XXVIII International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC 2013) IOP Publishing
Journal of Physics: Conference Series **488** (2014) 032004 doi:10.1088/1742-6596/488/3/032004

Exterior complex scaling method in TDDFT: HHG of Ar atoms in intense laser fields

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Synopsis Exterior complex scaling (ECS) method is applied in the framework of the time-dependent density functional theory to study high-order harmonic generation (HHG) of multielectron atoms in intense laser fields. ECS allows to impose correct (outgoing-wave) boundary conditions on the wave functions at large distances. In the present work, ECS is combined with the time-dependent generalized pseudospectral method for accurate and efficient solution of the time-dependent Kohn-Sham equations. Results for HHG of Ar atoms are presented.

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 imposed correctly with the help of the complex-scaling transformation. Exterior complex scaling (ECS) [1] may have advantages when applied to more complex systems with potentials which behave non-analytically (or defined only numerically) in the interior region of the coordinates.

In this work, we implement ECS in the time-dependent density functional theory (TDDFT) calculations of multielectron atoms in intense laser fields. To solve 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:

$$r = R(x)\exp[i\alpha(x)], \qquad (1)$$

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 $\alpha(x)$ along with 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 α_0 and then remains constant at longer distances.

We apply the TDDFT–ECS approach to study high-order harmonic generation (HHG) of Ar atoms in intense laser fields. In our calculations, we use laser pulses with the wavelength of 800 nm, sine-squared envelope, and pulse duration of 20 optical cycles (full width at half maximum is about 27 fs).

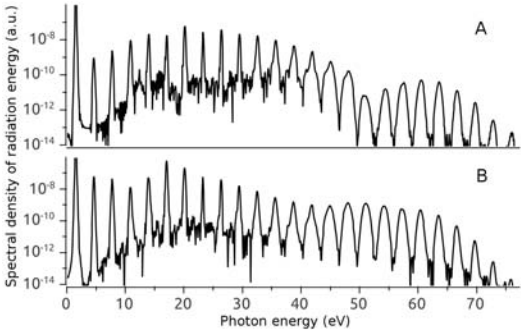

Figure 1. Spectral density of harmonic radiation energy for the peak intensity 2×10^{14} W/cm^2: (A) TDDFT–ECS; (B) frozen-core potential model.

Fig. 1 shows HHG spectra of Ar for the peak intensity of the laser pulse 2×10^{14} W/cm^2. To estimate significance of multielectron effects in HHG, we have also performed calculations within the frozen-core potential model where, unlike TDDFT, dynamic multielectron response to the external field is not taken into account. Both the TDDFT–ECS and frozen-core potential model spectra exhibit a minimum which is closely related to the well-known Cooper minimum observed in photoionization cross sections of Ar. In the TDDFT–ECS spectrum, this minimum is clearly seen near the photon energy of 51 eV. In the frozen-core potential model spectrum, however, the minimum is less pronounced and shifted to lower energies ($\sim$ 45 eV). Thus we conclude that dynamic multielectron effects are quite important in shaping of the HHG spectra in Ar.

References

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