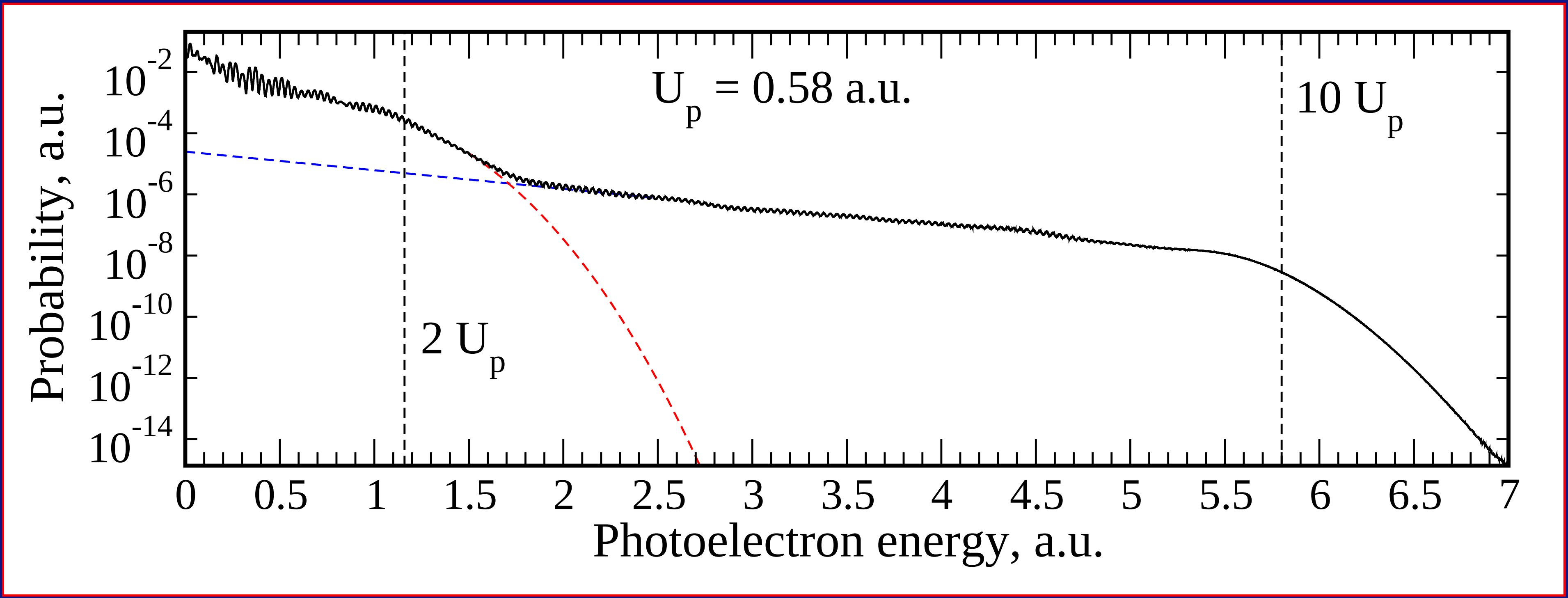
Example electron spectrum (ATI)



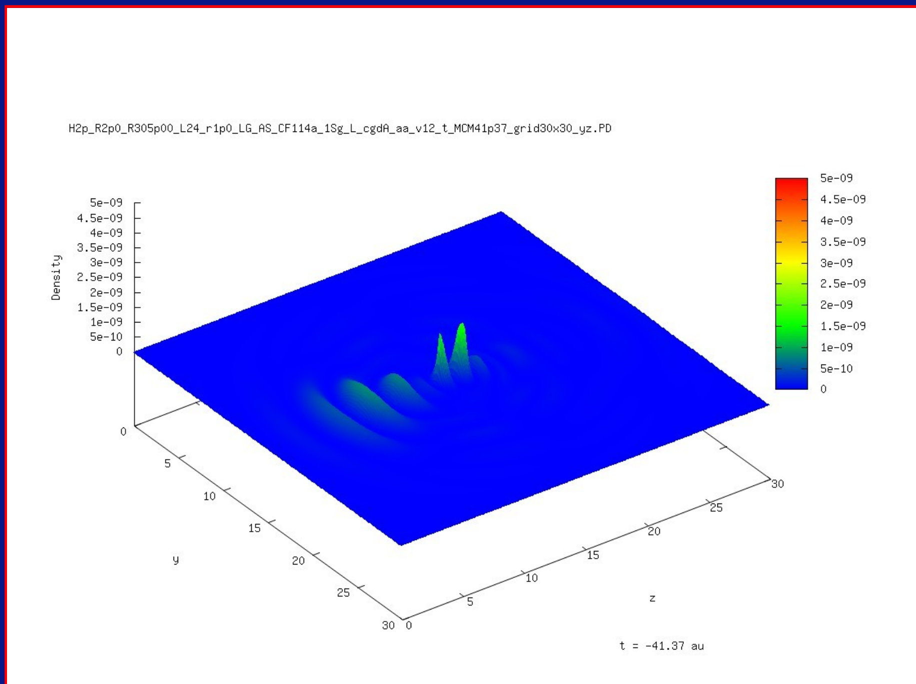
Hydrogen atom

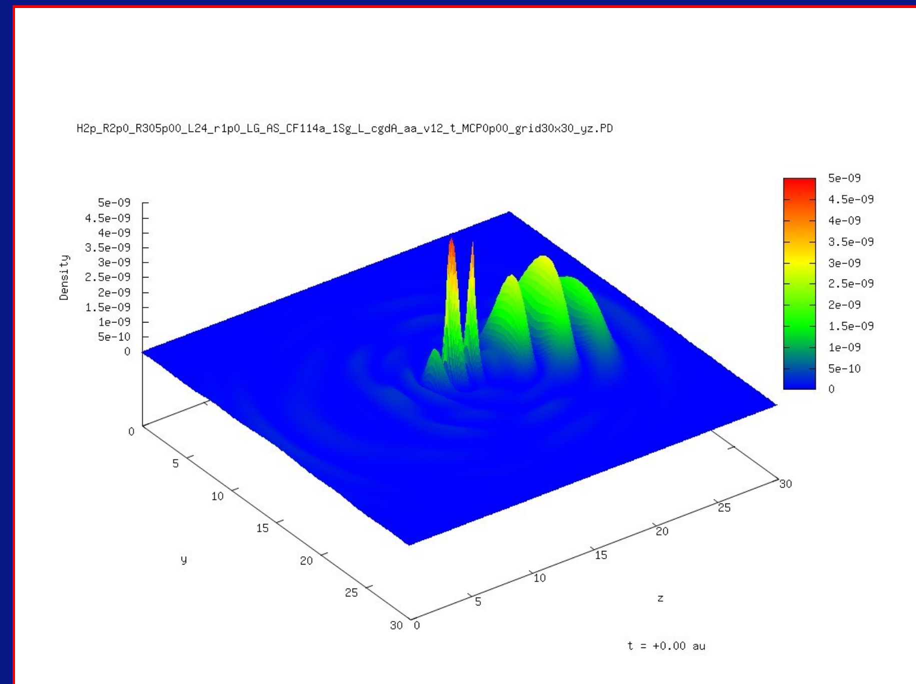
Laser parameters: 1300 nm; 6 cycles; cos^2; $I_{\max} = 10^{14}$ W/cm^2.

Direct electrons: 0 to about 2 times the ponderomotive energy $\mathrm{U_p} = I/(4\omega^2)$.

Rescattered electrons: dominate spectrum beyond 2 $\mathrm{U_p}$.

Example electronic wavepacket (H_2^+)

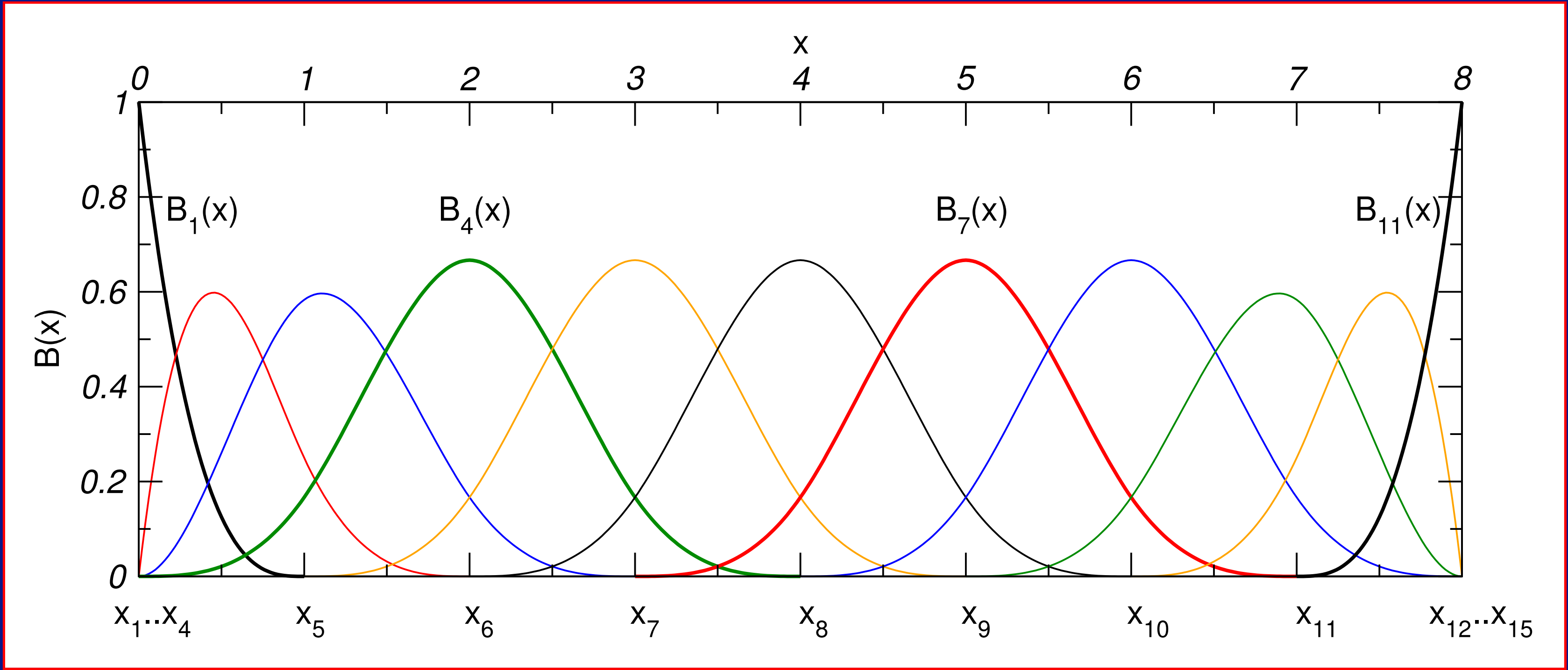




Electronic wavepacket at two different times within a 2-cycle laser pulse.

