

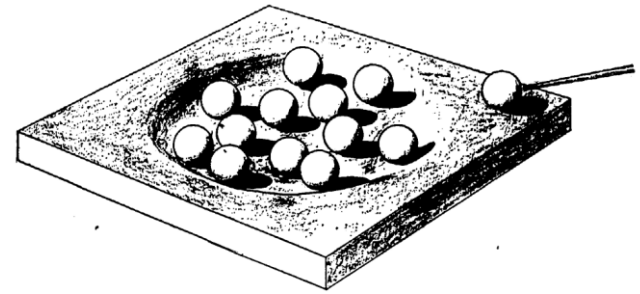
Towards Inclusion of Dissipation in TDDFT

A progress report...

Dissipative mechanisms
in finite quantum systems

An old story...

neutron on nucleus



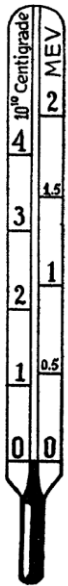
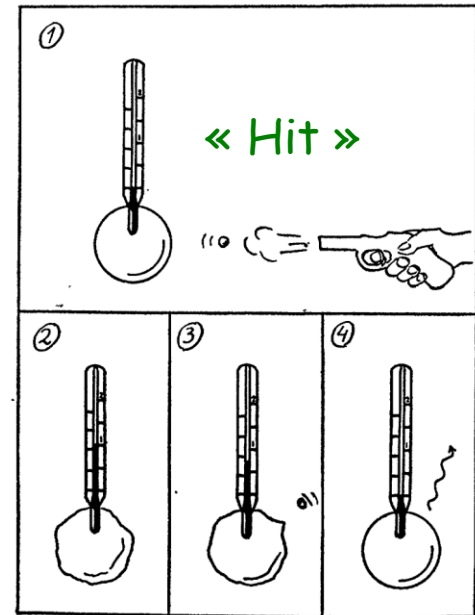
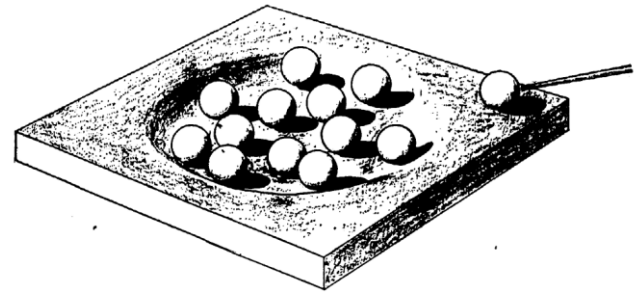
Towards Inclusion of Dissipation in TDDFT

A progress report...

Dissipative mechanisms
in finite quantum systems
An old story...

Dissipation
Dynamical picture
Microscopic description
Finite systems

neutron on nucleus



N. Bohr, Science, 1937

← compound nucleus →

← neutron cooling →

← radiative cooling →



Fusion in nuclear collisions (1980's...)

Nuclear collision

Hot compound nucleus

Deexcitation via

Fission

Neutron emission (Bohr)

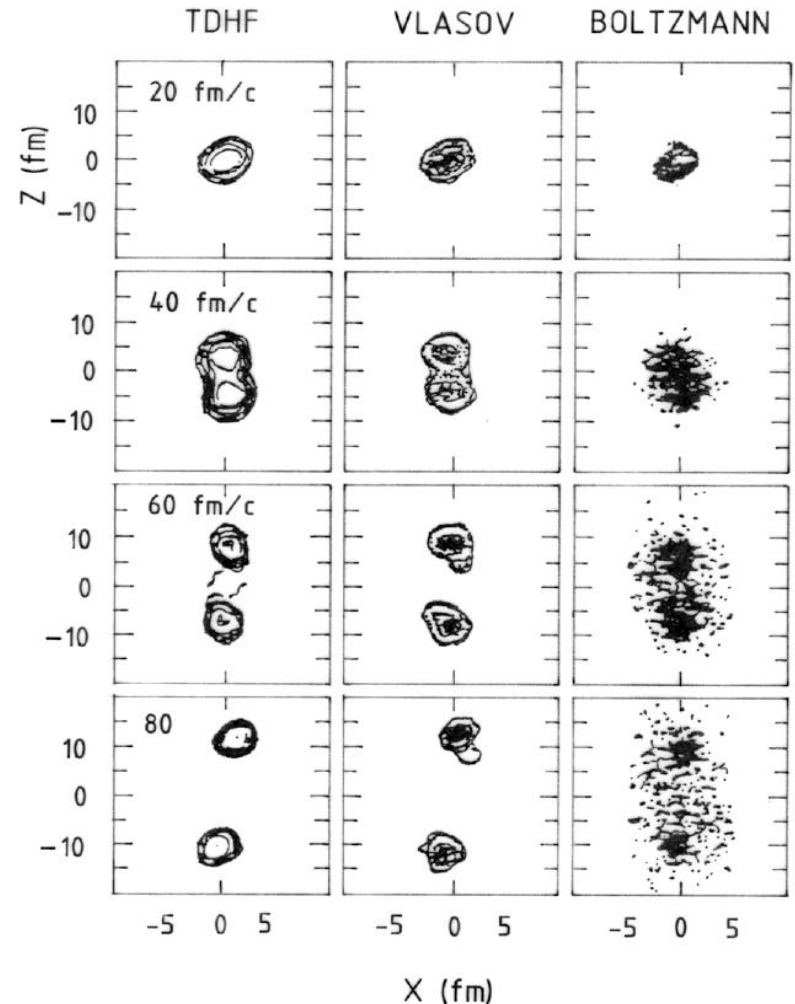
...

Finite temperature

Statistical emission (Weisskopf)

- Exponential energy slope $\rightarrow \tau$
- Isotropic emission

$^{12}\text{C} + ^{12}\text{C}$ $b = 0$ $v \sim$ Fermi veloc.



Nuclear fission and dissipation

Measure

- i) number of emitted neutrons
 - ii) angular distribution
- 1 nucleus : « isotropic »
2 nuclei : « anisotropic »



