# Exterior complex scaling method in TDDFT: MPI and HHG of Ar atoms in strong laser fields

Ksenia E. Sosnova[1], Dmitry A. Telnov[1], Efim Rozenbaum[1], Shih-I Chu[2]

[1]Department of Physics, St. Petersburg State University, St. Petersburg 198504, Russia
[2]Department of Chemistry, University of Kansas, Lawrence, Kansas 66045, USA
ks.sosnova@gmail.com

Atomic systems subject to laser fields can be ionized. At large distances from the core, only outgoing wave components (describing ionization) should be present in the wave function. The outgoing-wave boundary conditions can be correctly imposed with the help of the complex-scaling transformation. Exterior complex scaling (ECS) may have advantages when applied to more complex systems described by potentials with non-analytical behaviour (or defined only numerically) in the interior region of the coordinates.

In this project, we implement ECS in the time-dependent density functional theory (TDDFT) calculations of multielectron atoms in strong laser fields. For solving the time-dependent Kohn-Sham equations, we apply the time-dependent generalized pseudospectral method in the spherical coordinates. Smooth ECS is introduced by the mapping transformation of the radial coordinate: $r = R(x) \cdot exp[i\alpha(x)]$, where $R(x)$ is a real monotonous function which maps the interval $[-1,1]$ to the radial coordinate range $[0, R_b]$, where $R_b$ is the end point. The phase $\alpha(x)$, its first and second derivatives are continuous functions of $x$. In the interior domain, $x < x_0$, $\alpha(x) = 0$; in the exterior domain, $x > x_0$, $\alpha(x)$ gradually increases to reach the maximum value of $\alpha_0$ and then remains constant at longer distances.

Using TDDFT–ECS approach, we studied high-order harmonic generation (HHG) and multiphoton ionization (MPI) of Ar atoms in intense laser fields. Namely, the laser pulses with the wavelength of $800$ nm, $\sin^2$ envelope, and pulse duration of $20$ optical cycles (FWHM is about $27$ fs) are considered.

In Fig.1, we show HHG spectra of Ar for the laser pulse with peak intensity of $2 \cdot 10^{14}$ W/cm$^2$. The frozen-core potential model calculations (not including dynamic response of the electron density) were also performed to estimate significance of multielectron effects in HHG. Both the TDDFT–ECS and frozen-core potential model spectra have a minimum closely related to the well-known Cooper minimum observed in photoionization cross sections of Ar. This minimum is clearly seen near the photon energy of $51$ eV in the TDDFT–ECS spectrum. In the frozen-core potential model spectrum, it is less pronounced and shifted to lower energies ($\sim 45$ eV). The MPI probabilities calculated within the frozen-core potential model significantly overestimate those obtained by TDDFT for the same parameters of the laser field. We conclude that dynamic multielectron effects play an important role in both HHG and MPI processes in Ar.

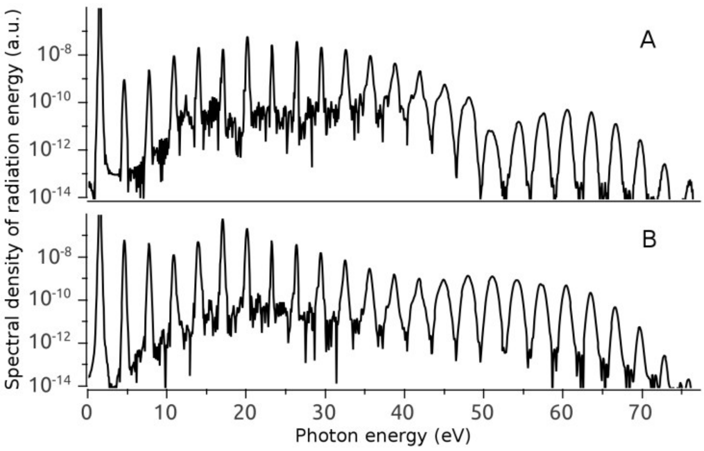


**Figure 1. Spectral density of harmonic radiation energy for the peak intensity 2·10$^{14}$ W/cm$^2$: (A) TDDFT-ECS; (B) frozen-core potential model.**