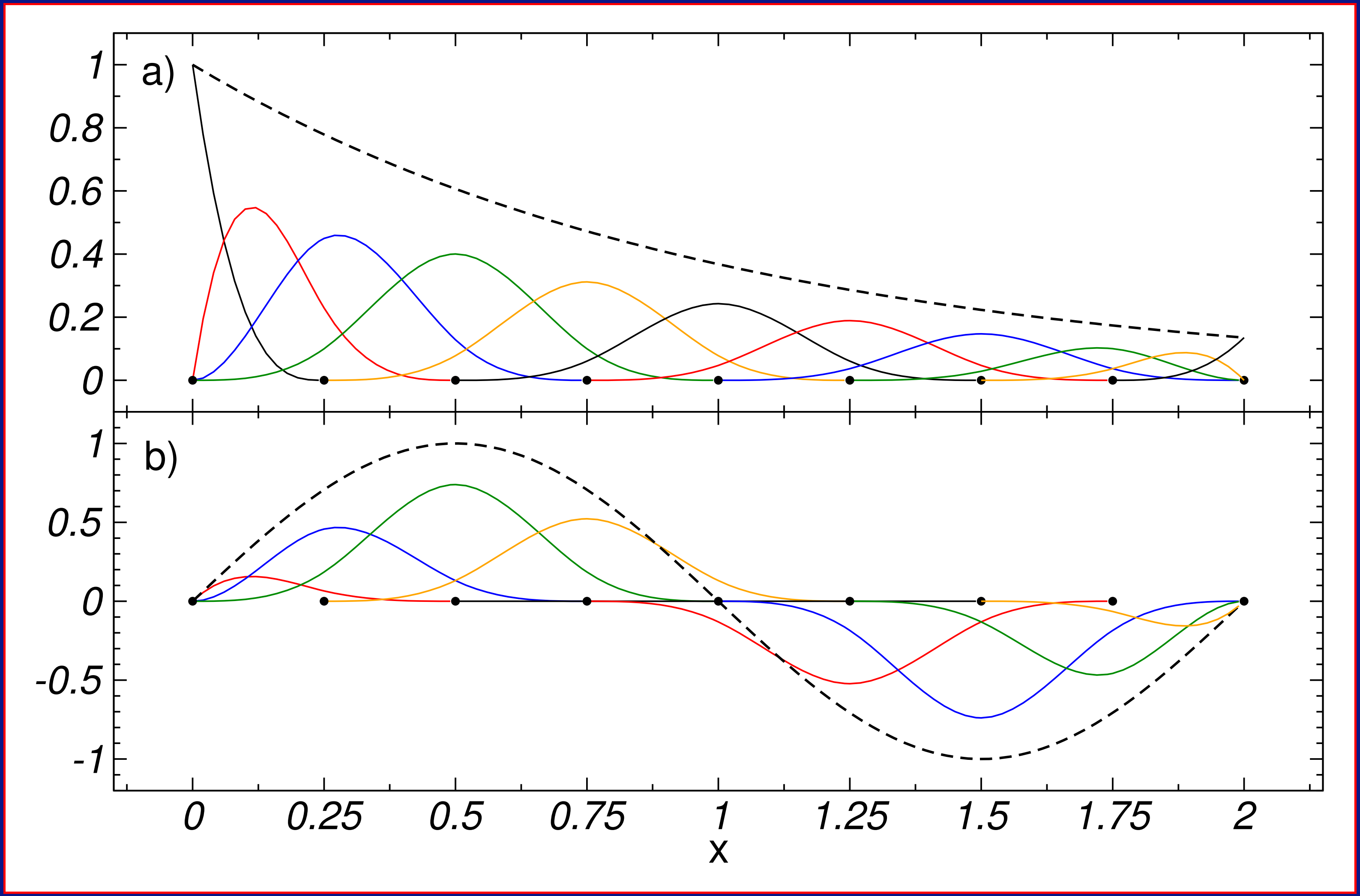
(Only the continuum part is shown.)

B-spline properties (I)



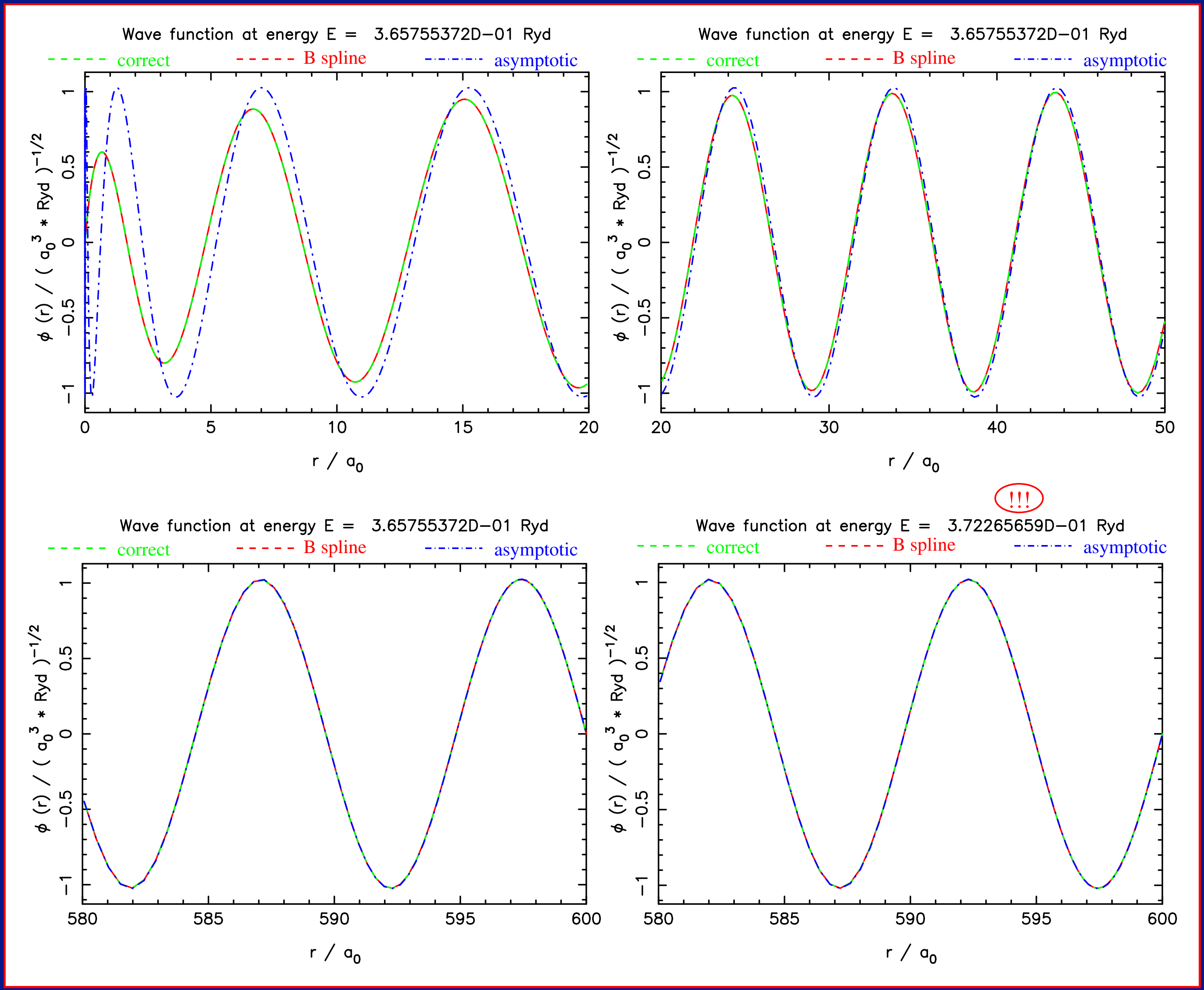
All 11 B splines of order $k = 4$ for knot sequence $\{t_i\} = \{0, 0, 0, 0, 1, 2, 3, 4, 5, 6, 7, 8, 8, 8, 8\}$.

B-spline properties (II)

