Processus Compton stimulé à deux couleurs en champ X intense et bref

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SFP 2023

Compton Scattering – 100 years

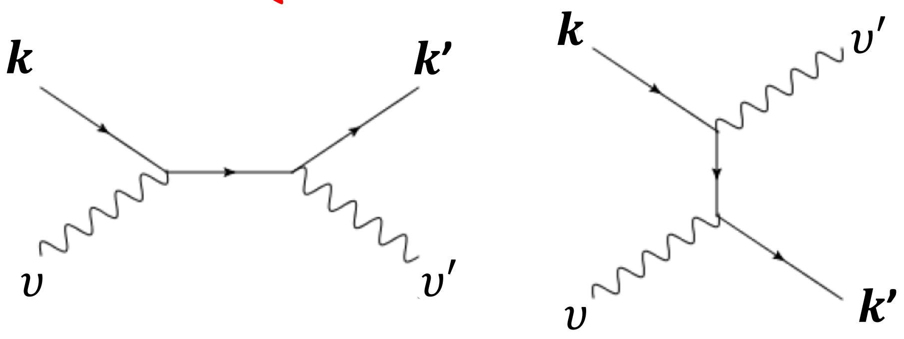
Classical view point (relativistic)

$$\lambda_s - \lambda -= \frac{h}{mc}\left(1 - Cos(\theta)\right) = \lambda_c\left(1 - Cos(\theta)\right)$$

A Quantum Theory of the Scattering of X-rays by Light Elements
A. H. Compton *Phys. Rev.* **21**, 483-502 (1923)

λ_c= 0,0024 nm = 500keV

Quantum version QED



Same result as for the classical calculation

Quantum version « classical »

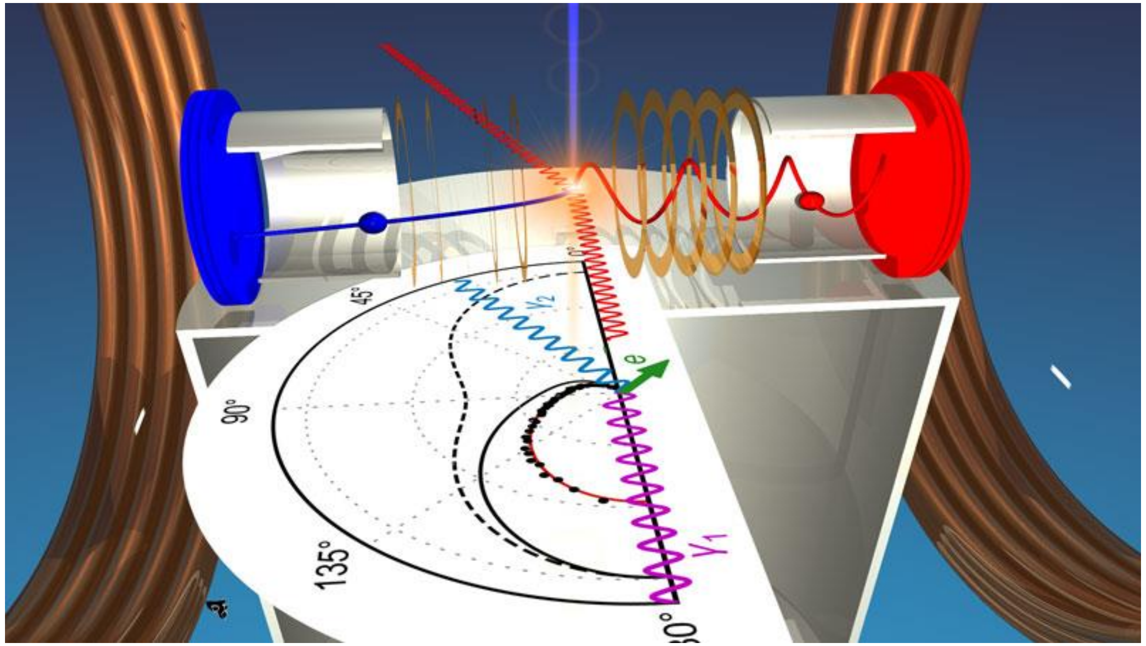
$$T = \int d\tau \, \langle \boldsymbol{k}, \tau | \boldsymbol{A}_s(\boldsymbol{r}, \tau) . \boldsymbol{A}_0(\boldsymbol{r}, \tau) | 0, \tau \rangle$$

We assume $\frac{\delta\lambda}{\lambda} \ll 1 \Leftrightarrow \lambda_c \ll \lambda$