i) Fission time

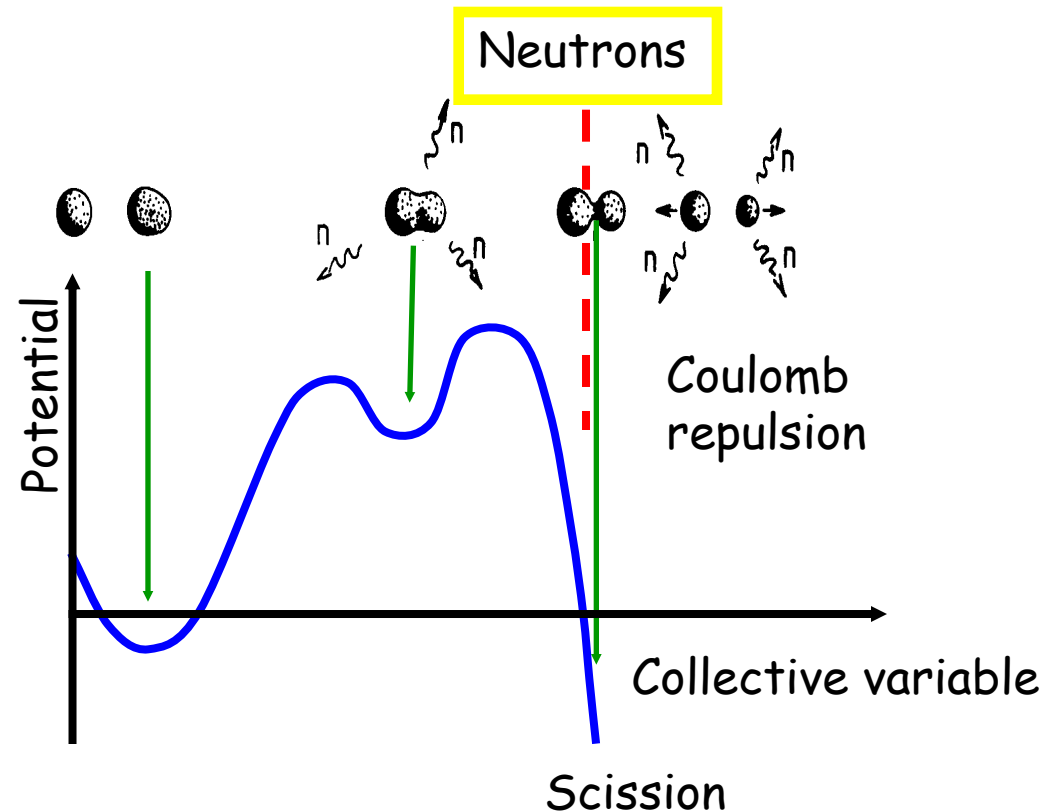
$$\tau \sim 10^{-20} \text{ s}$$

ii) Nuclear viscosity

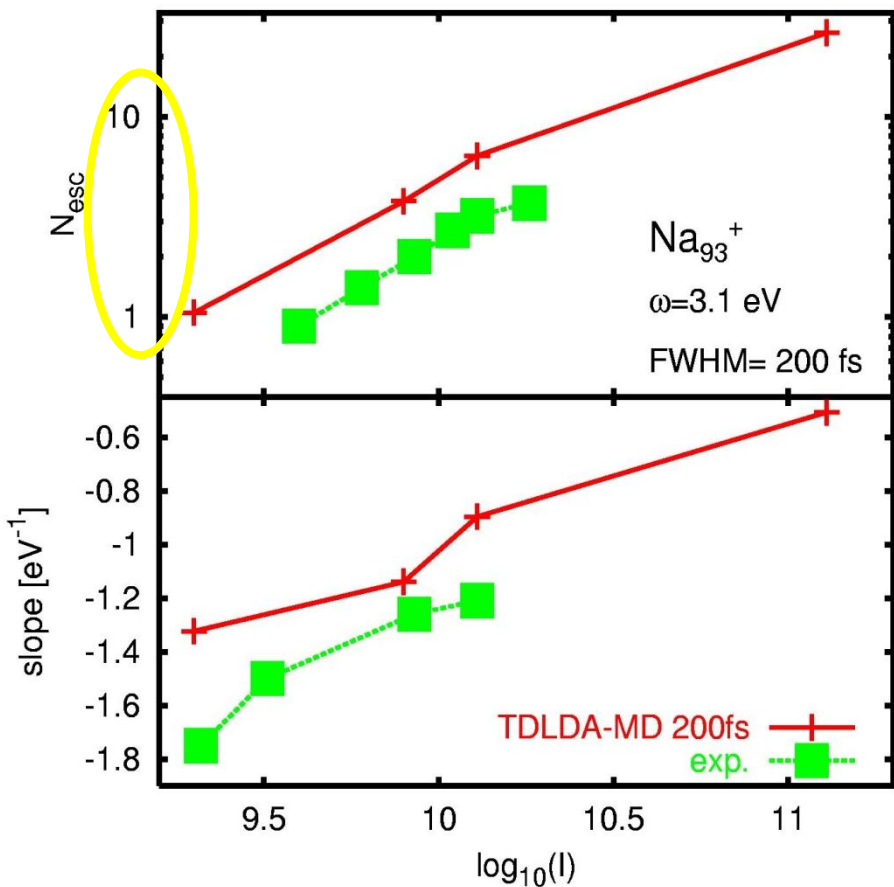
Fission of a hot nucleus

1 source

2 sources



PhotoElectron Spectroscopy (PES)



Pohl et al, JPB 2004

Exp. Freiburg

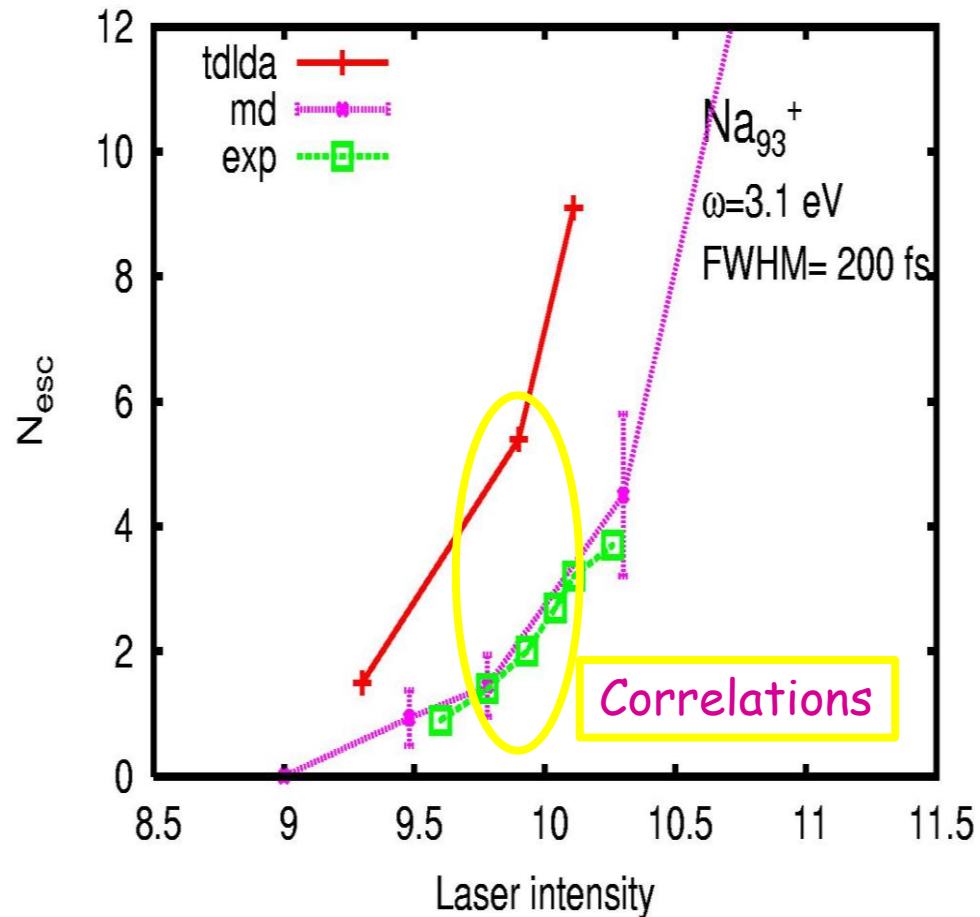
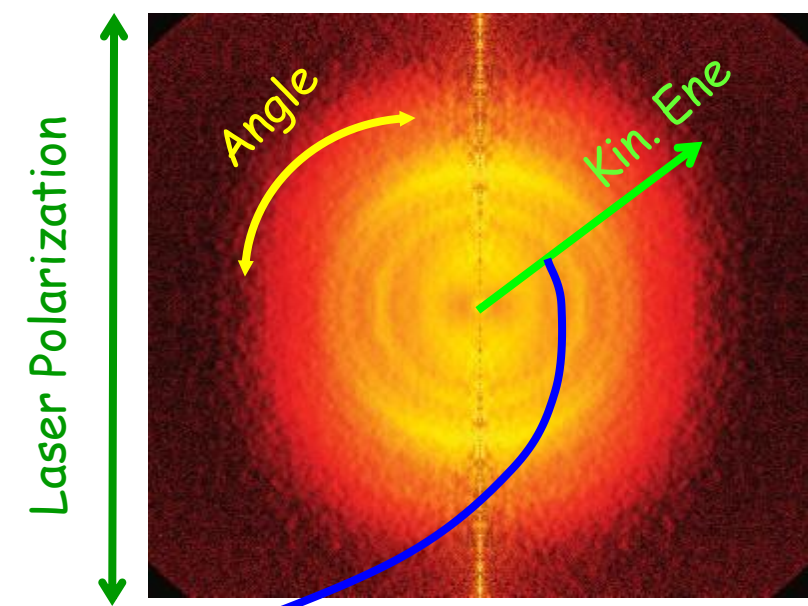
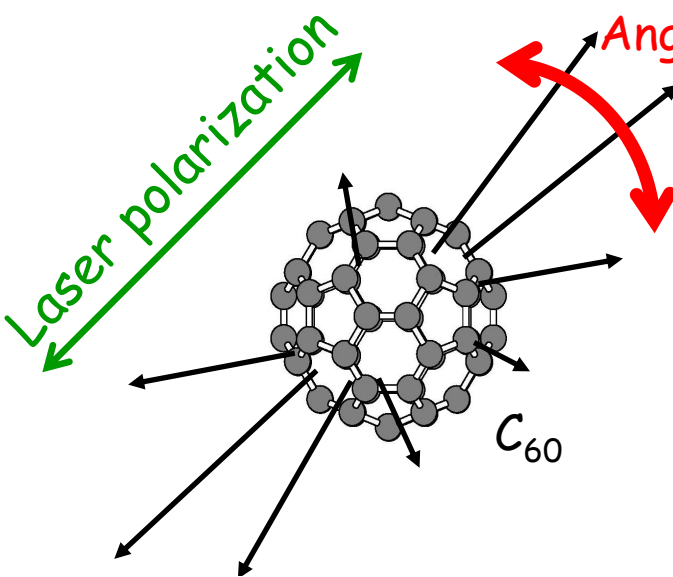
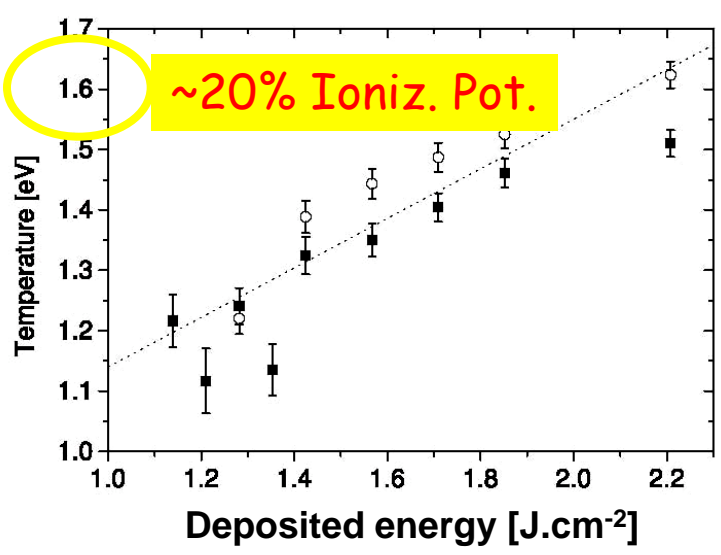


