ATOMIC IONIZATION by INTENSE XUV LASER PULSES of SHORT DURATION

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2. Analytic aspects
3. Numerical results
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Motivations and objectives I

- Motivations

  The interaction between intense laser pulses and matter - a subject which received considerable interest along the years. Special attention - given to photoionization: an electron of an atomic system exposed to such a pulse can absorb enough energy to quit the system and to escape to infinity.

  A recent and interesting experiment, done at the new free-electron laser in Hamburg (FLASH): Sorokin *et al.*, Phys. Rev. Lett. **99**, 213002 (2007).
  The photoionization phenomenon - studied by focusing XUV pulses with duration of ≈10 fs, wavelength of ≈13 nm and irradiance levels between 10^{12} and 10^{16} W/cm^2, on

Motivations and objectives II

free xenon atoms. To produce the ion charges recorded in experiment, a large number of photons is required. Particularly up to 57 photons (in a single shot) for the highest recorded ion charge, Xe^{21+}.
Maximum irradiance level used:
$I \approx 7.8 \times 10^{15}\mathrm{W/cm}^2 \approx I_0/4.5$, $I_0 \approx 3.51 \times 10^{16}\mathrm{W/cm}^2$

From documents of ELI project presentation:
-"ELI will provide a new generation of compact accelerators delivering ultra short (10^{-15}-10^{-18}s) pulses of radiation from EUV to γ-ray and energetic particles beams for European scientists".

Related experience in our group:

Motivations and objectives III

- Dondera, Muller and Gavrila, Phys. Rev. A **65**, R31405 (2002)

- Boca, Muller and Gavrila, J. Phys. B: At. Mol. Opt. Phys. **37**, 147 (2004)

Both papers - dedicated to the study of *atomic stabilization*, with emphasis on its dynamic version.

Present work: for the same range of frequencies but for intensities lower than those implied in stabilization and focused on photoelectron properties.

- Atomic photoionization: the road towards a quantitative description

  The exact nonpert. study of the phenomenon, in the nonrelativistic quantum mechanics frame, involves:

Motivations and objectives IV

- To accurately describe the time evolution of the state of the atomic system in interaction with the laser pulse
- (The state at every time moment being known) to extract with precision the measurable quantities, as photoelectron distributions in energies and directions - in order to make new predictions or comparisons with experimental results

Both problems - difficult to solve, even for the atom with only one electron!

The asymptotic region

- The wave function: continuum superposition of outgoing spherical waves (after the laser pulse end)

  $$\text{Reduced w. func.:} \qquad F(\boldsymbol{r},t) \equiv r\,\psi(\boldsymbol{r},t) \qquad (1)$$

  $$F(\boldsymbol{r},t) = \int_0^\infty f(E,\boldsymbol{n})\, e^{i(kr-Et)}\, dE\,, \quad r \to \infty \qquad (2)$$

  $$\boldsymbol{n} = \boldsymbol{e}_r = \boldsymbol{r}/r\,, \quad k = \sqrt{2E}$$

  Ingoing spherical waves - negligible contribution for $r \to \infty$ (they would descr. el. coming from ∞ towards the origin).

- The amplitudes f - determ. by inv. Fourier transf., from the w. func. as func. of time, for a fixed large value of the rad. r

Photoelectron distributions

- The total probability for the electron to cross the surface element $d\boldsymbol{S} = r^2 d\Omega \boldsymbol{e}_r$, in a time interval $(t_1, t_2) \Leftarrow$ from the usual interpretation of $\boldsymbol{J}$ vector

$$dp = \Im \left[\int_{t_1}^{t_2} F^*(\boldsymbol{r}, t) \frac{\partial F(\boldsymbol{r}, t)}{\partial r} dt \right] d\Omega \qquad (3)$$

- The most detailed probability distribution

$$d^2 p = \frac{k}{2\pi} \left| \int_{t_1}^{t_2} F(\boldsymbol{r}, t)\, e^{iEt}\, dt \right|^2 dE\, d\Omega \quad (r \to \infty) \qquad (4)$$