Provides the same result as for the other approaches

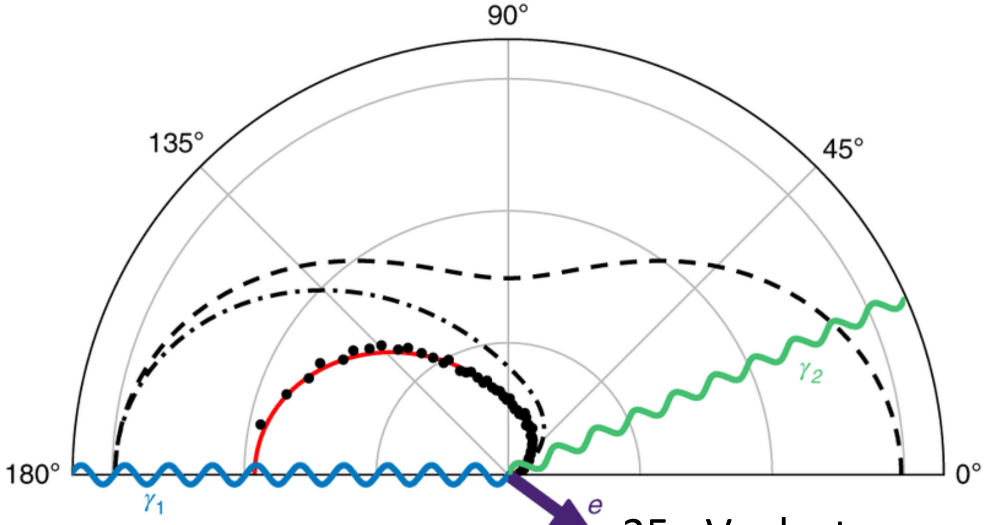
Compton scattering – PES

COLTRIM – Coincidence measurement electron/ion



$h\nu$ =2,5 keV
P04 beamline at PETAIII,DESY

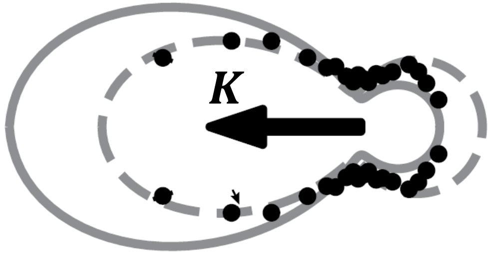
M. Kircher *et al.* Nature Physics **16**, 756–760 (2020)



25 eV; electron energy

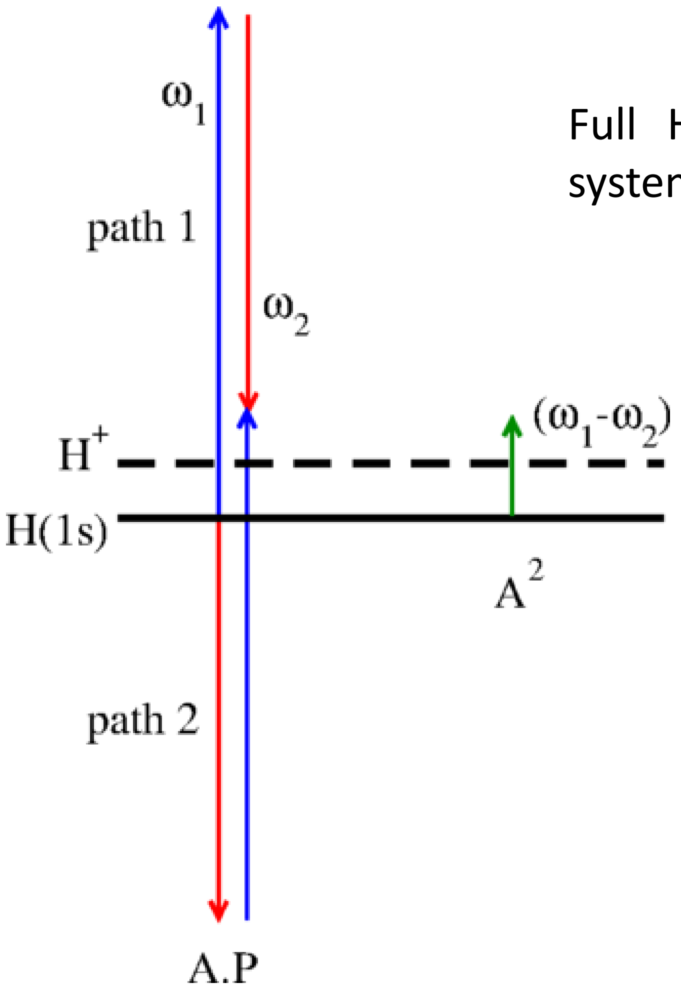
$$T = \int d\tau \, \langle \boldsymbol{k}, \tau | \boldsymbol{A}_s(\boldsymbol{r}, \tau) . \boldsymbol{A}_0(\boldsymbol{r}, \tau) | 0, \tau \rangle$$