Photo Angular Distributions (PAD)



Exp. Lund



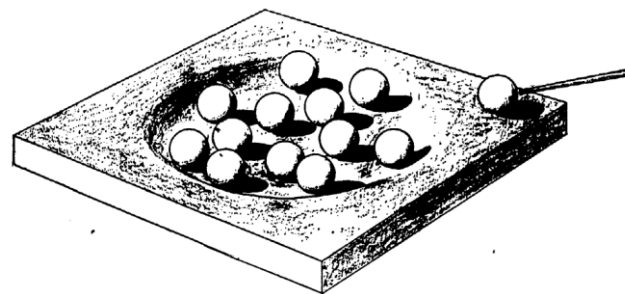
PAD → PES $\int d\Omega (d\sigma/d\Omega dE) = d\sigma/dE$

Thermalization
Dissipation:
collective (laser) → thermal



Towards Inclusion of Dissipation in TDDFT

neutron on nucleus



N. Bohr, Science, 1937

To do list (~exp.)

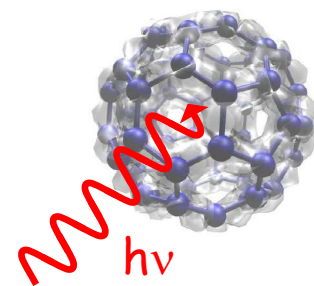
Cart (~theo.)

Photo Electron Spectra PES

Exponential slope

Photo Angular Distribution PAD

Isotropic



Model (cluster/molecule)

➤ Electrons

- **Time Dependent Density Functional Theory (TDDFT)**

Ensemble of orbitals (1 electron) / no correlation $\{\phi_i(\mathbf{r}), i = 1, \dots\}$

One body density $\rho(\mathbf{r}) = \sum_j |\phi_j(\mathbf{r})|^2$

Effective mean field theory (**Kohn-Sham**)

$$i\hbar \frac{\partial \phi_i}{\partial t} = h[\rho] \phi_i$$

$$h[\rho] = -\frac{\hbar^2}{2m} \Delta + U_{\text{KS}} + U_{\text{ext}}(\mathbf{r}, t)$$

Kohn-Sham potential

Ions + ext.

- **Local Density Approximation (LDA)**

$$U_{\text{KS}} = U_{\text{H}} + U_{\text{xc}}[\rho]$$

- + **Self Interaction Correction (SIC)** ...

Coulomb direct

Exch. + Corr.

- Semi-classical theory available (**Vlasov, VUU**)

- Explicit ions via **pseudo potentials**

➤ Ions

- Detail of structure + ionic **Molecular Dynamics (MD)**

➔ **TDLDA-MD : coupled non adiabatic electrons + ions dynamics**

Model (cluster/molecule)

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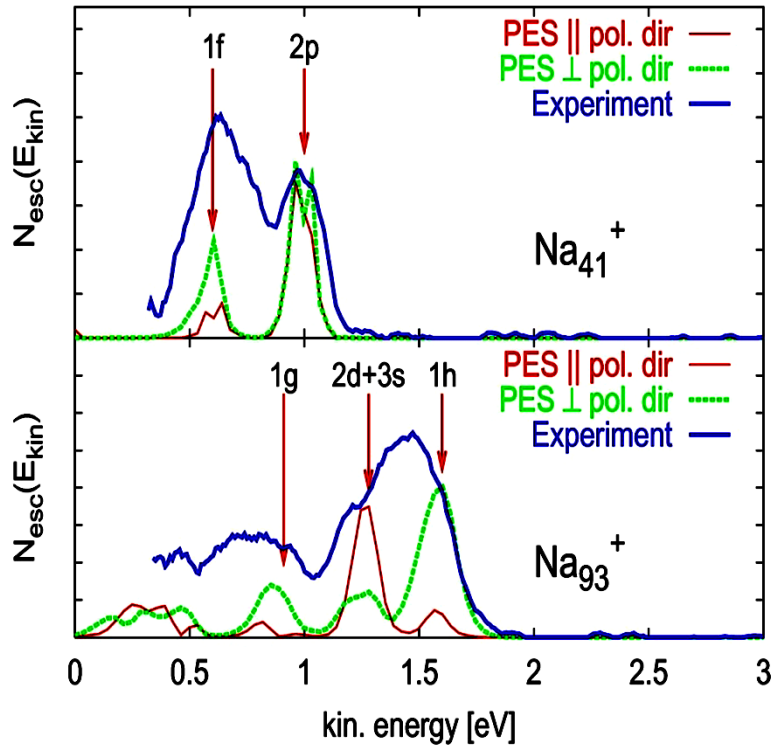
fs

