Formation of doubly excited states by XUV excitation and Auger spectra in presence of strong IR fields

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Doubly excited states do not have a strict mathematical correspondence in standard quantum mechanics. Rather, their energies are associated with poles of the scattering matrix in the complex plane. The time-honored method of (global) complex scaling (GCS) has been offering easy and mathematically well-defined access to these states: they can be related to square-integrable eigenfunctions of an analytically continued, non-hermitian Hamiltonian (see [1] for a recent discussion in a broader context). In the variant of "exterior complex scaling" (ECS) the method can be applied when the Hamiltonian can be analytically continued only outside a finite range. Both methods use the coordinate transformation

$$\vec{x} \to \vec{z}_{R_0,\theta}(x) = \begin{cases} \vec{x} & \text{for} \quad |\vec{x}| < R_0 \\ \left[e^{i\theta}(|\vec{x}| - R_0) + R_0\right] \hat{x} & \text{for} \quad |\vec{x}| > R_0 \end{cases} ,$$

where GCS corresponds to $R_0 = 0$.

GCS has rarely been applied to time-dependent problems, because the complex continued wave function cannot easily be associated with a physical counterpart. For ECS, only recently comprehensive numerical evidence was presented that the wave function $\Psi_{R_0,\theta}(\vec{x},t)$ resulting from propagation with the complex scaled Hamiltonian $H_{R_0,\theta}(t)$ agrees with the exact solution on $|\vec{x}| < R_0$. Also, with "infinite range" ECS (irECS) a particularly efficient discretization was found [2].

Using irECS, we are able perform *ab initio* calculations of formation of doubly excited states of He and other two-electron atoms by XUV pulses. In addition, fully differential (3d) photo-electron momentum spectra were calculated by the newly developed time-dependent surface flux (tSURFF) method [2]. Dependence of the Auger spectra on time-delayed IR fields will be shown.

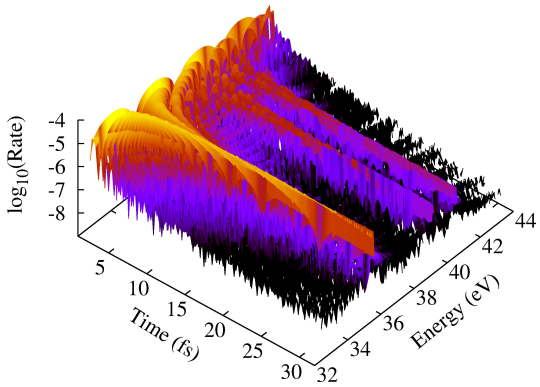

Figure: Buildup rate $d\sigma(E,t)/dt$ for the Fano-profile in the photo-emission spectrum of the lowest few doubly excited $L = 1$ states of Helium after excitation by an attosecond XUV pulse.

[1] N. Moiseyev, *Non-Hermitian Quantum Mechanics*, Cambridge University Press (2011).

[2] A. Scrinzi, *New. J. Phys.* 14:085008 (2012); A. Scrinzi, *Phys. Rev. A*, 81:053845 (2010).