- Less detailed distributions, in energies *or* directions - can be obtained by appropriate integrations of eq. (4)
- Other possibilities do exist - Madsen *et al.*, Phys. Rev. A **76**, 063407 (2007)

System, numerical procedure and simulations I

- System: hydrogenlike atom, initially in a stationary state of the type nlm with $m = 0$, in interaction with an XUV laser pulse, linearly polarized, described by the vector potential

$$\boldsymbol{A}(t) = \frac{F_0}{\omega}\, \boldsymbol{e}_z\, s(t) \cos \omega t \,, \tag{5}$$

where F_0 is the electric field amplitude and ω is the laser frequency.
Pulse: flat top. The envelope $s(t)$ increases from zero to one as $\cos^2(\pi t/2\tau_{on})$ for $-\tau_{on} < t < 0$, remains constant (equal with one) for a duration τ_{flat}, then decreases to zero as $\cos^2[\pi(t - \tau_{flat})/2\tau_{on}]$ for $\tau_{flat} < t < \tau_{on} + \tau_{flat}$. The parameters τ_{on} and τ_{flat} are chosen as integer multiples of the laser period $T = 2\pi/\omega$.

System, numerical procedure and simulations II

- Numerical procedure
  The corresp. TDSE - solved on an uniform space-time grid (spherical coordinates r and θ, and time t), using an approximation of the evolution operator. The propagation in time of the wave func. - continued (after the pulse end) until the wave function becomes again "zero". Photoelectron distributions - calculated with eqs. (3) and (4).
- Conditions for numerical simulations
  Values of parameters:

  $Z : 1, 3$

  Initial states: $1s$, $2s$, $2p$, $3s$, $3p$, $3d$
  $Z = 1$: $E_1 = -0.5$, $E_2 = -0.125$, $E_3 = -0.05555$
  $E_1 + \omega = 2.92 > 0$ (a.u.!)

System, numerical procedure and simulations III

$Z = 3$: $E_1 = -4.5$, $E_2 = -1.125$, $E_3 = -0.5$
$E_1 + \omega = -1.08$, $E_2 + 2\omega = 2.34 > 0$

$I : I_0/4.5,\ I_0,\ 10I_0,\ 100I_0$

ω: 3.42 $a.u. \approx 93$ eV

$\tau_{on} = \tau_{off} = 5T$, $\tau_{flat} = 40T$.
Total duration: $50T \approx 2.22$ fs

For the highest intensity, $I = 100I_0$,

$\alpha_0 \approx 0.85$ a.u.

