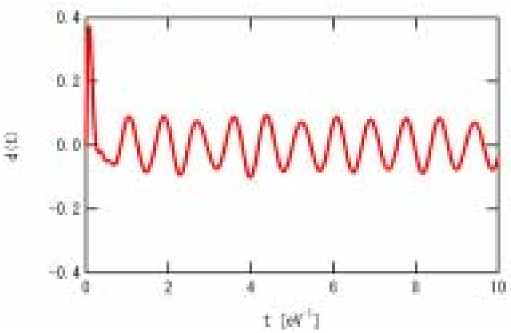


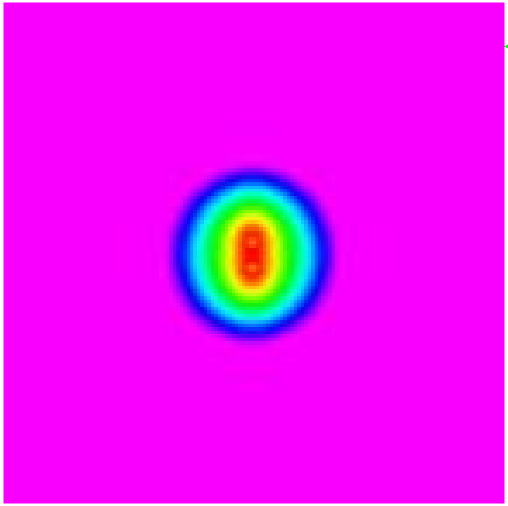
1. External perturbation t=0

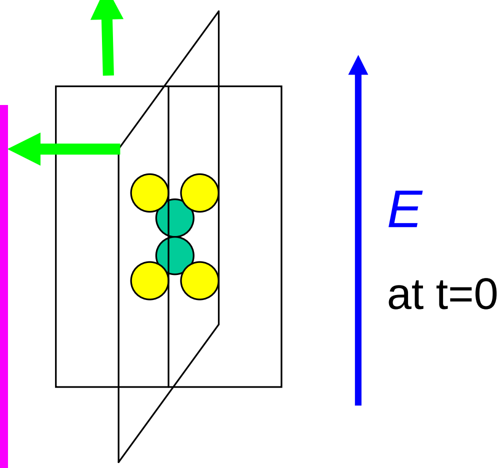
$$V_{ext}(\mathbf{r},t) = -\varepsilon r_i \delta(t), \quad i = x, y, z$$

2. Time evolution of dipole moment

$$d_i(t) \propto \int r_i \rho(\mathbf{r},t)$$



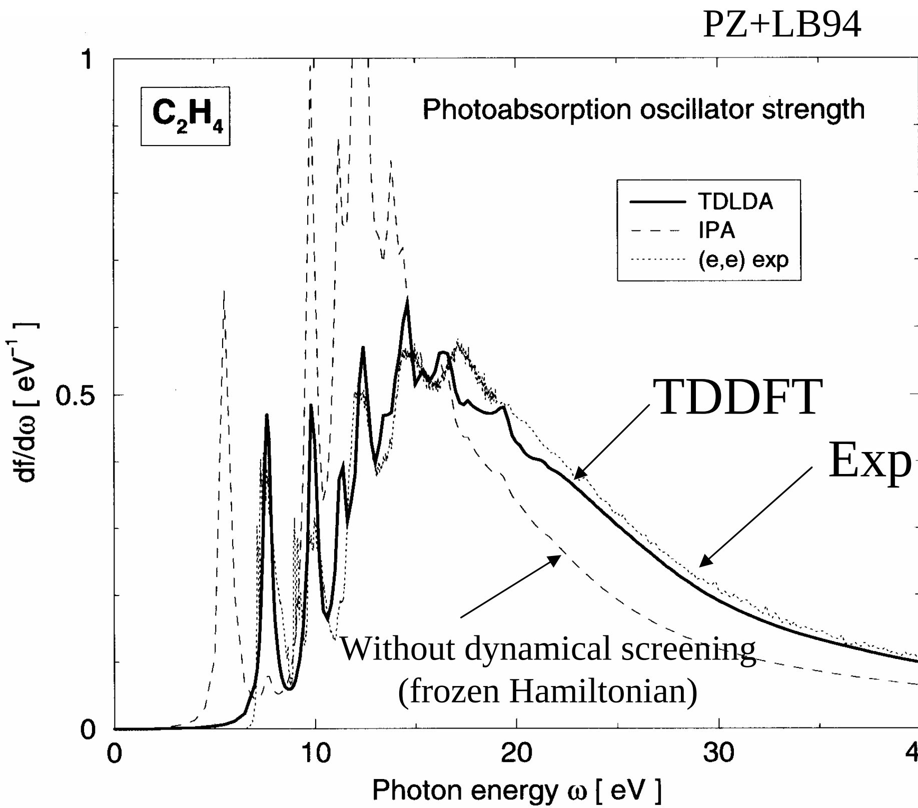




Ethylene molecule

Comparison with measurement (linear optical absorption)