Polar plot in the frame of the photon-momentum transfer $\boldsymbol{K}$



Angular asymetry due to the momentum transfer

Stimulated Compton Scattering
Application to H



H. Bachau *Phys. Rev. Lett.* **112**, 073001 (2014)

Full Hamiltonian of the system including the field $\mathcal{H} = H_{at} + \boldsymbol{A}(\boldsymbol{r},t).\boldsymbol{P} + \frac{1}{2}\boldsymbol{A}^2(\boldsymbol{r},t)$ $\quad \boldsymbol{\nabla}.\mathbf{A} = 0$

$\boldsymbol{A}(\boldsymbol{r},t) = \boldsymbol{A}_1(\boldsymbol{r},t) + \boldsymbol{A}_2(\boldsymbol{r},t)$ Total field is the sum of the two fields

$\boldsymbol{A}_i(\boldsymbol{r},t) = A_i(t - \alpha\boldsymbol{n}_i.\boldsymbol{r})\boldsymbol{e}_z \approx (A_i(t) + \alpha F_i(t)\boldsymbol{n}_i.\boldsymbol{r})\boldsymbol{e}_z$ Non-dipole contribution

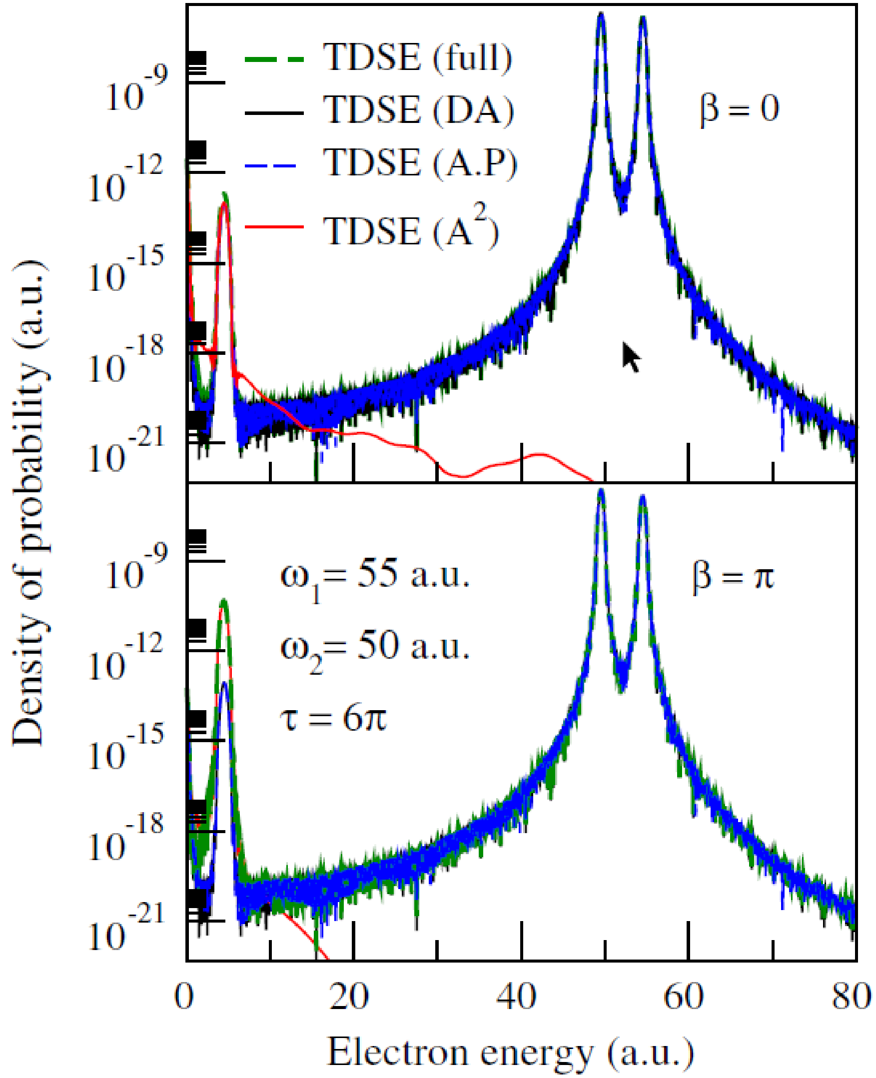
$$\mathcal{H} = H_{at} + H_{DA} + H_{RET}^{AP} + H_{RET}^{A^2}$$

$$H_{DA} = \mathrm{A(t)}\mathbf{P}.\boldsymbol{e}_z \quad H_{RET}^{AP} = \alpha\boldsymbol{F}_{pol}(t).\mathbf{rP}.\boldsymbol{e}_z \quad H_{RET}^{A^2} = \alpha\boldsymbol{F}_{prop}(t).\mathbf{r}\mathrm{A(t)}$$

