Acceleration and twisting of neutral atoms by laser fields

V.S. Melezhik

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SOUTH AFRICA - JINR Workshop, 23 - 27 June 2025, Dubna, Russia

hydrogen atom + EM pulse

- **Nondipole effects (NDE) in interaction of atoms with short-wave EM radiation**

- **NDE → nonseparability of CM and electron variables**
  → 6D Schr. Eq.

hydrogen atom + EM pulse

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  Quantum-quasiclassical method → **6D Schr. Eq.**

hydrogen atom + EM pulse

- Nondipole effects (NDE) in interaction of atoms with short-wave EM radiation

- NDE → nonseparability of CM and electron variables → 6D Schr. Eq.

  Quantum-quasiclassical method → 6D Schr. Eq.

- Acceleration and «twisting» of atoms by circularly polarized EM pulse

  ↓

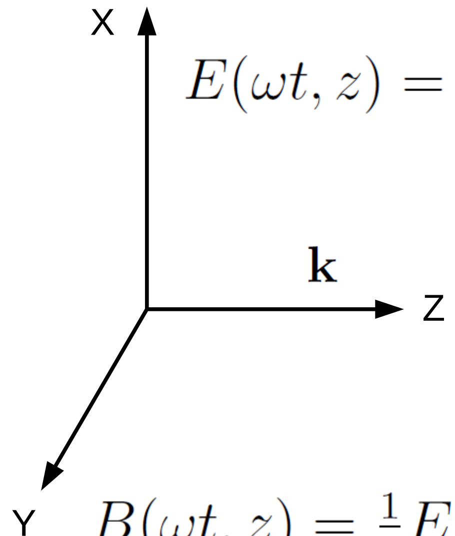
  electron vortex beams to study: chirality, magnetization mapping, transpher of angular momentum to nanoparticls ...

  several proposals to create vortex beams of composite particles (neutrons, protons and atoms)

- Conclusion & perspectives

Non-dipole effects

electromagnetic wave + atom



$$E(\omega t, z) = E_0 \cos(\omega t - kz) = E_0 \cos(\omega t - \frac{\omega}{c} z)$$

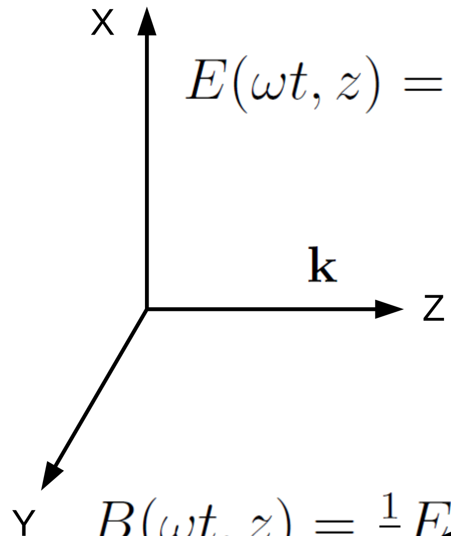
$$B(\omega t, z) = \frac{1}{c} E(\omega t, z) \qquad \frac{1}{c} = \alpha = \frac{1}{137}$$

optical range $\quad \lambda \sim 500\text{nm} \quad \omega \sim 10^{-1} a.u.$

$$\frac{\omega}{c} \simeq \frac{10^{-1}}{137} \to 0$$

Non-dipole effects

electromagnetic wave + atom



$$E(\omega t, z) = E_0 \cos(\omega t - kz) = E_0 \cos(\omega t - \cancel{\tfrac{\omega}{c} z})$$

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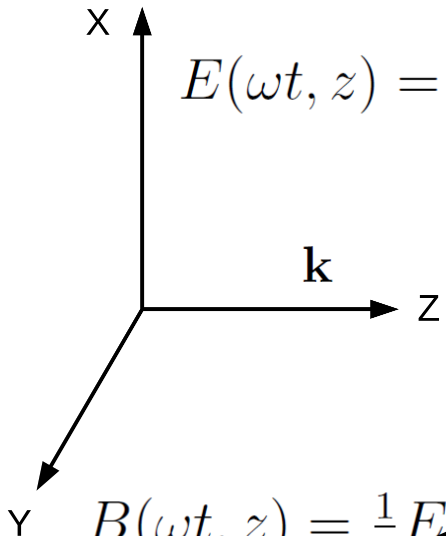
dipole approximation

Non-dipole effects

electromagnetic wave + atom



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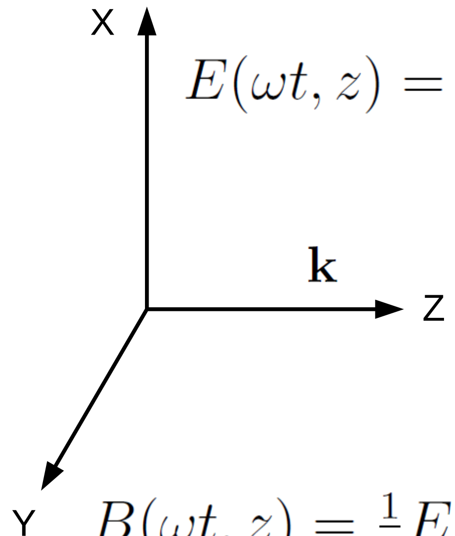
$$\frac{\omega}{c} \simeq \frac{10^{-1}}{137} \to 0$$ dipole approximation

X-ray $\lambda \sim (10^2 - 10^{-3}) nm \quad \omega \sim (1 - 10^4) a.u. \quad \frac{\omega}{c} \sim \frac{1}{137} - 10^2$

Non-dipole effects

electromagnetic wave + atom



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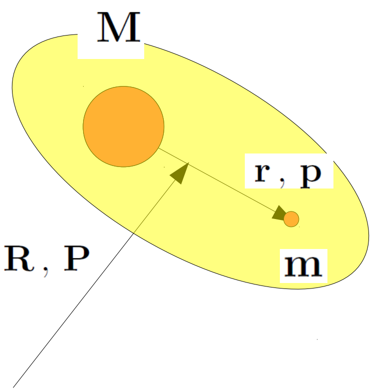
Hydrogen atom in strong laser field (non-dipole effects)



$M \gg m$

$P = MV \gg p = mv$

$$H(\boldsymbol{r},\boldsymbol{R},t) = \frac{\boldsymbol{P}^2}{2M} + h_0(\boldsymbol{r}) + V_1(\boldsymbol{r},t) + V_2(\boldsymbol{r},\boldsymbol{R},t)$$

$$h_0(\boldsymbol{r}) = \frac{\hat{\boldsymbol{p}}^2}{2\mu} - \frac{1}{r}$$

$$V_1(\boldsymbol{r}) = E_0 f(t)\{\cos(\omega t)x + \frac{1}{c}[\cos(\omega t)\hat{l}_y + \omega\sin(\omega t)xz]\},$$

$$V_2(\boldsymbol{r},\boldsymbol{R}) = \frac{1}{c}E_0 f(t)\{\cos(\omega t)[Z\hat{p}_x - X\hat{p}_z] + \omega\sin(\omega t)[xZ + zX]\}$$

Hydrogen atom in strong laser field
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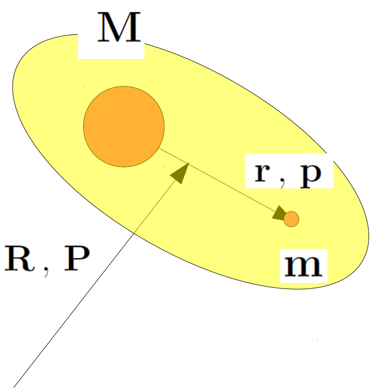

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2D

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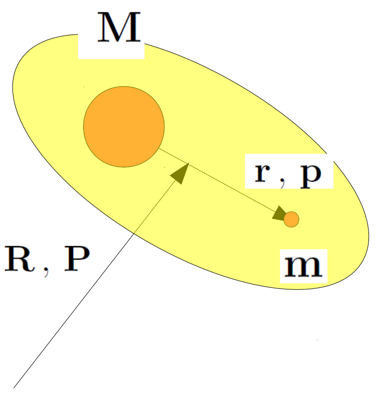

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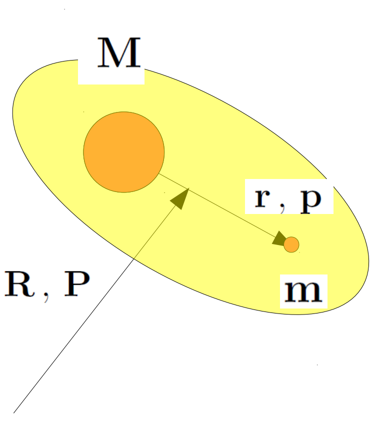

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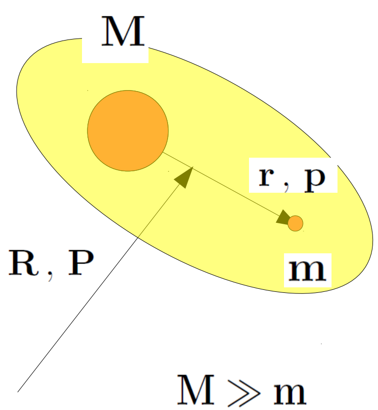
non-separable variables of CM and electron ~ $\frac{1}{c}$, $\frac{\omega}{c}$

Hydrogen atom in strong laser field (quantum-quasiclassical method)



$$\mathrm{M} \gg \mathrm{m}$$

$$\mathbf{P} = \mathbf{MV} \gg \mathbf{p} = \mathbf{mv}$$

classical ideal gas perfectly describes gas laws

$$\lambda_{dB} = \frac{h}{MV} \rightarrow 0$$

$$i\hbar\frac{\partial}{\partial t}|\psi(\mathbf{r},t)\rangle = [H_0(\mathbf{r}) + V(\mathbf{r},\mathbf{R}(t))]|\psi(\mathbf{r},t)\rangle$$

$$H_{cl}(\mathbf{P},\mathbf{R},t) = \frac{\mathbf{P}^2}{2M} + \langle\psi(\mathbf{r},t)|V(\mathbf{r},\mathbf{R}(t))|\psi(\mathbf{r},t)\rangle$$

$$\frac{d}{dt}\mathbf{P} = -\frac{\partial}{\partial\mathbf{R}}H_{cl}(\mathbf{P},\mathbf{R},t)$$

$$\frac{d}{dt}\mathbf{R} = \frac{\partial}{\partial\mathbf{P}}H_{cl}(\mathbf{P},\mathbf{R},t)$$

$$\psi(\boldsymbol{r},t=-n_TT/2)=\phi_{nlm}(\boldsymbol{r}),$$

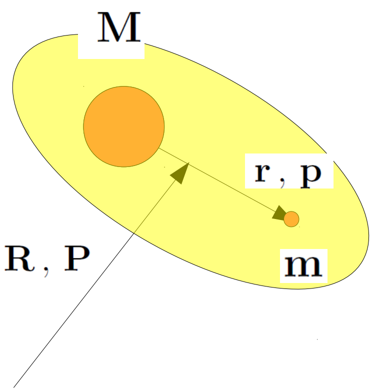
$$\boldsymbol{R}(t=-n_TT/2)=\boldsymbol{R}_0\ ,\ \boldsymbol{P}(t=-n_TT/2)=\boldsymbol{P}_0,$$

IOP Publishing — Journal of Physics A: Mathematical and Theoretical
J. Phys. A: Math. Theor. **56** (2023) 154003 (15pp) https://doi.org/10.1088/1751-8121/acc0e9

Quantum-quasiclassical analysis of center-of-mass nonseparability in hydrogen atom stimulated by strong laser fields*

Vladimir S Melezhik

Hydrogen atom in strong laser field (non-dipole effects)



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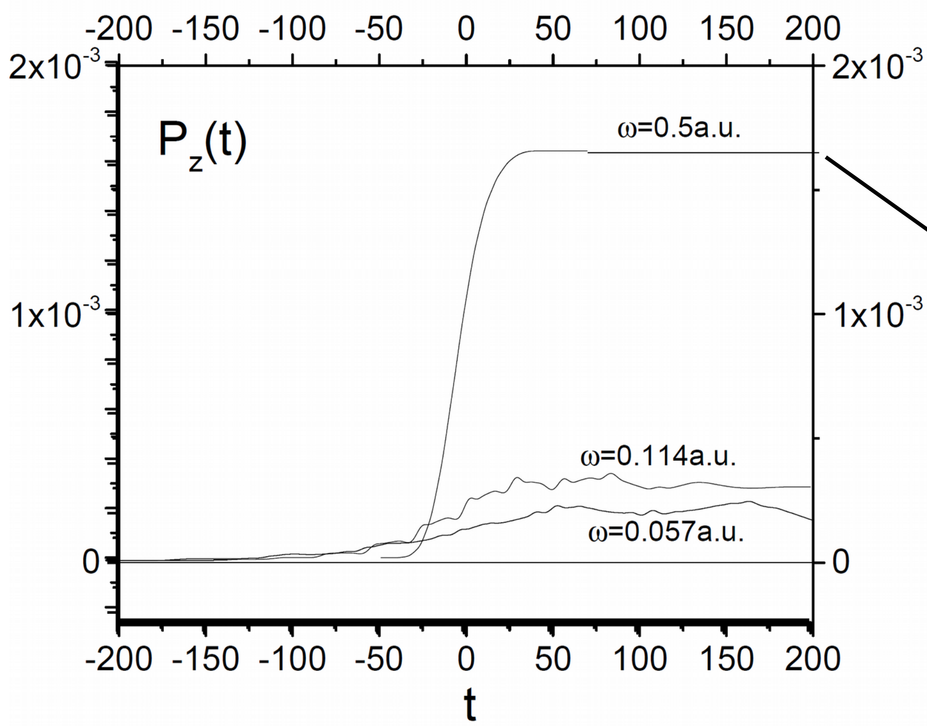
generally accepted: in the IR, optical and UV spectroscopies

the dipole approximation is well justified

Promising tasks: acceleration of atoms by strong EM pulses



$10^{14}\ \frac{W}{cm^2}$ ~10fs

$E_{kin} \sim 10^{-8}\ eV \sim 10^{-4} K$

$a \sim 10^{15} g$

Vol 461 | 29 October 2009 | doi:10.1038/nature08481 nature

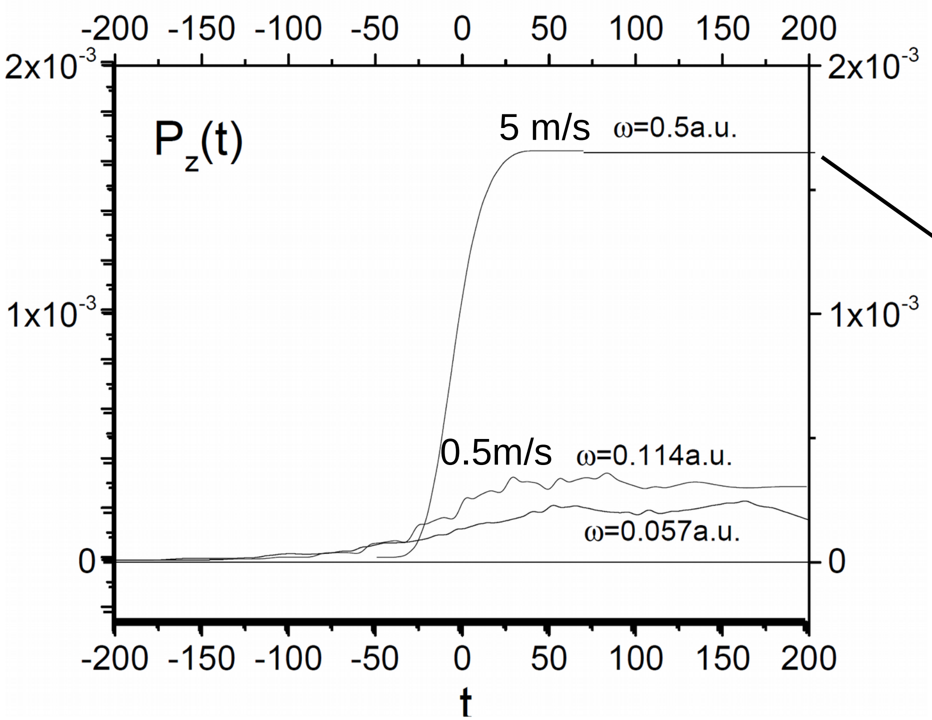
Acceleration of neutral atoms in strong short-pulse laser fields

U. Eichmann[1,2], T. Nubbemeyer[1], H. Rottke[1] & W. Sandner[1,2]

$a_{exp} \sim 10^{14} g$

$8 \times 10^{15} \frac{W}{cm^2}$, $(700 - 1100) nm$, $(40 - 100) fs$, He, Ne atoms

Promising tasks: acceleration of atoms by strong EM pulses



$10^{14}\ \frac{W}{cm^2}$ ~10fs

E_{kin}~10^{-8} eV~10^{-4}K

a ~ 10^{15}g

in IR, optics and UV energy range: non-dipole effects (CM non-separability)

↓

considerable acceleration of atom

Mechanisms of acceleration of atoms by EM pulses

photonics

Photonics **2023**, *10*, 1290.