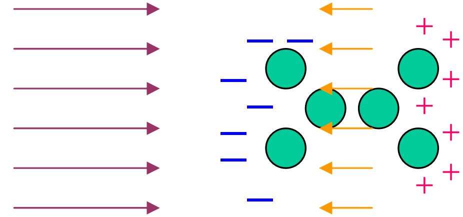
TDDFT accurately describe optical absorption
Dynamical screening effect is significant



$$i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t) = h[n(\vec{r},t)]\psi_i(\vec{r},t)$$

with
without
Dynamical screening

$$i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t) = h[n_0(\vec{r})]\psi_i(\vec{r},t)$$



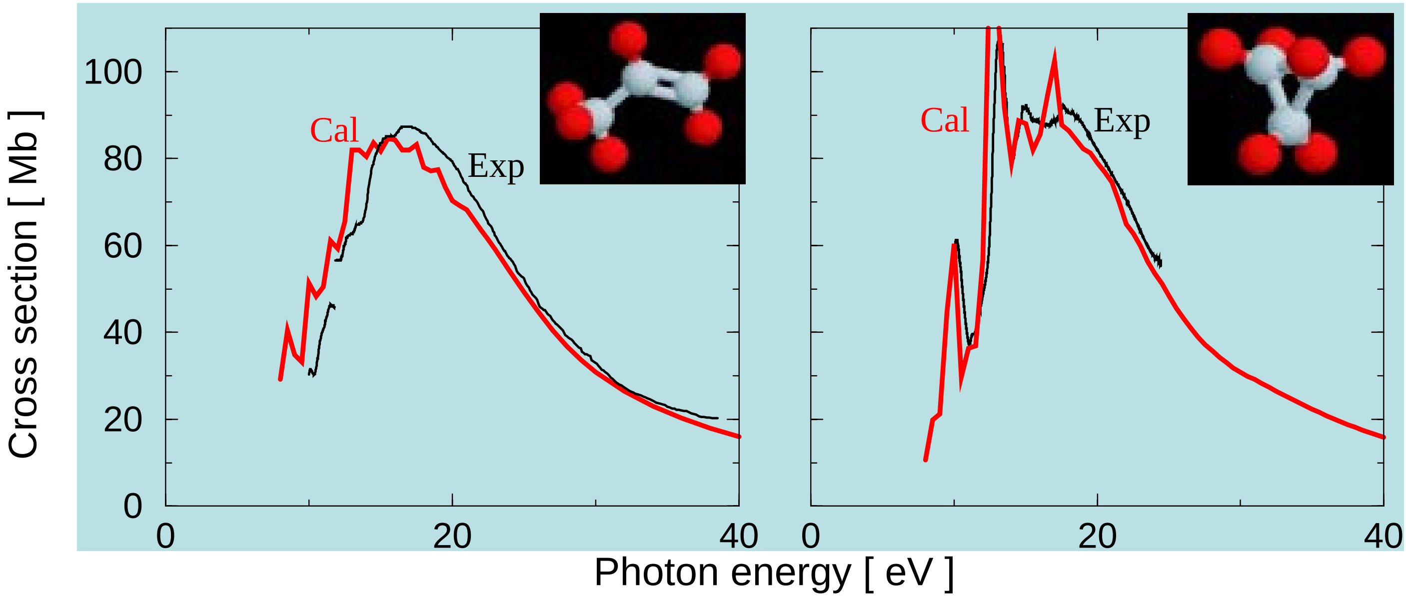
$E_{ext}(t)$ $E_{ind}(t)$

T. Nakatsukasa, K. Yabana, J. Chem. Phys. 114(2001)2550.

Photoabsorption cross section in C_3H_6 isomer molecules

Nakatsukasa & Yabana, Chem. Phys. Lett. 374 (2003) 613.

- TDLDA cal with LB94 in 3D real space
- 33401 lattice points (r < 6 Å)
- Isomer effects can be understood in terms of symmetry and anti-screening effects on bound-to-continuum excitations.