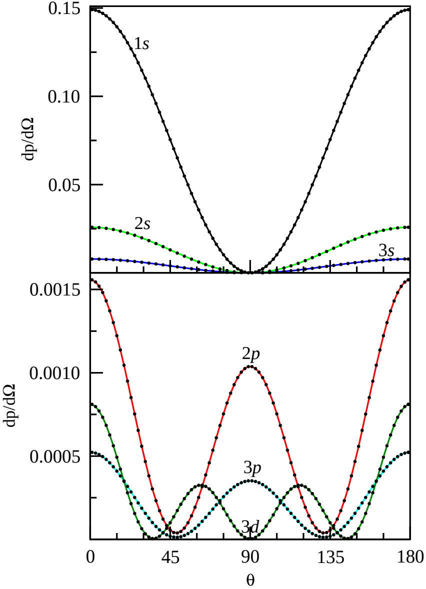
$a_0 \approx 0.02 \ll 1$

$$\alpha_0 = \frac{\sqrt{I}}{\omega^2}$$

$$a_0 \equiv \alpha\frac{\sqrt{I}}{\omega}$$

Figure 1.i Photoelectron distributions: $Z = 1$, $I = 10 I_0$

Left: angle distribution



Right: energy spectrum

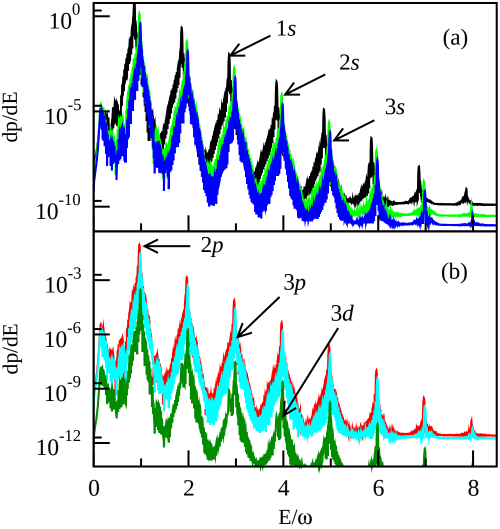
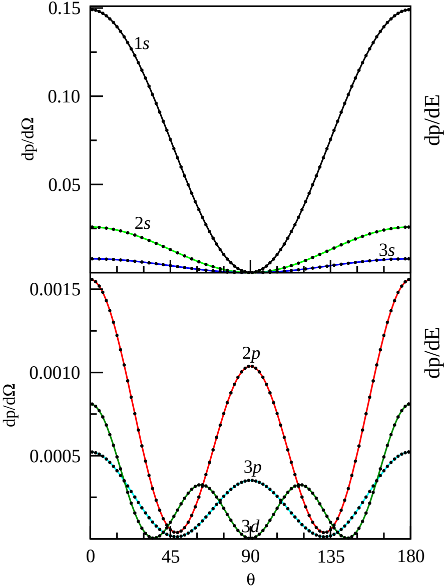


Figure 1.ii Photoelectron distributions: $Z = 1$, $I = 10 I_0$

Left: angle distribution



Right: energy spectrum

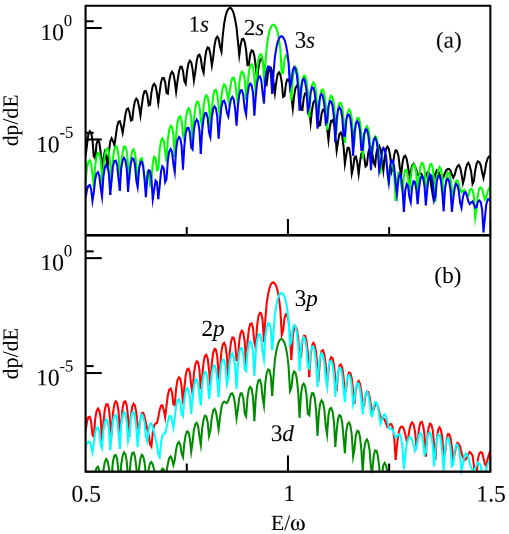


Figure 2. Photoelectron angular distributions

Left: $Z = 1$ Initial states: 1*s*, 2*p* and 2*s* Right: $Z = 3$

Intensities: $I = I_0/4.5$ (a), $I = I_0$ (b)

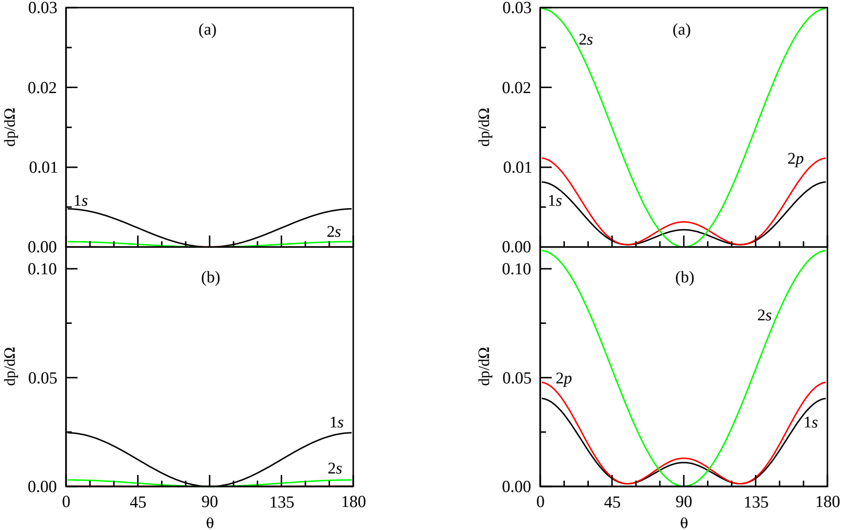
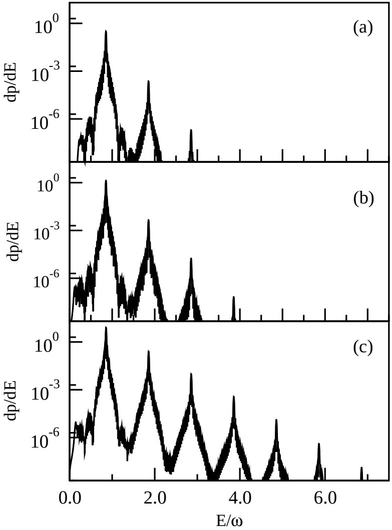