ps



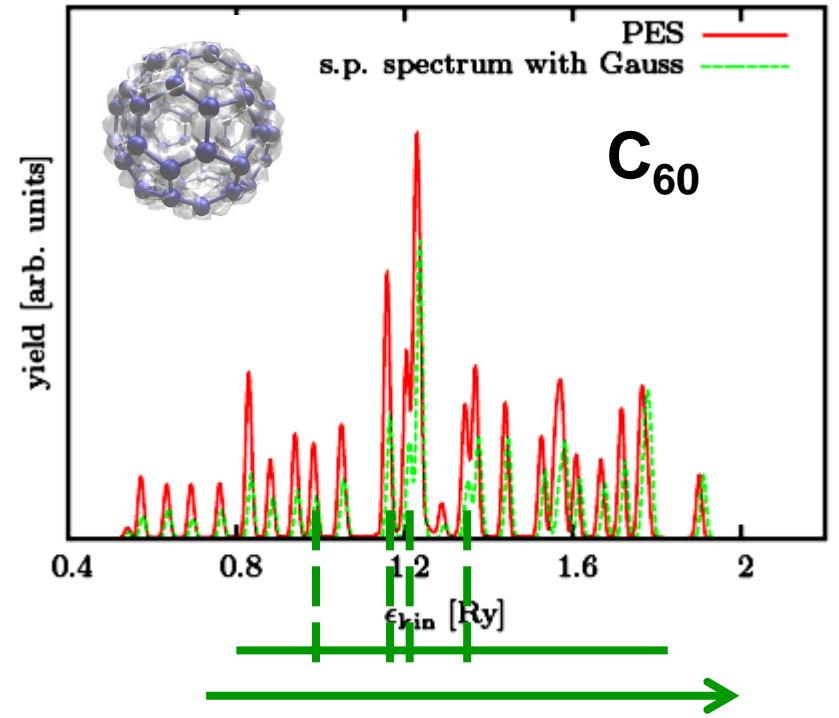
TDLDA-MD : coupled non adiabatic electrons + ions dynamics

Photoelectron Spectroscopy (PES)



Pohl et al, PRA 2003

Exp. Freiburg



Electron spectrum + $\omega = 2.5$ Ry

Th/Exp : IP, HOMO-LUMO 5%



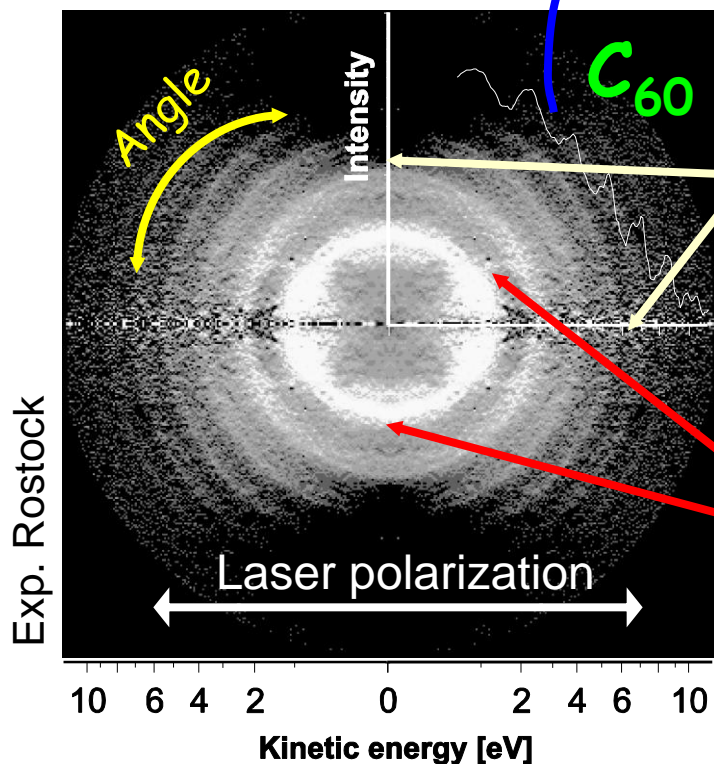
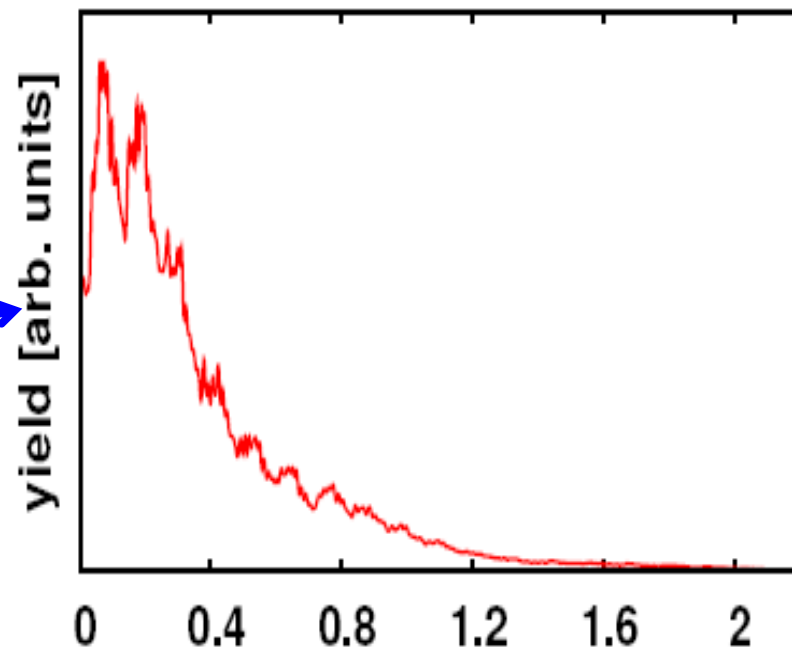
Spectroscopic accuracy
Dynamical features

Energy resolved angular distributions

The orientation Problem...

Angle-energy correlation

$$\rightarrow d\sigma/d\Omega dE$$



Directed emission

Isotropic emission

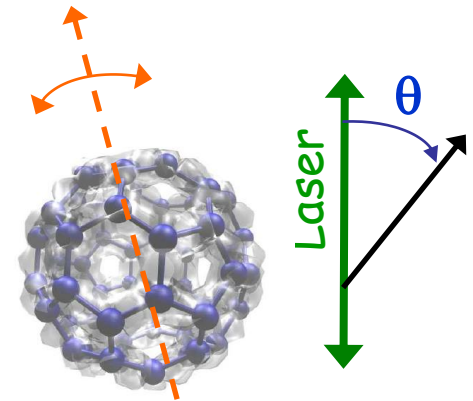
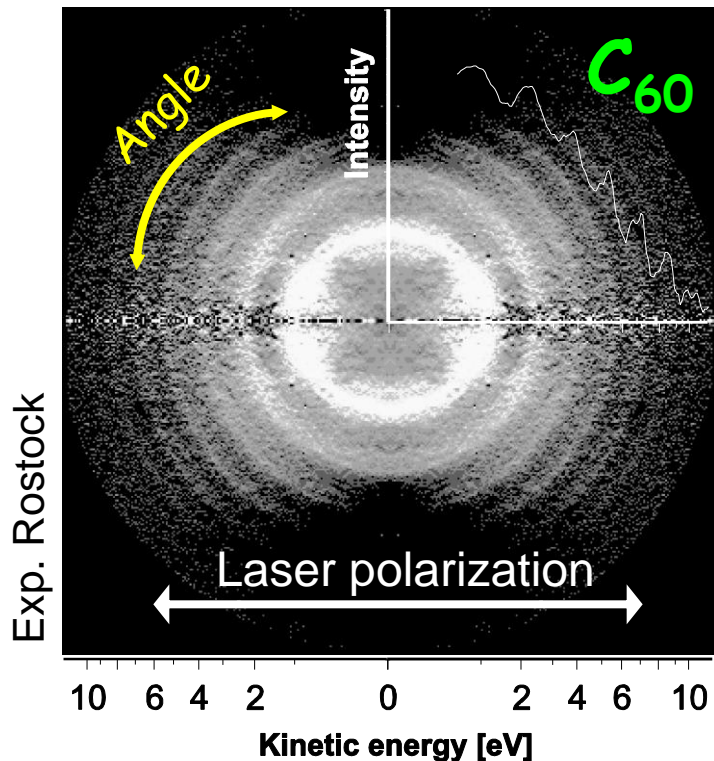