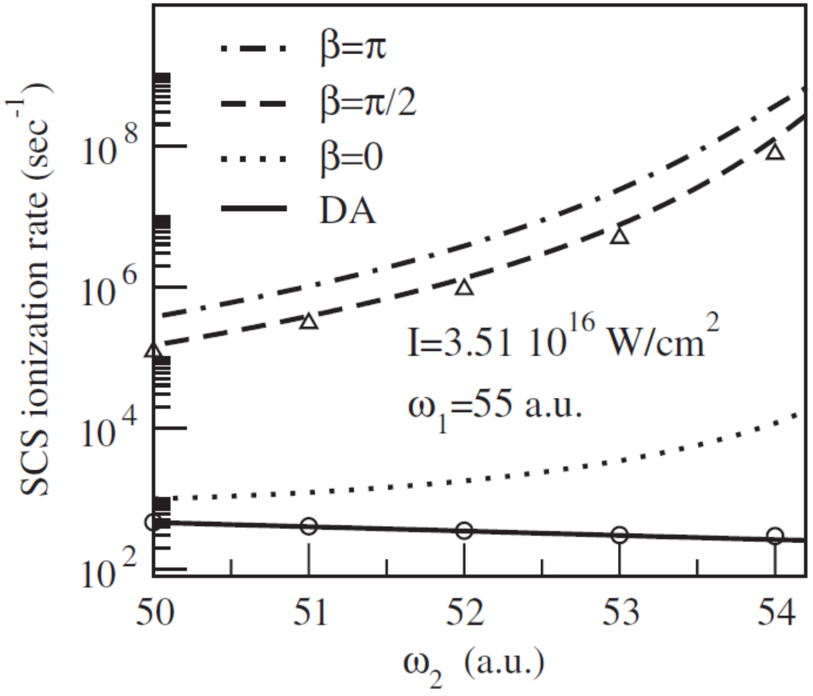
The eigenstates of the field-free Hamiltonian are computed (bound and continnum) to generate the coupling matrix of the field operator. The **Time Dependent Schrödinger equation** is then solved **numerically** in the Interaction picture.

Stimulated Compton Scattering

Two-Color Ionization of H in keV regime



$\beta = \widehat{\boldsymbol{n}_1, \boldsymbol{n}_2}$

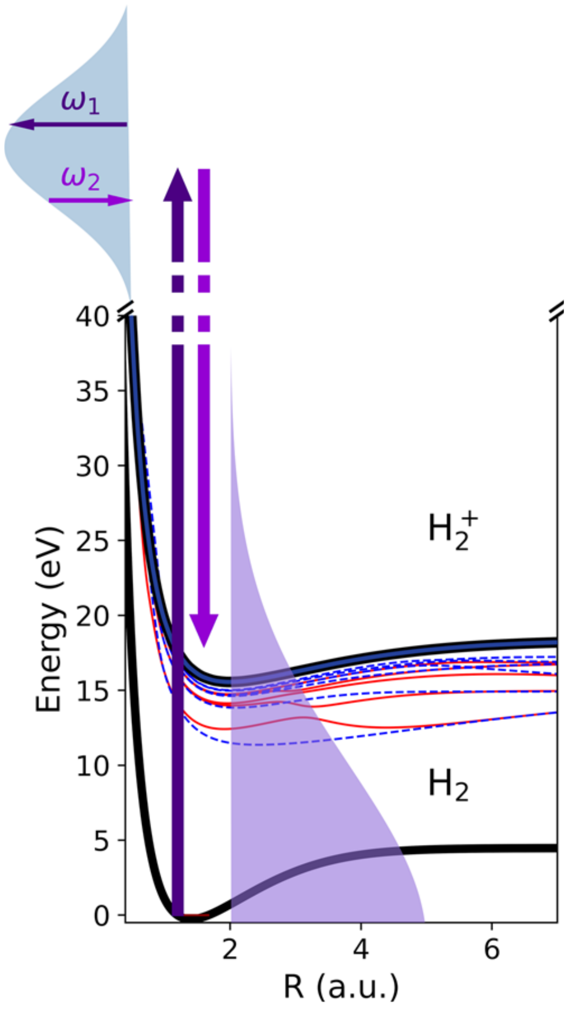


Field parameters

ω_1 = 55 a.u. (1496 eV)
ω_2 = 50 a.u. (1360 eV)
$\tau_1 = \tau_2$ = 6π a.u. (452 as)
$I_1 = I_2 = I_0$, where $I_0 \approx 3.51 \times 10^{16}$ W/cm^2.