Figure 3.i Photoelectron energy spectra

Left: $Z = 1$ Initial state: $1s$ Right: $Z = 3$

Intensities: $I = I_0/4.5$ (a), $I = I_0$ (b), $I = 10I_0$ (c)



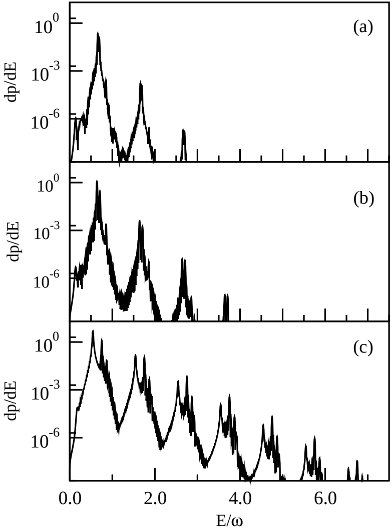


Figure 3.ii Photoelectron energy spectra

Left: $Z = 1$ Initial state: $2p$ Right: $Z = 3$

Intensities: $I = I_0/4.5$ (a), $I = I_0$ (b), $I = 10 I_0$ (c)

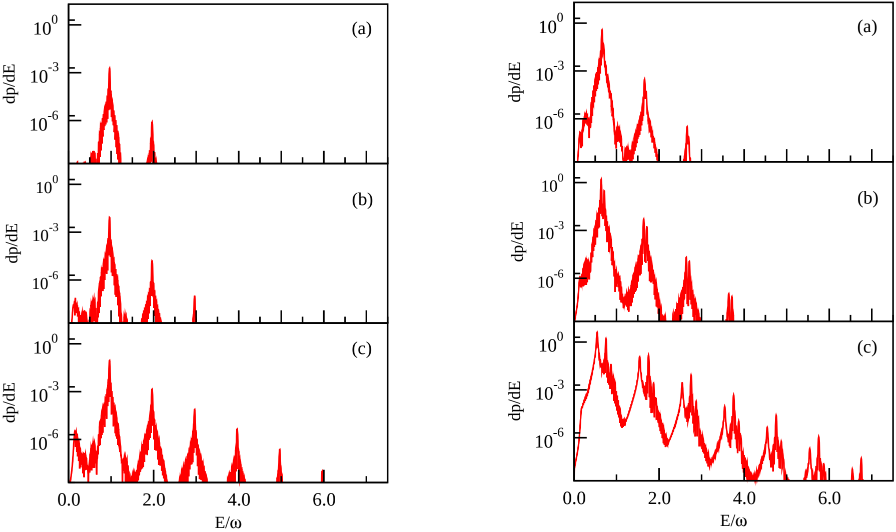
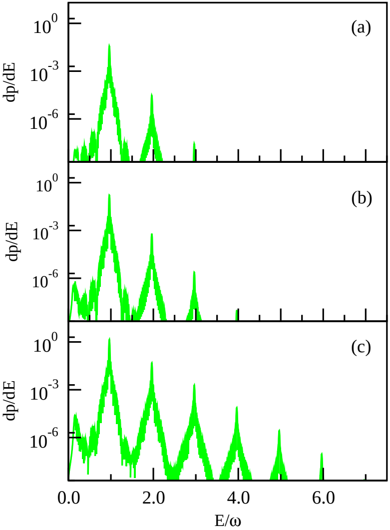