MDPI

Article

Acceleration of Neutral Atoms by Strong Short-Wavelength Short-Range Electromagnetic Pulses

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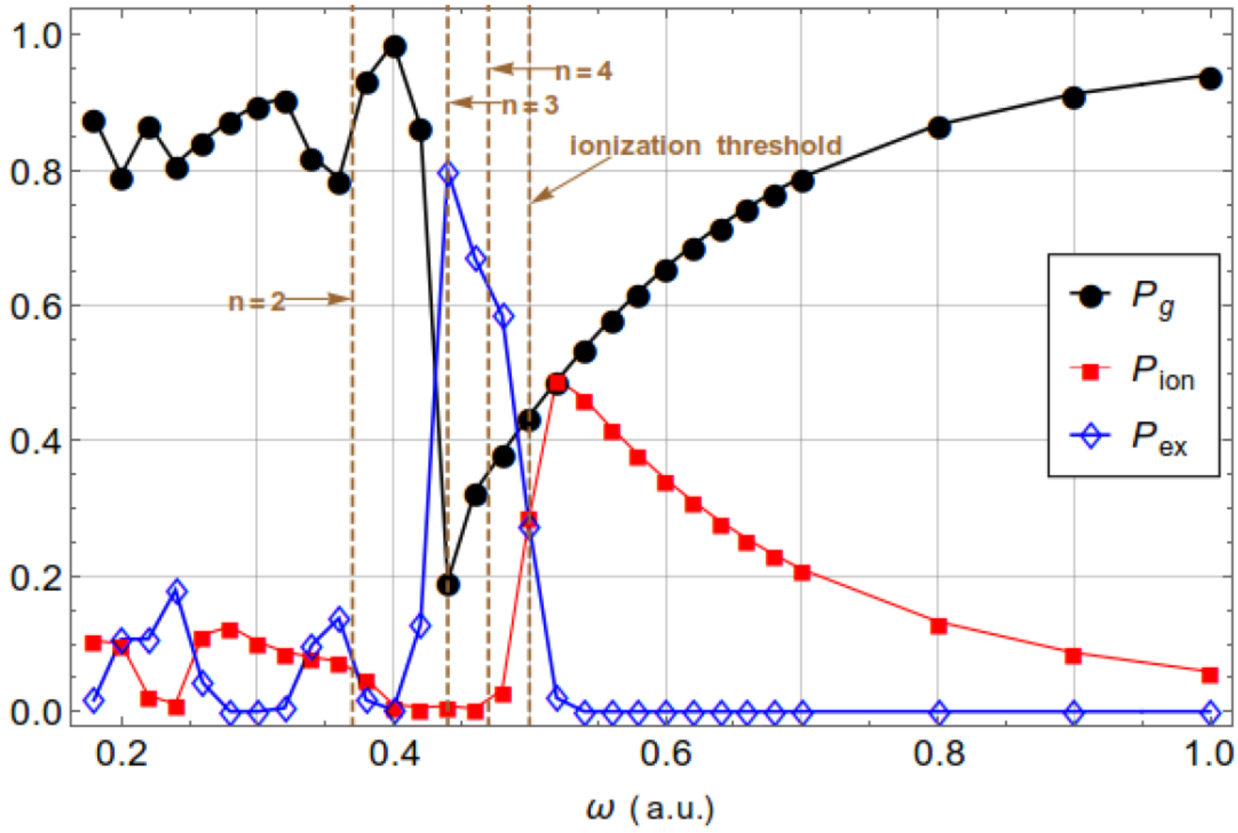
[1] Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, Moscow Region 141980, Russian Federation

[2] Dubna State University, 19 Universitetskaya Street, Dubna, Moscow Region 141982, Russian Federation



10^{14} W/cm^2

8 fs

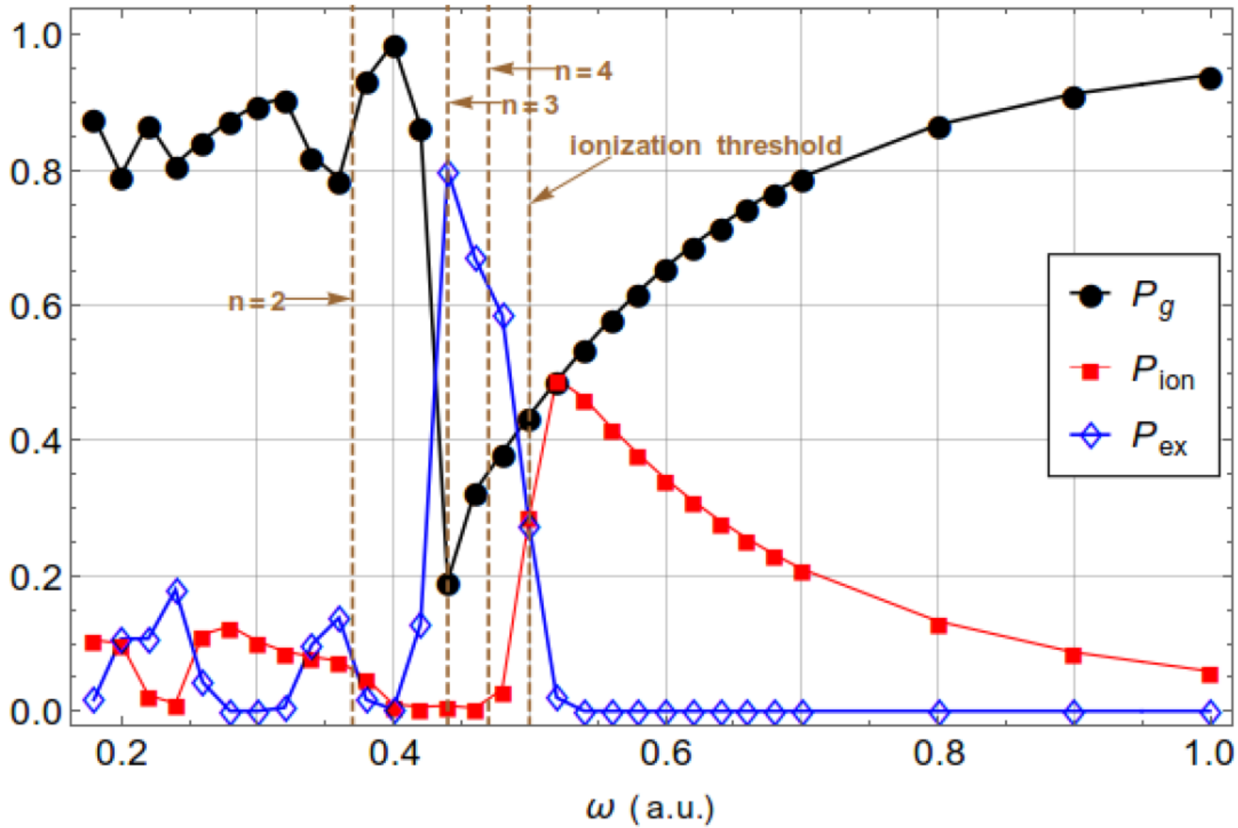
$$P_g(\omega) = |\langle\psi|\phi_{100}\rangle|^2 = \left|\int \psi(\mathbf{r},\omega,T_{out})\phi_{100}(\mathbf{r})d\mathbf{r}\right|^2$$

$$P_{ex} = \sum_{n=2}^{\infty} P_n = \sum_{n=2}^{N'} P_n + \sum_{n=N'+1}^{\infty} P_n$$

$$P_{ion} = \int_0^{+\infty} \frac{dP}{dE} dE$$

$$\sum_{n=1}^{\infty} P_n + \int_0^{+\infty} \frac{dP}{dE} dE = 1$$

Shadmehri, S.; Melezhik, V.S. *Laser Phys.* **2023**, *33*, 026001.

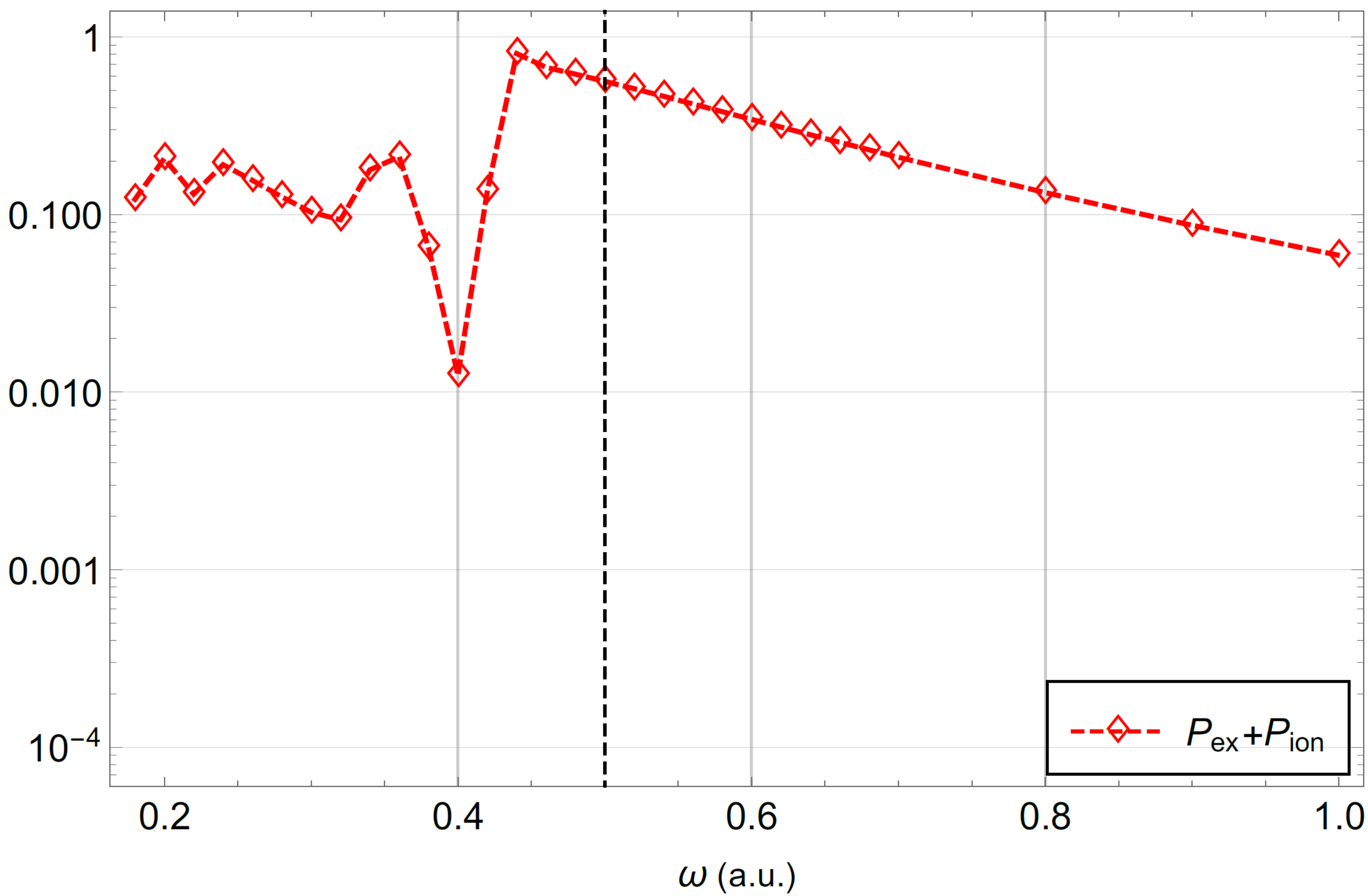


10^{14} W/cm^2

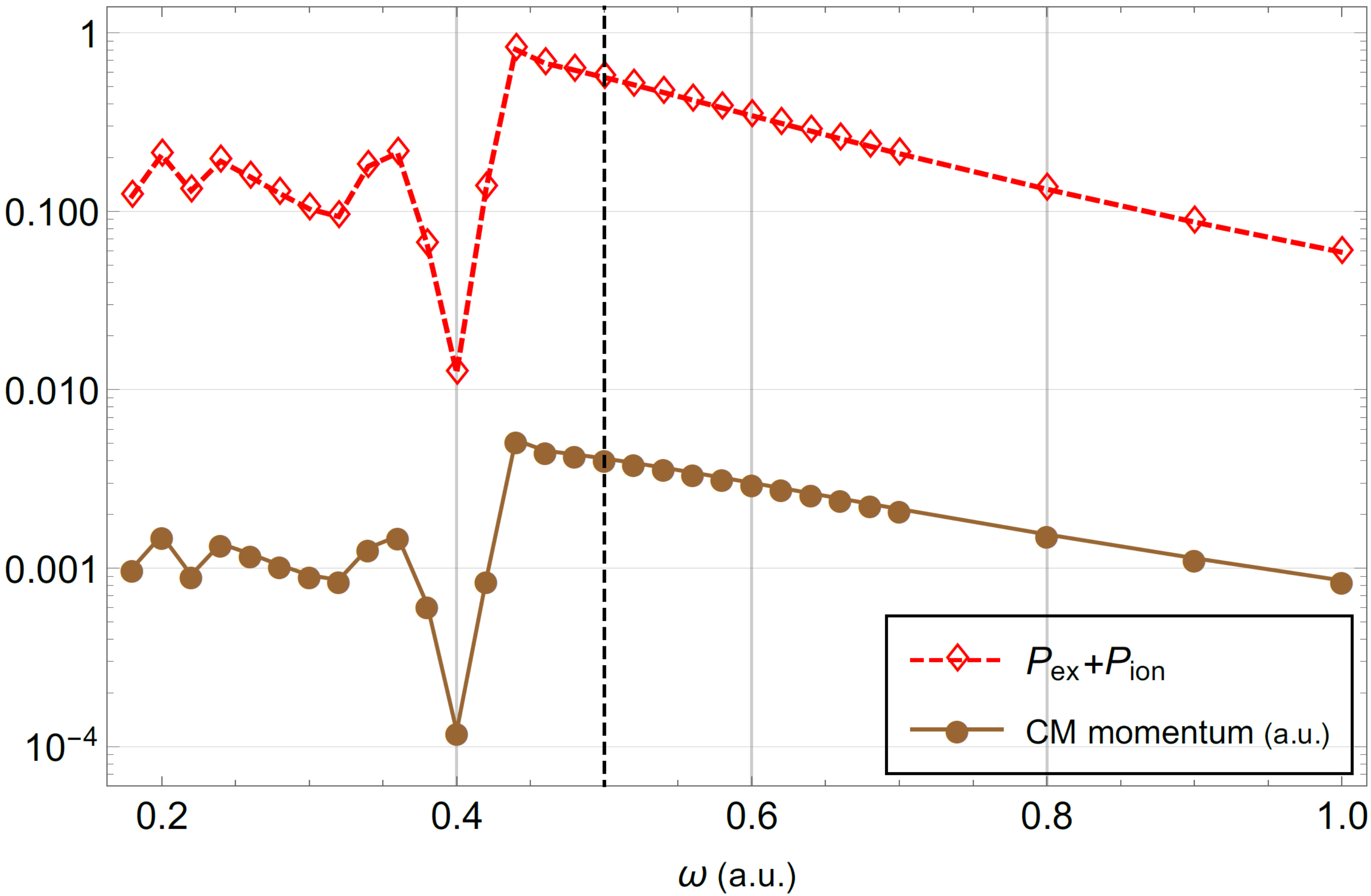
8 fs

	P_g			P_{ex}		
ω	**Dipole**	**Nondipole**	$\lvert\Delta P\rvert$ [1]	**Dipole**	**Nondipole**	$\lvert\Delta P\rvert$ [1]
0.30	0.896815	0.896805	1.05×10^{-5}	6.3410×10^{-5}	6.3414×10^{-5}	6.59×10^{-5}
0.40	0.987600	0.987599	1.34×10^{-6}	2.3058×10^{-3}	2.3052×10^{-3}	2.51×10^{-4}
0.48	0.382308	0.382294	3.54×10^{-5}	5.8582×10^{-1}	5.8568×10^{-1}	2.37×10^{-4}
0.52	0.488483	0.488465	3.74×10^{-5}	1.9974×10^{-2}	1.9984×10^{-2}	4.84×10^{-4}
0.80	0.867150	0.867131	2.20×10^{-5}	4.6748×10^{-7}	4.6756×10^{-7}	1.64×10^{-4}
1.00	0.941058	0.941045	1.39×10^{-5}	4.8210×10^{-7}	4.8218×10^{-7}	1.68×10^{-4}

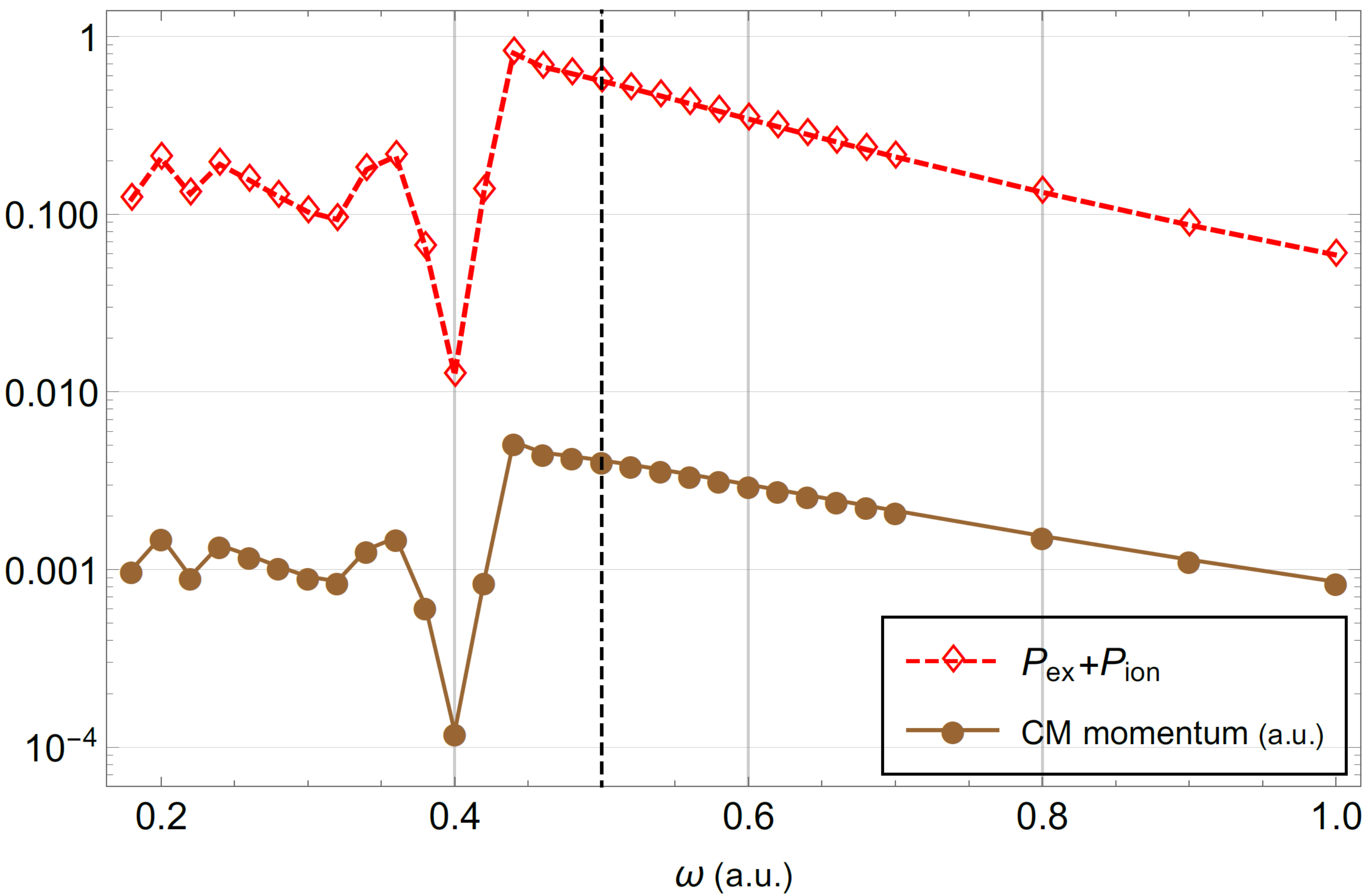
[1] $\lvert\Delta P\rvert = \left|\frac{P_{Dipole} - P_{Nondipole}}{P_{Dipole}}\right|$.