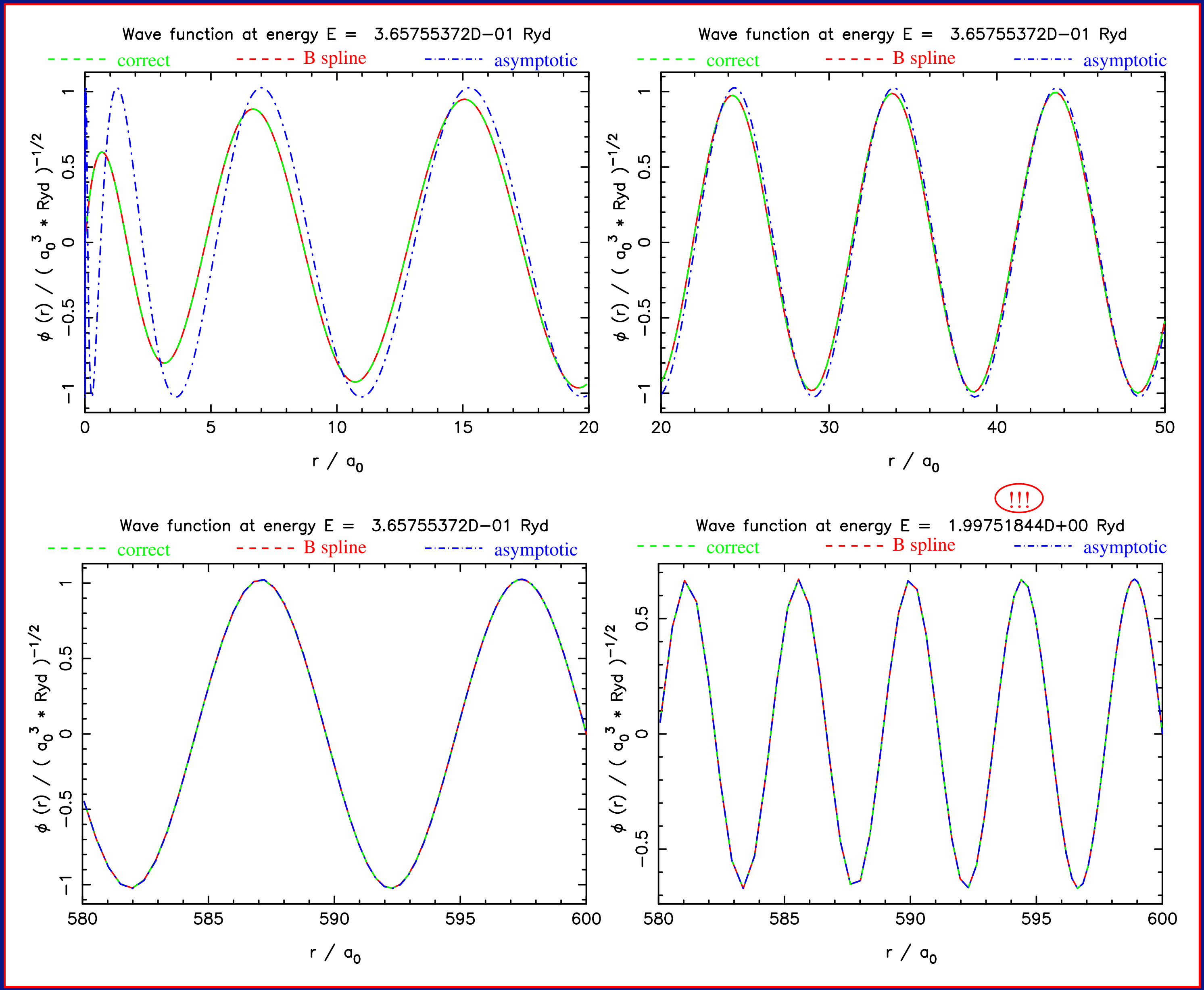


Fitting (a) e^{-x} or (b) $\sin(\pi x)$ with B splines (order $k = 4$ and $s = 8$ knot points).

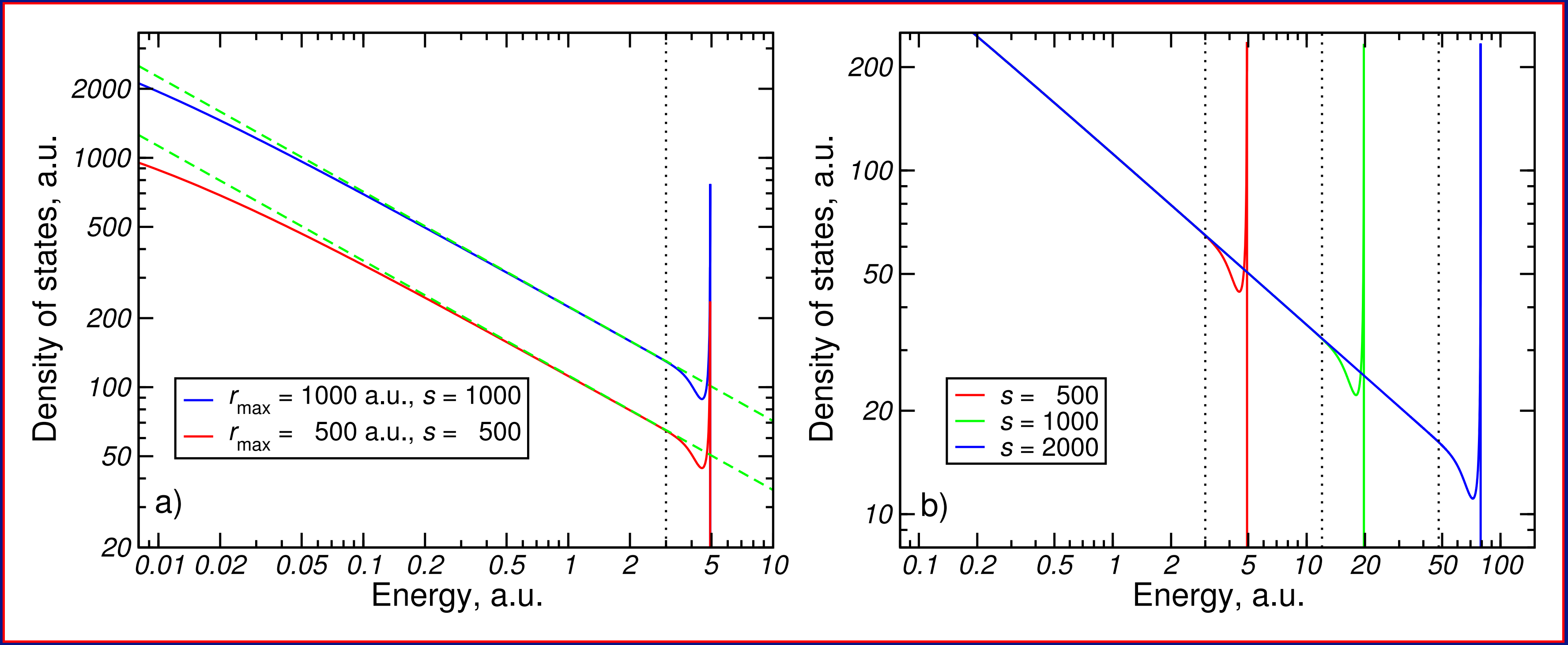
Example: continuum wavefunctions for H atom (I)



Example: continuum wavefunctions for H atom (II)



Box discretization with B splines



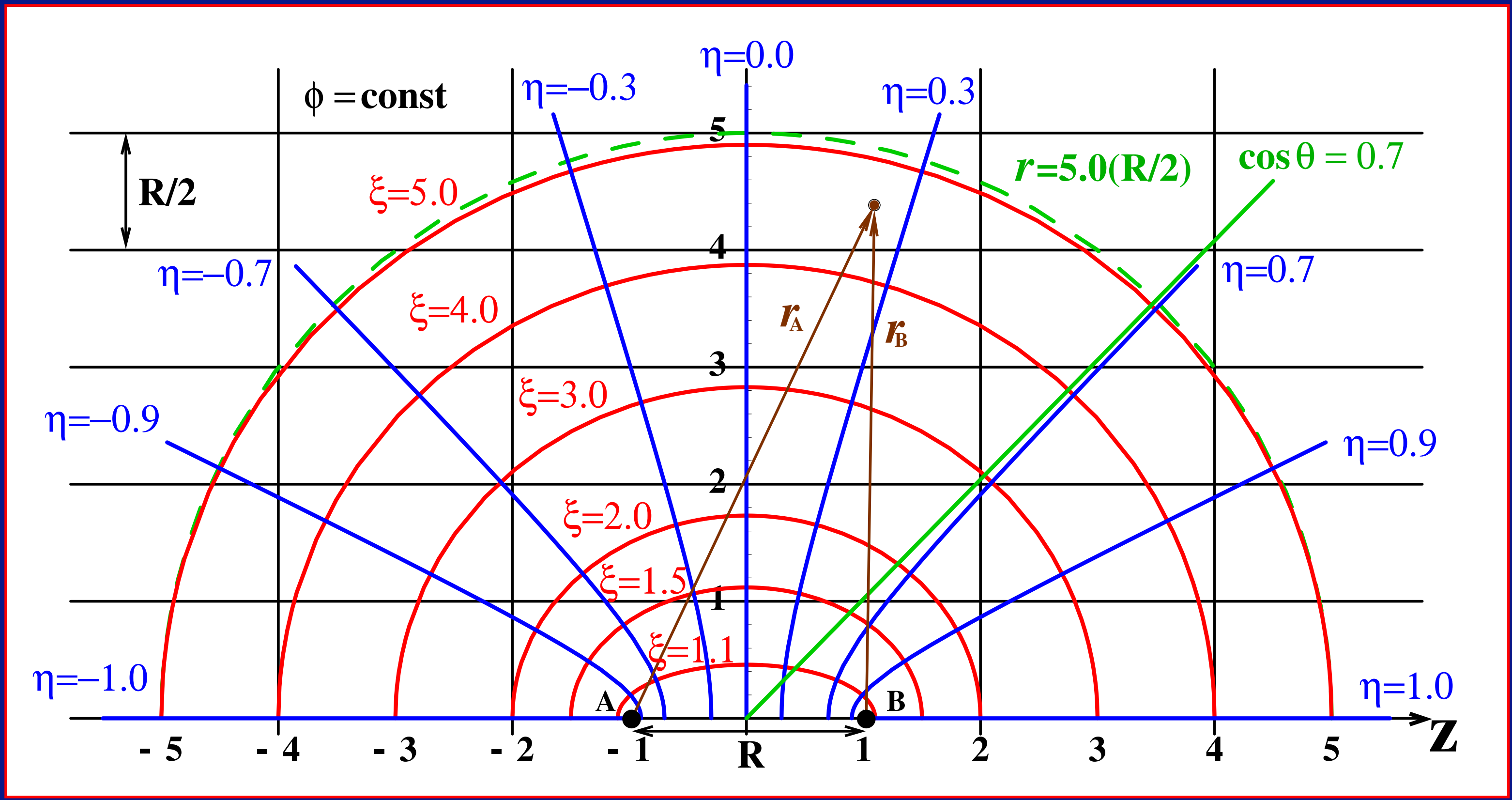
Size of the (radial) "box": $r_{\max}$

Number of (radial) knot points: s

(a): same knot spacing;

(b): variable knot spacing ($r_{\max} = 500\, a_0$).