Skyrme TDHF in real space

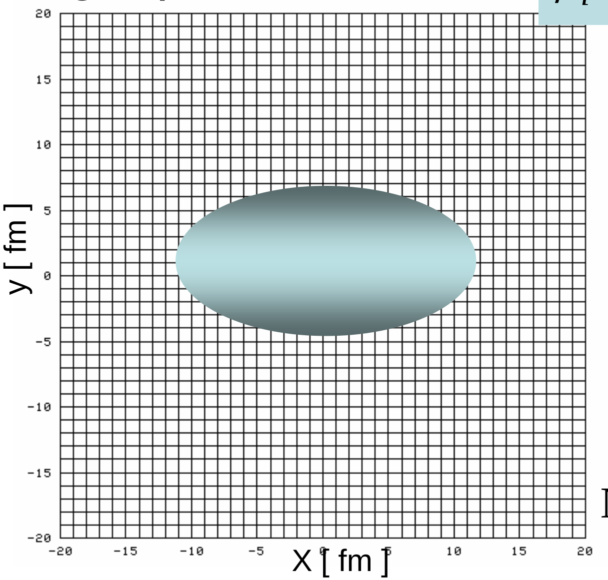
Time-dependent Hartree-Fock equation

$$- i \tilde{\eta}(r)$$

$$i \frac{\partial}{\partial t} \psi_i(\mathbf{r}\sigma\tau, t) = \left(h_{\mathrm{HF}}[\rho, \tau, \mathbf{j}, \mathbf{s}, \overleftrightarrow{\mathbf{J}}](t) + V_{\mathrm{ext}}(t) \right) \psi_i(\mathbf{r}\sigma\tau, t)$$

3D space is discretized in lattice

Single-particle orbital: $\varphi_i(\mathbf{r}, t) = \{\varphi_i(\mathbf{r}_k, t_n)\}_{k=1,\cdots Mr}^{n=1,\cdots Mt}, \quad i = 1, \cdots, N$



N: Number of particles

Mr: Number of mesh points

Mt: Number of time slices

Spatial mesh size is about 1 fm.

Time step is about 0.2 fm/c

Nakatsukasa, Yabana, Phys. Rev. C71 (2005) 024301

Real-time calculation of response functions

1. Weak instantaneous external perturbation

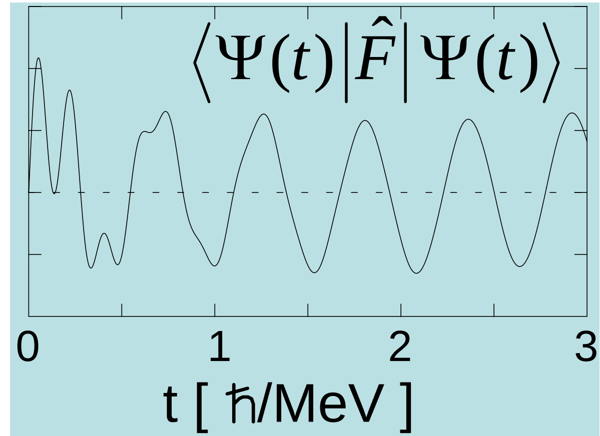
$$V_{\text{ext}}(t) = \hat{F}\delta(t)$$

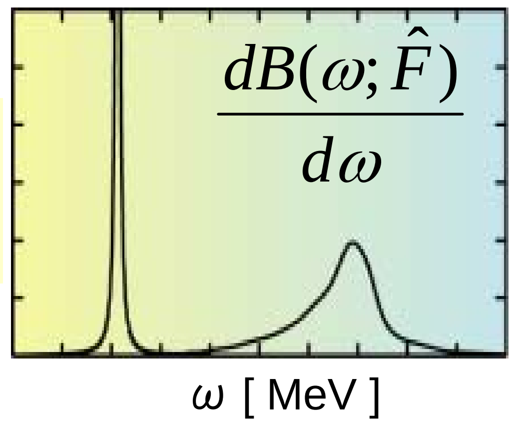
2. Calculate time evolution of

$$\left\langle \Psi(t) \middle| \hat{F} \middle| \Psi(t) \right\rangle$$

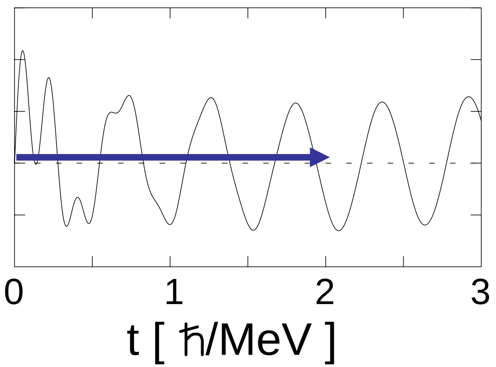
3. Fourier transform to energy domain

$$\frac{dB(\omega;\hat{F})}{d\omega} = -\frac{1}{\pi}\,\mathrm{Im}\int \left\langle \Psi(t) \middle| \hat{F} \middle| \Psi(t) \right\rangle e^{i\omega t}\,dt$$