Same behavior for most atoms investigated in particular for the angular distribution. Is it a universal pattern?

Stimulated Compton Scattering in H_2



A. Sopena *Phys. Rev. A* **105**, 033104 (2022)

A. Sopena *Nat. Com.* **4**, 253 (2021)

Selection rules in the molecule due to the different channels:

- A.P contributions

$$X^1\Sigma_g^+ \xrightarrow{\epsilon_z} {}^1\Sigma_g^+$$

$$X^1\Sigma_g^+ \xrightarrow{\epsilon_x/\epsilon_y} {}^1\Sigma_g^+,\ {}^1\Delta_g$$

Axis of quantization : polarisation axis

- A^2 contributions

$$X^1\Sigma_g^+ \xrightarrow{n_z} {}^1\Sigma_u^+$$

$$X^1\Sigma_g^+ \xrightarrow{n_x/n_y} {}^1\Pi_u.$$

Axis of quantization : propagation axis

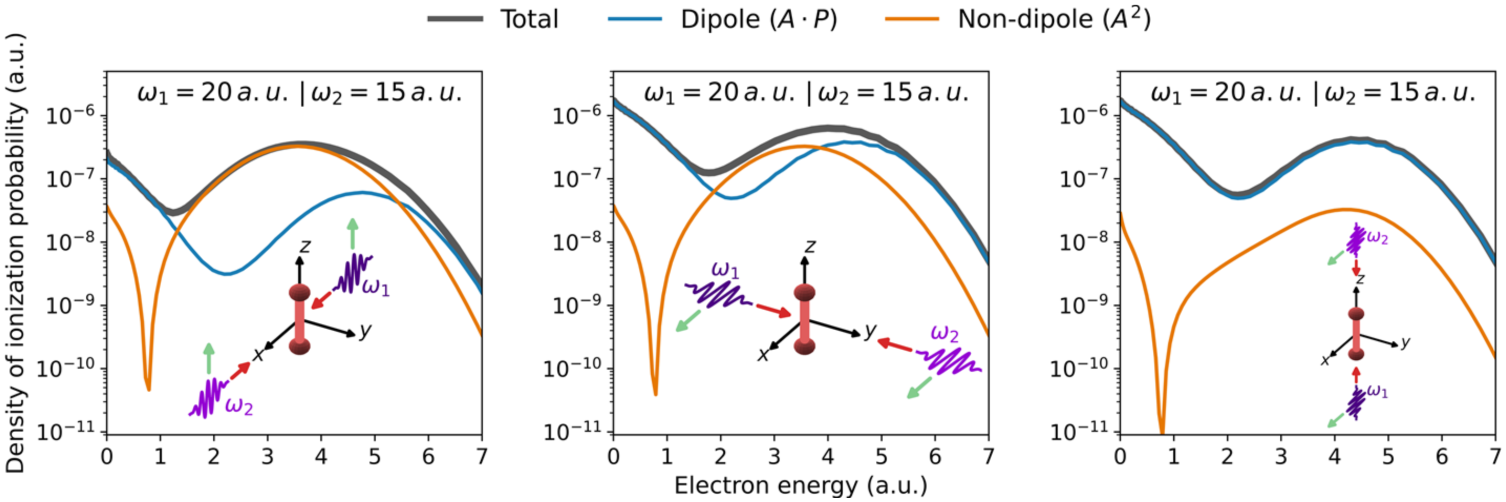
Angle integrated energy distribution + MFPAD in H_2

Two-pulse configuration

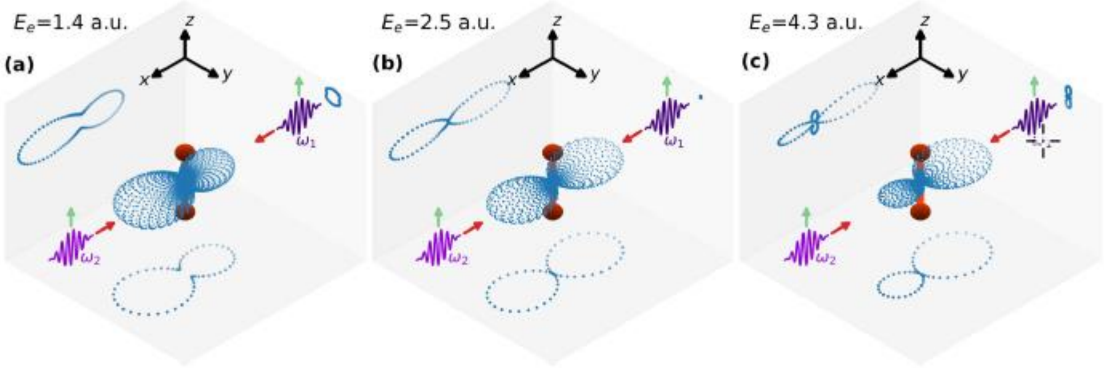
ω_1 = 20 a.u. (544 eV) and ω_2 =15 a.u. (408 eV)