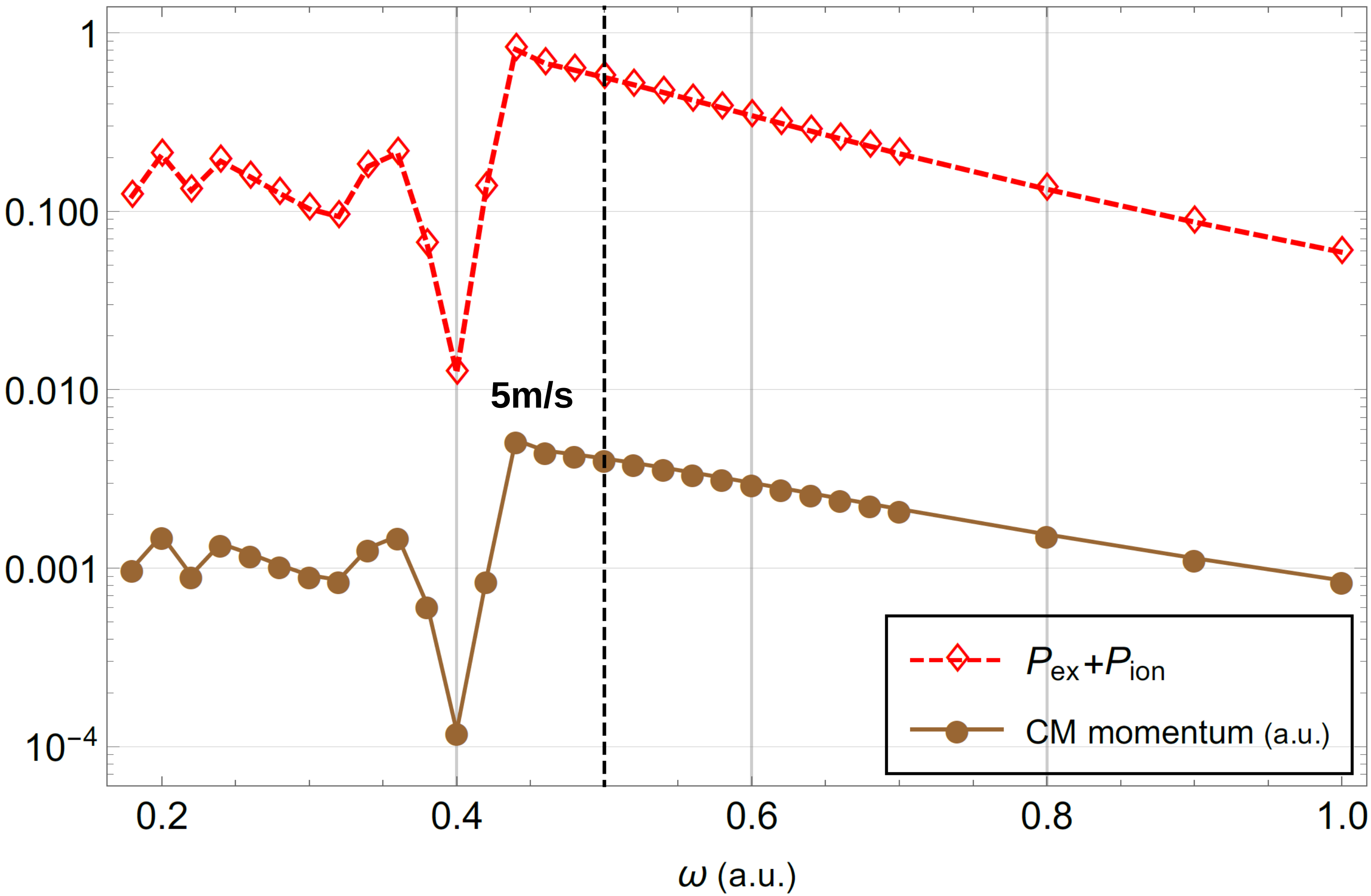
1
0.100
0.010
0.001
10^−4
0.2
0.4
0.6
0.8
1.0
ω (a.u.)
P_ex+P_ion



1
0.100
0.010
0.001
10^{-4}
0.2
0.4
0.6
0.8
1.0
ω (a.u.)
$P_{ex}+P_{ion}$
CM momentum (a.u.)



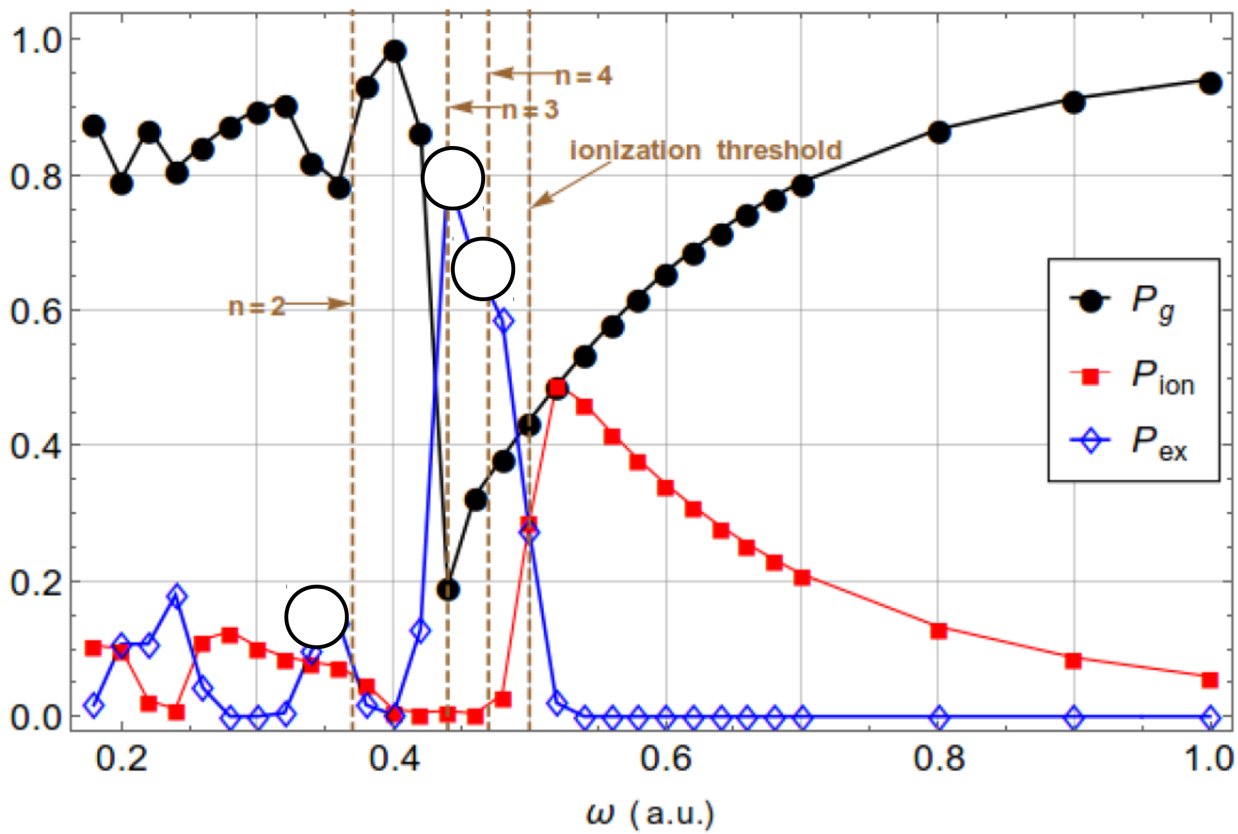
strong correlation between $P_{ex} + P_{ion}$ and V_y (CM momentum $= MV_y$)



strong correlation between $P_{ex} + P_{ion}$ and V_y (CM momentum $= MV_y$)

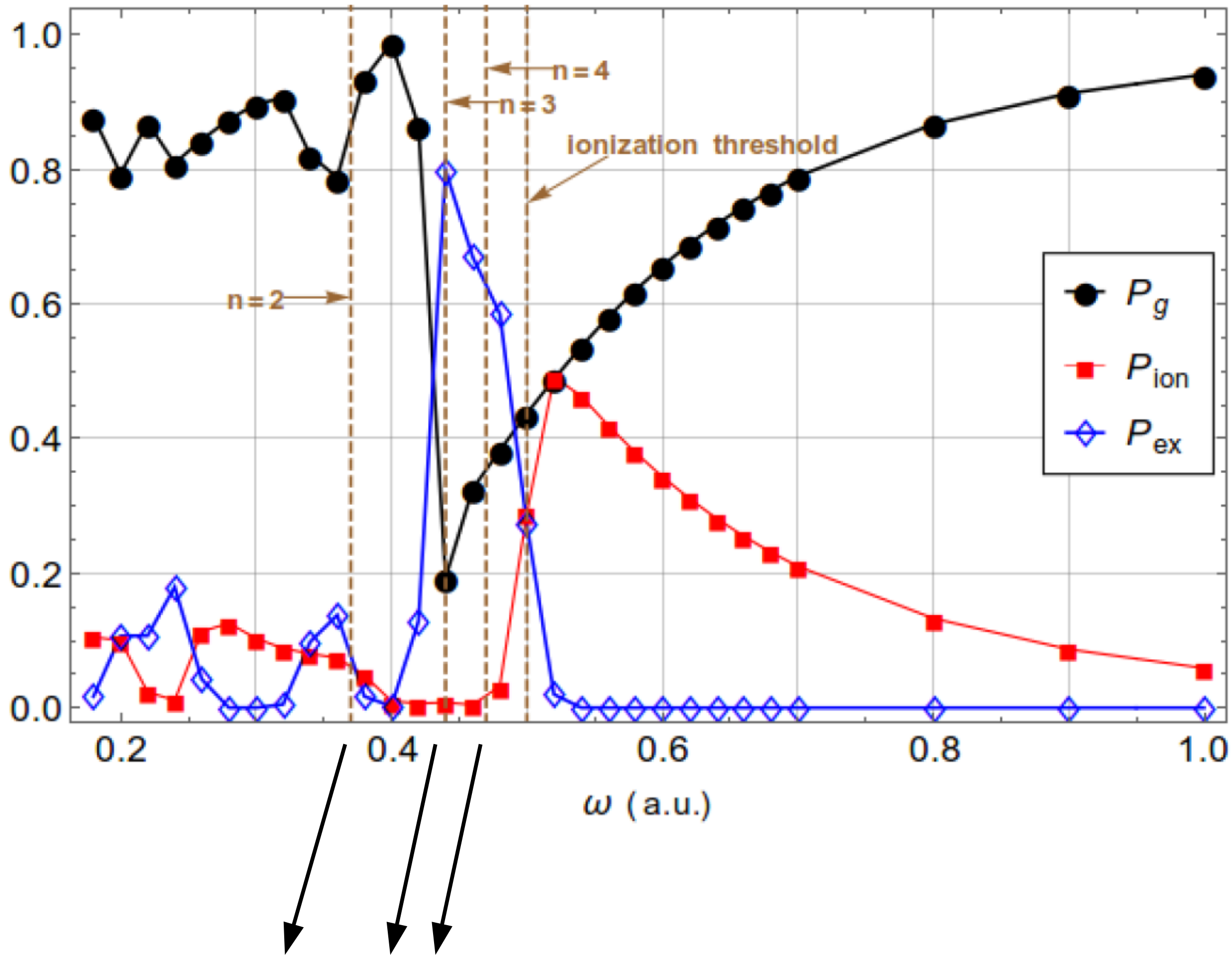
mechanism of CM acceleration:

generation of nonzero dipole between proton and electron cloud
transferred either to excited states of atom or to its continuum



10^{14} W/cm^2

8 fs



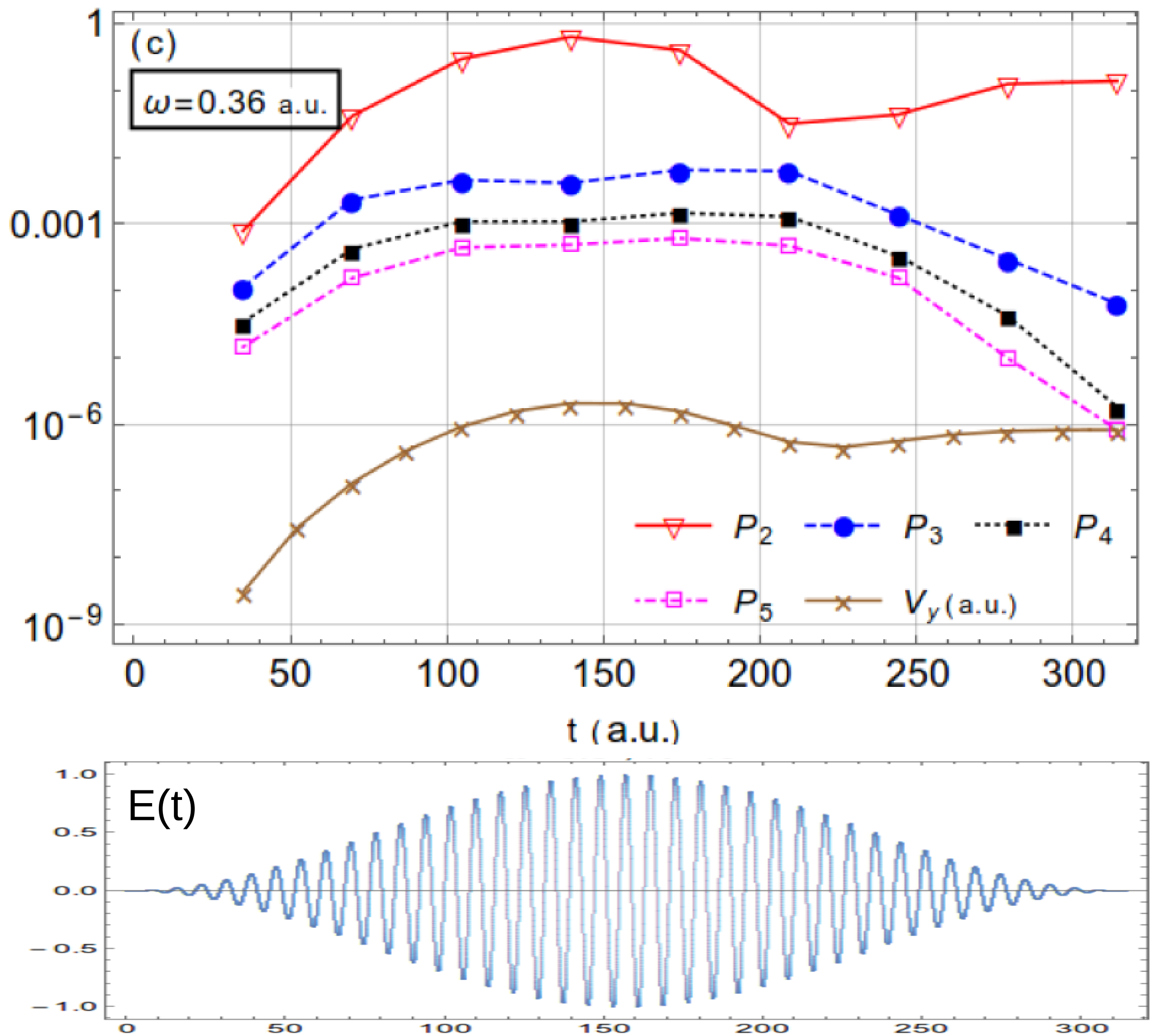
10^{14} W/cm^2

8 fs

$$H_{n=1} + \hbar\omega \rightarrow H_{n'}\,, \quad n' = 2, 3, 4$$

$$\hbar\omega = \frac{1}{2n^2} - \frac{1}{2n'^2} \qquad \omega = 0.38,\ 0.44,\ 0.47\ \text{(a.u.)}$$

