README file for ”Angularly resolved Atomic Time Delays”

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December 22, 2022

1 Time-Dependent Schrödinger Equation (TDSE) calculations

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1.1 Files

1. Angular_delays_TDSE_0_4_0_0_180_2.dat
2. Angular_delays_TDSE_20_4_0_0_180_2.dat
3. Angular_delays_TDSE_40_4_0_0_180_2.dat
4. Angular_delays_TDSE_60_4_0_0_180_2.dat
5. Angular_delays_TDSE_80_4_0_0_180_2.dat
6. Angular_probs_TDSE_4_0_0_60_20_0_180_2.dat

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1.2 Description

Files with name pattern *Angular_delays_TDSE_Θ_4_0_0_180_2.dat* contain the angularly resolved atomic time delays $\tau_{at}(\theta)$ we obtain from TDSE simulations of RABBITT spectra for hydrogen atoms initially in the $1s$ ground state. Each file contains the results for the relative polarization angle $\Theta = 0°$, $20°$, $40°$, $60°$, and $80°$ between the polarization vectors of pump and probe pulses. The first column indicates the photoelectron emission angle in the xy-plane measured from the positive x-axis, the polarization direction of the attosecond pulse train (see Fig. 1 in Ref. [1]). The following columns in the data file contain the angularly resolved time delays $\tau_{at}(\theta)$ for SBs 12 to 26.

The file with name Angular_probs_TDSE_4_0_0_60_20_0_180_2.dat contains the results for the fitting parameter A for SBs 12 to 26, as a function of the electron emission angle and for each relative polarization angle Θ. Again, we obtain these results from TDSE simulations of RABBITT spectra for hydrogen atoms initially in the $1s$ ground state.

1.3 Method

Utilizing the Qprop code [2], we numerically solve the TDSE for each angle Θ and 41 different values of the delay τ between the attosecond pulse train and the infrared (IR) laser. These delays span one IR period, and allow us to find the dependence of angle-resolved RABBITT spectra on the delay τ. Then, we fit the signal for each sideband with the general expression $I_{2q} = A + B\cos(2\omega_0\tau - \phi_{at})$, from which we obtain the angular dependence of the parameters A and B, and the atomic time delay $\tau_{at} = \phi_{at}/2\omega_0$.

The relevant parameters to reproduce the TDSE simulations are the following (values in atomic units unless otherwise stated):

- Radial grid step: 0.24
- Cutoff radius: 850
- T-surff radius: 1700
- Number of angular momenta in expansion: 4
- Time step for propagation: 0.06
- IR intensity: 0.05 TW/cm^2
- IR angular freq. ω_0: 0.056954190
- IR pulse duration: 10 IR-cycles
- XUV pulse duration: 3 IR-cycles
- XUV Harmonic orders: 11 to 27

1.4 Observations

The relative time delays $\Delta\tau_{at}(\theta)$ in Figs. (2) and (3) from Ref. [1], are obtained by taking the difference $\tau_{at}(\theta) - \tau_{at}(0°)$ from the datasets above.

2 Second-order perturbation theory (SOPT) calculations

Author(s): D.I.R. Boll and L. Martini

2.1 Files

1. Angular_delays_SOPT_0_0_180_2.dat
2. Angular_delays_SOPT_20_0_180_2.dat
3. Angular_delays_SOPT_40_0_180_2.dat
4. Angular_delays_SOPT_60_0_180_2.dat
5. Angular_delays_SOPT_80_0_180_2.dat

2.2 Description

Files with name pattern *Angular_delays_SOPT_Θ_0_180_2.dat* contain the angularly resolved atomic time delays $\tau_{at}(\theta)$ we obtain from SOPT calculations for hydrogen atoms initially in the $1s$ ground state. Each file contains the results for the relative polarization angle $\Theta = 0°$, $20°$, $40°$, $60°$, and $80°$ between the polarization vectors of pump and probe pulses. The first column indicates the photoelectron emission angle in the xy-plane measured from the positive x-axis, the polarization direction of the attosecond pulse train (see Fig. 1 in Ref. [1]). The following columns in the data file contain the angularly resolved time delays $\tau_{at}(\theta)$ for SBs 12 to 26.