Prolate spheroidal coordinates (for diatomics)



$\xi \in [1, \infty)$

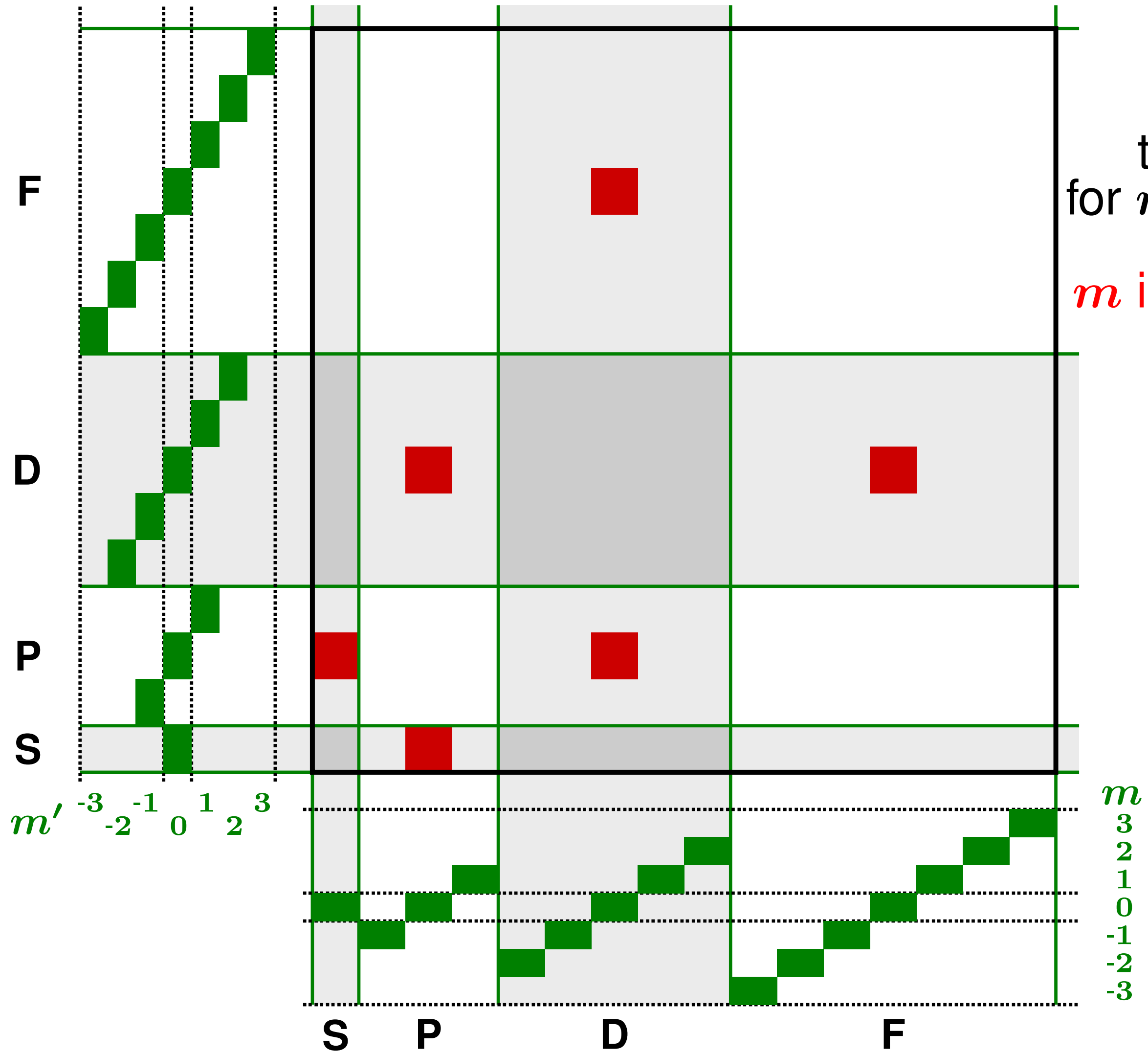
$\eta \in [-1, 1]$

$\phi \in [0, 2\pi)$

$$\xi = \frac{r_A + r_B}{R} \qquad r = \frac{R}{2}\sqrt{\xi^2 + \eta^2 - 1} \xrightarrow{\xi \gg 1} \frac{R}{2}\xi$$

$$\eta = \frac{r_A - r_B}{R} \qquad \cos\theta = \frac{\xi\eta}{\sqrt{\xi^2 + \eta^2 - 1}} \xrightarrow{\xi \gg 1} \eta$$

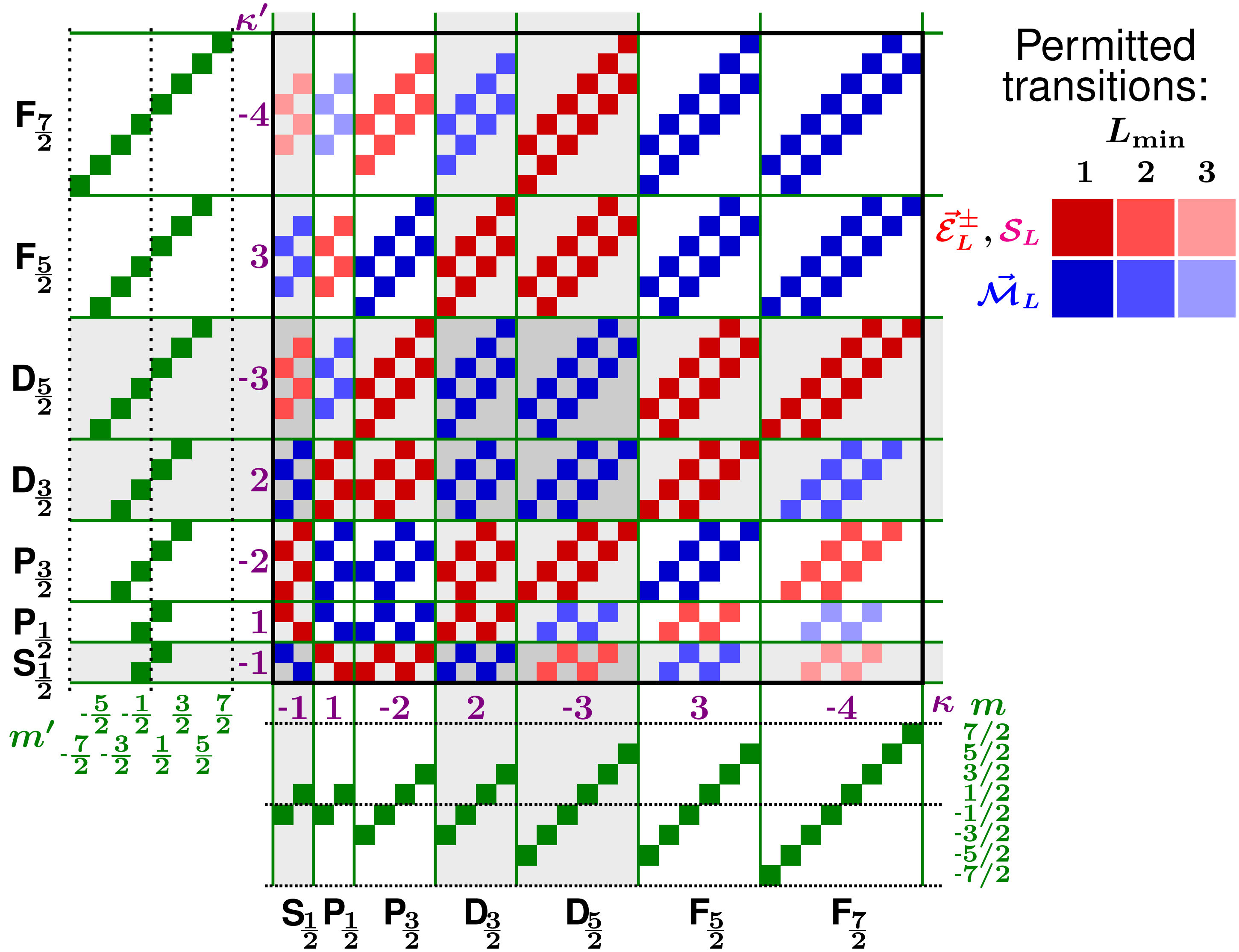
Transitions within non-relativistic dipole approximation



Permitted dipole transitions for $m' = m = 0$.

m is conserved!

Transitions within relativistic beyond-dipole treatment



Normalization of continuum states

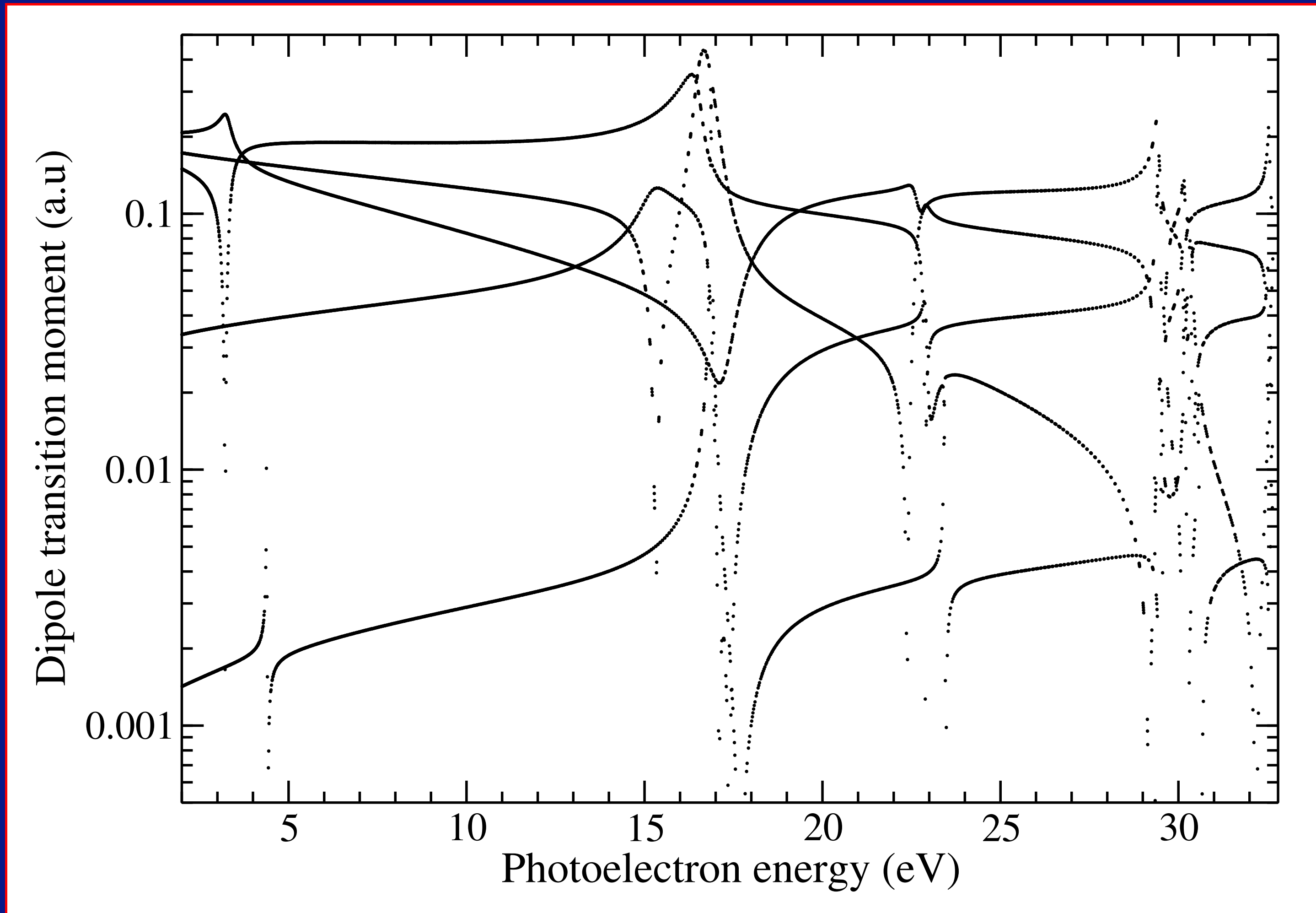
Uncoupled continuum states:

- separable potential (H_2^+): channels are separately obtained,
- normalization (of originally) box-discretized states via density of states or asymptotic behaviour.