Figure 3.iii Photoelectron energy spectra

Left: $Z = 1$ Initial state: $2s$ Right: $Z = 3$

Intensities: $I = I_0/4.5$ (a), $I = I_0$ (b), $I = 10I_0$ (c)



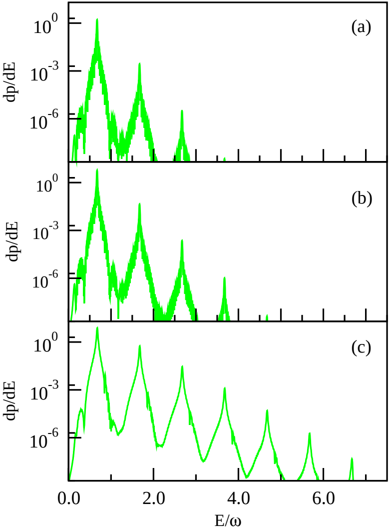


Figure 3.iv Photoelectron energy spectra (excerpts)

Left: $Z = 1$ Initial states: 1*s*, 2*p* and 2*s* Right: $Z = 3$

Intensities: $I = I_0/4.5$ (a), $I = I_0$ (b), $I = 10I_0$ (c)

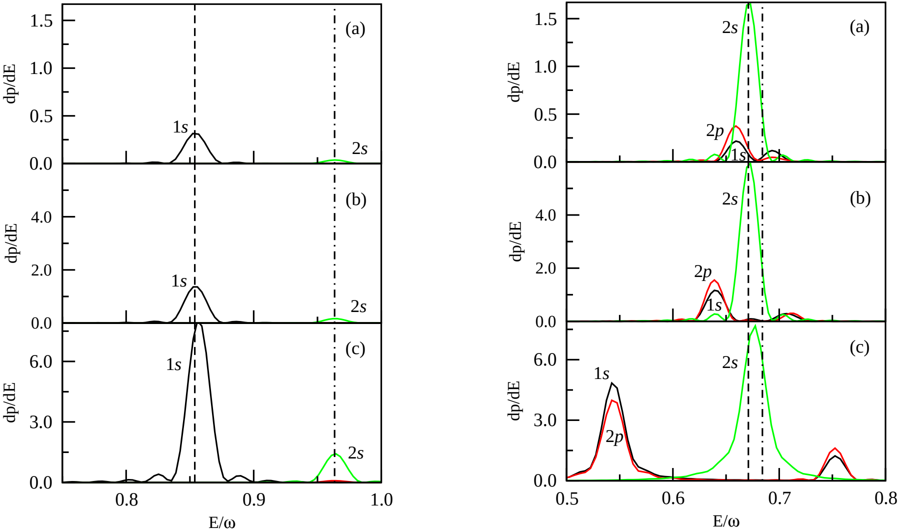
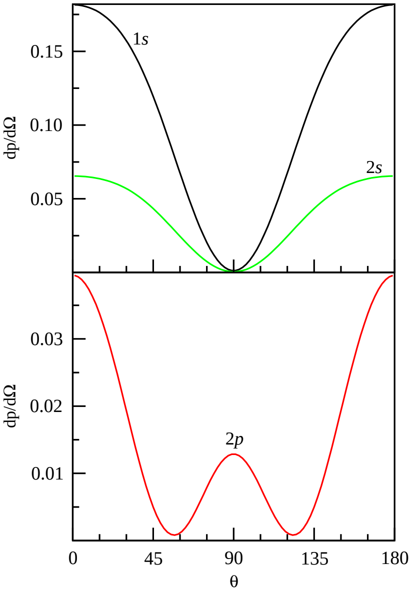