$$P_n(\omega, t) \xrightarrow{t \to T_{out}} P_n(\omega)$$



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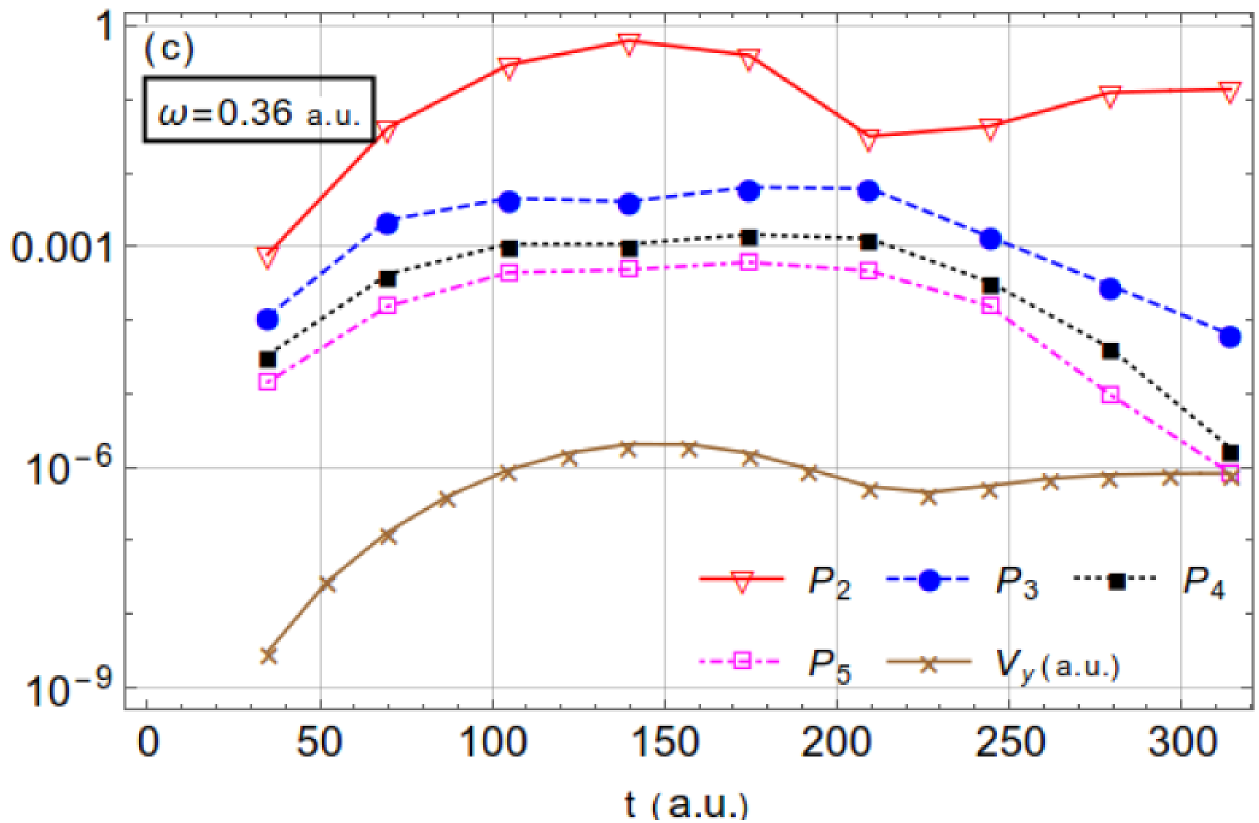
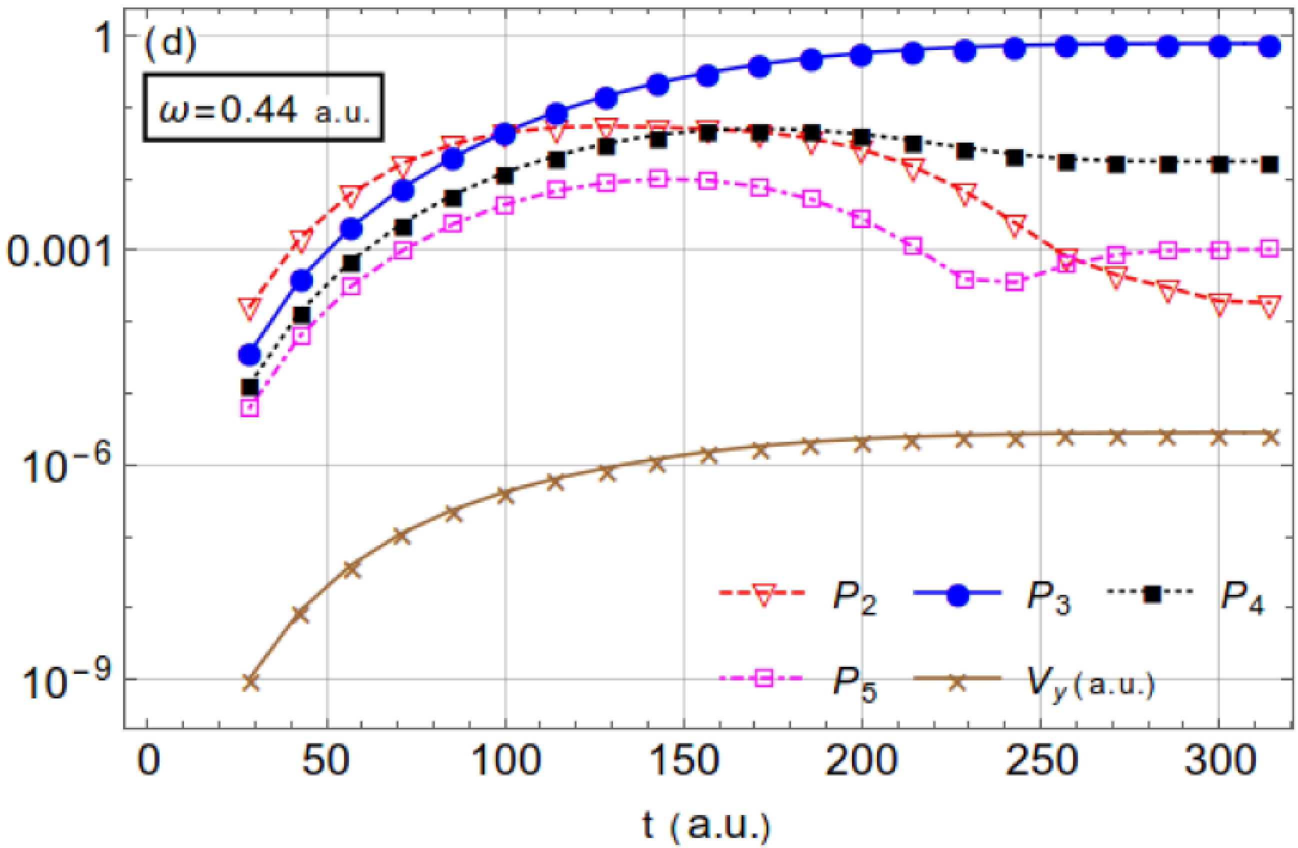
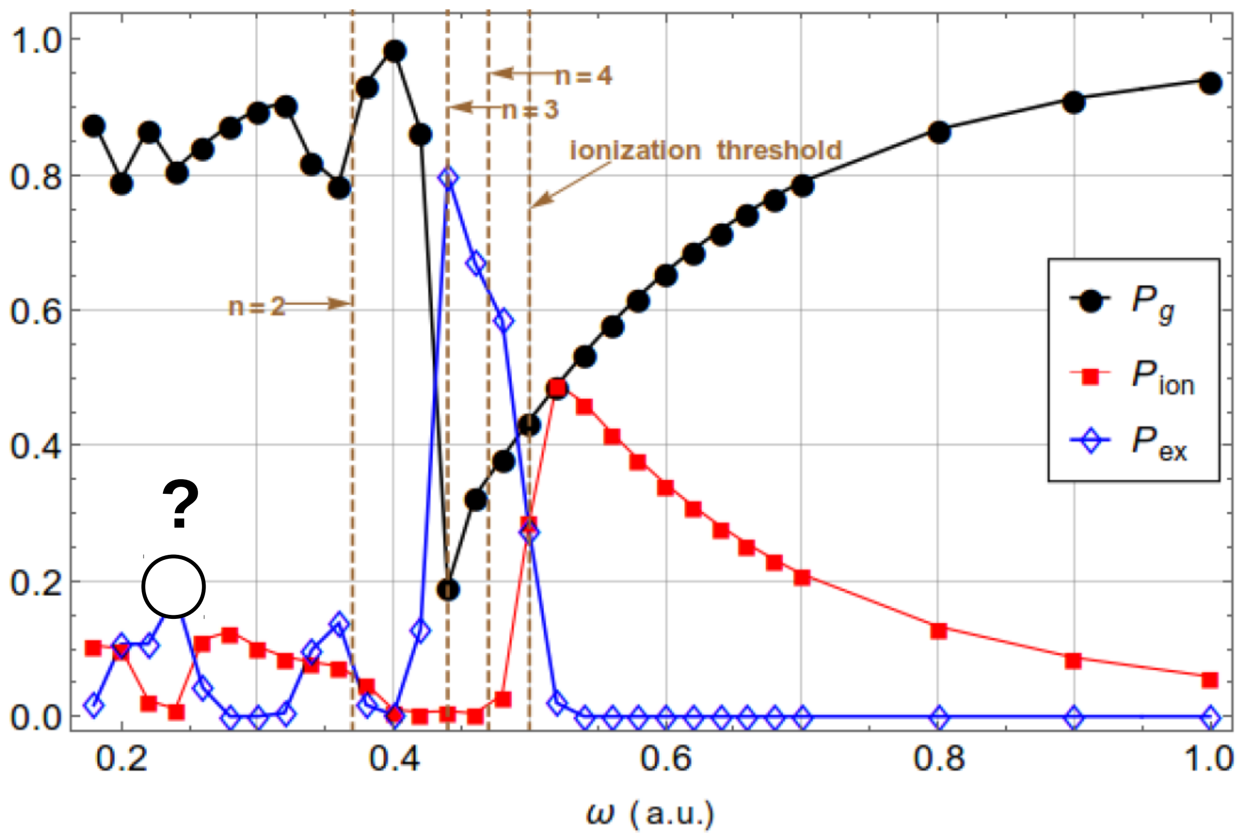


$$H_{n=1} + \hbar\omega \to H_{n'}, \quad n' = 2,$$

$$P_n(\omega, t) \xrightarrow{t \to T_{out}} P_n(\omega)$$

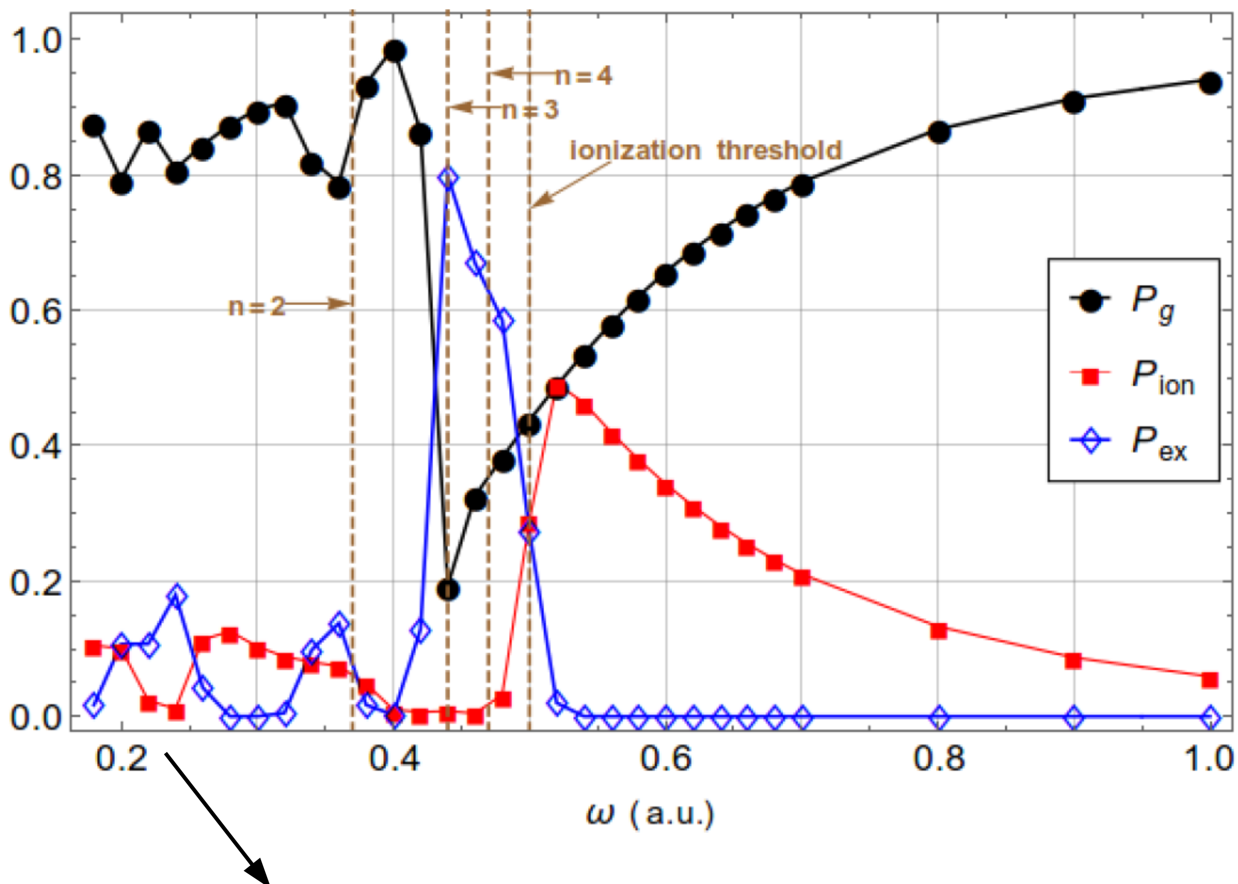


$$H_{n=1} + \hbar\omega \to H_{n'} \quad n' = 3.$$



10^{14} W/cm^2

8 fs



10^{14} W/cm^2

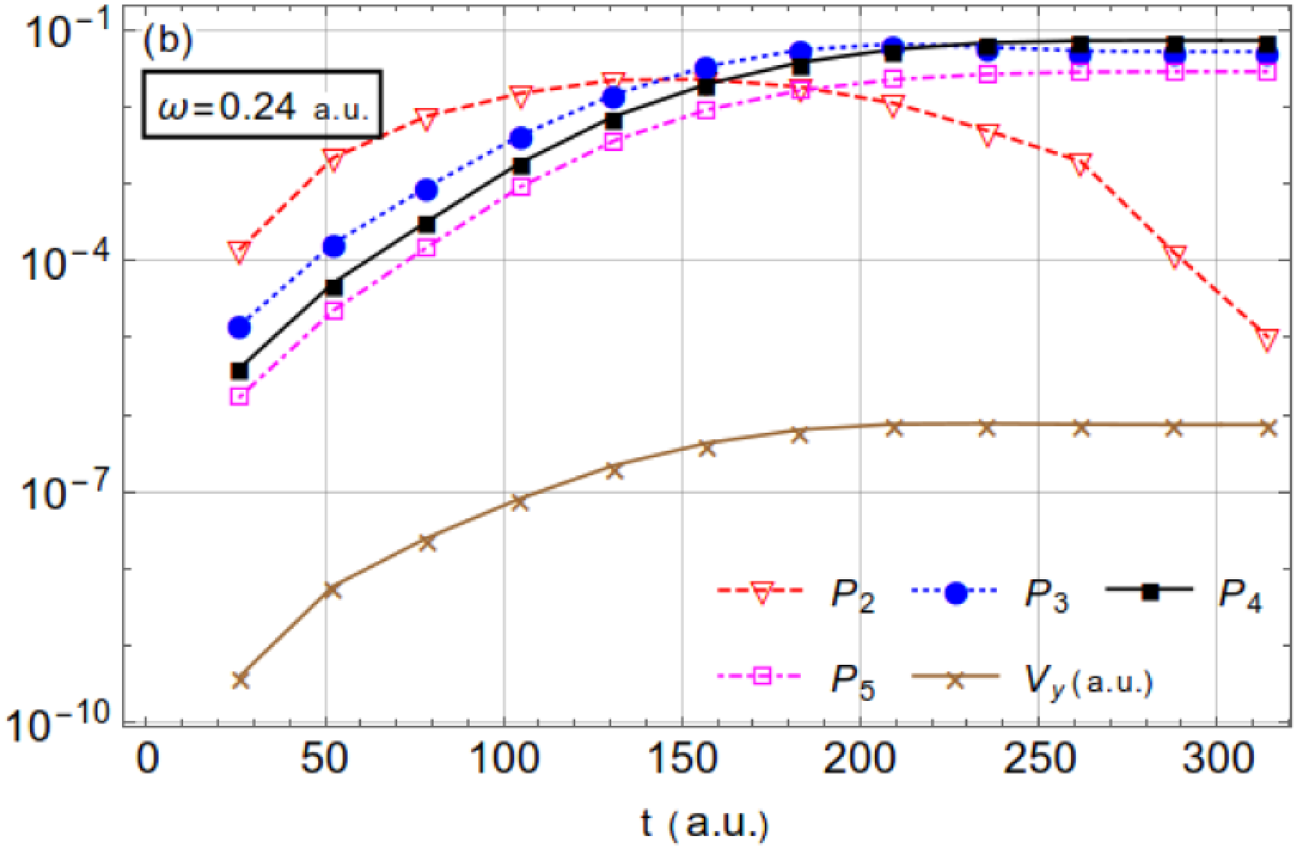
8 fs

$$H_{n=1} + 2\hbar\omega \rightarrow H'_n \qquad 2\hbar\omega = \frac{1}{2n^2} - \frac{1}{2n'^2}$$

two-photon transition $2\hbar\omega \approx 0.47$ a.u. for $n = 1$ and $n' = 4$

peak in $P_{ex}(\omega)$ at $\omega = 0.24$ a.u.