Coupled continuum states:

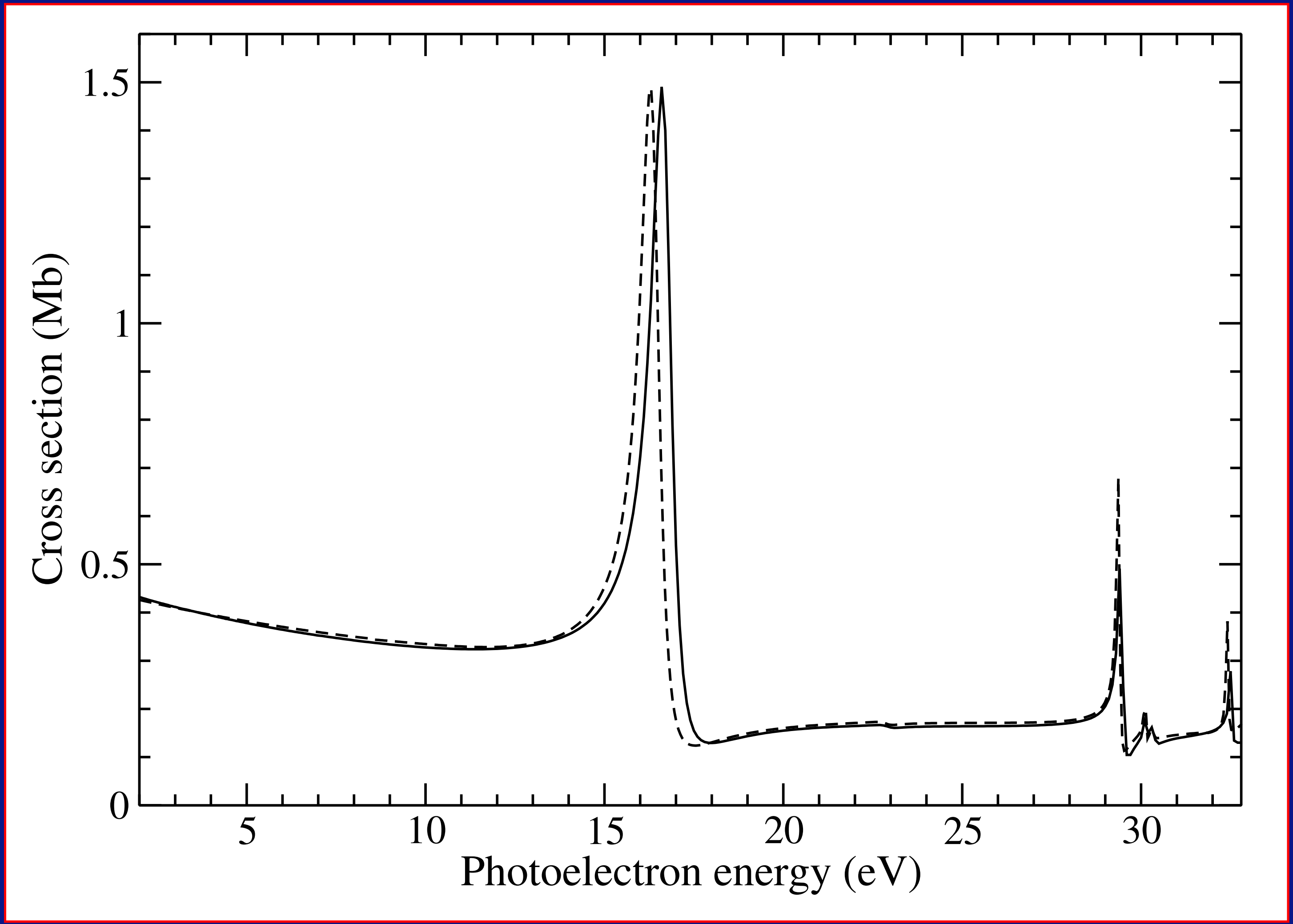
- non-separable potential (like Na_2^+) or two-electron case,
- **Note:** this differs from atoms (and larger molecules) where the electron-electron interaction does not break a symmetry!
- analysis of leading configurations (two-electron case): [Apalategui & Saenz, *J. Phys. B* **35**, 1909 (2002)].
- asymptotic analysis in terms of linear combinations of spherical harmonics (more robust): [Vanne & Saenz, *J. Phys. B* **37**, 4101 (2004)].

Continuum transition moments for HeH^+



$$X\,^1\Sigma \rightarrow ^1\Sigma \; (R = 1.45\, a_0)$$

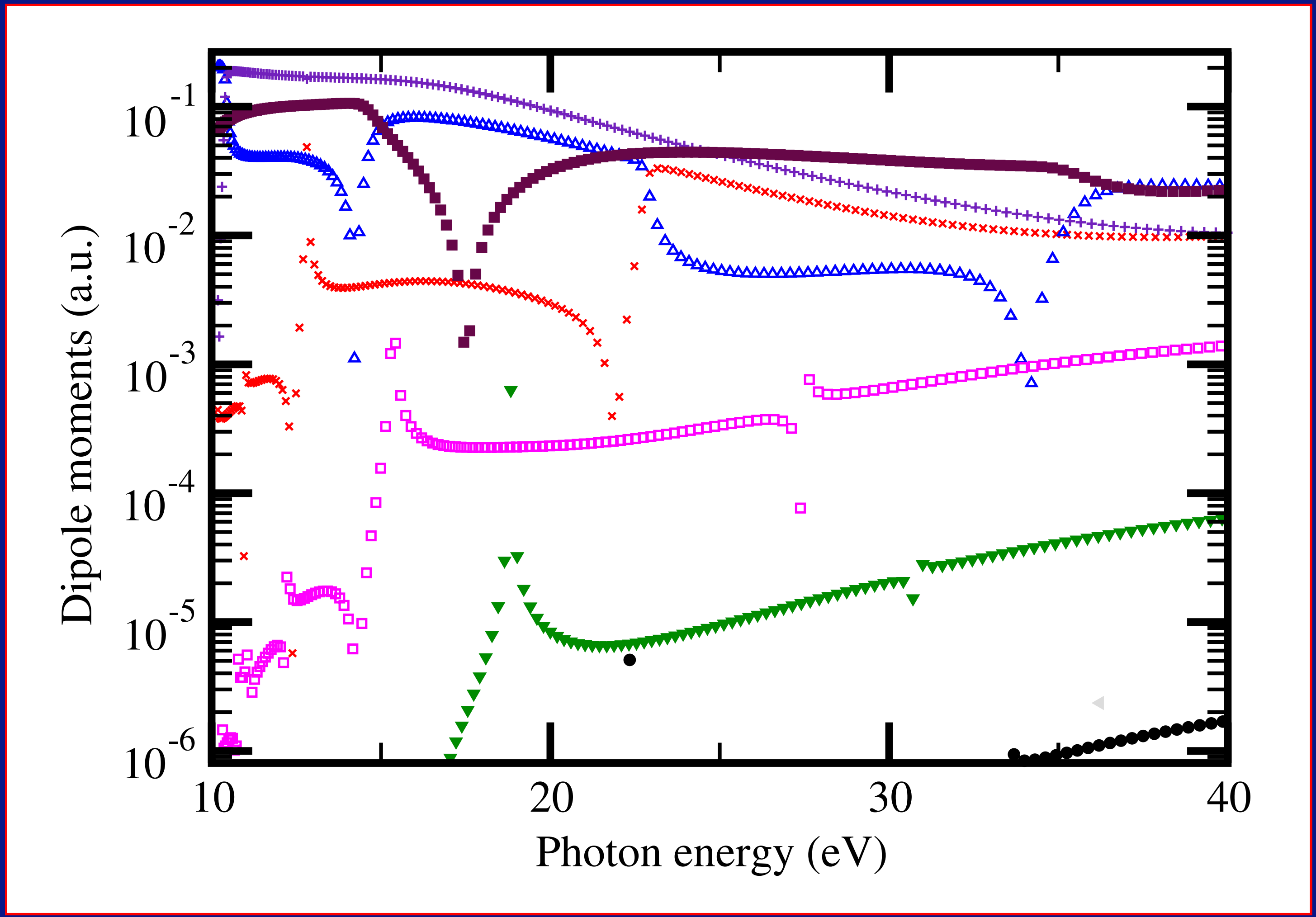
Partial photoionization cross-section for HeH^+



