# *Ab initio* simulations of multielectron dynamics in intense laser fields with infinite-range exterior complex scaling

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**Synopsis** We report successful implementation of infinite-range exterior complex scaling as an efficient absorbing boundary to the time-dependent complete-active-space self-consistent field method. This substantially reduces computational costs of *ab initio* simulations of multielectron dynamics in intense laser fields and attosecond light pulses; $\sim 80\%$ cost reduction, e.g., for the case of high-harmonic generation from Ne.

Recent developments of laser technology with intense laser pulses and attosecond pulses have provided new research interest of strong-field phenomena and ultrafast electronic dynamics. Though various theoretical methods have been developed to explore these phenomena [1], *ab initio* simulations of multielectron dynamics in intense laser fields are still a challenging task. In order to realize simulations of larger systems, we have recently formulated the time-dependent complete-active-space self-consistent field (TD-CASSCF) method, which enables compact and accurate simulations [2] and implemented it for atoms and molecules [3, 4]. In these implementation we have used the mask function method as an absorbing boundary to avoid unphysical reflections of departing electrons at the simulation box boundary.

In this study, to further reduce computational costs we introduce a more efficient absorbing boundary of infinite-range exterior complex scaling (irECS) [5]. irECS efficiently prevents unphysical reflection by analytically continuing wave functions into the complex plane and, furthermore, enables simulations over the entire space by using a infinitely-extending scaled (absorption) region. However, application of irECS, originally developed for single-electron cases, to multielectron systems has never been reported, to our knowledge. Here we successfully implement irECS to the TD-CASSCF method. The results of irECS calculated with a quite small number of discretization grid points perfectly agree with exact results calculated with a sufficiently large box (Figs. 1 and 2). Accurate simulations are possible even in an extremely strong-field case where double ionization yield reaches 50% (Fig. 2). The computational costs required by these calculations with irECS are reduced by 66% (Fig. 1) and 80% (Fig. 2), compared to the previous implementation with the mask function. Our achievements will open a way to *ab initio* simulations of larger systems, relevant to real-world

experiments and applications.
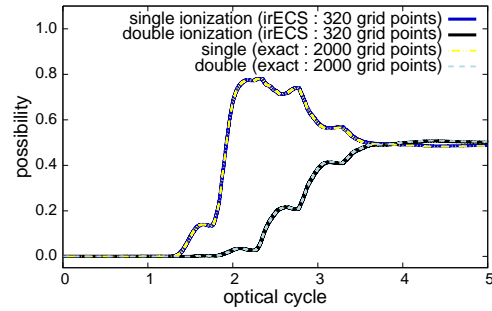


**Figure 1**. Temporal evolution of ionization probabilities of a Beryllium atom exposed to a laser pulse with a wavelength of 800 nm and duration of 5 optical cycles at a peak intensity of $3 \times 10^{14}$ W/cm$^2$.
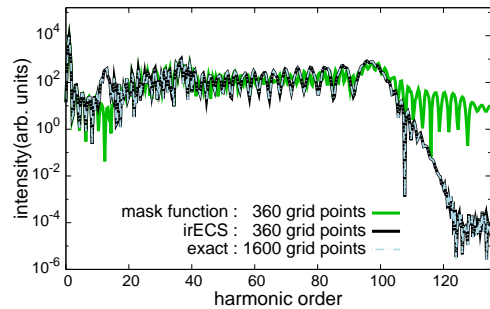


**Figure 2**. High harmonic spectra of a Neon atom exposed to a laser pulse with a wavelength of 800 nm and duration of 3 optical cycles at a peak intensity of $8 \times 10^{14}$ W/cm$^2$. The mask function method under the same condition as irECS fails to reproduce the exact result.

## References

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