IS octupole resonances in ^{16}O



BKN interaction

External field: $r^3 Y_{30}$

IS transition density

$$\delta\rho(t) = \rho(t) - \rho_0$$

Absorbing BC

Vanishing BC

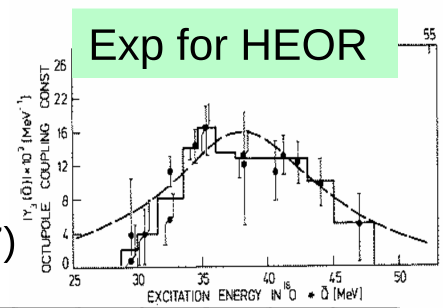
@ xz-plain (y=0)

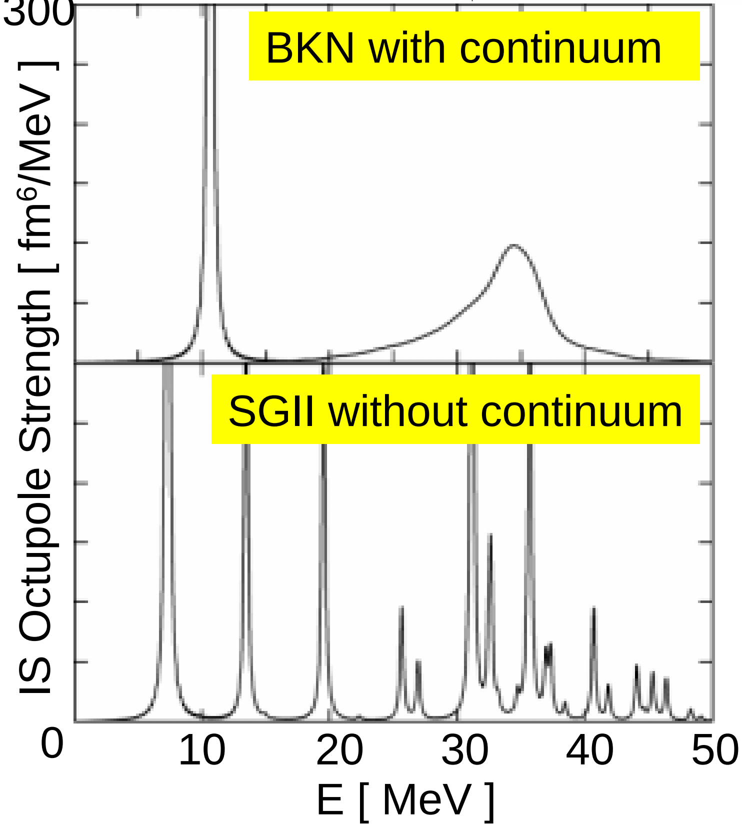
$\delta\ \rho > 0$

$\delta\ \rho < 0$

LEOR & HEOR in ^{16}O

Perrin et al. (1977)