2.3 Method

For initial atomic s states, in Ref. [1] we show that angularly resolved atomic phase imprinted on RABBITT sidebands is given by

$$\tan(\phi_{at}) = \frac{\sum_{L,L'} |T_L^+||T_{L'}^-| g_{L,L'} \sin(\phi_{L'}^- - \phi_L^+)}{\sum_{L,L'} |T_L^+||T_{L'}^-| g_{L,L'} \cos(\phi_{L'}^- - \phi_L^+)}, \tag{1}$$

where $|T_L^\pm|$ and $\phi_L^\pm$ are the modulus and phase of (pseudo) radial matrix elements contributing to final states with angular momentum L, from absorption (+) and emission (−) channels, respectively. The full angular dependence of atomic phase ϕ_{at} is contained in the $g_{L,L'}$ functions (see appendix in Ref. [1]). Therefore, to obtain the angularly-resolved atomic time delays from SOPT calculations we substitute into Eq. (1) the results for radial matrix elements $T_L^\pm$ obtained from Second-order Perturbation Theory (SOPT), reported previously [3].

2.4 Observations

The relative time delays $\Delta\tau_{at}(\theta)$ in Figs. (2) and (3) from Ref. [1], are obtained by taking the difference $\tau_{at}(\theta) - \tau_{at}(0°)$ from the datasets above.

3 Model calculations

Author(s): D.I.R. Boll

3.1 Files

1. Angular_delays_Model_0_0_180_2.dat
2. Angular_delays_Model_20_0_180_2.dat
3. Angular_delays_Model_40_0_180_2.dat
4. Angular_delays_Model_60_0_180_2.dat
5. Angular_delays_Model_80_0_180_2.dat

3.2 Description

Files with name pattern *Angular_delays_Model_Θ_0_180_2.dat* contain the angularly resolved atomic time delays $\tau_{at}(\theta)$ we obtain from ACC-RME model [4] calculations for hydrogen atoms initially in the 1s ground state. Each file contains the results for the relative polarization angle $\Theta = 0°$, $20°$, $40°$, $60°$, and $80°$ between the polarization vectors of pump and probe pulses. The first column indicates the photoelectron emission angle in the xy-plane measured from the positive x-axis, the polarization direction of the attosecond pulse train (see Fig. 1 in Ref. [1]). The following columns in the data file contain the angularly resolved time delays $\tau_{at}(\theta)$ for SBs 12 to 26.

3.3 Method

We obtain the angularly-resolved atomic time delays from model calculations by substituting into Eq. (1) the results for radial matrix elements $T_L^{\pm}$ obtained from ACC-RME model [4], reported previously [3].

3.4 Observations

The relative time delays $\Delta\tau_{at}(\theta)$ in Figs. (2) and (3) from Ref. [1], are obtained by taking the difference $\tau_{at}(\theta) - \tau_{at}(0°)$ from the datasets above.

4 Changelog

References

[1] D. I. R. Boll, L. Martini, and O. A. Fojón. Two-color polarization control on angularly resolved attosecond time delays. *Physical Review A*, submitted.

[2] Vasily Tulsky and Dieter Bauer. Qprop with faster calculation of photoelectron spectra. *Computer Physics Communications*, 251:107098, 2020.

[3] D.I.R. Boll, L. Martini, and O.A. Fojón. Two-photon two-color transition matrix amplitudes. Repositorio Institucional CONICET Digital. http://hdl.handle.net/11336/156629, 2022. Creation date: 2022/05/05.

[4] D. I. R. Boll, L. Martini, and O. A. Fojón. Analytical model for attosecond time delays and fano's propensity rules in the continuum. *Phys. Rev. A*, 106:023116, Aug 2022.