Time-dependent method in the laser-atom interactions

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Abstract

We introduce a recent developed time-dependent method used in the study of laser-atom interactions. The key ingredients of the method are that (1) we propagate the wave function in real space in a finite region. The region is split into two parts, an inner-region and an outer-region. Once the electron moved into the outer-region, the wave function is projected into momentum space and propagated analytically to avoid the reflection from the boundary. (2) To increase the numerical accuracy and make the physical processes more transparent, we solve the time-integral Schrödinger equation, instead of time-differential equation. Then we apply the method to study the infrared laser assisted photoionization of helium by a coherent extreme-ultraviolet light. The ionization process can be controlled by tuning the time delay between the two pulses.

Keywords: time-propagator, Intense laser, Infrared laser assisted photoionization,

Numerical simulation plays an important role in the laser-atom interactions. Although there are some simple models, like rescattering model [1, 2], which can be used to explain some experiment observations qualitatively, we have to rely on the full numerical simulation to explain them quantitatively. Numerical simulation can also help us to dig out the detailed intermediate information, like the rescattering electron energy [3] and space distribution [4], which are very important quantities to understand the dynamics and cannot yet be observed in experiment. Directly solving the time-dependent Schrödinger equation for a single electron system is still not a simple work, although the computational power increases dramatically in recent years due to the advances of the computer technology. The main difficulties in the simulation of laser-atom interactions are that (1) the number of continuum states involved in the process is infinite and (2) the continuum wave function extends to infinite in space while a simulation has to be done in a limit region, (3) in some cases, the wave function of a dynamical process is very small, and it is embedded into a large useless background wave function in the simulation.

Taking infrared (IR) laser assisted photoionization of helium atoms by a coherent extreme-ultraviolet (EUV) light as an example, we show a method to circumvent the above difficulties. Instead of solving the time-differential equation, we solve the time-integral equation as (atomic units, $m = \hbar = e = 1$, are used hereafter unless otherwise stated),

$$\Psi(t) = -i\int_{-\infty}^{t} e^{-i\int_{t'}^{t} H(t'')dt''} V^{ext}(t') e^{-iH_0 t'} \Psi_g dt' + e^{-iH_0 t}|\Psi_g> . \quad (1)$$

Here Ψ_g is the ground state of , H_0 is the atomic Hamiltonian with the model potential $V(r)$ [5], $V^{ext}(t)$ is the interaction of the electron with external light fields, and the total Hamiltonian $H(t) = H_0 + V^{ext}(t)$. Note that $V^{ext}(t)$ could be any type of time-dependent or time-independent external potential. The wave function in Eq. (1) is propagated by the split-operator-method in the energy representation [6] using a generalized pseudospectral method. We first diagonalize the Hamiltonian H_0 in an L^2 integrable basis set [7]. In principle, all the functions in this finite region can be expanded using the basis. The time-propagation mainly involves matrix-matrix and matrix-vector multiplications, which are calculated using the basic linear algebra subprograms (blas). In this way we can use the computer more effectively.

The numerical simulations are performed in a finite box. To avoid the unphysical reflection at the boundary, we separate the space into two regions within the box [8, 9], the inner region and the outer region. When

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the time-dependent wave function in space reaches the outer region, we project the outer region wave function into momentum space (Volkov state) and remove it from the wave function in real space. The wave function in the inner-region is propagated numerically in real space and the wave function in the outer-region is propagated in momentum space analytically. In doing so, we ignore the electron parent core interaction in the outer region. This approximation is reasonable so long as the outer region is far enough. In the present calculation, we choose the outer region starts from 150 a.u. where the electron laser field interaction is orders of magnitude larger than the electron-nucleus Coulomb interaction. This procedure allows us to keep all the phase information for a long time-propagation without the reflection from the boundary. The details of the numerical procedure can be found in our previous papers [10, 11]. When the pulses are over, the total wave function is separated into two parts. One is the wave function in momentum space (or the outer region) which describes the ionization process and the other is located in the inner region in real space and describes the excitation process. The second term of Eq. (1) does not contribute to any dynamical process. To improve the numerical accuracy, we drop this part in the calculation. The wave function in momentum space after the pulse provides all the information of the ATI spectra. Integrating the ATI spectra we get the total ionization probability.

