Spin-Orbit Interaction Activated Correlations (SOIAC) in Dipole and Quadrupole Photoionization

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**Photoionization: Observables**

**Cross Section**

**Angular Distribution**

**Asymmetry Parameters**

**Spin Polarization Parameters**

**Differential Cross Section**, \( \frac{d\sigma}{d\Omega} \propto \left| \langle \psi_f | e^{ik \cdot r} \hat{e} \cdot \vec{\nabla} | \psi_i \rangle \right|^2. \)

\( e^{ik \cdot r} = 1 + ik \cdot r + \ldots \approx 1 + ik \cdot r, \)

\[
\frac{d\sigma}{d\Omega} = \frac{\sigma_{nl}}{4\pi} \left[ 1 + \frac{\beta}{2} (3\cos^2 \theta - 1) + (\delta + \gamma \cos^2 \theta) \sin \theta \cos \phi \right]
\]

\( \beta: \) E1 angular distribution parameter \{Interference of E1 amplitudes\}

\( \gamma, \delta, \zeta = \gamma + 3\delta: \) E2 angular distribution parameters

\{Interference of E1 & E2 amplitudes\}
What is Interchannel Coupling?

**Neon 2p photoionization**

Various dipole channels arising from 2p, 2s and 1s:

\[
\begin{align*}
2p_{3/2} & \rightarrow s \\
2p_{3/2} & \rightarrow d_{3/2} \\
2p_{3/2} & \rightarrow d_{5/2} \\
2p_{1/2} & \rightarrow s \\
2p_{1/2} & \rightarrow d_{3/2} \\
2s & \rightarrow p_{1/2} \\
1s & \rightarrow p_{1/2}
\end{align*}
\]

Ionization thresholds: $2p: \sim 22$ eV, $2s: \sim 53$ eV, $1s: \sim 870$ eV

All the channels contribute significantly around the ionization threshold of 1s.

Truncated RRPA allows to couple channels selectively.

Channels from different levels interact with each other modifying energy dependence of photoionization parameters.

Truncated RRPA (Relativistic Random Phase Approximation) enables one the inclusion of select channels, thereby including correlations in a controlled way.

Most often, inner shells contribute only a little to outer-shell photoionization (frozen core).
3d photoionization: E1


Second maximum in 3d\(_{5/2}\) cross section results from the coupling among channels arising from 3d\(_{5/2}\) and 3d\(_{3/2}\): A purely many-body effect, i.e., a correlation effect (no single particle analogue).

* SPRPAE: Spin-Polarized Random Phase Approximation with Exchange

Spin-orbit splitting ~ 10 eV
3d photoionization: E1

SOIAC effect similar to what is observed in Xe3d

Spin-orbit splitting ~ 14 eV

The structures in the circles are the result of SOIAC effect.
The bell-shaped structure results due to SOIAC effect.

SOIAC effect similar to what is observed in Xe3d, but the structure is below 3d_{3/2} threshold.

Spin-orbit splitting ~ 15 eV

HF calculation


Richter et al, PRL 2007

The bell-shaped structure results due to SOIAC effect.
The dip in 3d cross section just above 3d cross section is a SOIAC effect. There is no significant effect on $\beta$.

Spin-orbit splitting $\sim 93$ eV

The dip in 3d$_{5/2}$ cross section just above 3d$_{3/2}$ cross section is a SOIAC effect. There is no significant effect on $\beta$. 

3d photoionization: E1

Present RRPA
Coupling affects overall behavior of the cross section. 

$\beta$ also gets affected?

Spin-orbit splitting $\sim 2$ eV.
4d photoionization: $E_1$

Splitting of $3d_{5/2}, 3d_{3/2}$ components: signature of SOIAC

Present RRPA

$\beta_{4d}$

With coupling

Without coupling

$\beta_{4d}$

Photoelectron Energy (au)

Photoelectron Energy (au)
Flat behavior of branching ratio confirms Spin-Orbit Interaction Activated Interchannel Coupling effect.
Again coupling affects overall behavior of the cross section. \( \beta \) also gets affected.

Spin-orbit splitting \( \sim 5 \) eV.

\[ \text{Structures due to SOIAC} \]

\[ \text{Spin-orbit splitting} \sim 5 \text{ eV.} \]
When channels from $4d_{3/2}$ are coupled with those from $4d_{5/2}$, the matrix elements get modified; especially matrix elements involving $f$-waves resulting from $4d_{5/2}$.

$f$-waves see strong centrifugal barrier so that corresponding matrix elements go through large shape resonance.
**4p photoionization: E2**

First observation of SOIAC in E2 photoionization parameters:

The second maximum in the $4p_{5/2}$ cross section results due to SOIAC.

The measurable quantity $\zeta$ has a noticeable structure corresponding to the second maximum in the cross section.

Spin-orbit splitting $\sim 7$ eV.
Rn 5p\textsubscript{3/2} also displays a structure, though feeble, corresponds to the SOIAIC effect.

Spin-orbit splitting \(\sim 34 \text{ eV}\).
Physics behind the phenomenon

- Channels arising from inner shells with \( j = l + \frac{1}{2} \) mix with those from \( j = l - \frac{1}{2} \) of the same subshell often leads to dramatic results.

- Overlap between the wave functions corresponding to \( j = l + \frac{1}{2} \) and \( j = l - \frac{1}{2} \) will be quite large because spin-orbit interaction leaves the radial wave functions nearly identical.

- Large overlap can produce dramatic change in the photoionization parameters of one or both of the spin-orbit split components.

- A weak channel gets modified appreciably in the region of a much stronger channel. This is the reason for the second maximum in 3d partial cross sections of Xe, Cs and Ba and that in 4p E2 cross section of Xe 4p.

- In the case of E1 photoionization of Xe 4d, Rn 5d, and E2 photoionization of Rn 5p, it is a complex mixing of channels which modifies photoionization parameters.
Conclusions

- The SOIAC is a purely correlation effect which should be present with photoionization of all subshells with $l > 0$.

- In most cases, it is significant if there is a shape resonance in one or both of the components of a subshell.

- The effect can be significant if the spin-orbit splitting is so large that the $j=l+1/2$ cross section is smaller than $j=l-1/2$ cross section in the vicinity of $j=l-1/2$ maximum. That’s why the effect is scarcely visible with outer shell photoionization, where splitting is so small.

- As the effect modifies most of matrix elements, it may not be visible in the angular distribution asymmetry parameters.

- It has been observed, for the first time, in E2 photoionization parameters.