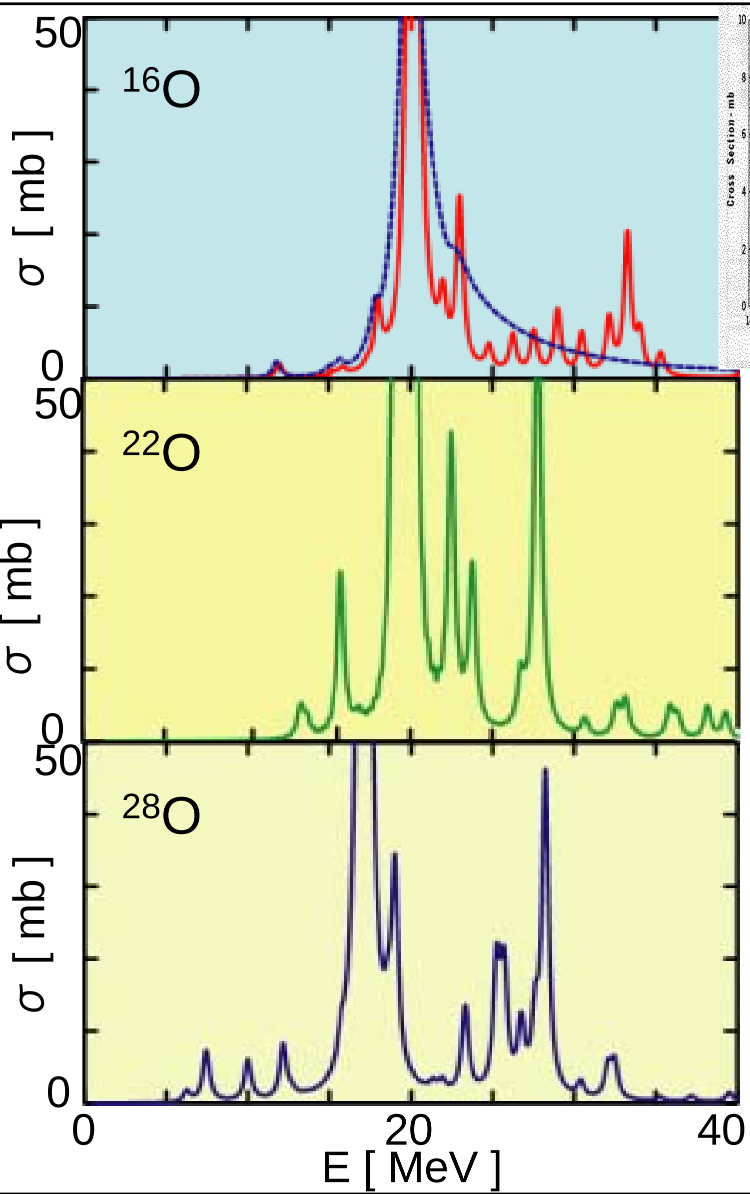


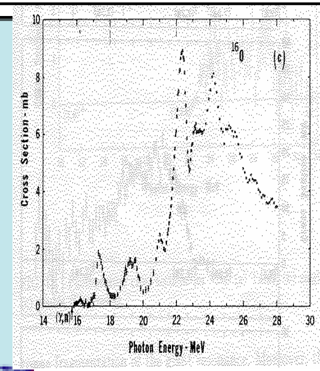
Low-lying 3^- state

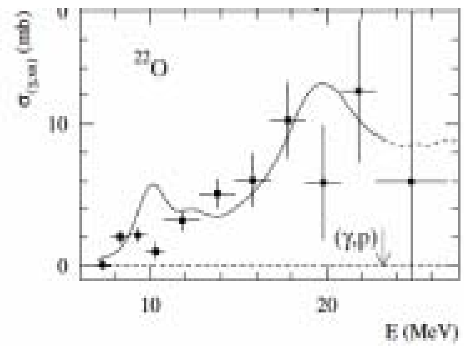
BKN int.→ E ≈ 10 MeV

SGII int.→ E ≈ 7, 13, 14 MeV

Exp . → E ≈ 6.1, 11.6, 13, 14 MeV







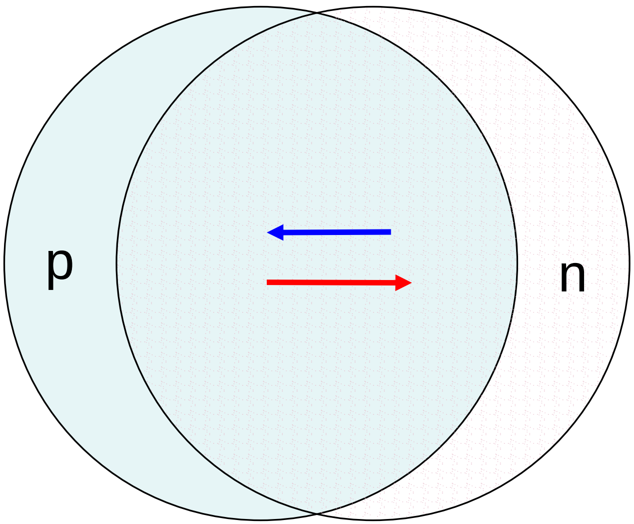
SGII parameter set

$\Gamma = 0.5$ MeV

Note: Continnum is NOT taken into account !