$$\mathrm{X}\,^1\Sigma \rightarrow ^1\Sigma \;(R = 1.45\,a_0)$$

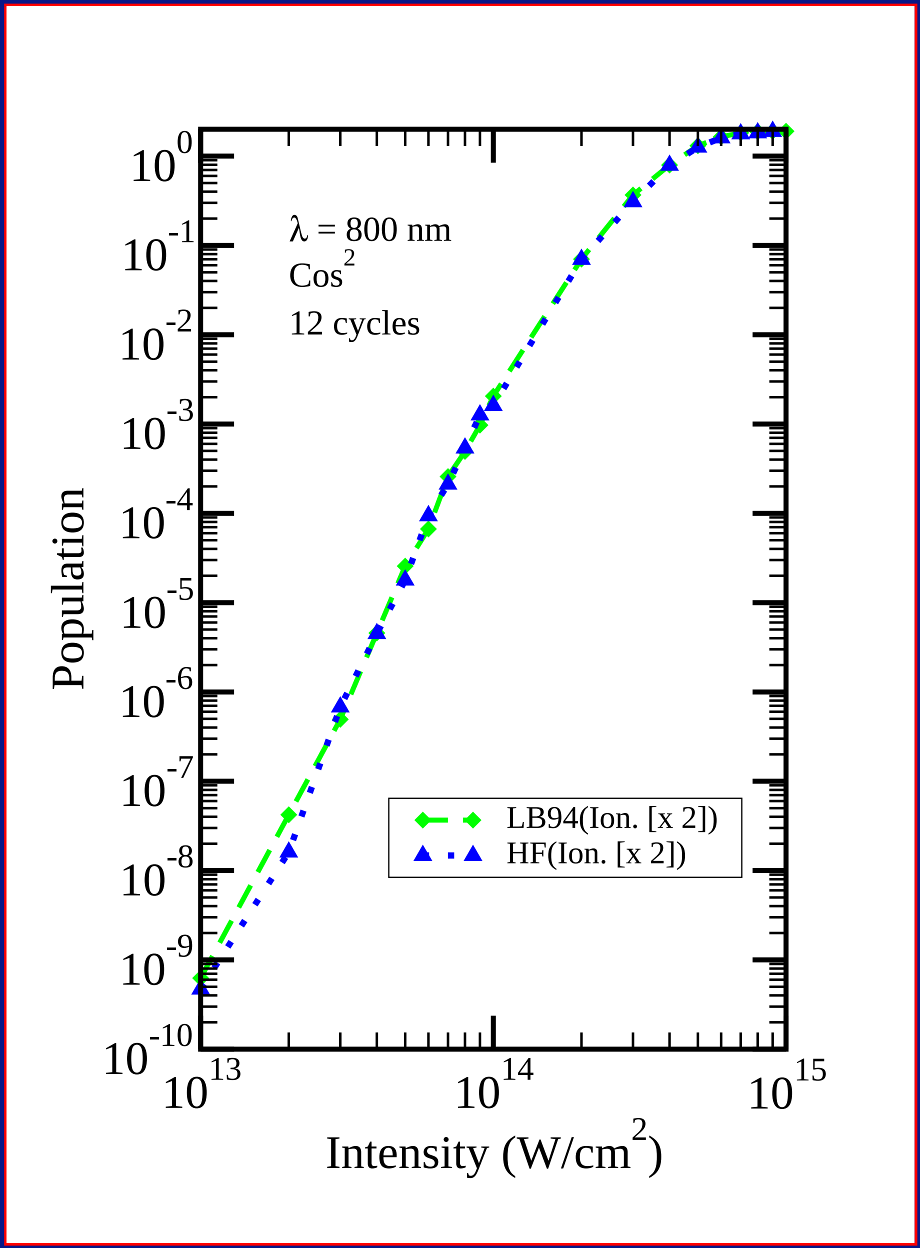
Solid: this method, **dashed:** explicitly-correlated basis functions + CSM [Saenz, *Phys. Rev. A* **67**, 033409 (2003)].

Continuum transition moments for Na_2^+



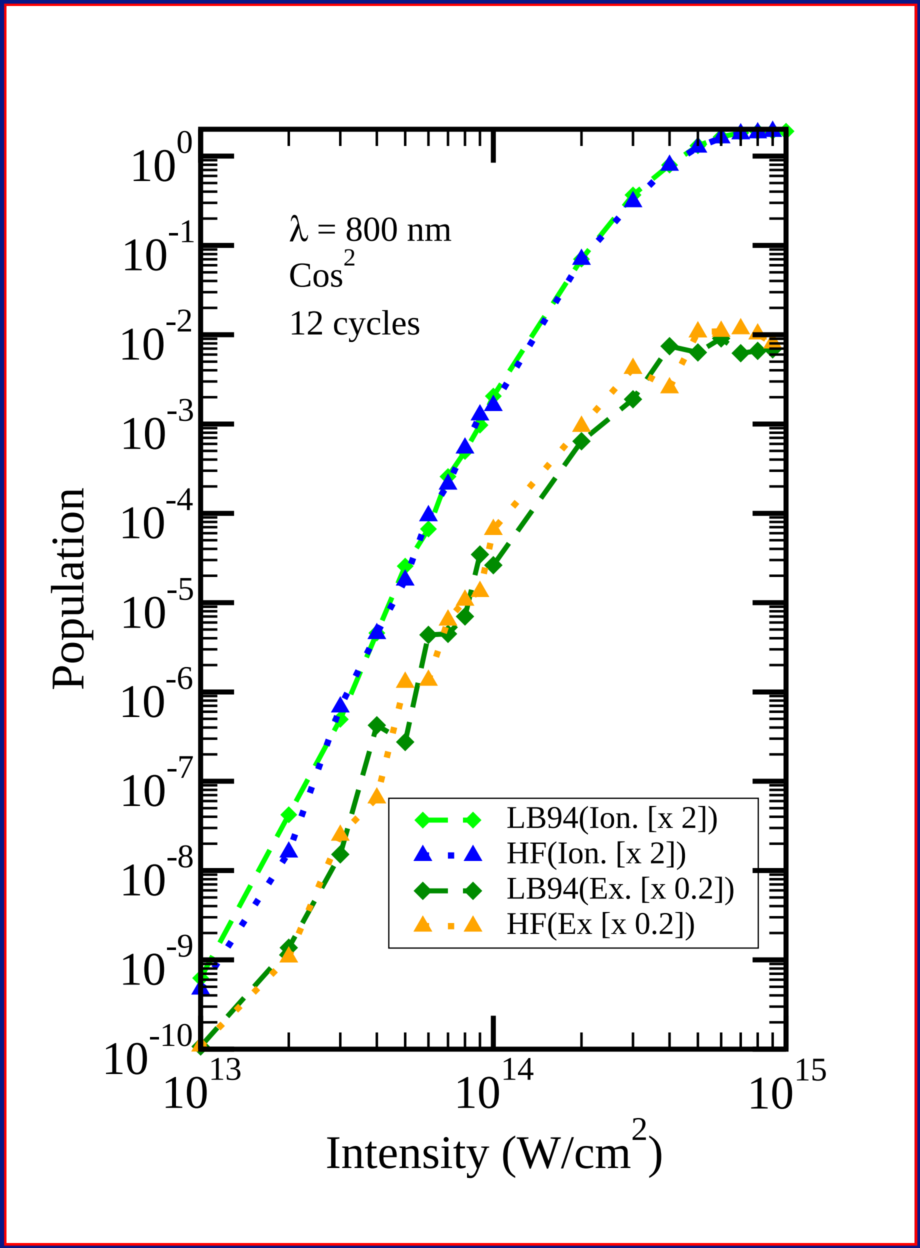
$$\mathsf{X}\,{}^2\Sigma_g \rightarrow {}^2\,\Sigma_u\;(R = 6.75\,a_0)$$

H_2: Hartree-Fock vs. DFT core (ionization)



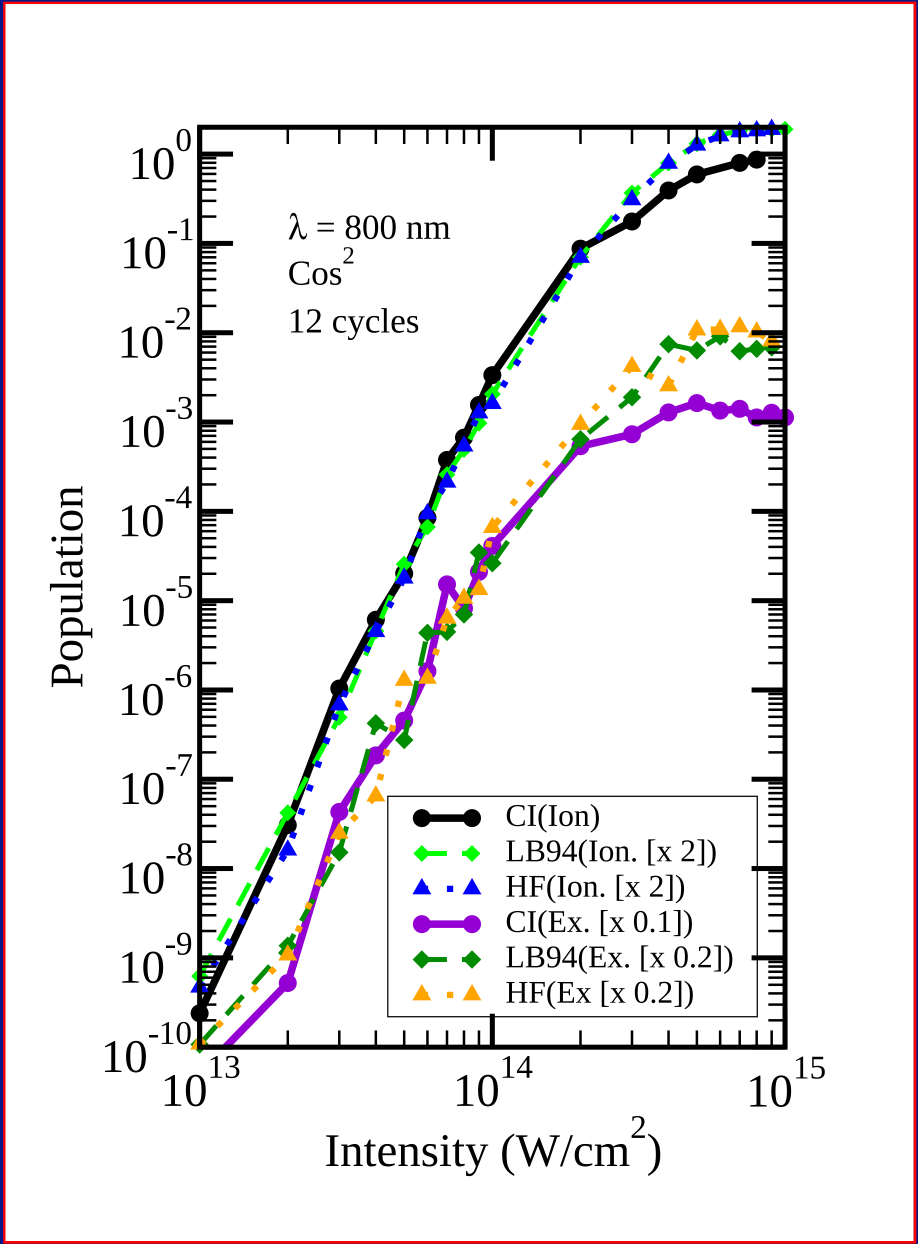
M. Awasthi et al.
PRA **77**, 063403 (2008)