Figure 4.i Photoelectron distributions: $Z = 1$, $I = 100 I_0$

Left: angle distribution

Right: energy spectrum



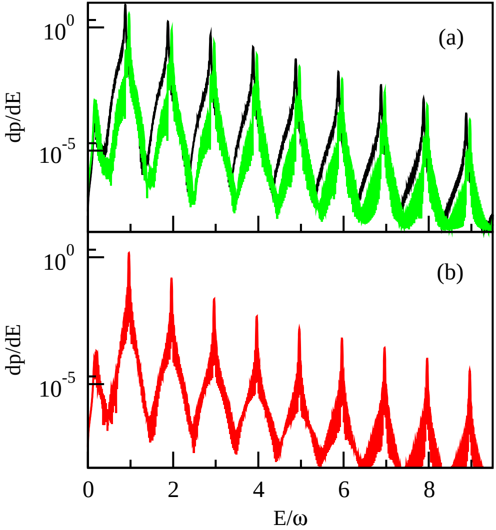
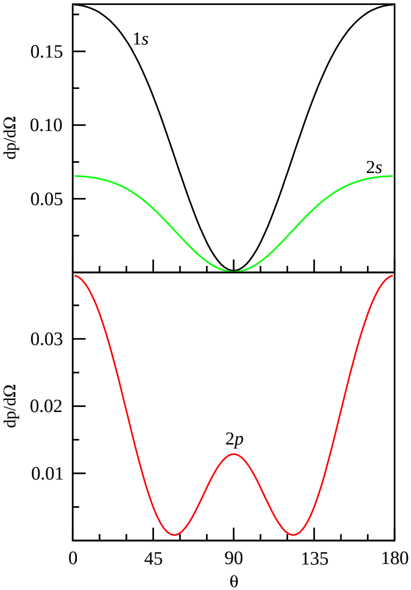


Figure 4.ii Photoelectron distrib.: $Z = 1$, $I = 100 I_0$

Left: angle distribution



Right: energy spectrum

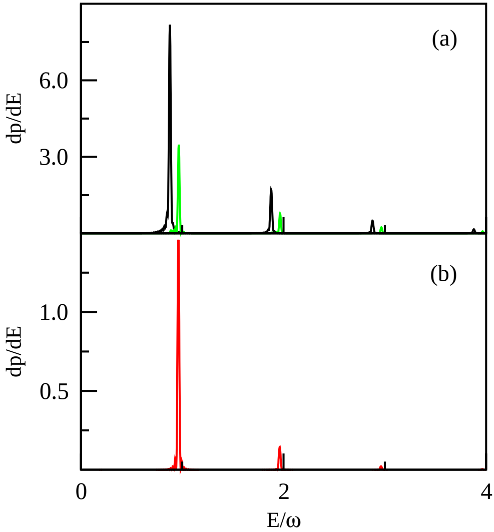


Figure 5.i Energy *and* angle distributions

Initial state: 1*s*
Intensity: $10 I_0$
Angles:
1° (a), 31° (b),
45° (c), 91° (d)

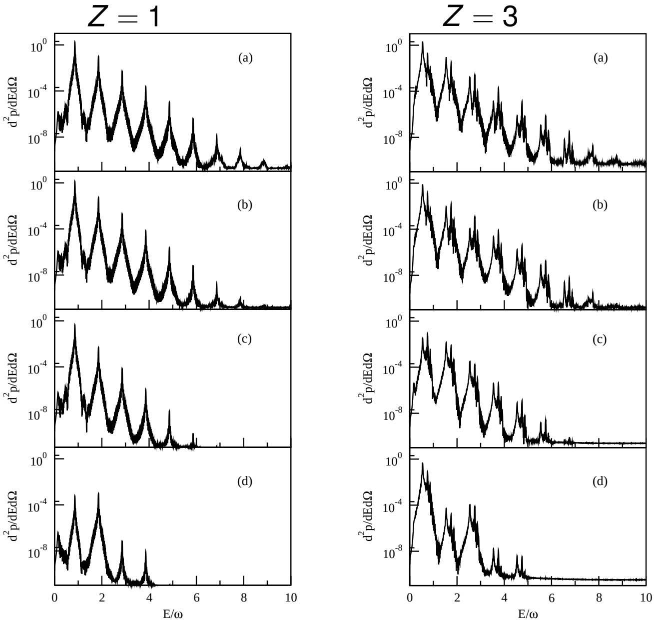


Figure 5.ii Energy *and* angle distributions

Initial state: 2*p*
Intensity: $10I_0$
Angles:
1° (a), 31° (b),
45° (c), 91° (d)