$$P_n(\omega, t) \xrightarrow{t \to T_{out}} P_n(\omega)$$



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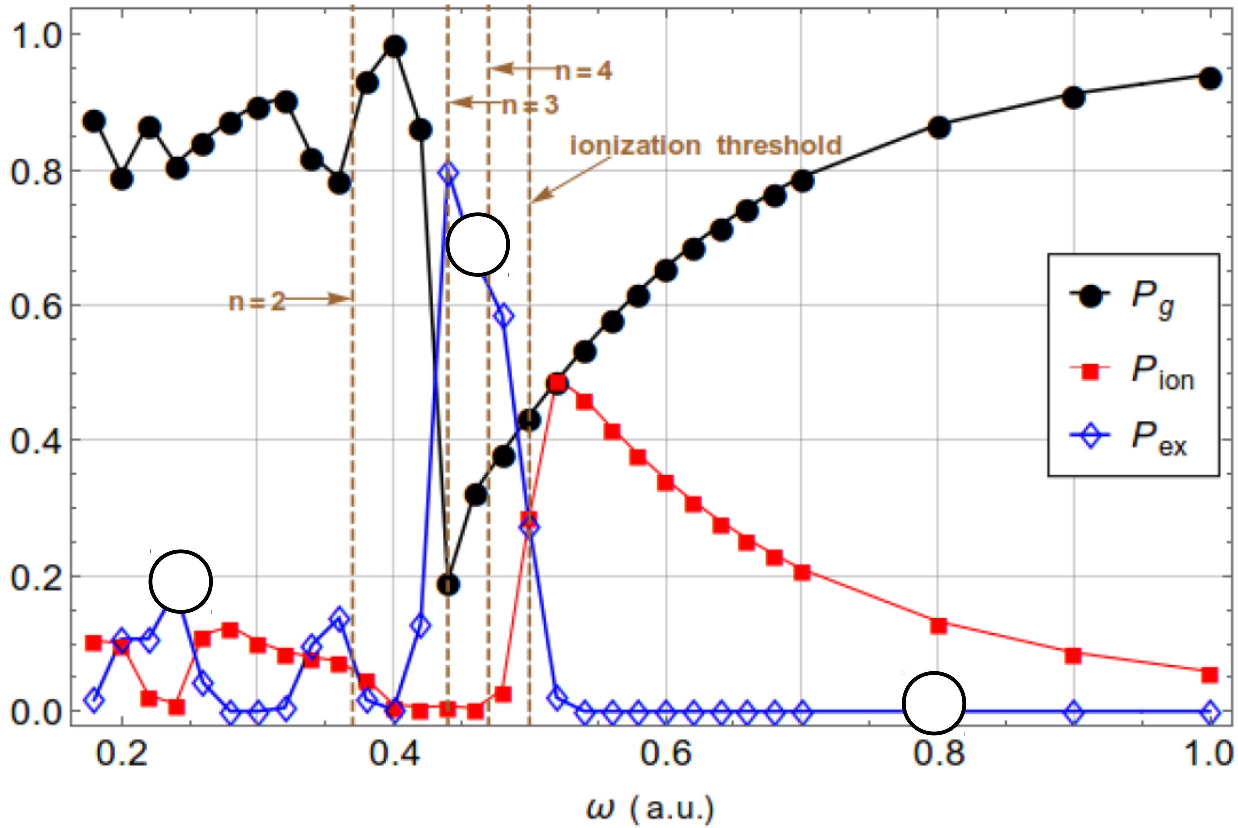
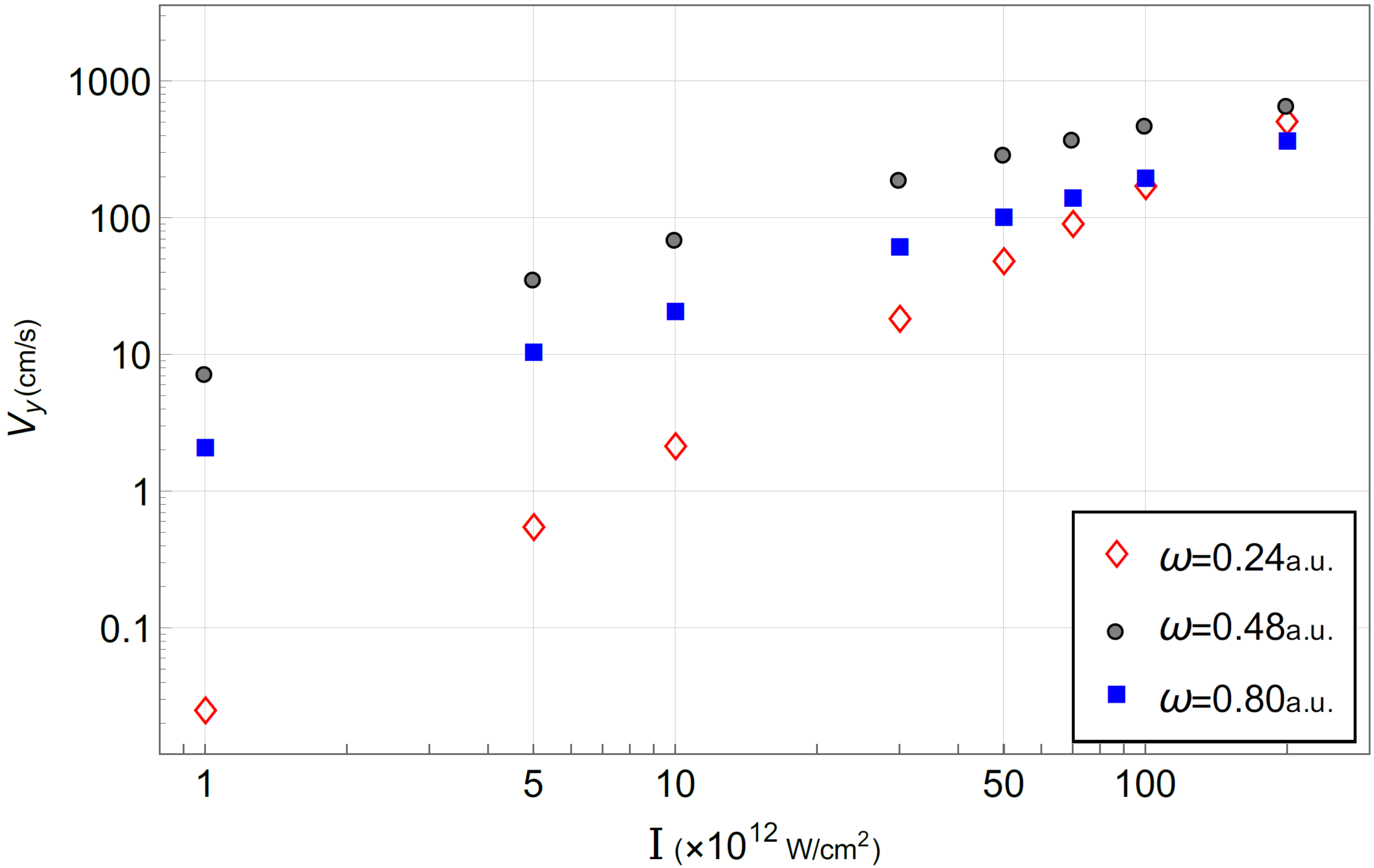


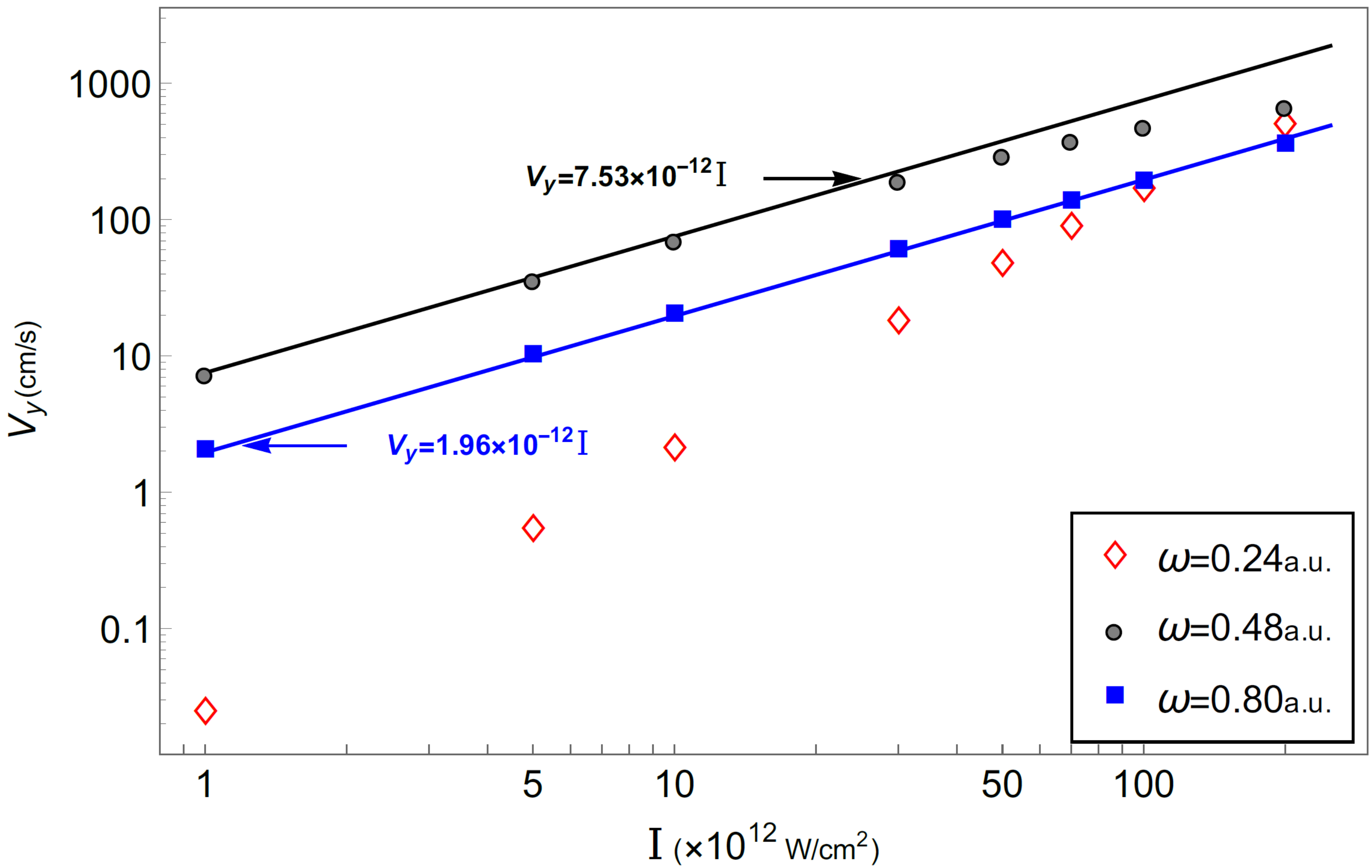
$\omega = 0.48$a.u. one-photon resonant transition $n = 1 \rightarrow n' = 4$

$\omega = 0.24$a.u. two-photon resonant transition $n = 1 \rightarrow n' = 4$

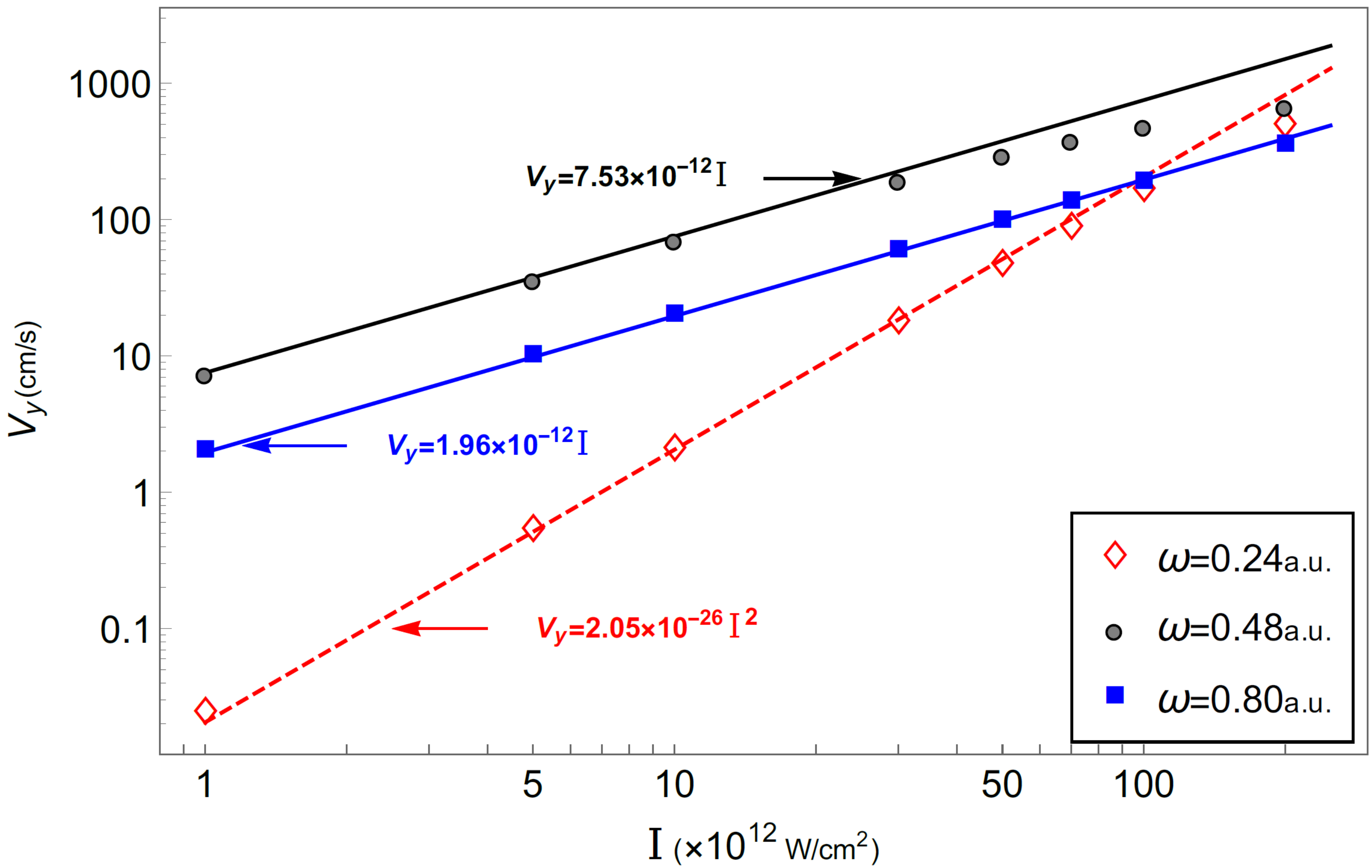
$\omega = 0.8$a.u. non-resonant mechanism



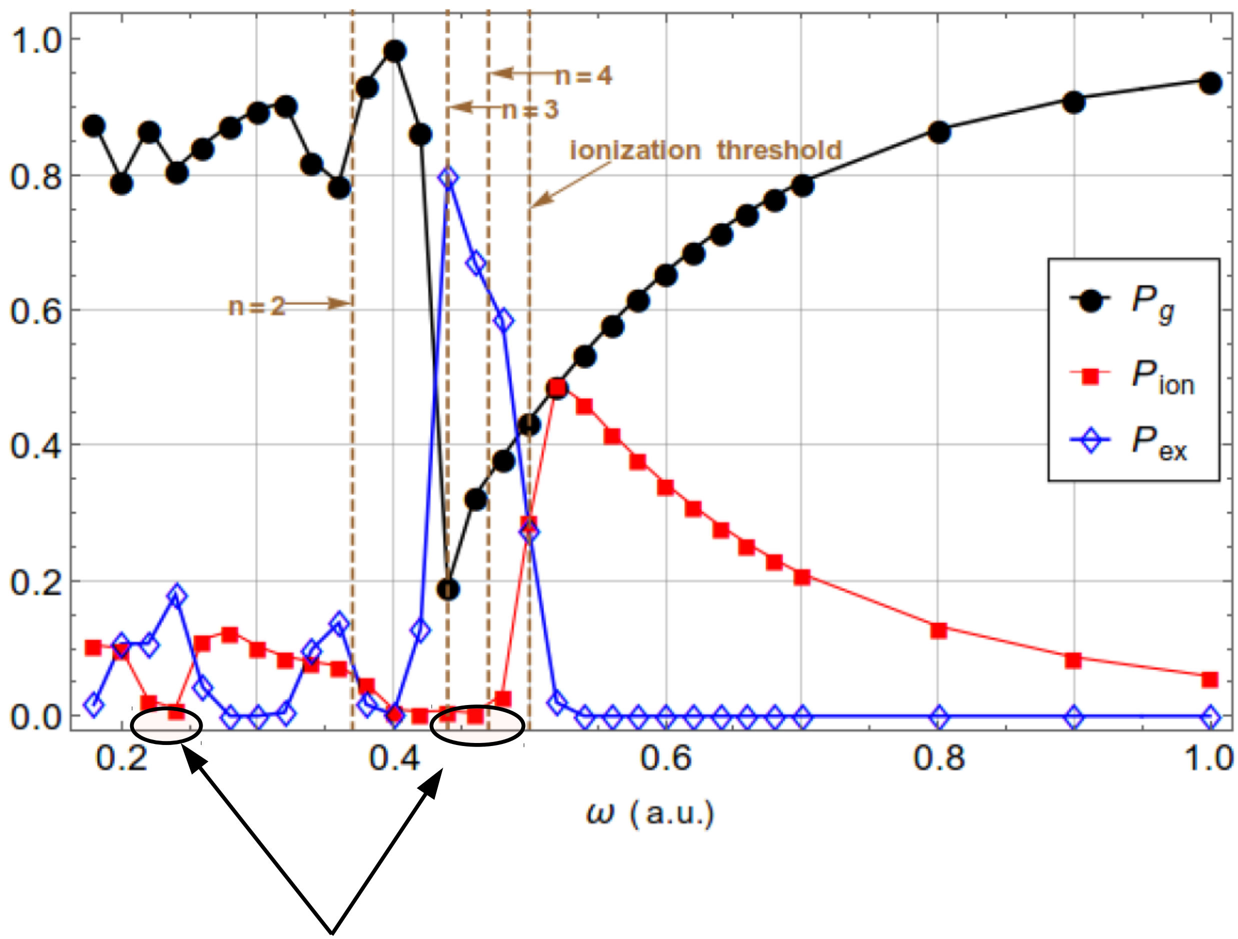
1000
100
10
1
0.1
V_y(cm/s)
1
5
10
50
100
I (×10^12 W/cm^2)
ω=0.24a.u.
ω=0.48a.u.
ω=0.80a.u.