Energy resolved angular distributions

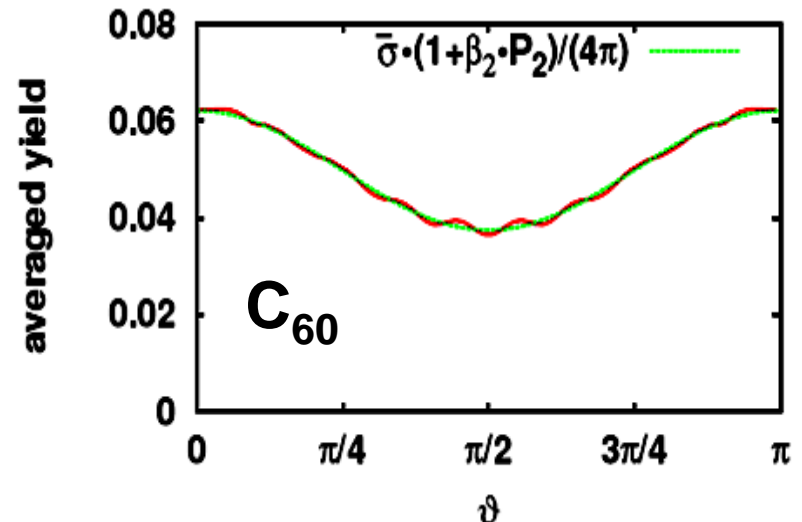
The orientation Problem...

Angle-energy correlation

→ $d\sigma/d\Omega dE$



Anisotropy parameter β_2
 $d\sigma/d\theta \propto 1 + \beta_2 P_2(\cos \theta)$



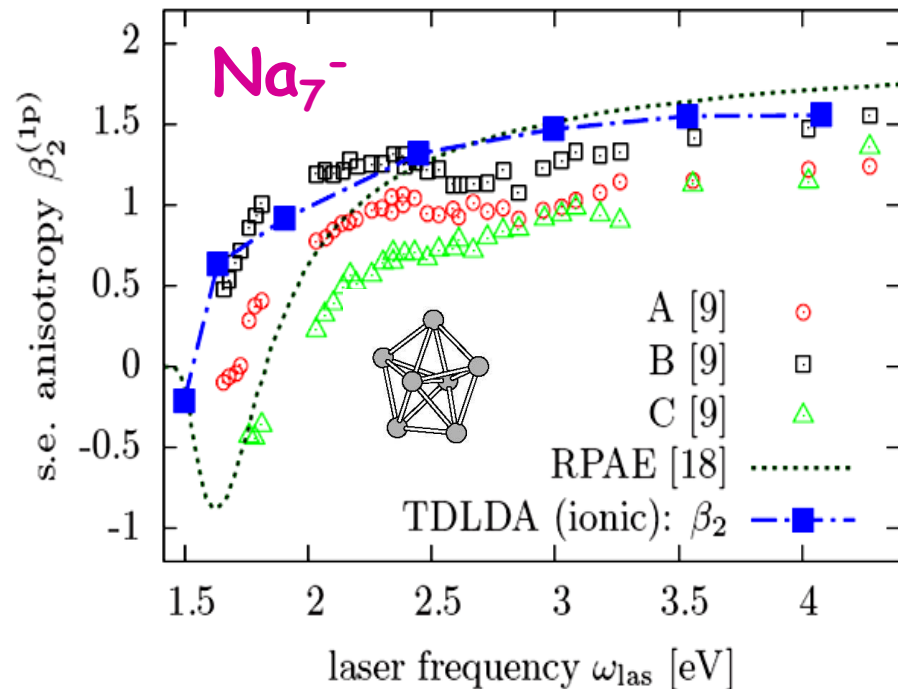
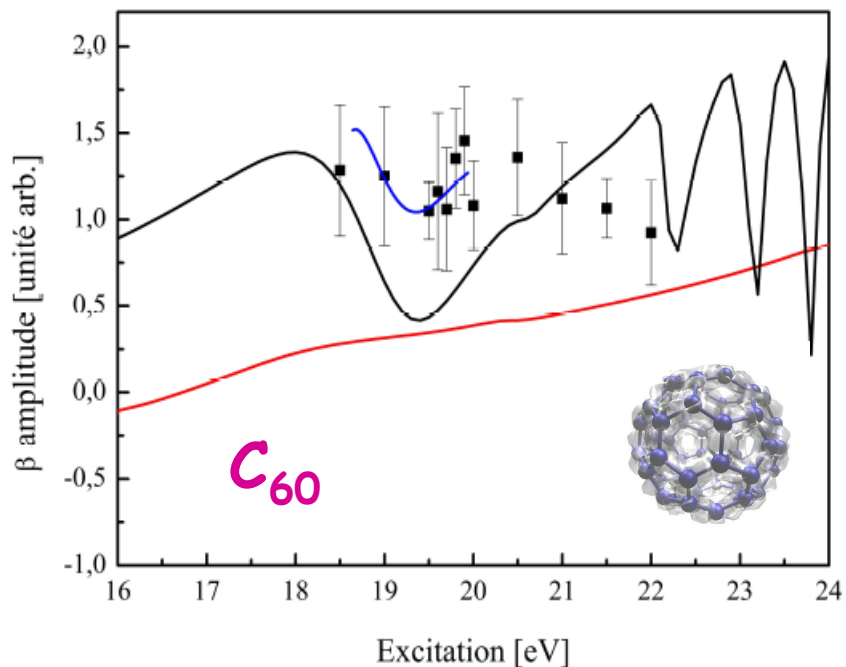
Th/Exp : $\beta_2 \sim 5\%$

↪ | Good agreement ! (?)

Laser frequency dependence of PAD

Anisotropy parameter β_2 as a function of laser frequency ω

Exp. Lyon



Exp. Freiburg

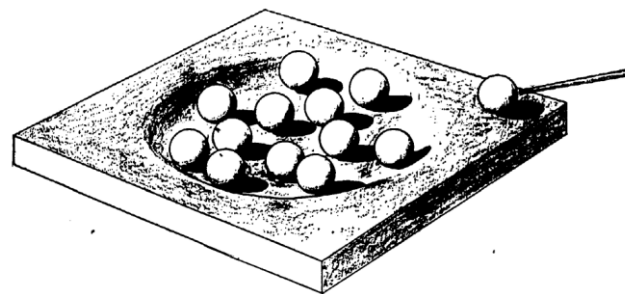


Extremely sensitive observable $\beta_2(\omega)$

Requires a highly elaborate theory

Towards Inclusion of Dissipation in TDDFT

neutron on nucleus



N. Bohr, Science, 1937

To do list (~exp.)

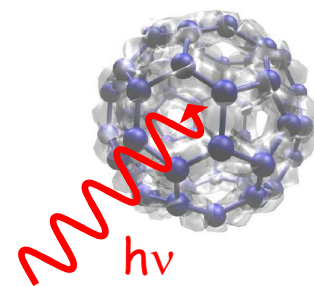
Cart (~theo.)