$\tau_1 = \tau_2$ = 200 as

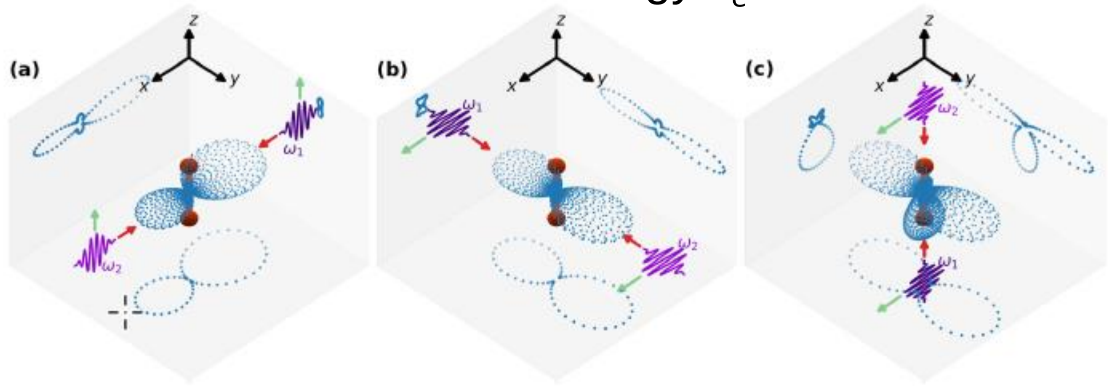
$I_1 = I_2 = 10^{18}$ W/cm^2



Fixed field configuration



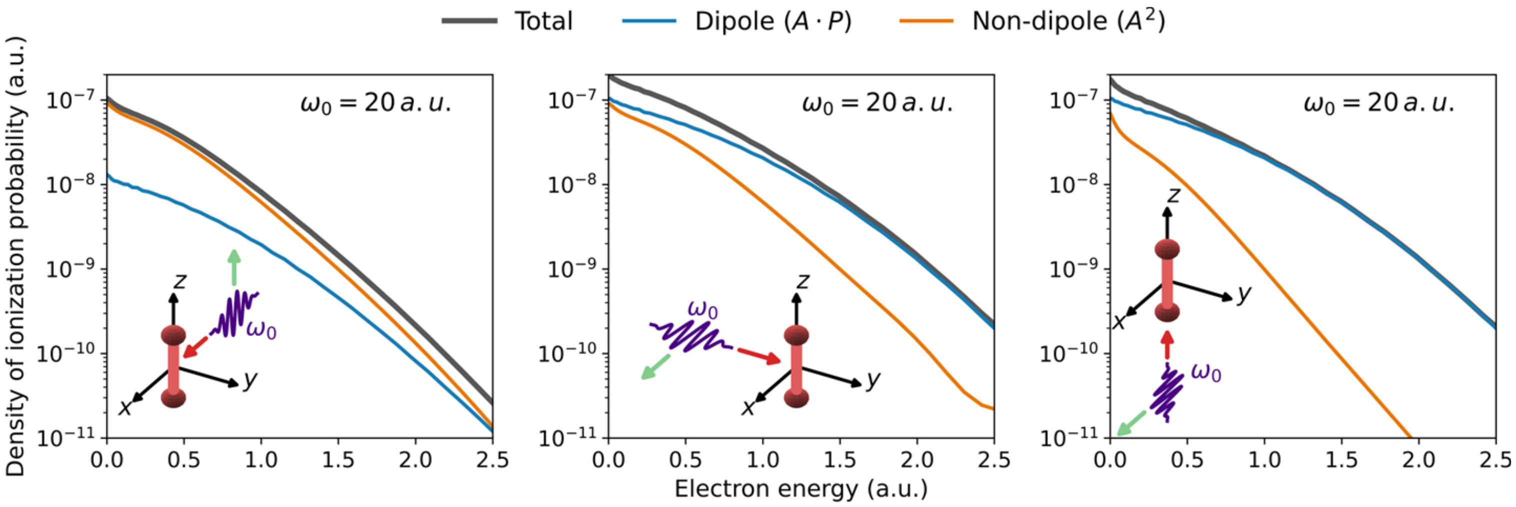
Fixed electron energy E_e = 4 a.u.