E1 resonances in ^{16,22,28}O

Giant dipole resonance in stable and unstable nuclei



Classical image of GDR

Neutrons

$$\delta\rho_n(t) = \rho_n(t) - \left(\rho_0\right)_n$$

Time-dep. transition density

^{16}O

$\delta\ \rho > 0$

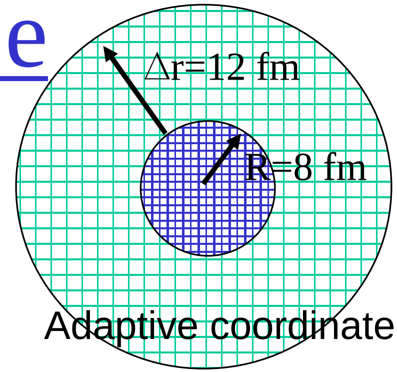
$\delta\ \rho < 0$

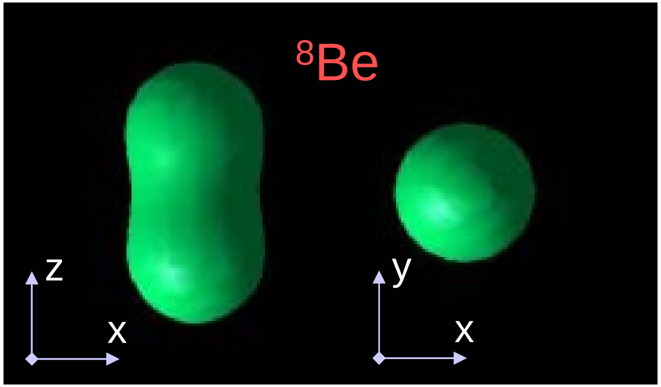
^{28}O

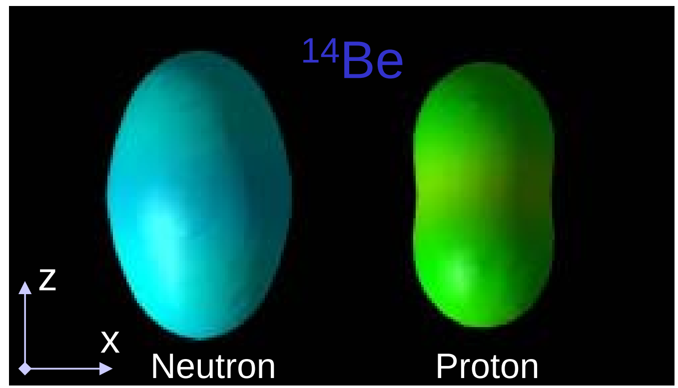
$$\delta\rho_p(t) = \rho_p(t) - \left(\rho_0\right)_p$$

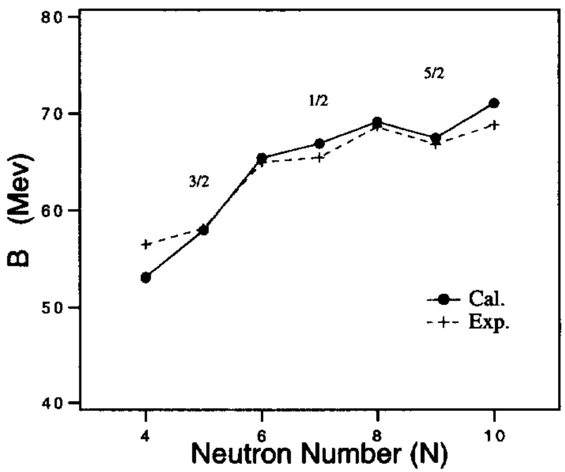
Protons

Skyrme HF for ^{8,14}Be









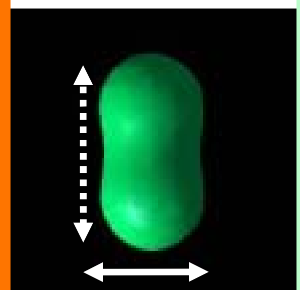
S.Takami, K.Yabana, and K.Ikeda, *Prog. Theor. Phys*. **94** (1995) 1011.

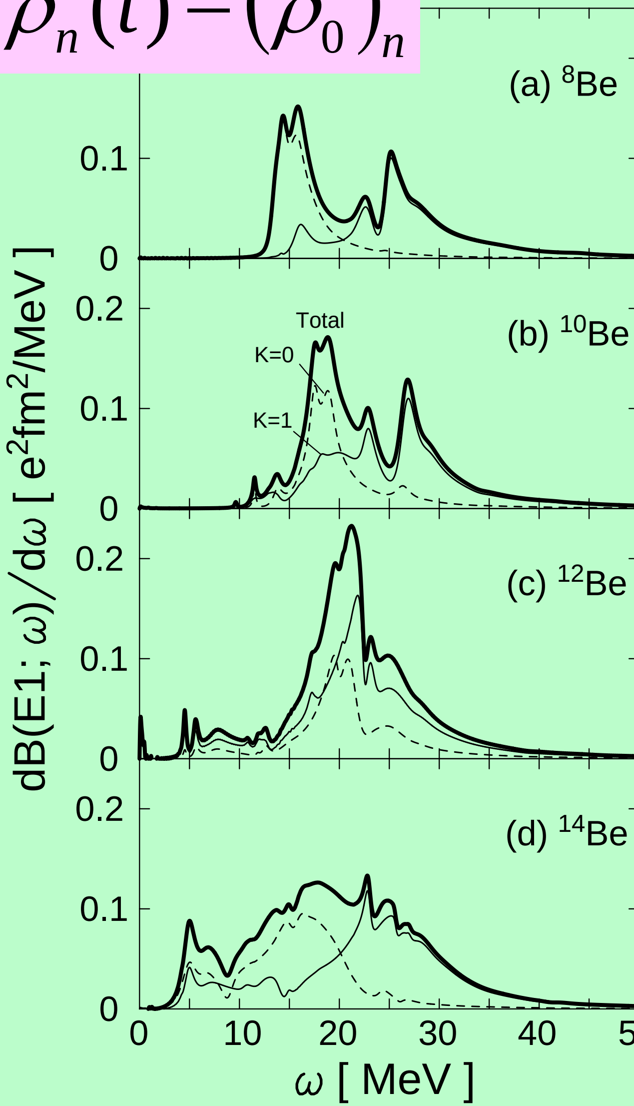
$$\delta\rho_n(t) = \rho_n(t) - \left(\rho_0\right)_n$$

