# Theory of x-ray absorption by laser-dressed atoms

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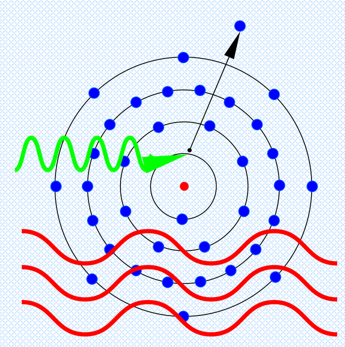
## Laser dressing and x-ray absorption

### X-ray probe of laser-dressed atoms

- Atoms are in the field of an optical laser, 800 nm (Ti:Sapphire)
- Probed by x rays
- Laser dressing barely influenced by x rays
- Laser is of moderately high intensity $10^{13}$ W cm$^{-2}$
  - Ground state atomic electrons are neither excited nor ionized
  - Only final states are modified
- Keldysh parameter for Rydberg orbitals (here Ne $3p$): $\gamma=\sqrt{I_{3p}/(2U_p)}=1.5$ => Strong field regime



### Quantum electrodynamic description of atoms

- Non-relativistic quantum electrodynamics in electric dipole approximation

$$\hat H=\hat H_{AT}+\hat H_{EM}+\hat H_L+\hat H_X+\hat W=\hat H_0+\hat H_1$$

- Hartree-Fock-Slater one-electron model

$$\hat H_{AT}=-\frac{1}{2}\vec\nabla^2+V_{HFS}(r)$$

- Free electromagnetic field for two-modes (laser plus x rays)

$$\hat H_{EM}=\omega_L\hat a_L^\dagger\hat a_L+\omega_X\hat a_X^\dagger\hat a_X$$

- Interaction of electrons with laser- or x-ray-light $\lambda=L, X$

$$\hat H_\lambda=\vec x\cdot i\sqrt{2\pi V^{-1}\omega_\lambda}\,[\vec e_\lambda\hat a_\lambda-\vec e_\lambda^{\,*}\hat a_\lambda^\dagger]$$

### Resonance energies using complex absorbing potentials (CAPs)

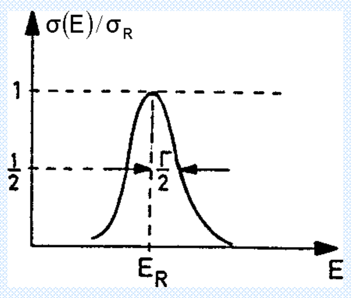
- CAP added to the Hamiltonian $\hat W$
- CAP derived from smooth exterior complex scaling
- Absorbs photoelectron (continuum electron)
- Decaying state becomes a bound state with a complex Siegert energy

$$E_{res}=E_R-i\frac{\Gamma}{2}$$

- Wave function

$$\psi\propto e^{-iE_{res}t}\propto e^{-iE_R t}e^{-\frac{\Gamma}{2}t}$$

- Resonance position $E_R$ and width $\Gamma$; lifetime $1/\Gamma$




### Laser-atom interaction

- Hamiltonian for the atom in the laser field [no x rays so far]

$$\hat H_0=\hat H_{AT}+\hat H_{EM}+\hat H_L+\hat W$$

- Direct product basis set of atomic orbitals $\psi_{n,l,m}(\vec r)$ and laser Fock states with $\mu$ laser photons absorbed $\mu>0$ (emitted $\mu<0$)

$$|\Phi_{nlm\mu}\rangle=|\psi_{n,l,m}\rangle\,|N_L-\mu\rangle$$

- Diagonalization yields laser-dressed atomic energy levels

$$(\boldsymbol H_0^{(m)})_{nl\mu,n'l'\mu'}=\langle\Phi_{nlm\mu}|\hat H_0|\Phi_{n'l'm\mu'}\rangle$$

$$\boldsymbol H_0^{(m)}\vec c_F^{\,(m)}=E_F^{(m)}\vec c_F^{\,(m)}$$

### X-ray photon absorption

- Decaying core excited state with complex Siegert energy
- Relaxes by Auger decay [Ne 2.4 fs] and x-ray fluorescence [Kr 240 as] => extra width $E_{F,0}^{(m)}=E_F^{(m)}-i\Gamma_{1s}^{exp}/2$
- X-ray probe $\hat H_1\equiv\hat H_X$ is a weak, one-photon process => Non-Hermitian Rayleigh-Schrödinger perturbation theory
- Initial state $|I\rangle=|\psi_{1,0,0}\rangle\,|N_L\rangle\,|N_X\rangle$ and laser-dressed, core-excited final states $|F^{(m)}\rangle=\sum_{n,l,\mu}c_{F,n,l,\mu}^{(m)}|\Phi_{nlm\mu}\rangle\,|N_X-1\rangle$

$$E_{I,0}=\langle I|\hat H_0|I\rangle,\qquad E_{I,1}=\langle I|\hat H_1|I\rangle=0$$

$$E_{I,2}=\sum_{F,m}\frac{\langle I|\hat H_1|F^{(m)}\rangle\langle F^{(m)}|\hat H_1|I\rangle}{E_{I,0}-E_{F,0}^{(m)}}$$

$$\Gamma=-2\,\mathrm{Im}[E_{I,0}+E_{I,1}+E_{I,2}]\ \Rightarrow\ \sigma_{1s}=2\frac{\Gamma}{J_X}$$