1000
100
10
1
0.1
V_y(cm/s)
V_y=7.53×10^{-12} I
V_y=1.96×10^{-12} I
ω=0.24a.u.
ω=0.48a.u.
ω=0.80a.u.
1
5
10
50
100
I (×10^{12} W/cm^2)



V_y(cm/s)
1000
100
10
1
0.1
V_y=7.53×10^{-12} I
V_y=1.96×10^{-12} I
V_y=2.05×10^{-26} I^2
ω=0.24a.u.
ω=0.48a.u.
ω=0.80a.u.
1
5
10
50
100
I (×10^{12} W/cm^2)



areas promising for accelerating atoms where ionization is suppressed

elliptical polarization of laser

$$\mathbf{A} = -\frac{E_0 f(t)}{\omega\sqrt{1+\varepsilon^2}}\left[\hat{\mathbf{x}}\sin(\omega t - \mathbf{k}\cdot\mathbf{r}) - \varepsilon\hat{\mathbf{y}}\cos(\omega t - \mathbf{k}\cdot\mathbf{r})\right]$$

$$f(t) = \sin^2\left(\frac{\pi t}{NT}\right), \quad 0 \le t \le T_{out} = NT = 100\pi$$

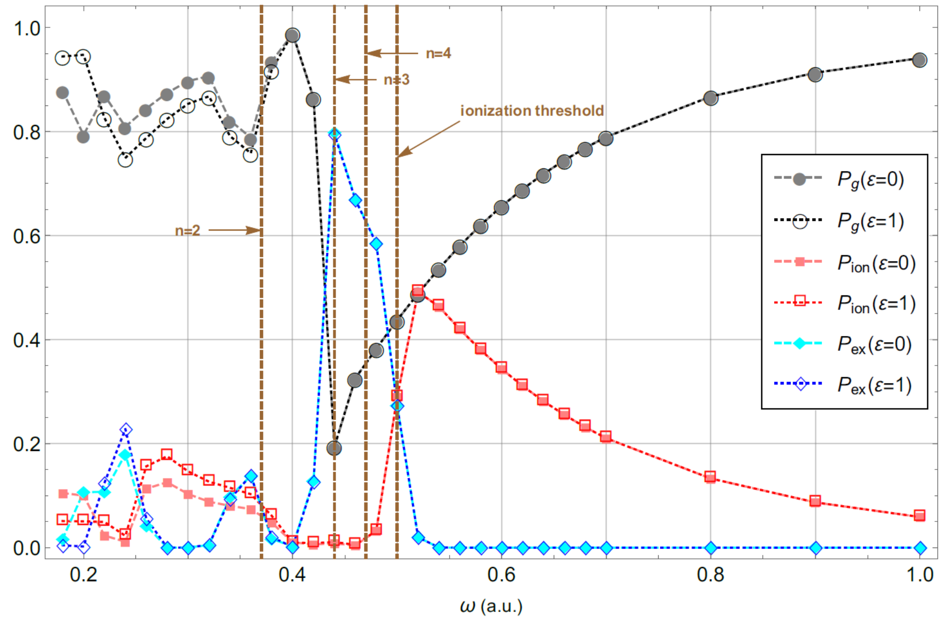
$$V(\mathbf{r},t) \Rightarrow V(\mathbf{r},t) + V_1(\mathbf{r},t) + V_2(\mathbf{r},\mathbf{R},t),$$

$$V(\mathbf{r},t) = E_0(t)\left\{\left[\cos(\omega t) + \frac{\bar{f}(t)}{2Nf(t)}\sin(\omega t)\right]x + \varepsilon\left[\sin(\omega t) - \frac{\bar{f}(t)}{2Nf(t)}\cos(\omega t)\right]y\right\},$$

$$V_1(\mathbf{r},t) = \frac{E_0(t)}{c}\left\{\omega\left[\sin(\omega t) - \frac{\bar{f}(t)}{2Nf(t)}\cos(\omega t)\right]zx - \varepsilon\omega\left[\cos(\omega t) + \frac{\bar{f}(t)}{2Nf(t)}\sin(\omega t)\right]zy + \left[\cos(\omega t)\hat{l}_y - \varepsilon\sin(\omega t)\hat{l}_x\right]\right\}$$

$$V_2(\mathbf{r},\mathbf{R},t) = \frac{E_0(t)}{c}\left\{\omega\left[\sin(\omega t) - \frac{\bar{f}(t)}{2Nf(t)}\cos(\omega t)\right](zX + xZ) - \varepsilon\omega\left[\cos(\omega t) + \frac{\bar{f}(t)}{2Nf(t)}\sin(\omega t)\right](zY + yZ) + \left[\cos(\omega t)(Z\hat{p}_x - X\hat{p}_z) + \varepsilon\sin(\omega t)(Z\hat{p}_y - Y\hat{p}_z)\right]\right\}$$

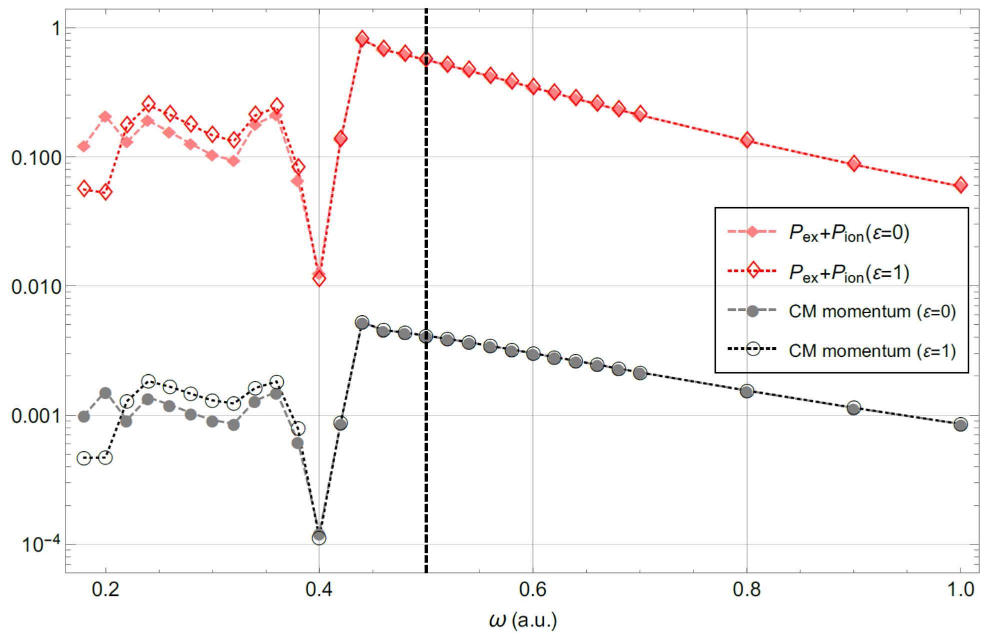
dependence on laser polarization



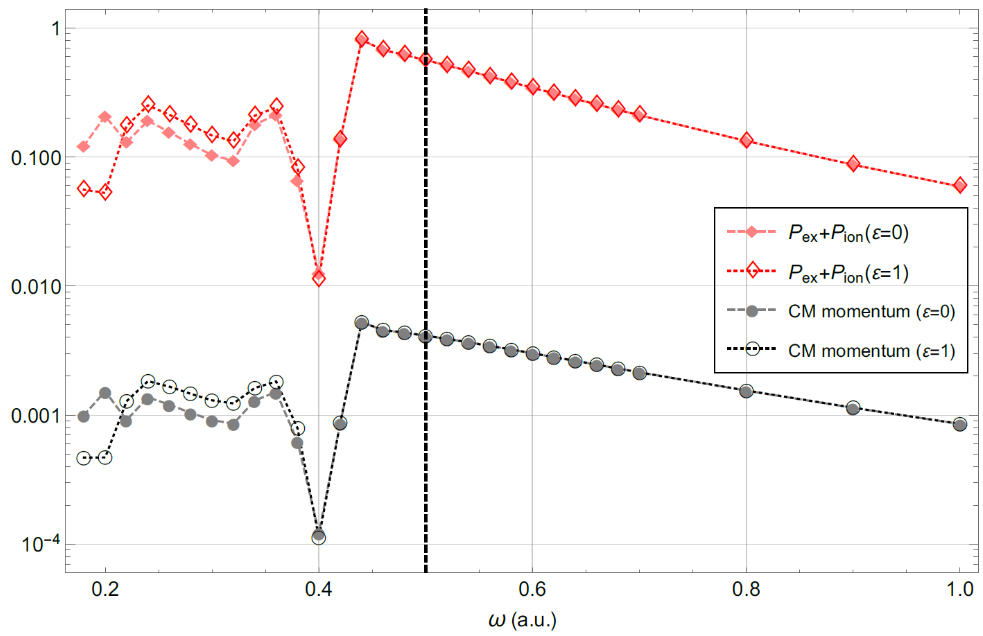
atom exitation and ionization weakly depend on polarization

Vladimir S. Melezhik ; Sara Shadmehri   *J. Chem. Phys.* 162, 174304 (2025)

dependence on laser polarization



dependence on laser polarization



atom acceleration weakly depends on polarization

However ...

Twisting of atoms by fork diffraction gratings

QUANTUM PHYSICS

Vortex beams of atoms and molecules

Alon Luski[1]†, Yair Segev[1]†‡, Rea David[1], Ora Bitton[1], Hila Nadler[1], A. Ronny Barnea[2], Alexey Gorlach[3], Ori Cheshnovsky[2], Ido Kaminer[3], Edvardas Narevicius[1]*

SCIENCE · 1 Sep 2021 · Vol 373, Issue 6559 · pp. 1105-1109

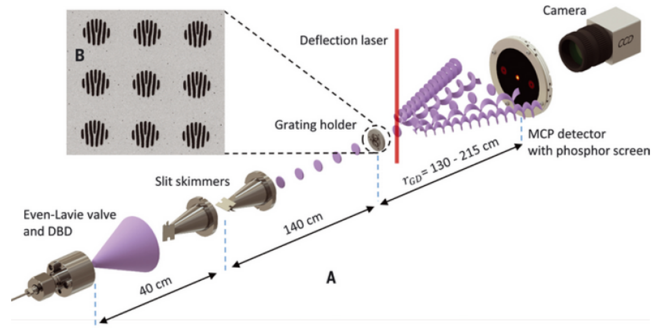


Fig. 2. Experimental setup for the production and detection of atomic and molecular vortex beams.

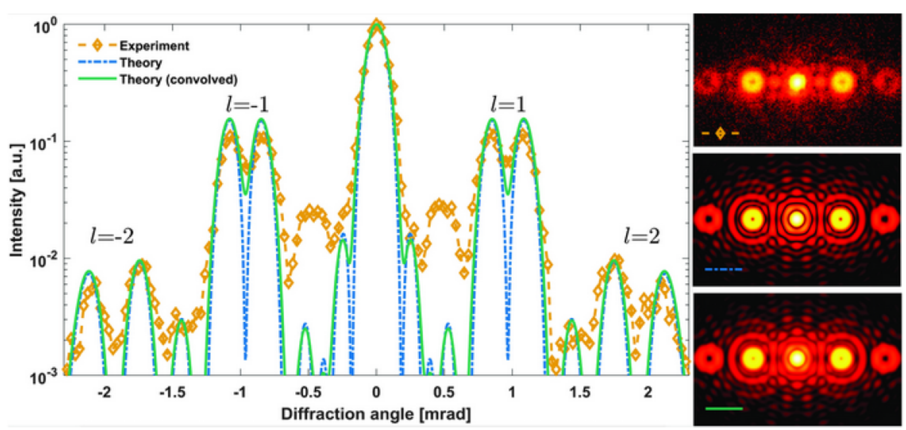


Fig. 4. Comparison of intensity measured in the experiment to theory, with simulated contribution of only the atoms.

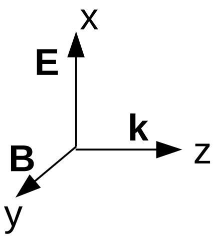
Luski *et al.*, *Science* **373**, 1105–1109 (2021) 3 September 2021

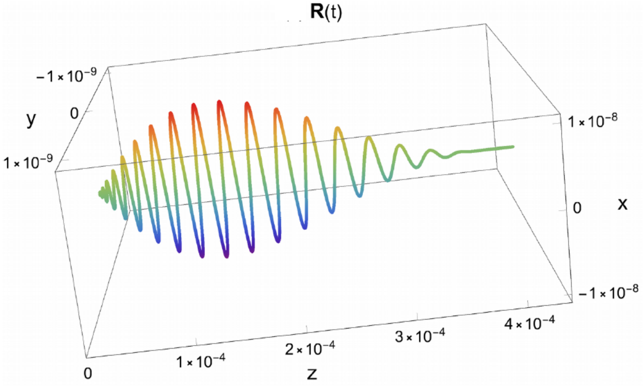
Alternative: twisting of atoms by EM pulses

10^{14} вт/см^2 , ~10фс, hν ~13эВ~ 0.48a.u.

Linear polarization (ϵ=0)

$$\mathbf{A} = \frac{E_0}{\omega\sqrt{2}} \sin^2(\frac{\pi t}{NT}) \left[-\hat{\mathbf{x}} \sin(\omega t - kz)\right]$$





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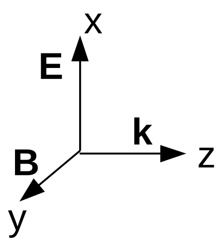
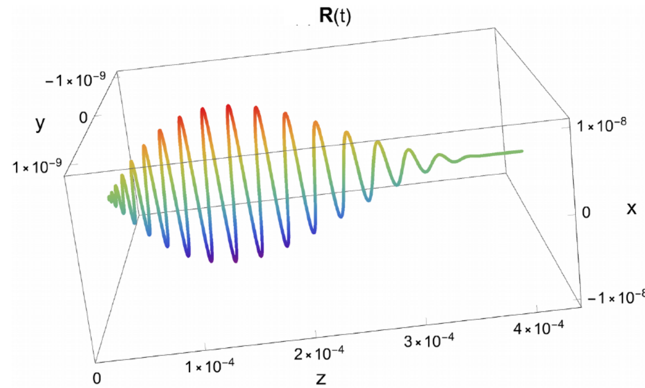
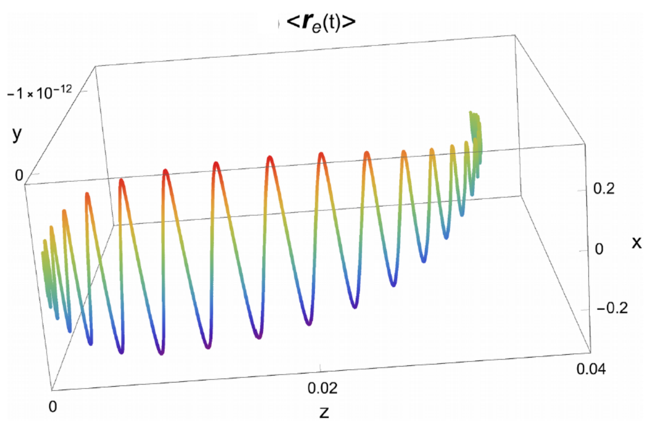
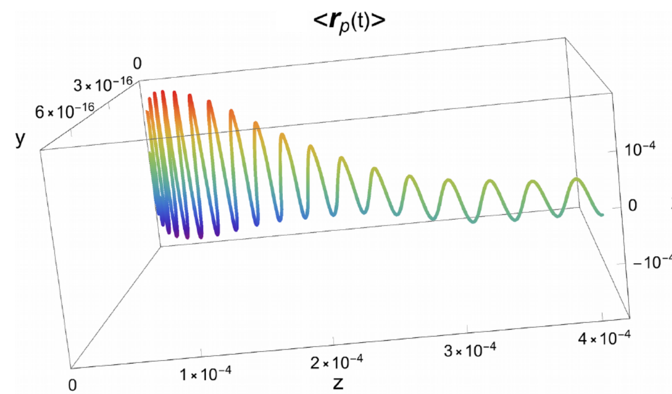




$$\langle x_e(t)\rangle = X_{cm}(t) + \frac{m_p}{M}\langle x(t)\rangle$$
$$\langle x_p(t)\rangle = X_{cm}(t) - \frac{m_e}{M}\langle x(t)\rangle$$





Alternative: twisting of atoms by EM pulses

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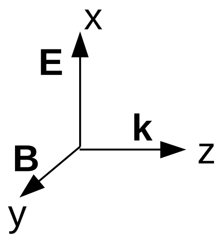
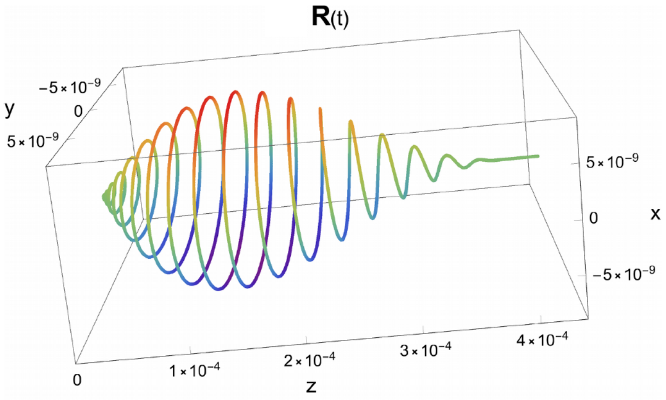
Circular polarization (ϵ=1)

$$\mathbf{A} = \frac{E_0}{\omega\sqrt{2}} \sin^2(\frac{\pi t}{NT}) \left[-\hat{\mathbf{x}} \sin(\omega t - kz) + \hat{\mathbf{y}} \cos(\omega t - kz)\right]$$





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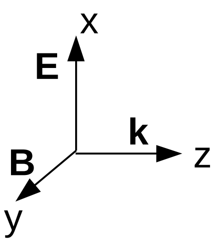

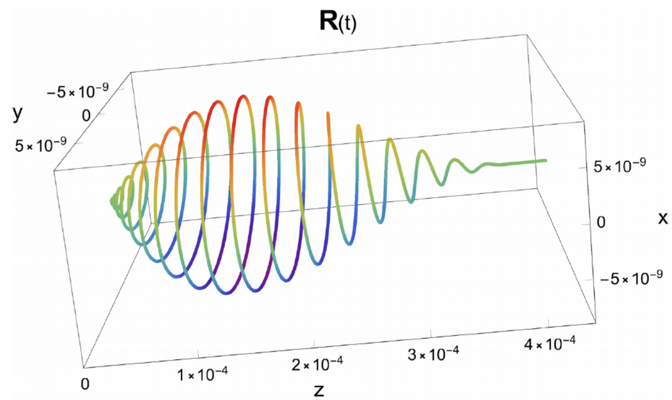

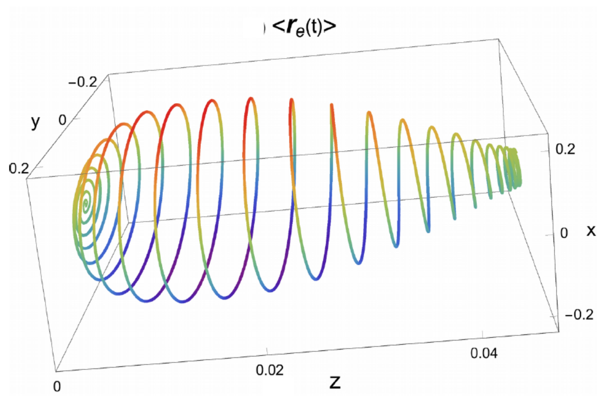

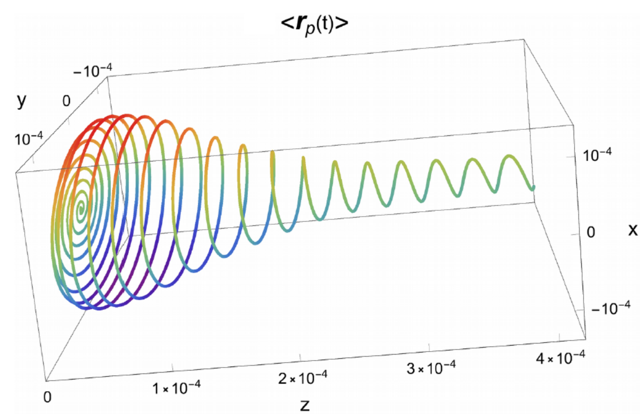

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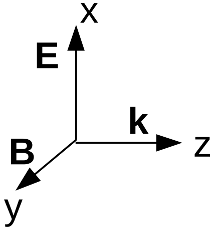
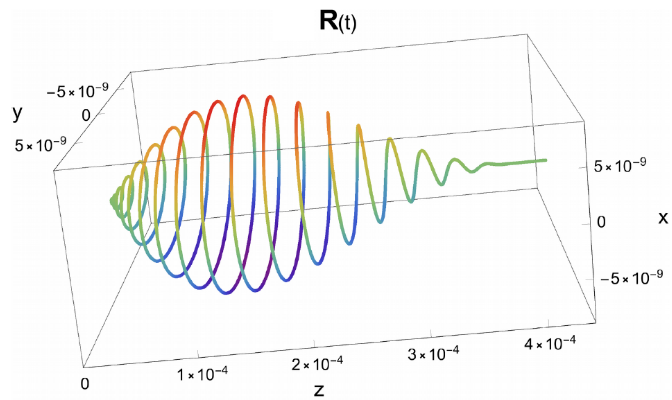
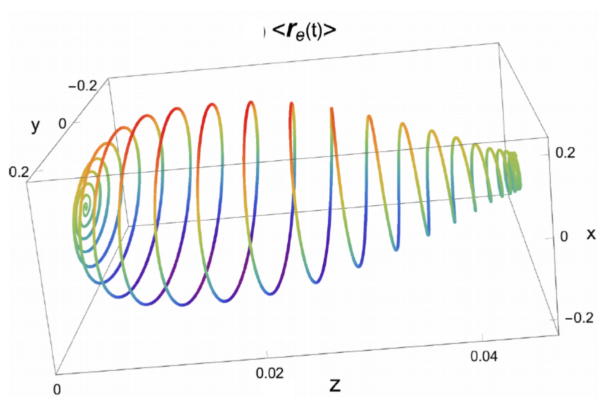
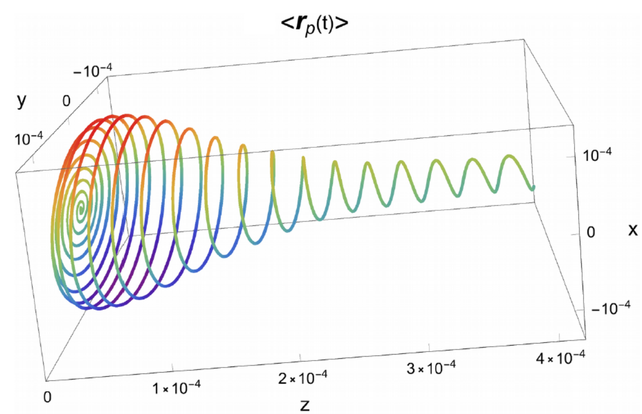