H_2: Hartree-Fock vs. DFT core (excitation)



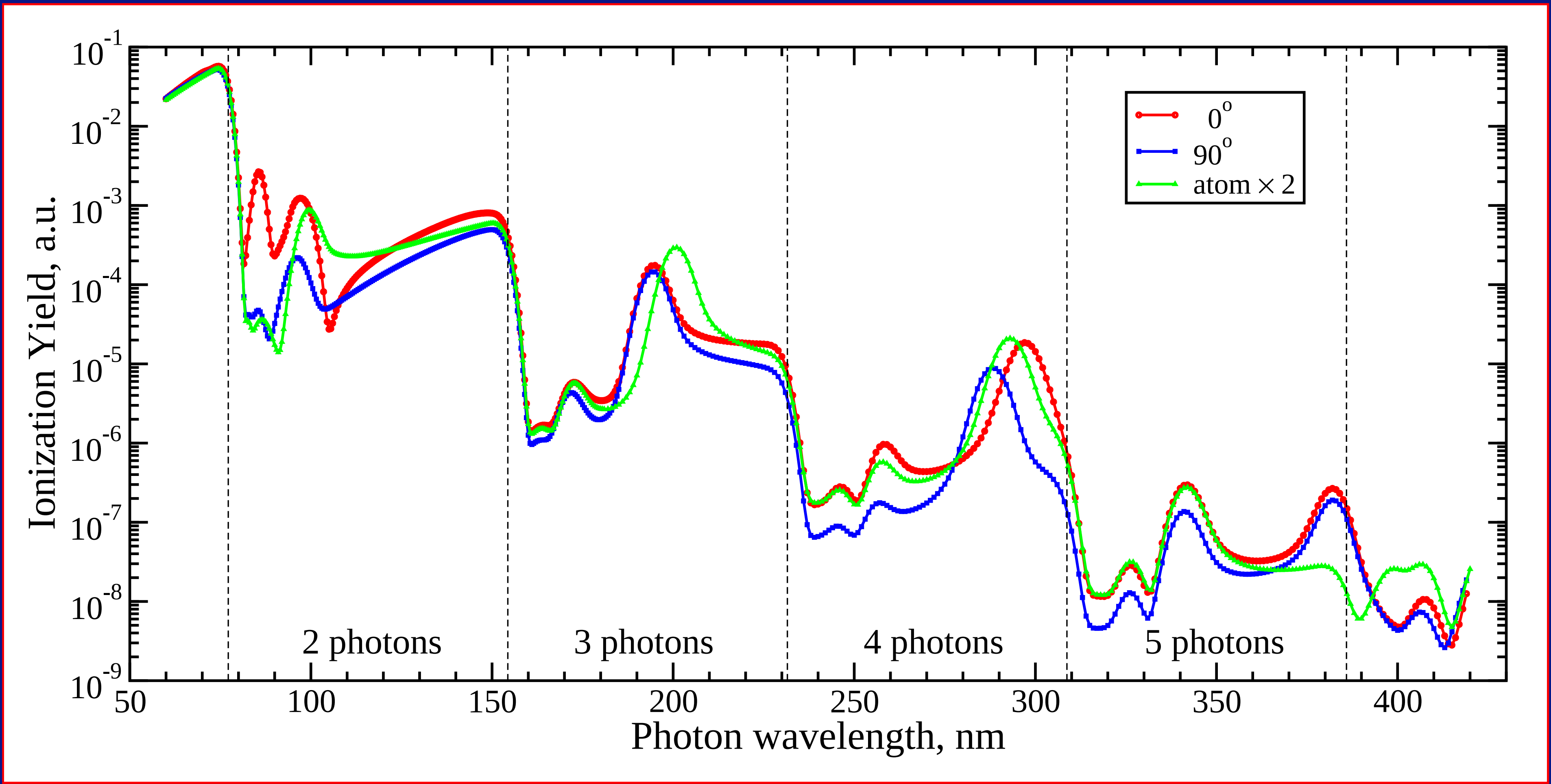
M. Awasthi et al.
PRA **77**, 063403 (2008)

Validity of the SAE approximation for H_2



M. Awasthi et al.
PRA **77**, 063403 (2008)

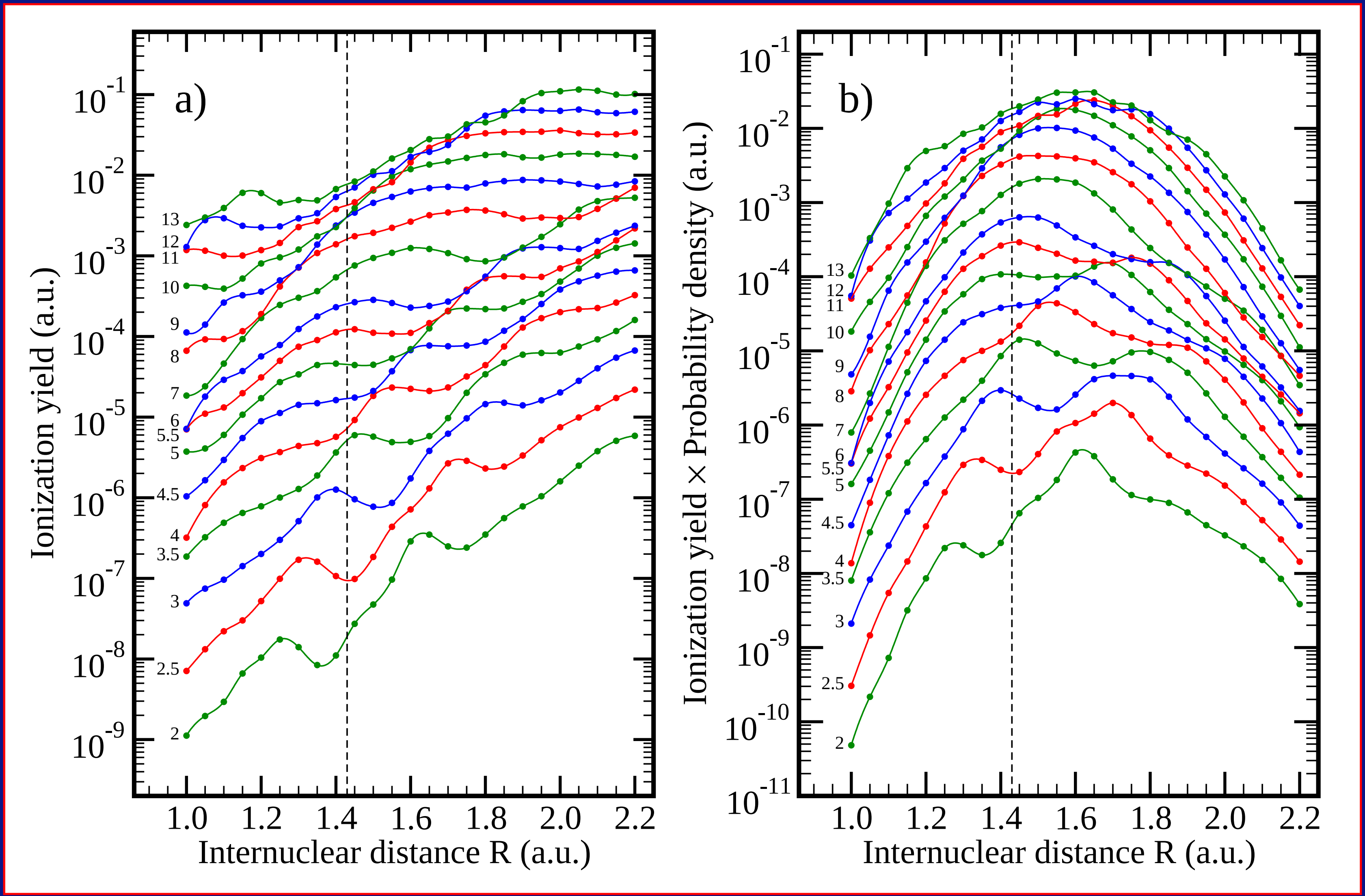
6D: Orientational dependent ion yield of H_2 ($R = 1.4\,a_0$)



Laser field: 30-cycle ($\cos^2$) pulses with peak intensity $I = 5 \cdot 10^{12}$ W/cm^2.

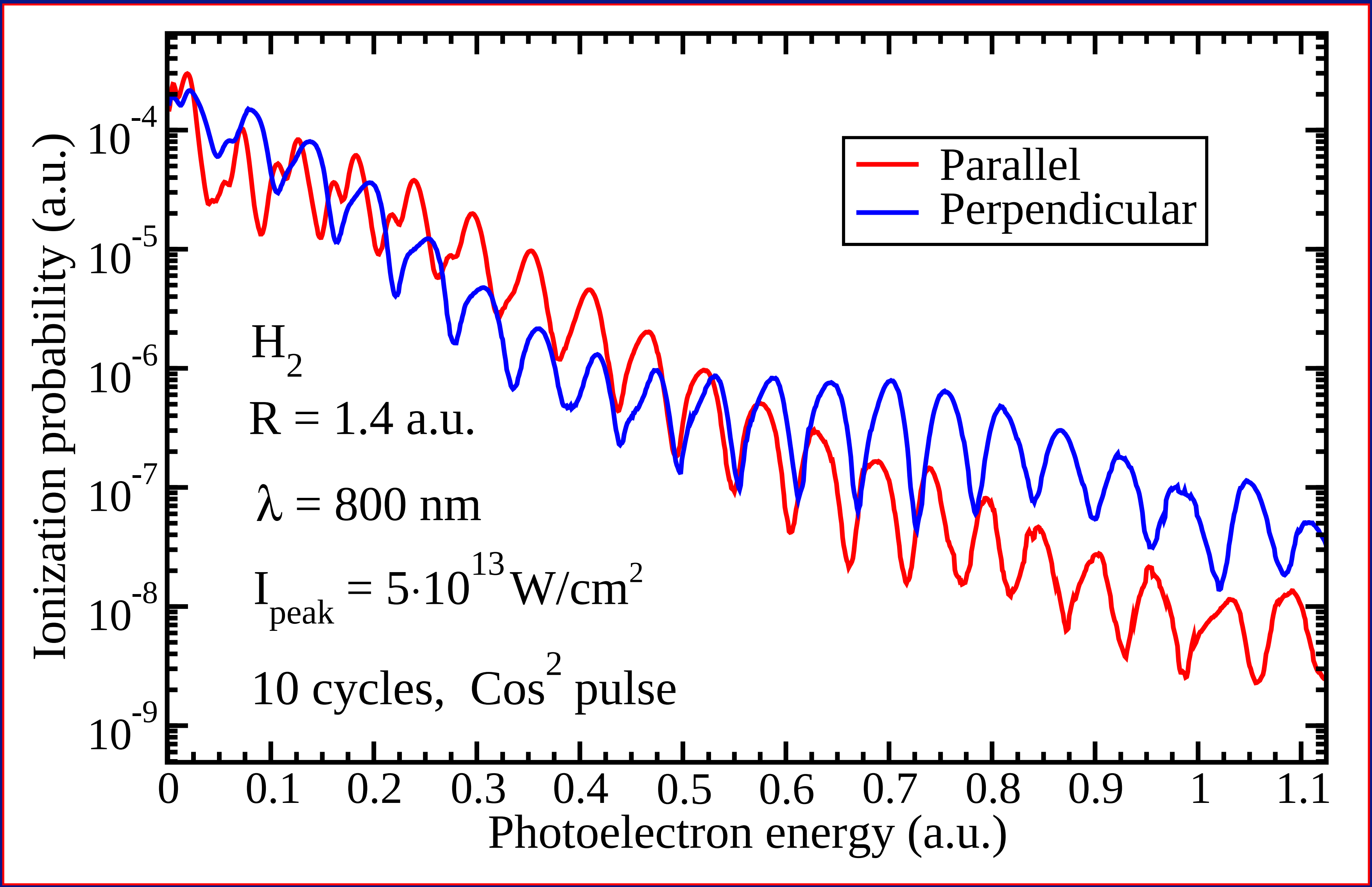
[Y. V. Vanne and A. Saenz, *J. Mod. Optics* **55**, 2665 (2008).]