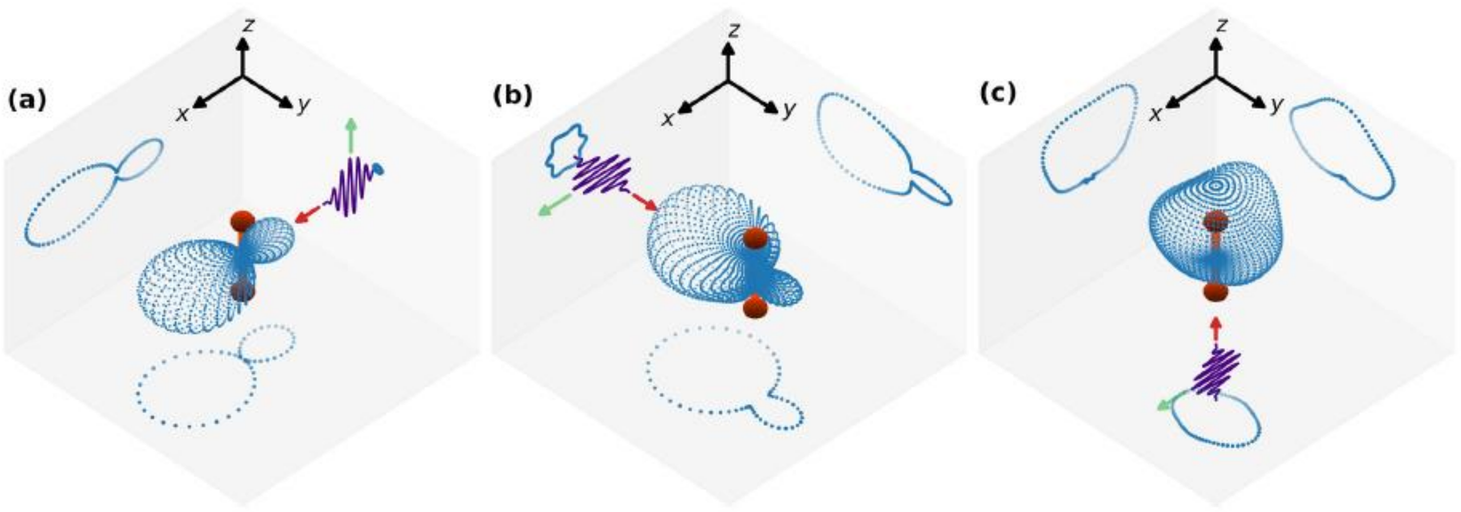
Angle integrated energy distribution + MFPAD in H_2

One-pulse configuration

ω = 20 a.u. (544 eV)
τ = 200 as
I = 10^{18} W/cm^2



E_e = [0, 1.4] a.u.



Conclusion and prospective

- We show the quantum nature of the process and in particular that the usual picture of momentum absorption is not sufficient + complex pattern in the molecular case

- Usage very intense X-ray pulses and ultrashort for intraband processes (The advance of FEL source allows for such configurations)

What's next ?

- Include more terms of the Taylor expansion and include the spin in the dynamics … under going

- Study the case of more complex fields in particular dichroism

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Modèle TDPT

Cross-section $$\frac{d\sigma}{dE_e d\Omega_e d\Omega_2} = r_e^2 p_e t |M|^2$$

With amplitude transition $$M(\mathbf{Q}, \mathbf{p}_e) = (\mathbf{e}_1 \cdot \mathbf{e}_2)\langle \Psi_{\mathbf{p}_e}^{(-)} | \sum_{j=1}^{N} e^{i\mathbf{Q}\cdot\mathbf{r}_j} | \Psi_0 \rangle$$

And final wave function $$\tilde{\Psi}_{\mathbf{p}_e}^{(-)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}\left[\psi_{\mathbf{p}_e}^{C}(\mathbf{r}_1)\psi_0^{\mathrm{He}^+}(\mathbf{r}_2) + \psi_{\mathbf{p}_e}^{C}(\mathbf{r}_2)\psi_0^{\mathrm{He}^+}(\mathbf{r}_1)\right]$$