J = L + l = 0 + l

J = l





Twisting of atoms by EM pulses

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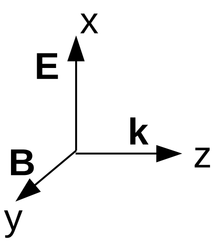
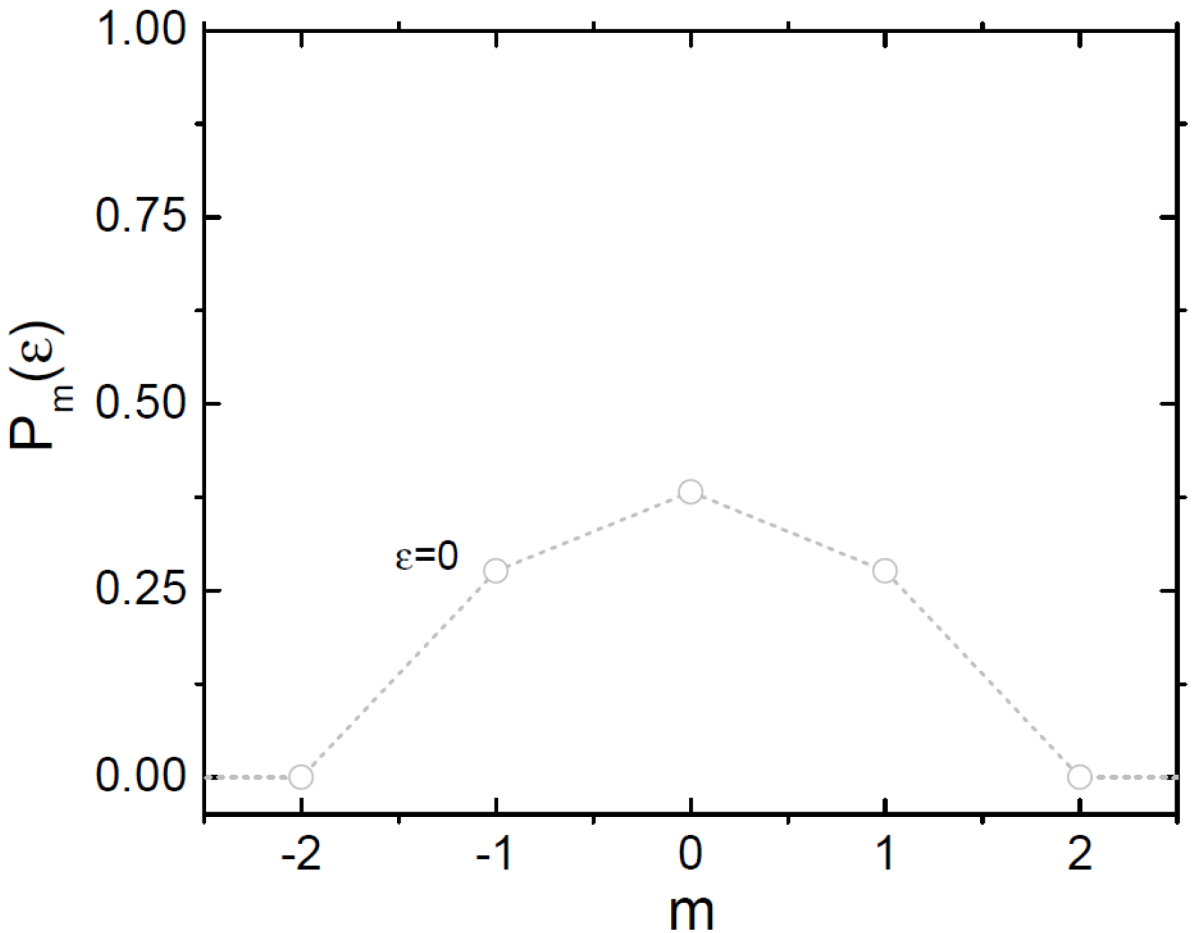
Elliptical polarization (ϵ=0-1)

$$P_m = \sum_{n=l+1}^{n_{max}} \sum_{l=|m|}^{n_{max}-1} |\langle \psi \mid \phi_{nlm} \rangle|^2$$





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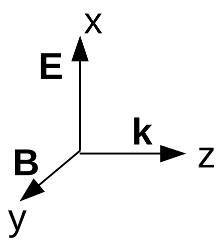

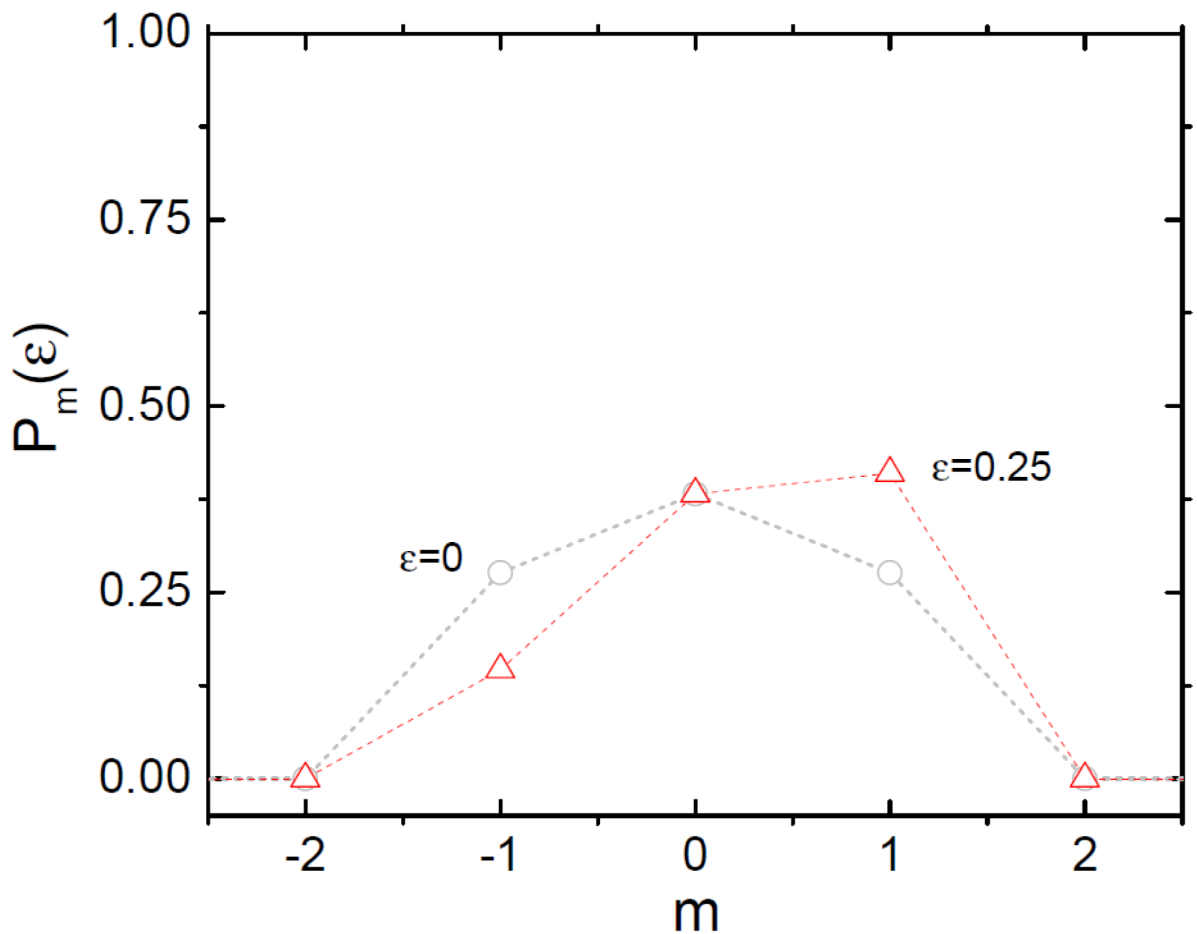

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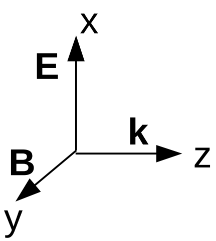

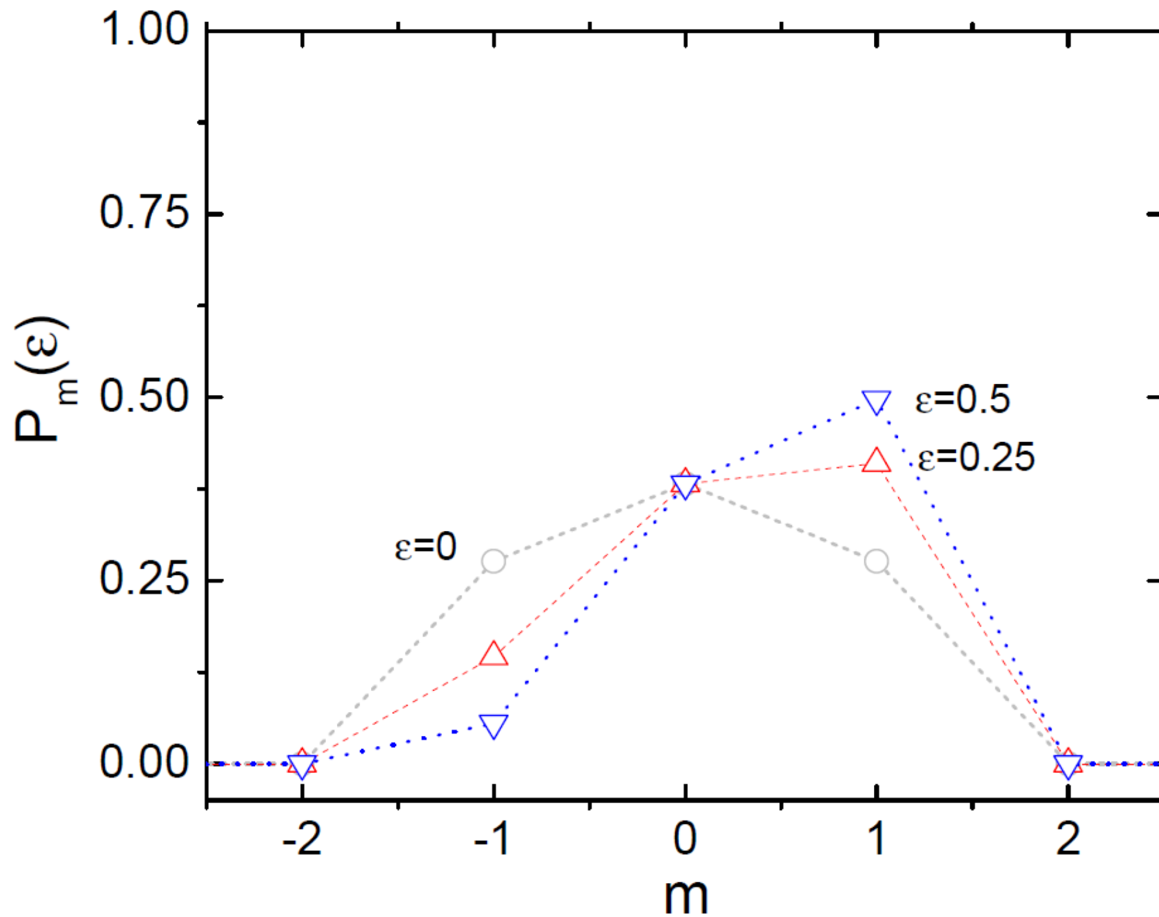

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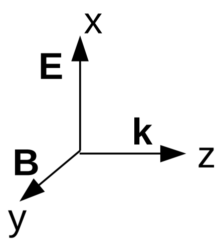

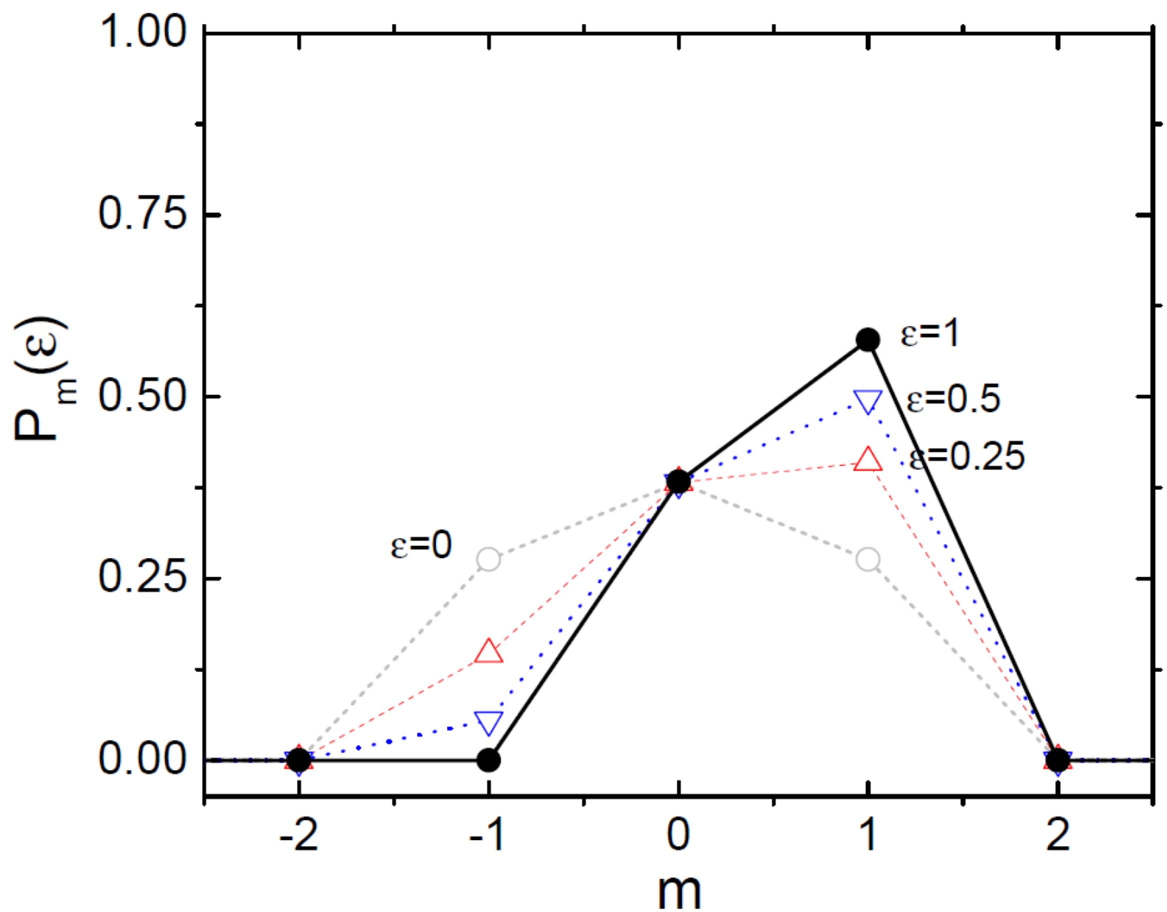

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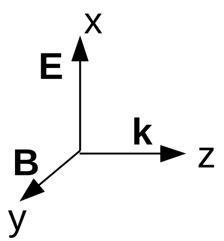
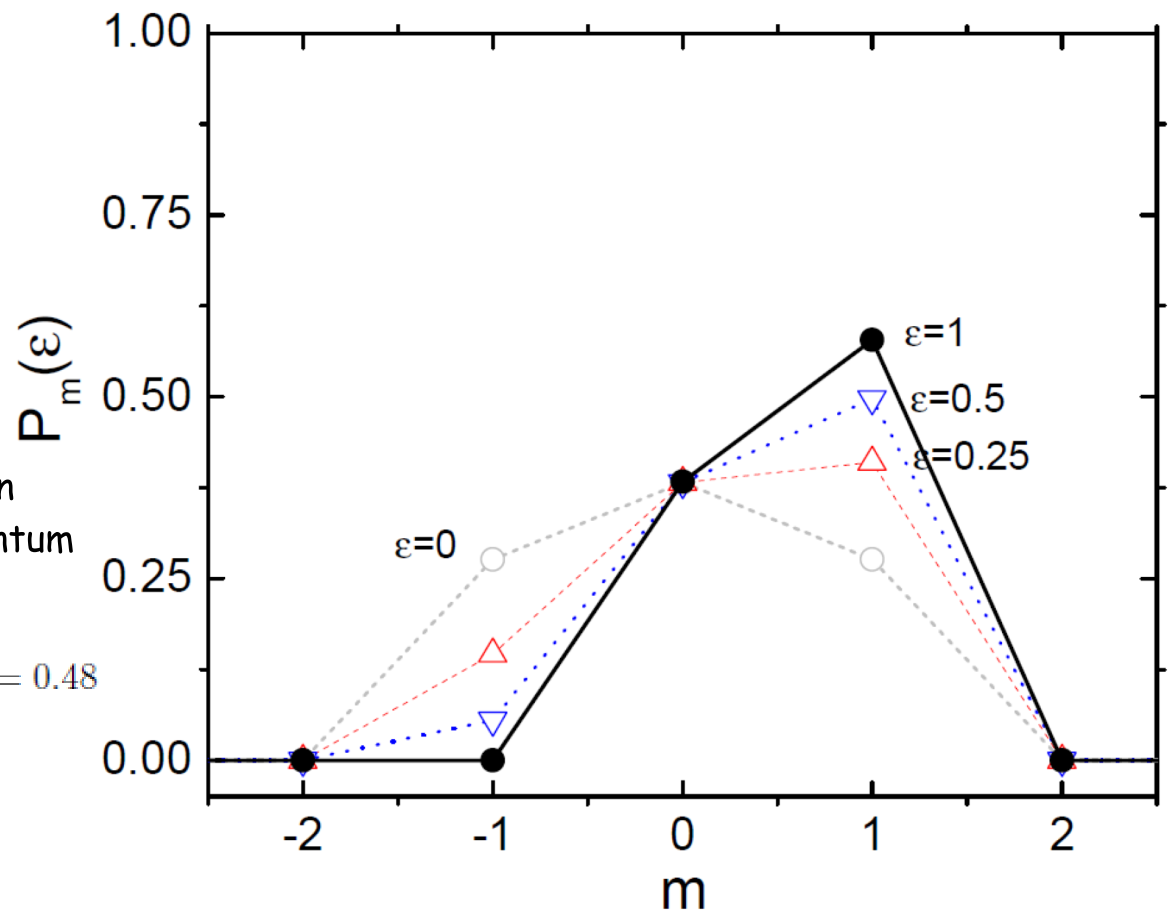


$$\langle \hat{l}_z \rangle = \sum_m P_m(\varepsilon) m$$

atom «twists» with transfer of photon helicity to atom orbital angular momentum l_z=+1

$$H_{n=1} + \hbar\omega \rightarrow H_{n'=4,5} \qquad \hbar\omega = \frac{1}{2n} - \frac{1}{2n'} = 0.48$$