Internuclear-distance dependent ion yields of H_2 (800 nm, perp.)

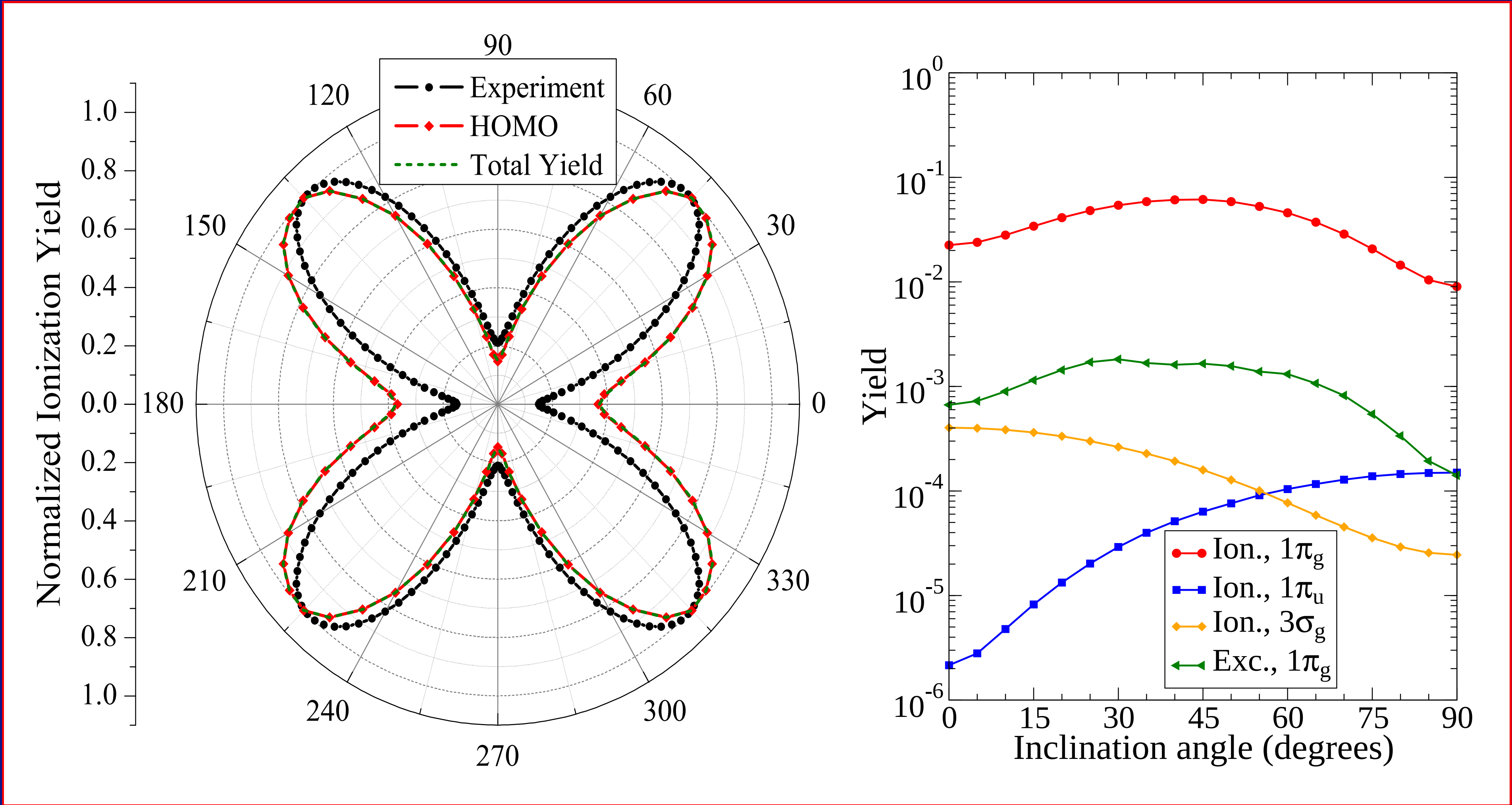


[for method see: Y.V. Vanne and A. Saenz, J. Modern Optics **55**, 2655 (2008); Phys. Rev. A **80**, 053422 (2009)]

Energy-resolved electron spectra (ATI)

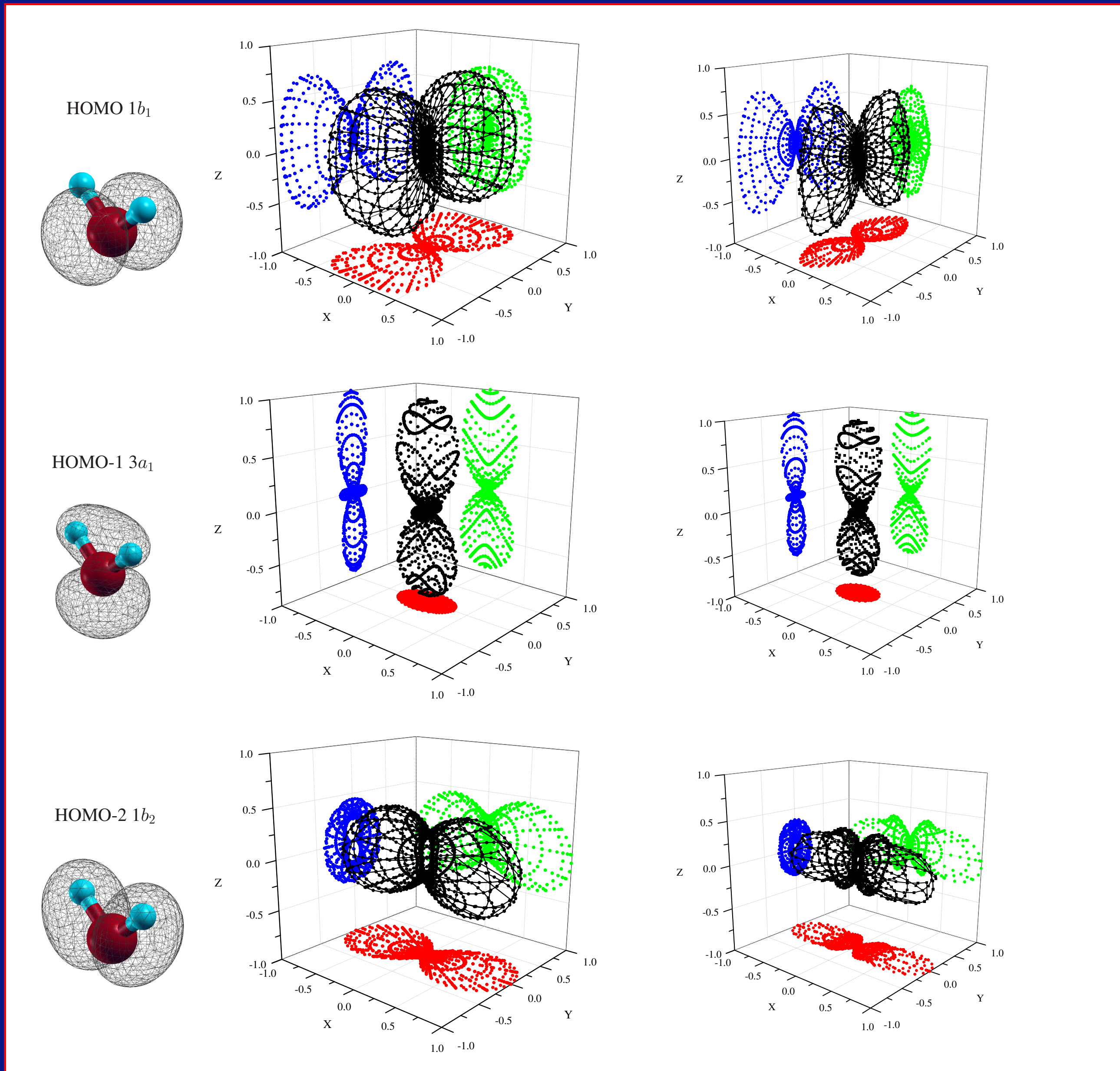


Imaging (I): Orientational-dependent ionization of O_2 molecules



[Exp.: Pavicic et al., PRL **98**, 243001 (2007); Theory: Petretti et al., PRL **104**, 223001 (2010)]

Imaging (II): Orientation-dependent ionization of H_2O molecules



Imaging:

enforced inversion symmetry.

Short pulses:

carrier-envelope effects (interesting by itself), but limits time resolution!

[*Chem. Phys.* (2012)]