For unpolarized field $$\frac{d\sigma}{dE_e d\Omega_e d\Omega_2} = \left(\frac{d\sigma}{d\Omega_2}\right)_{\mathrm{Th}} p_e t |M_e|^2$$ With $$\left(\frac{d\sigma}{d\Omega_2}\right)_{\mathrm{Th}} = \frac{1}{2} r_e^2 (1 + \cos^2\theta)$$

$$M_e(\mathbf{Q}, \mathbf{p}_e) = \langle \Psi_{\mathbf{p}_e}^{(-)} | \sum_{j=1}^{N} e^{i\mathbf{Q}\cdot\mathbf{r}_j} | \Psi_0 \rangle$$

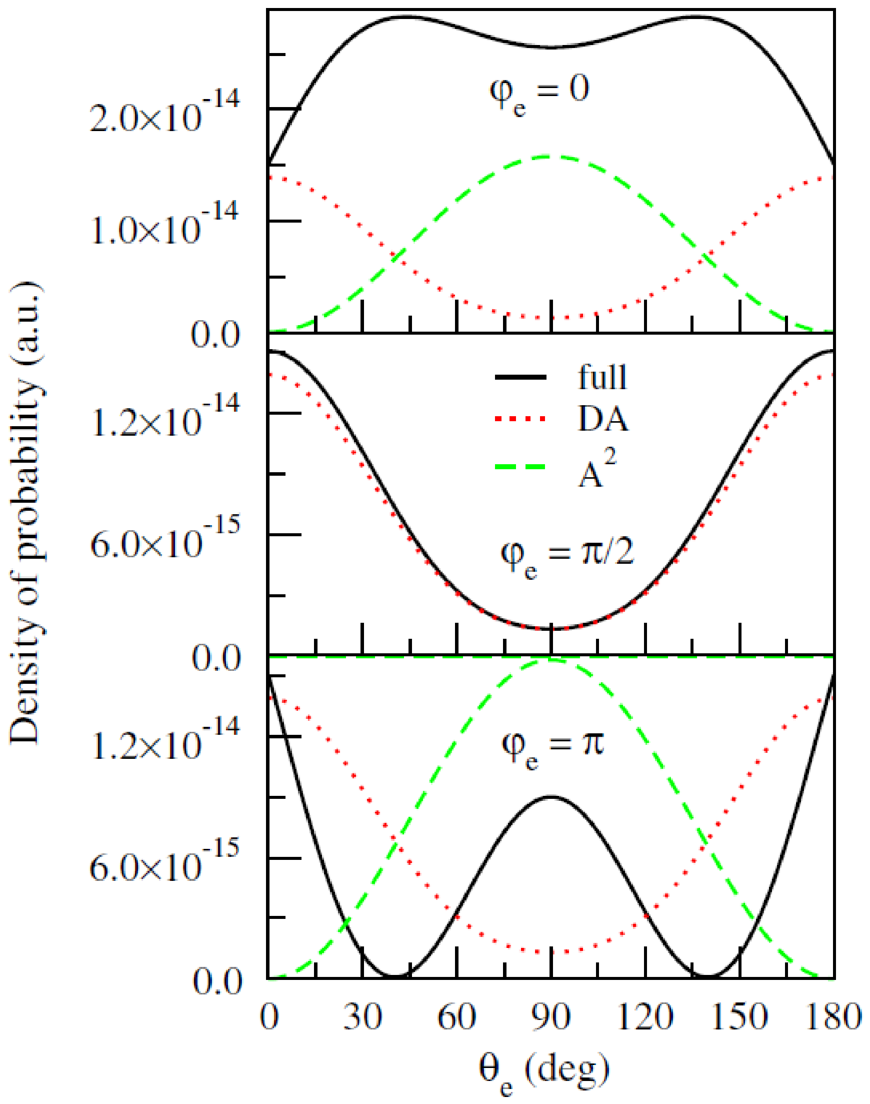
Modèle TDSE

- The wave function is expanded on a basis of 6880 correlated two-electron states described as linear combinations of anti-symmetrized products of H_2^+ orbitals

- The ionic orbitals wave function is represented in a basis of radial B-spline functions and spherical harmonics ($\ell_{max} = 16$) and a radial box size of up to 60 a.u.

- The total wf includes 280 of these functions. The typical number of configurations used for continuum states is 280 and for bound states, it varies between 390 and 700. The continuum states included in the expansion satisfy the proper incoming scattering boundary conditions

- The TDSE is solved using an RK4 predictor-corrector propagator.



Density of probability (a.u.)
2.0×10^-14
1.0×10^-14
0.0
φe = 0
1.2×10^-14
6.0×10^-15
0.0
full
DA
A^2
φe = π/2
1.2×10^-14
6.0×10^-15
0.0
φe = π
0
30
60
90
120
150
180
θe (deg)