Photo Electron Spectra PES

Exponential slope

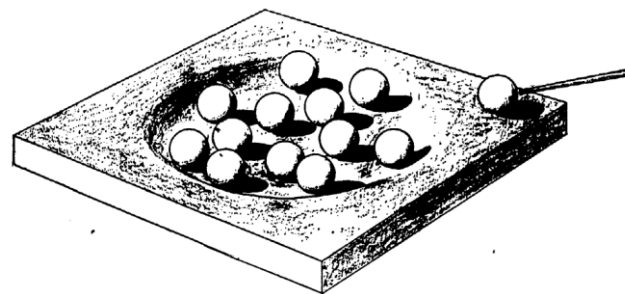
Photo Angular Distribution PAD

Isotropic



Towards Inclusion of Dissipation in TDDFT

neutron on nucleus



N. Bohr, Science, 1937

To do list (~exp.)

Cart (~theo.)

Photo Electron Spectra PES

Spectroscopic signal

Exponential slope

... not specific

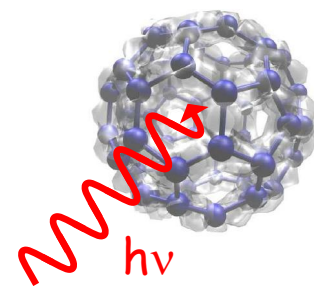
Photo Angular Distribution PAD

« Complex » signal

Isotropic

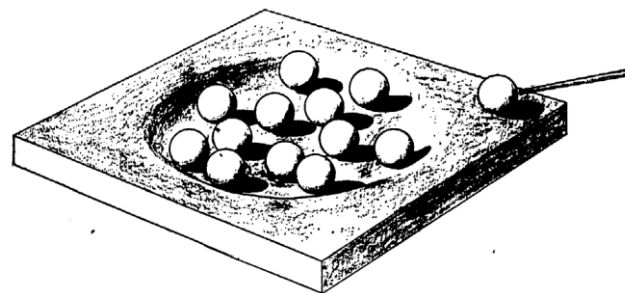
Orientation average

Laser frequency depend.



Towards Inclusion of Dissipation in TDDFT

neutron on nucleus



N. Bohr, Science, 1937

To do list (~exp.)

Cart (~theo.)

Photo Electron Spectra PES

Spectroscopic signal

TDLDA

→ Exponential slope
... not specific

~~X~~

Photo Angular Distribution PAD

« Complex » signal

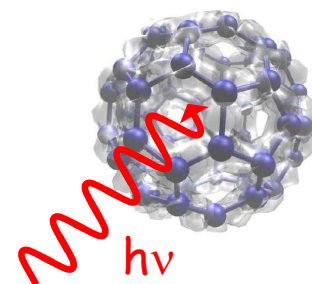
TDLDA

→ Isotropic
Orientation average
Laser frequency depend.

~~X~~


TDLDA

TDLDA



Vlasov and VUU

- Vlasov provides a sound basis for complementing mean-field by dynamical correlations (« Boltzmann-like » collision term)



$i\hbar\dot{\rho} = [h, \rho]$	TDDFT
$\dot{f} = \{h, f\}$	Vlasov
$\dot{f} = \{h, f\} + I_{coll}[f]$	VUU/BUU

- Semi classical kinetic equation (plasmas, nuclear physics...)
- Collision integral

$$I_{coll}[f] \sim \int d\mathbf{p}_2 d\mathbf{p}_3 d\mathbf{p}_4 \delta(\sum \mathbf{p}_i) \delta(\sum \epsilon_i) \frac{d\sigma}{d\Omega} \{f_1 f_2 (1 - f_3)(1 - f_4) - \dots\}$$

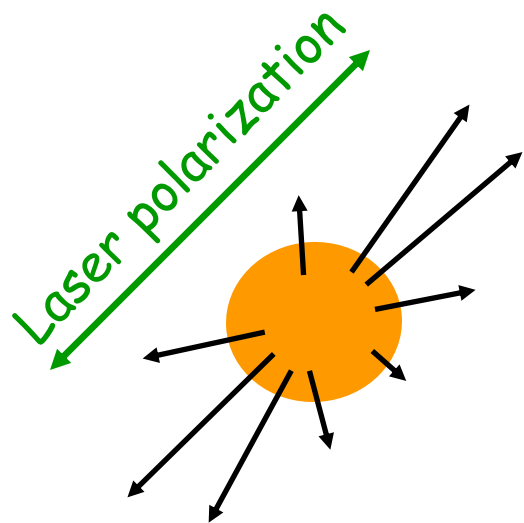
In medium cross section/
Screened Coulomb

Pauli blocking

Numerics : test particles



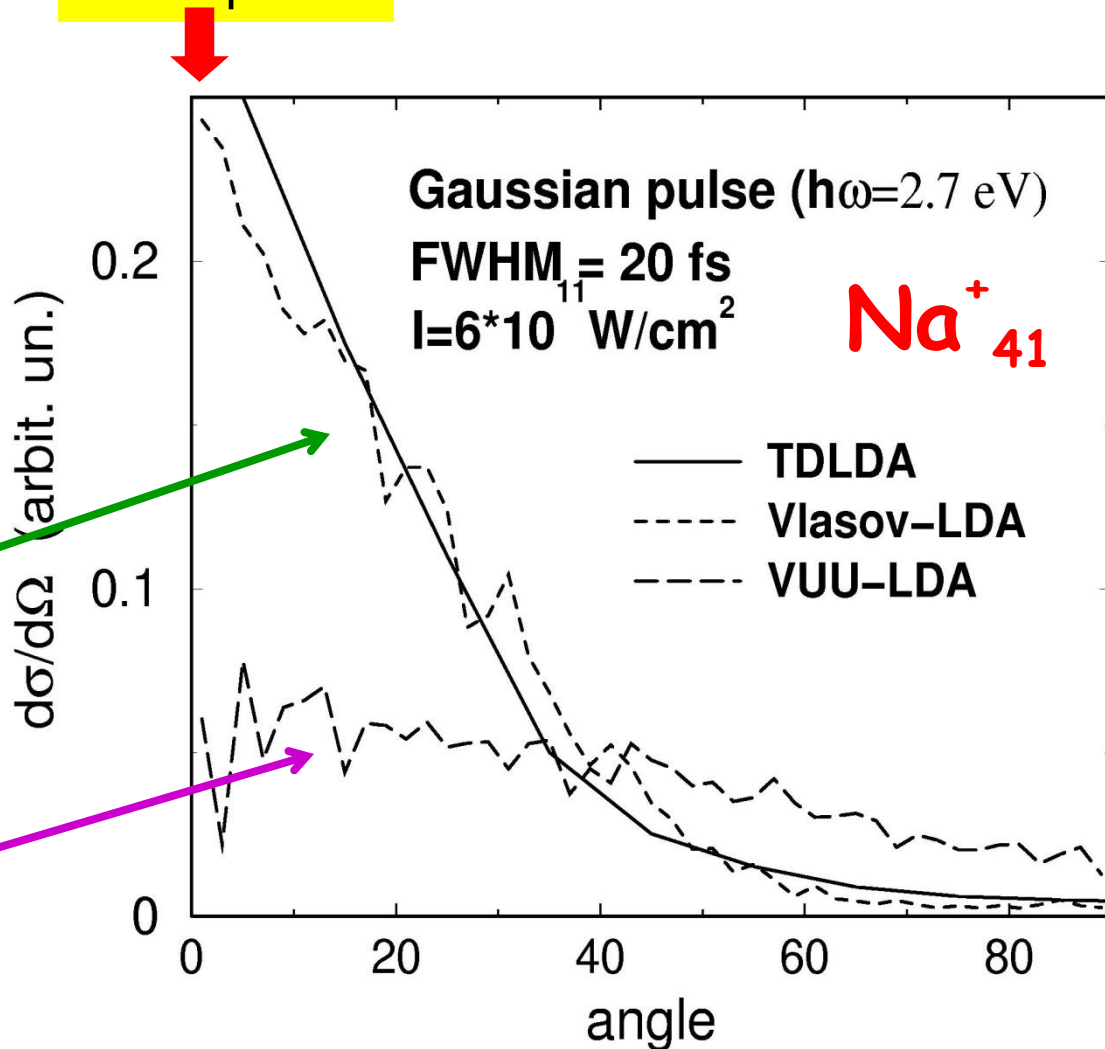
Angular distributions and (thermo)dynamics