### Total x-ray absorption cross section

$$\sigma_{1s}(\omega_X,\vartheta_{LX})=\sigma_{1s}^{\parallel}(\omega_X)\cos^2(\vartheta_{LX})+\sigma_{1s}^{\perp}(\omega_X)\sin^2(\vartheta_{LX})$$

$$\sigma_{1s}^{\parallel}(\omega_X)\equiv\sigma_{1s}^{0}(\omega_X),\qquad\sigma_{1s}^{\perp}(\omega_X)\equiv\sigma_{1s}^{1}(\omega_X)$$

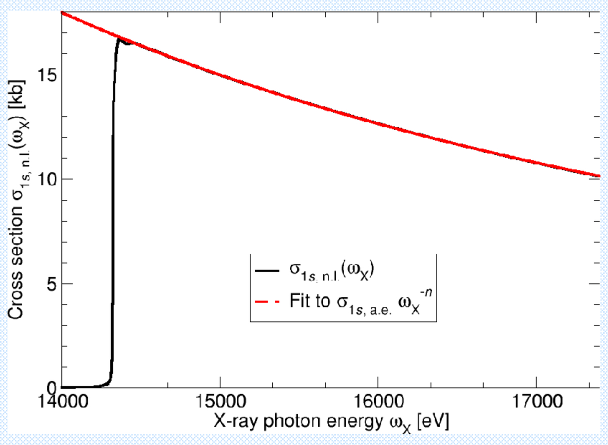
$$\sigma_{1s}^{|m|}(\omega_X)=\frac{8\pi}{3}\alpha\omega_X\,\mathrm{Im}\left[\sum_F\frac{(d_F^{|m|})^2}{E_{F,0}^{|m|}-E_{1s}-\omega_X}\right]$$

- Atom is cylindrically deformed along the laser axis
- Dependence on angle between polarizations $\vartheta_{LX}$
- Atomic properties described by $\sigma_{1s}^{\parallel}(\omega_X)$, $\sigma_{1s}^{\perp}(\omega_X)$
- Radial dipole matrix element between initial and dressed final state $d_F^{|m|}$; energy of *K* edge $E_{1s}$

## Krypton results

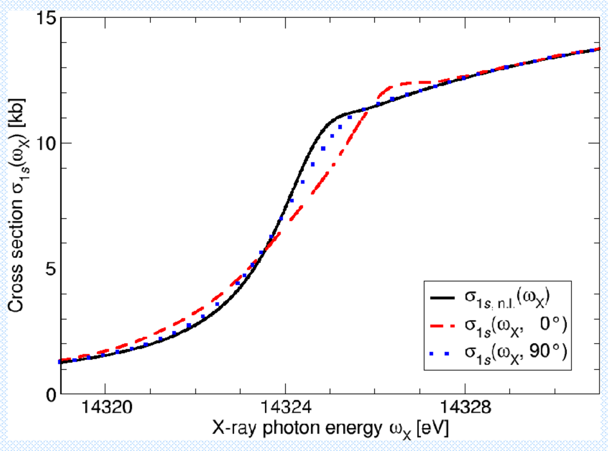
### Krypton above the K edge

- Without laser dressing; only x-ray absorption
- Above edge Bethe and Salpeter give $\sigma_{1s}(\omega_X)=\frac{\sigma_{1s,a.e.}}{\omega_X^n}$
- Non-linear fit $n=2.63$
- For hydrogen $n=2.\bar 6$
- Test of Hartree-Fock-Slater model, radial finite-element basis, and CAP method



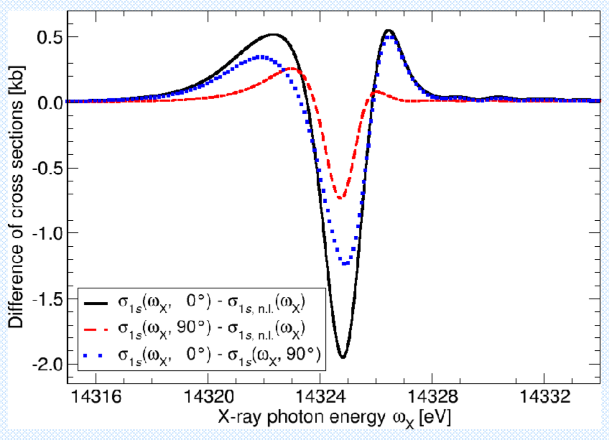

### Krypton K edge

- Laser dressing with 800 nm at $10^{13}$ W cm$^{-2}$
- Laser influences cross section in the vicinity of the *K* edge
- Depends on the angle between laser and x-ray polarizations
- Moderate effect (20%)