^{8}Be

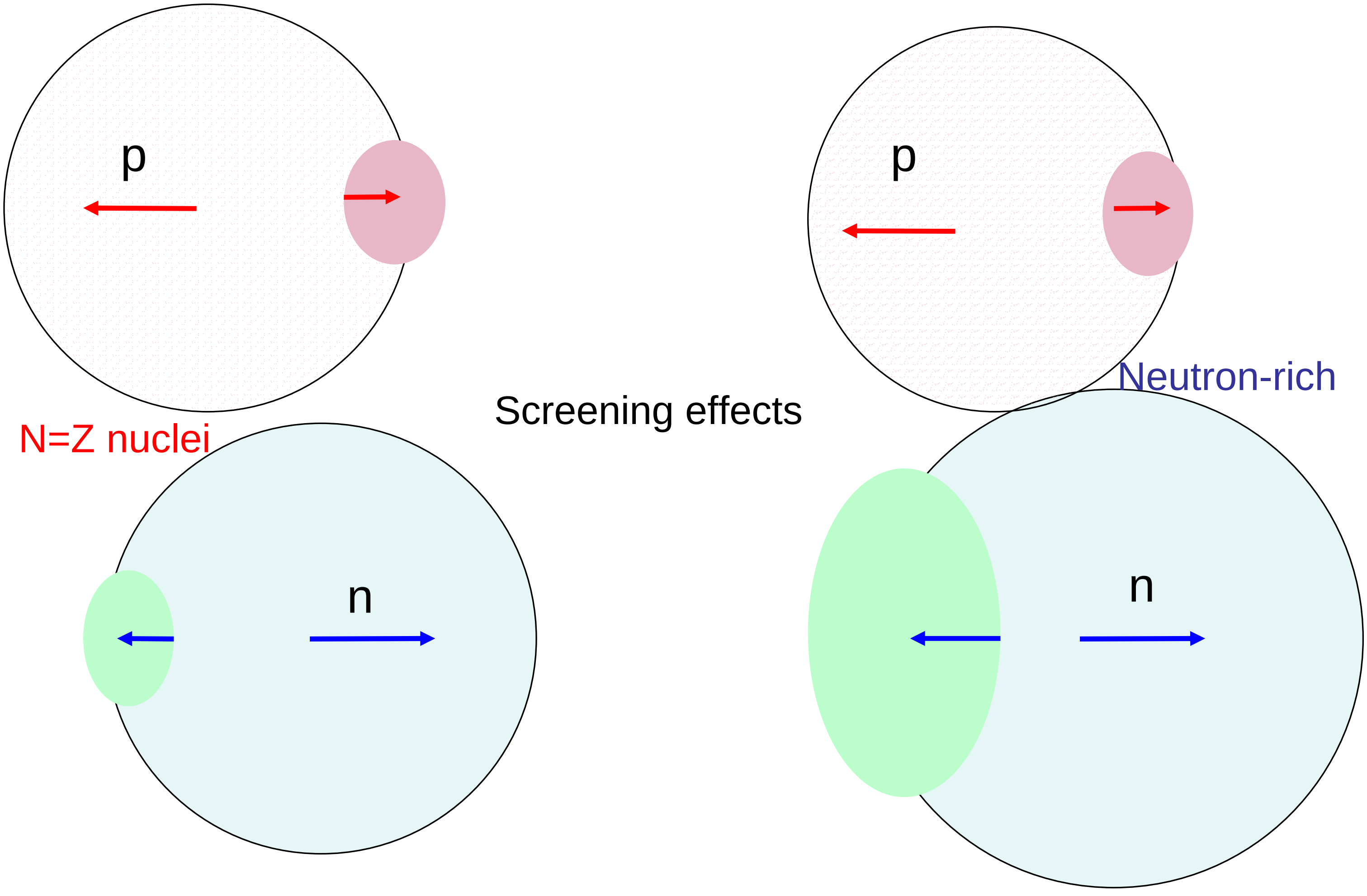
^{14}Be

Solid: K=1
Dashed: K=0

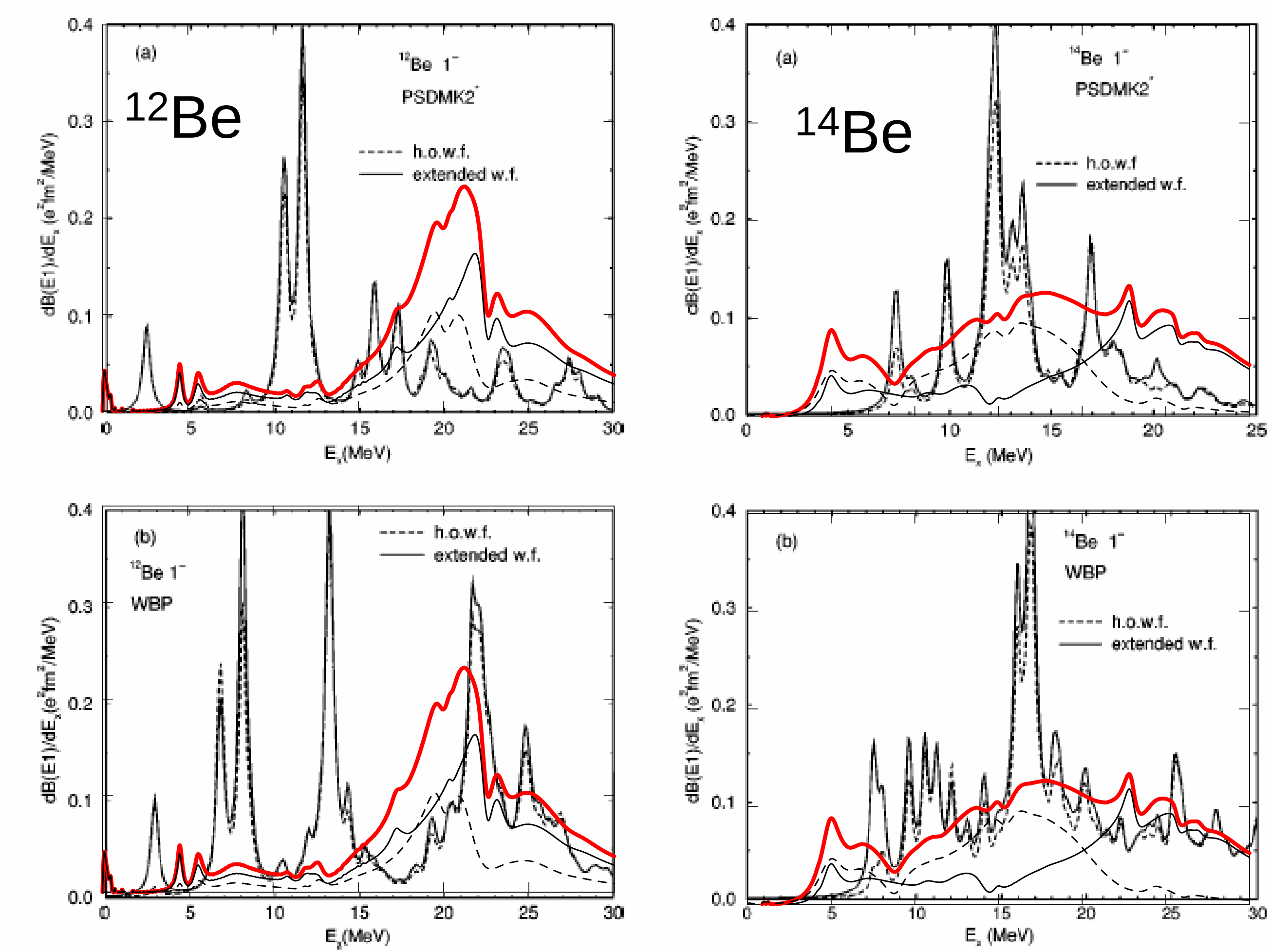




Giant dipole resonance



High-energy *E1* strengths



Sagawa, Suzuki, Iwasaki, Ishihara, PRC63 (2001) 034310

Summary

- TDHF+ABC to study dynamical aspects of nuclear response in the continuum
- GDR near the neutron drip line shows a large broadening, and strong low-energy E1
- Neutron-proton attractive correlation leads to a complex dipole motion (“screening”?)