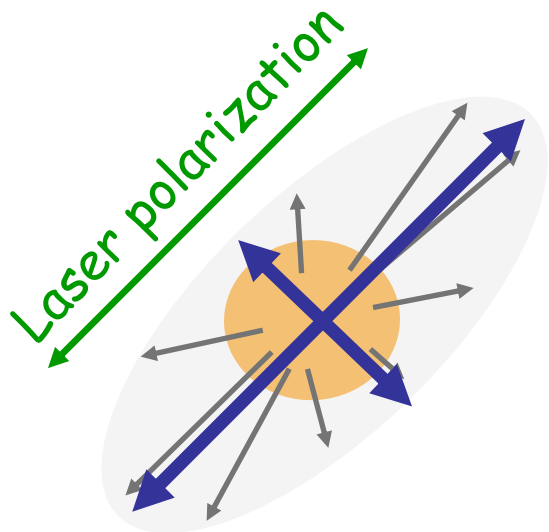
Mean field:
Directed emission

Mean-field + colls :
Isotropic emission

Laser polar.

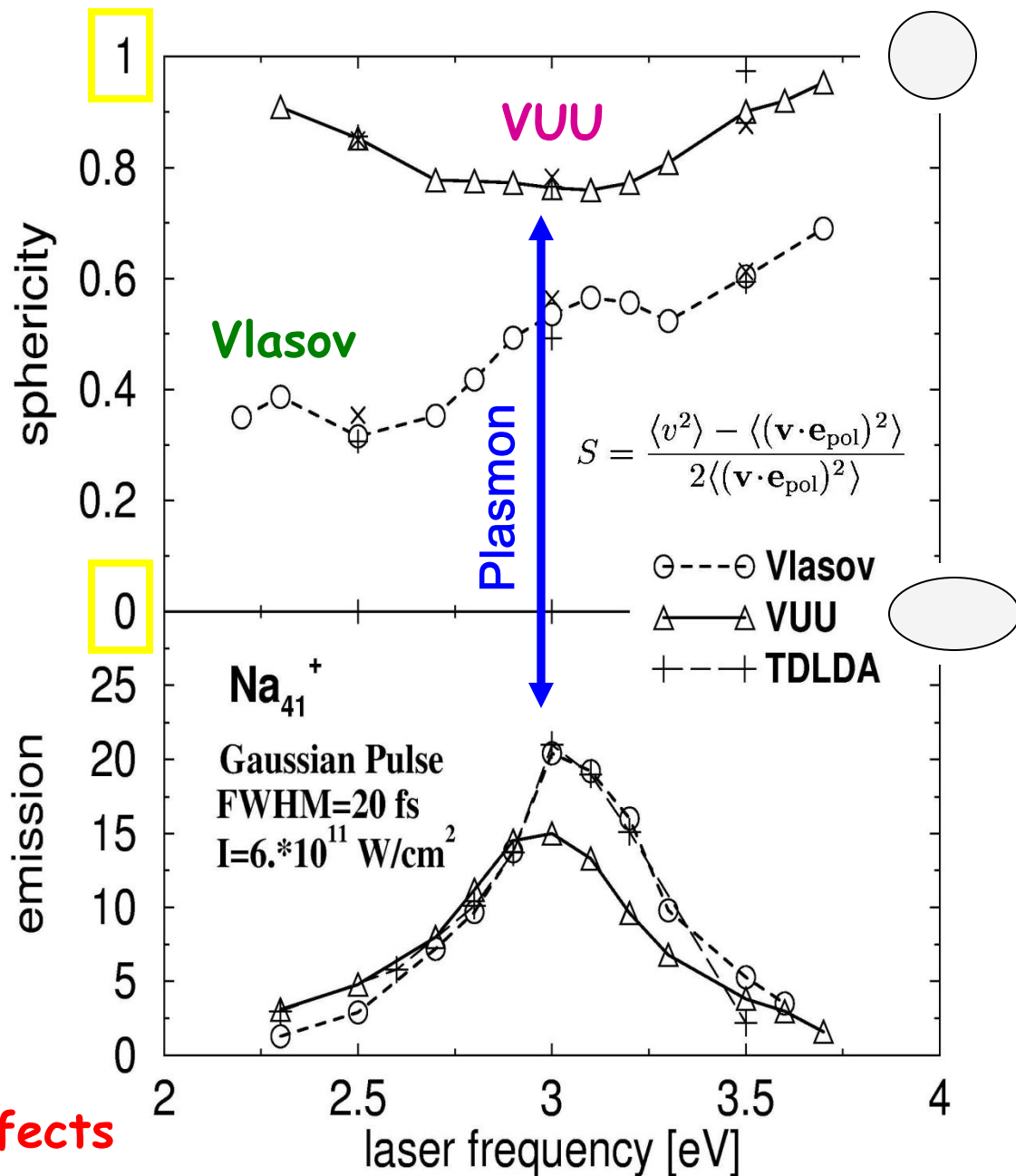


Sphericity analysis



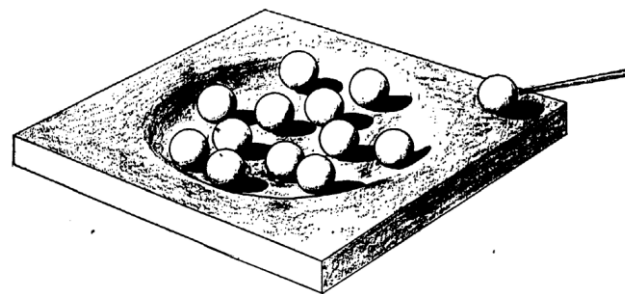
Sphericity:
alignment/laser ($S \sim 0$)
isotropy ($S \sim 1$)

↪ Role of resonance effects
Qualitatively sound



Towards Inclusion of Dissipation in TDDFT

neutron on nucleus



N. Bohr, Science, 1937

To do list (~exp.)

Cart (~theo.)

Photo Electron Spectra PES

Spectroscopic signal

Exponential slope
... not specific

TDLDA

Photo Angular Distribution PAD

« Complex » signal

Isotropic

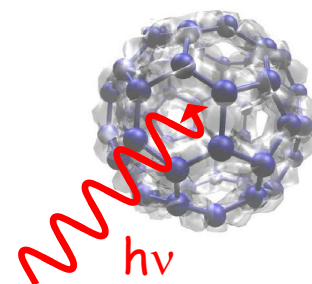
Orientation average

Laser frequency depend.

TDLDA

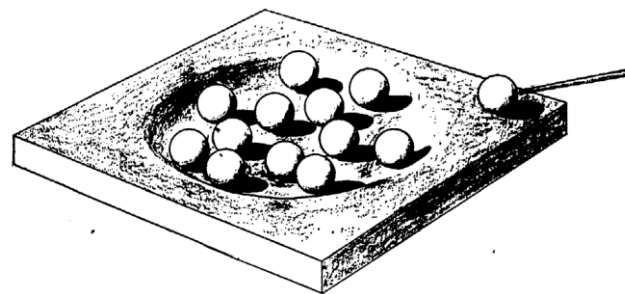
TDLDA

TDLDA



Towards Inclusion of Dissipation in TDDFT

neutron on nucleus



N. Bohr, Science, 1937

To do list (~exp.)