1-photon resonance mechamism twisting of atom

$$H_{n=1} + \hbar\omega \to H_{n'=4,5} \qquad \hbar\omega = \frac{1}{2n} - \frac{1}{2n'} = 0.48$$

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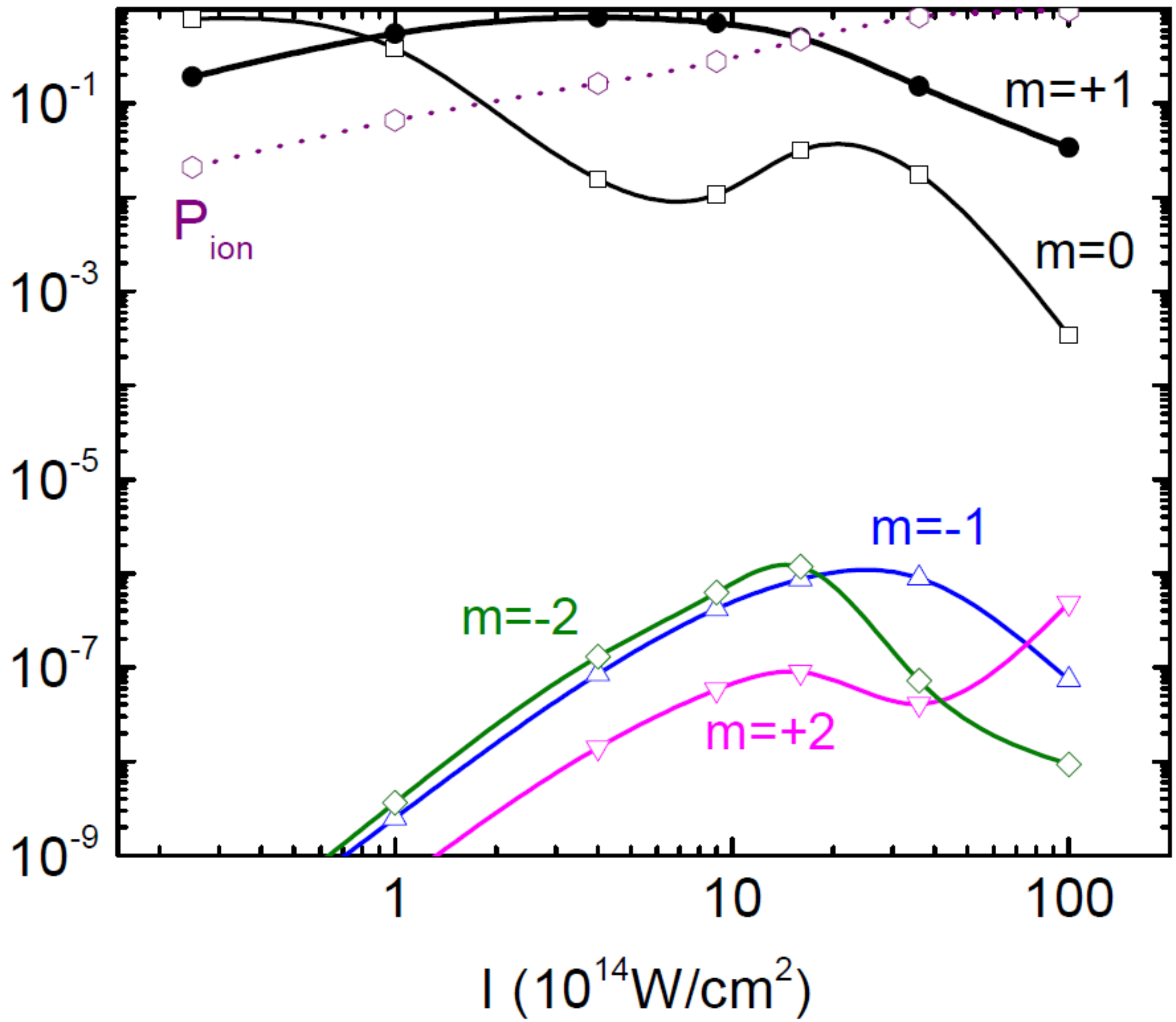
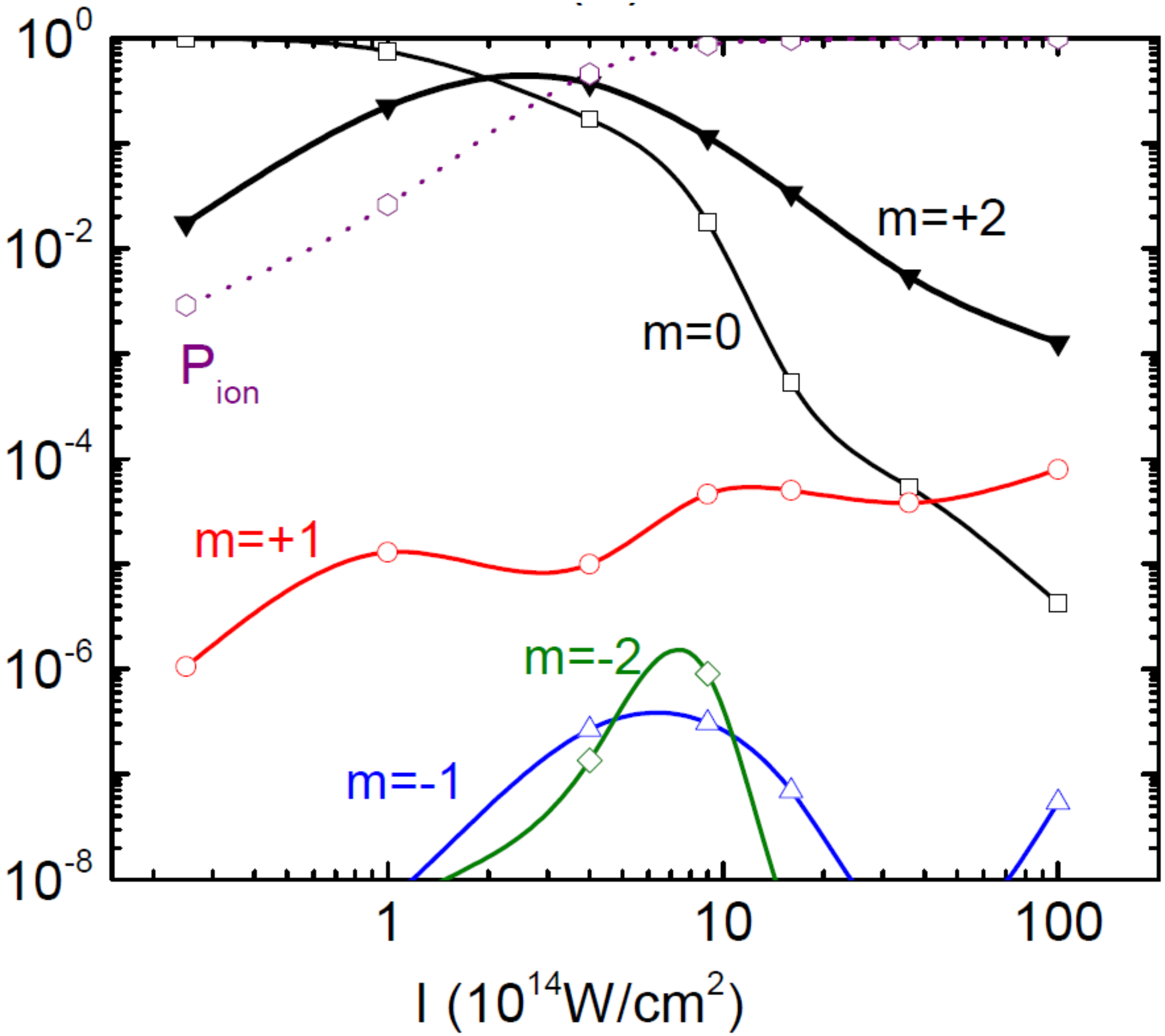


2-photon resonance mechamism twisting of atom

$$H_{n=1} + 2\hbar\omega \to H_{n'=4,5} \qquad \hbar\omega = \frac{1}{2n} - \frac{1}{2n'} = 0.48/2$$

2-photon resonance mechamism twisting of atom

$$H_{n=1} + 2\hbar\omega \rightarrow H_{n'=4,5} \qquad \hbar\omega = \frac{1}{2n} - \frac{1}{2n'} = 0.48/2$$

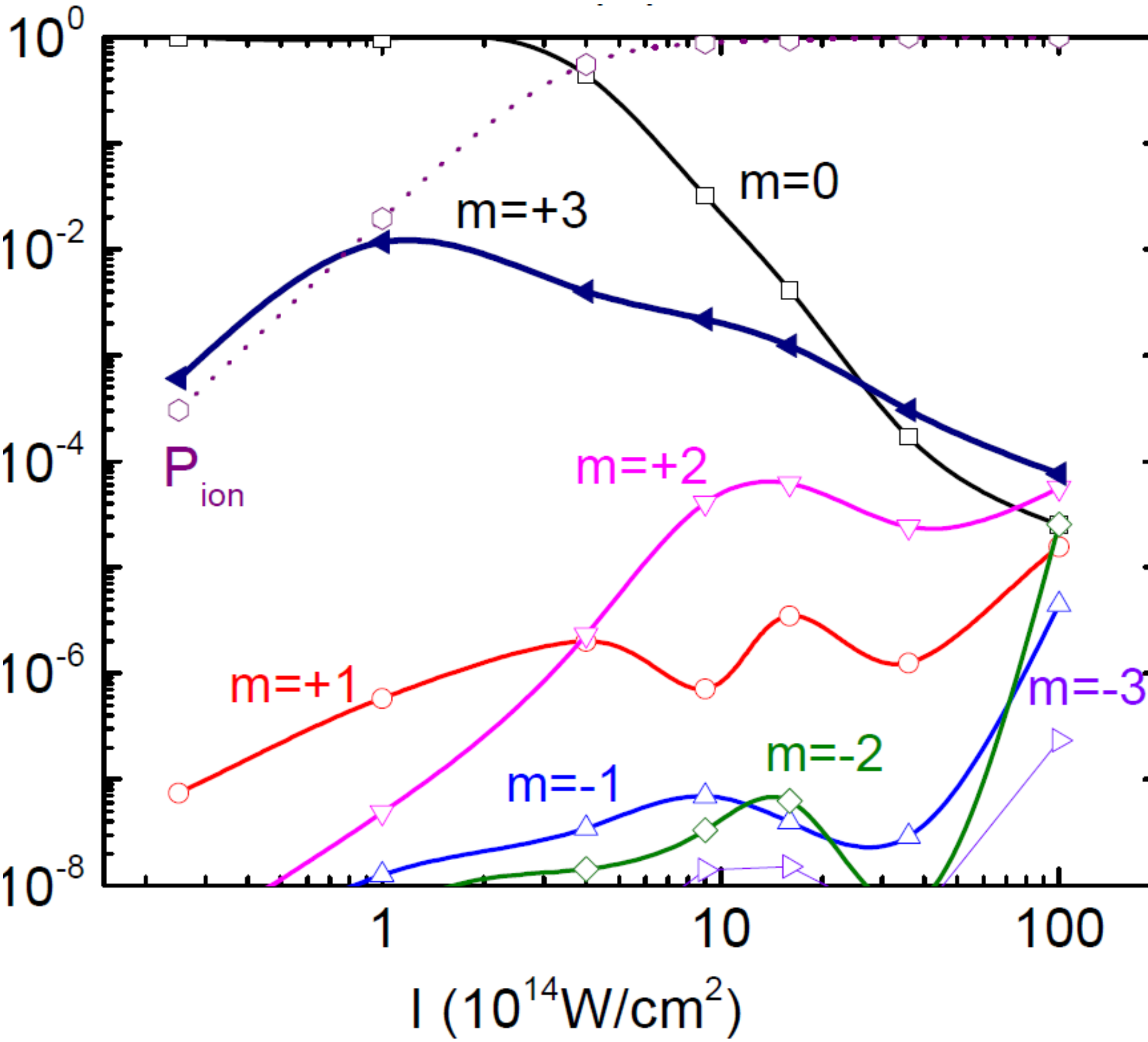


3-photon resonance mechamism twisting of atom

$$H_{n=1} + 3\hbar\omega \to H_{n'=4,5} \qquad \hbar\omega = \frac{1}{2n} - \frac{1}{2n'} = 0.48/3$$

3-photon resonance mechamism twisting of atom

$$H_{n=1} + 3\hbar\omega \to H_{n'=4,5} \qquad \hbar\omega = \frac{1}{2n} - \frac{1}{2n'} = 0.48/3$$



n-photon resonance mechamism twisting of atom

$$H_1 + n\hbar\omega \to H_{n'=4,5} \qquad \hbar\omega = \frac{1}{2} - \frac{1}{2n'} = 0.48/n$$

Conclusion & outlook

- acceleration of atom due to non-dipole corrections kr in EM wave and magnetic component B/c in it was invastigated
- strong correlation was found between V (MV) and $P_{ex} + P_{ion}$
- mechanism for n-photon resonant twisting of atom with transfer of helicity of photons from circularly polarized laser field to it was found

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TASKS:

1) using beams of twisted photons with internal orbital angular momentums for increasing efficiency of production twisted atoms

2) nuclear photonics: photoionization by hard x-rays and γ-radiation with including of nuclear motion

Conclusion & outlook

hybrid quantum-quasiclassical approach + DVR

S Shadmehri, V S Melezhik, Laser Phys. 33, 026001 (2023)

V Melezhik, J. Phys. A56, 154003 (2023)

V S Melezhik, S Shadmehri, Photonics 10(12), 1290 (2023)

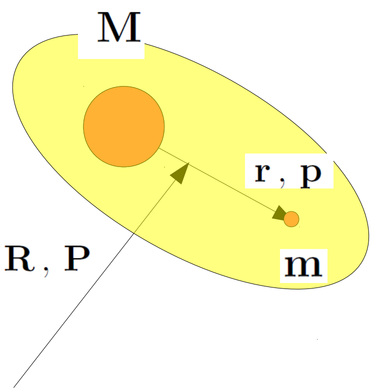
V S Melezhik, S Shadmehri, arXiv: 2408.08613; accepted to JETP
V S Melezhik, S Shadmehry, J Chem Phys 162, 174304 (2025)

Conclusion & outlook

- acceleration of atom due to non-dipole corrections kr in EM wave and magnetic component B/c in it was invastigated
- strong correlation was found between V (MV) and $P_{ex} + P_{ion}$
- two resonant mechanisms of atom acceleration were found: through single-photon and two-photon excitation of atom
- потенциальные приложения:

ускоренные атомы — литография микро-чипов для микро-электроники, диагностика плазмы в ТОКАМАК, ...
«закрученные» атомы — модификация фундаментальных взаимодействий, новый «инструмент» для исследования атомных столкновений, ...

Hydrogen atom in strong laser field
(non-dipole effects)



$$H(\boldsymbol{r},\boldsymbol{R},t)=\frac{\boldsymbol{P}^2}{2M}+h_0(\boldsymbol{r})+V_1(\boldsymbol{r},t)+\underline{V_2(\boldsymbol{r},\boldsymbol{R},t)}$$

$$h_0(\boldsymbol{r})=\frac{\hat{\boldsymbol{p}}^2}{2\mu}-\frac{1}{r}$$

PHYSICAL REVIEW LETTERS **124**, 233202 (2020)

Dissecting Strong-Field Excitation Dynamics with Atomic-Momentum Spectroscopy

A. W. Bray,[1,2,*] U. Eichmann,[2,†] and S. Patchkovskii[2,‡]
[1]*Australian National University, Canberra ACT 2601, Australia*
[2]*Max-Born-Institute, 12489 Berlin, Germany*

$\mathrm{P}=\mathrm{MV}\gg\mathrm{p}=\mathrm{mv}$

$$H(\mathbf{r},\mathbf{R},t)\to H_{eff}(\mathbf{r},t)=h_0(\mathbf{r})+V_{eff}(\mathbf{r},t)$$ **3D !!**

We propose using the c.m. degrees of freedom of atoms and molecules as a "built-in" monitoring device for observing their internal dynamics in nonperturbative laser fields.

detection of the internal electron quantum dynamics with CM-velocity spectroscopy.