Theoretical study of Coulomb tail effects on photoemission time delays in the low-energy regime

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Attosecond metrology based on high-harmonic generation enables measurements of photoemission time delays for gas-phase atoms and molecules in the extreme-ultraviolet range. The photoemission time delay is mainly caused by scattering with atomic or molecular potentials and described by the energy derivative of the scattering phase. Therefore, the photoemission time delay depends on the atomic species and molecular structure. For example, a delay difference of approximately 60 as at a photoelectron energy of ~10 eV has been reported between adamantane and naphthalene.[1]

Photoelectrons are scattered not only by short-range potentials V_{short} but also by long-range (Coulomb) potentials V_{long} arising from the electron–hole interaction. In the high-energy region, the following sum rule holds between the time delays t_{short} and t_{long} due to V_{short} and V_{long} respectively, and the time delay t_{tot} due to $V_{\text{short}} + V_{\text{long}}$:

$$t_{\text{tot}} \xrightarrow[\text{high energy limit}]{} t_{\text{short}} + t_{\text{long}} \, . \tag{1}$$

According to the point of view of Eq.(1), subtracting the reference photoemission time delay from the targeted photoemission time delay allows us to eliminate t_{long} and extract the system-specific time delay t_{short} in high energy region.

In this study, we focused on the low-energy region (0–30 eV) where photoemission time delay measurements have been reported and quantitatively verified the validity of Eq.(1) by performing numerical calculations of core-level photoemission time delays for simple spherically symmetric models in Fig.1(a). As shown in Fig.1(b), a difference of 24 as was found between $t_{\text{short}} + t_{\text{long}}$ and t_{tot} at a photoelectron energy of 10 eV and it was shown that the effect of Coulomb tail dominates the photoemission time delay in the low-energy region.

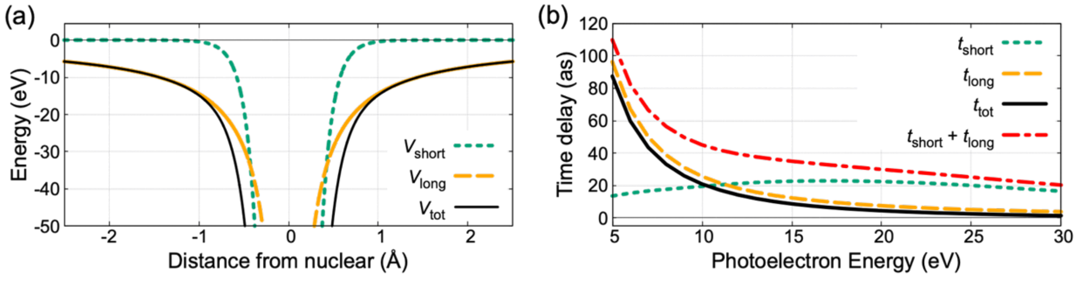

Figure 1. (a) Model potentials. (b) Numerical results of core-level photoemission time delay.

References

[1] V. Loriot *et al*., Nat. Phys. **20**, 765-769 (2024).