Cart (~theo.)

Photo Electron Spectra PES

Spectroscopic signal

Exponential slope
... not specific

VUU

TDLDA

Photo Angular Distribution PAD

« Complex » signal

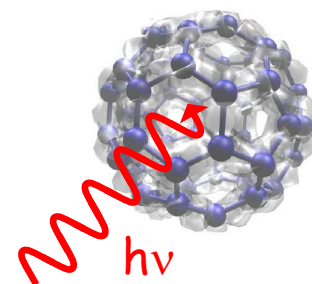
Isotropic
Orientation average
Lqser frequency depend.

VUU

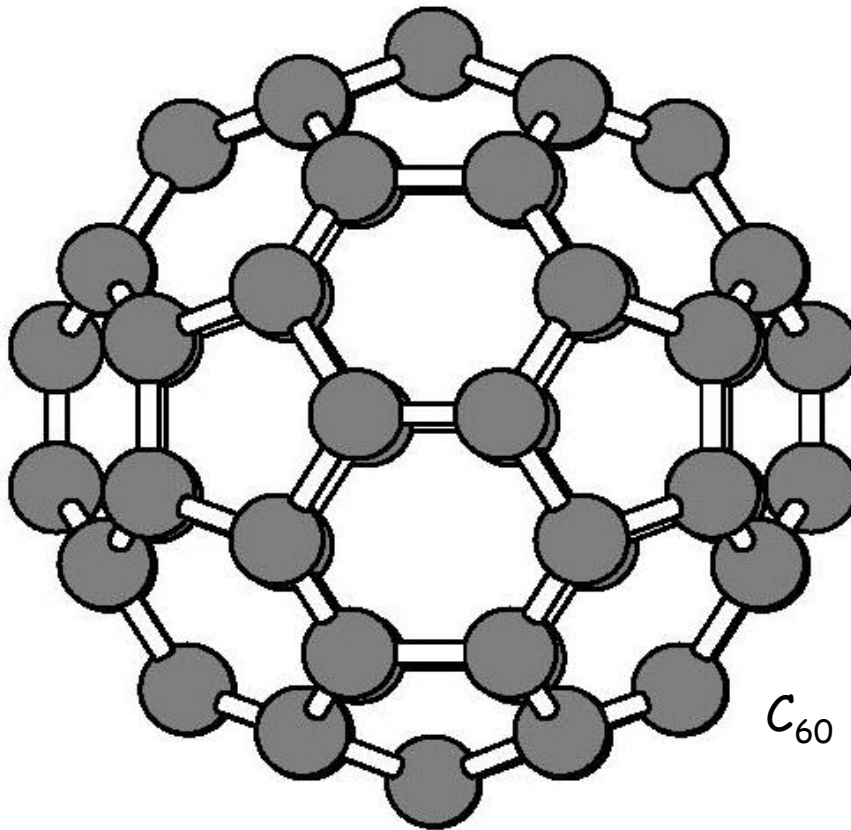
TDLDA

TDLDA

TDLDA



But...



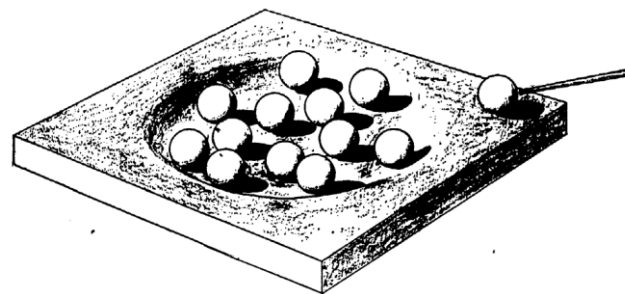
How to compute a
realistic
semi-classical
C₆₀?

Remind
Carbon atom
with
s and p states
Carbon
double and triple
bonds...

Well,
it just
does not work!

Towards Inclusion of Dissipation in TDDFT

neutron on nucleus



N. Bohr, Science, 1937

To do list (~exp.)

Cart (~theo.)

Photo Electron Spectra PES

Spectroscopic signal

Exponential slope
... not specific

VUU

TDLDA

Photo Angular Distribution PAD

« Complex » signal

Isotropic

Orientation average

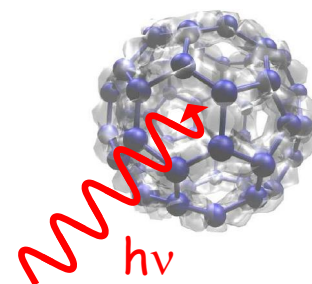
Lqser frequency depend.

VUU

TDLDA

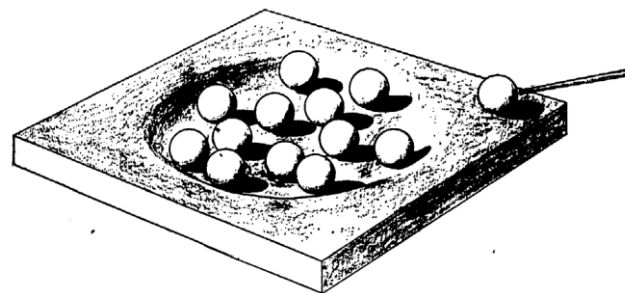
TDLDA

TDLDA



Towards Inclusion of Dissipation in TDDFT

neutron on nucleus



N. Bohr, Science, 1937

To do list (~exp.)

Cart (~theo.)

Photo Electron Spectra PES

Spectroscopic signal

Exponential slope
... not specific

VUU

TDLDA

Photo Angular Distribution PAD

« Complex » signal

Isotropic

Orientation average

Lqser frequency depend.

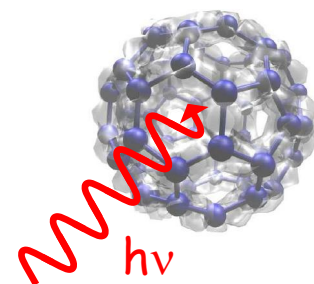
VUU

TDLDA

TDLDA + τ

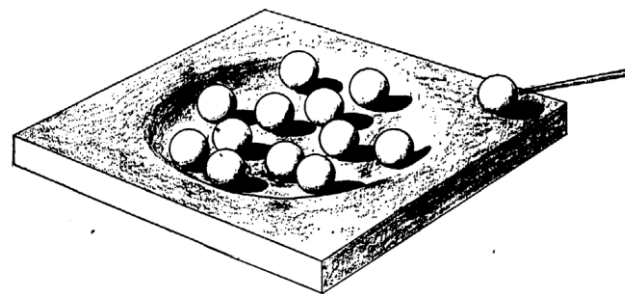
TDLDA

TDLDA



Towards Inclusion of Dissipation in TDDFT

neutron on nucleus



N. Bohr, Science, 1937

To do list (~exp.)

Cart (~theo.)

Next steps

Photo Electron Spectra PES

Spectroscopic signal

TDLDA

Exponential slope
... not specific

VUU

TDLDA + colls.

Photo Angular Distribution PAD

« Complex » signal

TDLDA

Isotropic

VUU

TDLDA + colls.

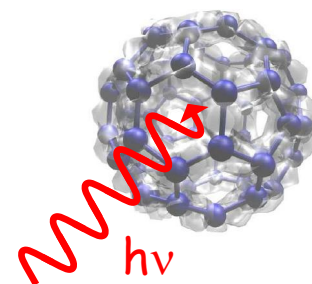
Orientation average

TDLDA

Lqser frequency depend.

TDLDA

Ions...





Thank you

for your

attention

« Palm tree »
Jacobins church, Toulouse

Thank you too...
to

People

P. G Reinhard
P. M. Dinh
P. Romaniello
P. Wopperer
F. Lépine
J. M. Escartin



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