### Differences of cross sections at the krypton K edge

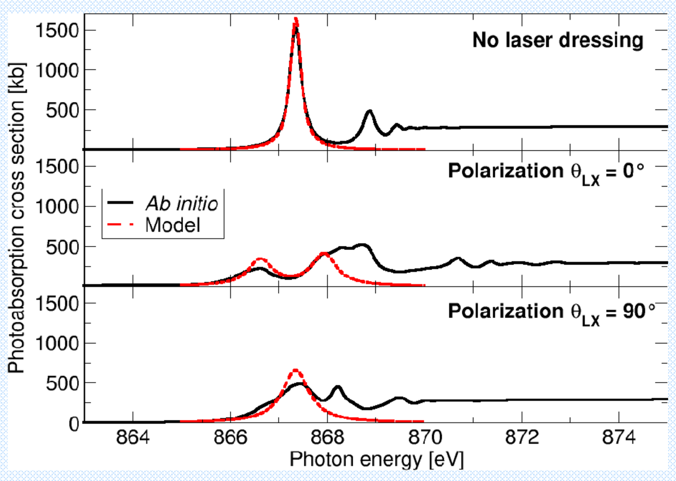
- Largest effect for parallel polarization in relation to no laser
- Transition $1s\to5p$ suppressed by laser
- Oscillator strength redistributed to $5s$ and $4d$
- Reason for moderate effect: the line width $\Gamma_{1s}=2.7$ eV




## Neon results

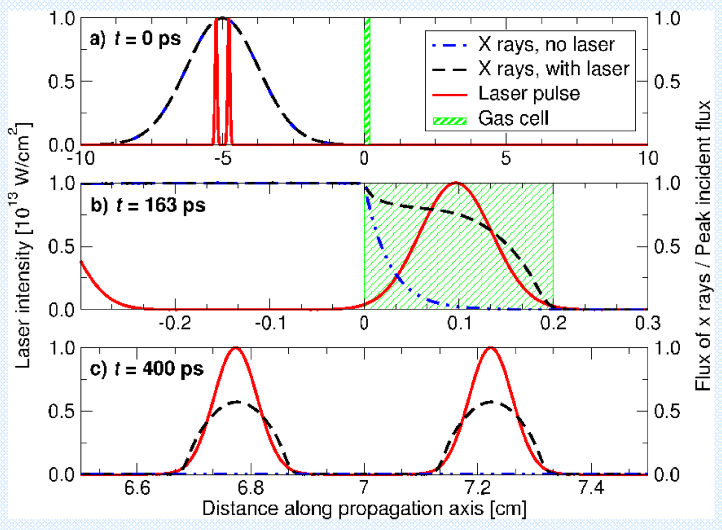
### Neon K edge

- Rydberg series clearly resolved due to a lower line width
- For parallel laser and x-ray polarizations transparency at the $1s\to3p$ transition
- Dominant physics from three levels: $1s$, $3s$, and $3p$



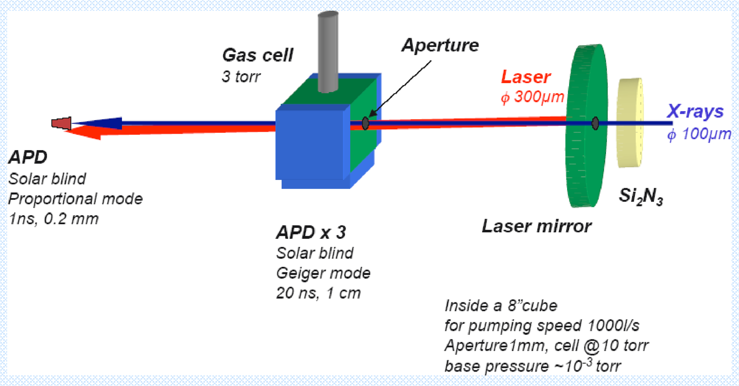

### Ultrashort pulse shaping of x rays

- Laser pulse shape is imprinted on x rays
- Femtosecond x-ray pulses
- All x-ray pump-probe experiments
- Amplitude modulation only




### Schematic experimental setup of two-color neon experiment

- Experiment under way at Lawrence Berkeley National Laboratory
- Overlap x rays and laser beams both in space and time
- Need ultrafast x-ray source for neon experiment




## Related talk

Electromagnetically induced transparency for x rays (DAMOP07-2007-000179) in session P5, (Interactions of Ultrashort Intense Light with Atoms, Molecules, and Plasmas) at 10:30 AM on Friday, 06/08/2007 in TELUS Convention Center, Macleod A3-A4 (room).

## References


1. Buth, Santra, Phys. Rev. A 75, 033412 (2007), arXiv:physics/0611122
2. Buth, Santra, Cederbaum, Phys. Rev. A 69, 032505 (2004), arXiv:physics/0401081
3. Buth, Santra, Young, Phys. Rev. Lett., accepted, arXiv:0705.3615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