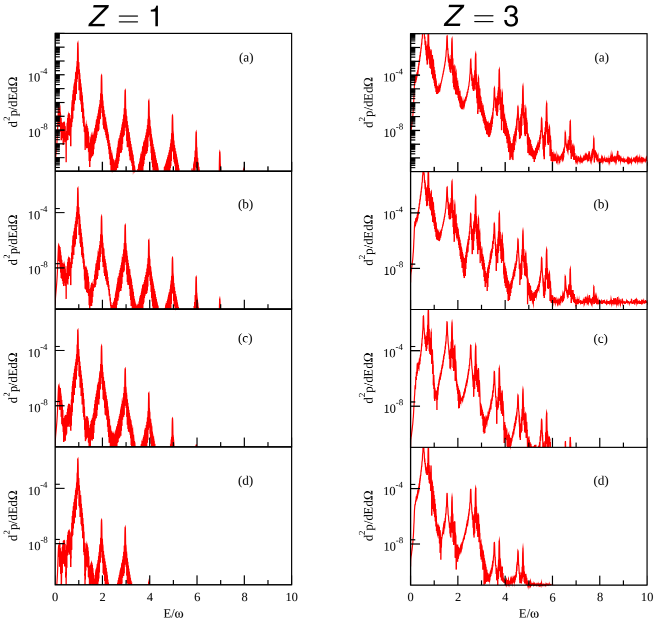
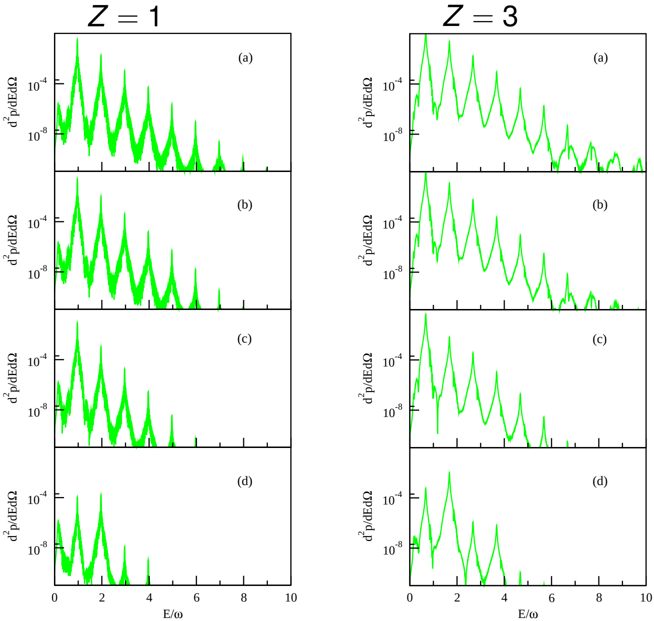


Figure 5.iii Energy *and* angle distributions

Initial state: $2s$
Intensity: $10I_0$
Angles:
1° (a), 31° (b),
45° (c), 91° (d)



Conclusions

- A recently developed method, based on the asymptotic behavior of the wave function, was applied to determine of photoelectron energy and angular distributions for a laser frequency belonging to XUV regime and intensities around or higher than the atomic unit of intensity.
- The results obtained for a hydrogenlike atom in interaction with an XUV laser pulse demonstrate that at intensities around I_0 (or lower) the photoionization is dominated by the absorption of the minimum number of photons (required to ionize the atom).
- Distinct features of photoionization are observed if the (quasi)resonance condition is or is not fullfiled.
- The excess photon ionization (EPI) becomes important for intensities signif. higher than the atomic unit of intensity.