If we choose the EUV light source of a combined field of the 13th and 15th harmonics, which are the major components in the APT used in the experiments [12, 13], created by the high-order harmonic generation of the same IR laser, we can write the time-dependent external potential as $V^{ext}(t) = -z[E_{IR}(t) + E_x(t)]$ with the IR laser field

$$E_{IR}(t) = F_{IR} e^{-2\ln 2\ (t-t_d)^2/\tau^2} \cos(\omega(t-t_d)), \quad (2)$$

where F_{IR} is the field strength of the IR laser, $\tau = 45$ fs is the full width half maximum (FWHM) of the IR pulse, ω is the center frequency , and t_d is the time delay between the IR pulse and the EUV pulse. The EUV pulse is written as

$$E_x(t) = e^{-2\ln 2\ t^2/\tau_x^2} F_x[\cos(13\omega t) + \cos(15\omega t)], \quad (3)$$

where F_x is the field strengths of the EUV light, $\tau_x = 10$ fs the FWHM of the EUV pulse. We assume that both the IR laser and EUV light are polarized along the z-direction. In the simulation, we choose the IR laser center wavelength as 800 nm.

Figure 1 shows the IR assisted photoionization of helium by the EUV light as a function of the time delay between the two pulses. The IR laser intensity is

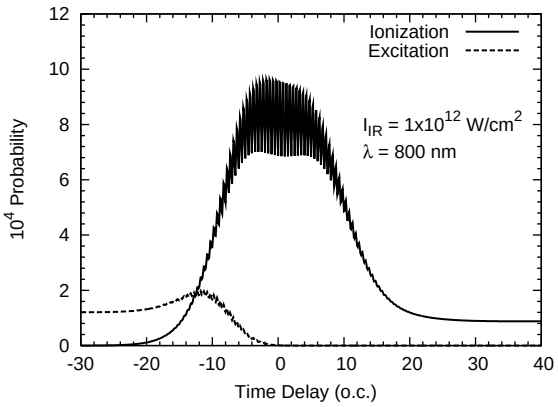

Figure 1: The IR assisted photoionization (solid line) and excitation (dashed line) of helium by the EUV light as a function of the time delay between the two pulses; o.c. denotes the optical cycle.

so low that it cannot ionize helium atoms without the EUV light and the EUV photon energies are below the ionization threshold so it cannot ionize helium atoms either without the IR laser. Thus when the IR pulse arrives well before the EUV laser as shown in Fig. 1, the ionization probability is almost zero and the excitation probability by the EUV is unchanged. The ionization probability increases as the IR pulse approaches the EUV pulse, and reaches a peak when the two overlap with each other while the excitation probability decreases instead. In this region, the ionization probability also oscillates rapidly. When the IR pulse arrives later than the EUV pulse, the ionization probability reduces significantly but does not approach zero, and the excitation probability vanishes. This is due to that although the EUV light cannot ionize the helium atoms, it can excite the helium atoms and the excited atoms can be ionized by the IR laser arrived later on. Note that the EUV can excite the atoms without the IR laser through resonance processes so the excitation probability is sensitive to the IR laser used to generate the EUV light. If we change the center wave length from 800 nm to 785 nm, the excitation probability can be enhanced dramatically, as observed in the recent experiment [13].

When the two pulses overlap with each other, the ionization probability is large and oscillates twice per optical cycle as shown in Fig. 2. This observation is consistent with the recent experiments [12, 13]. We see that the ionization probability is larger than the EUV excitation probability, which means that the IR does not only ionize the excited helium but also enhances the ionization probability by the EUV light from the ground state. Recently, We [14] proposed a general theory to explain the IR assisted photoionization processes. In the the-

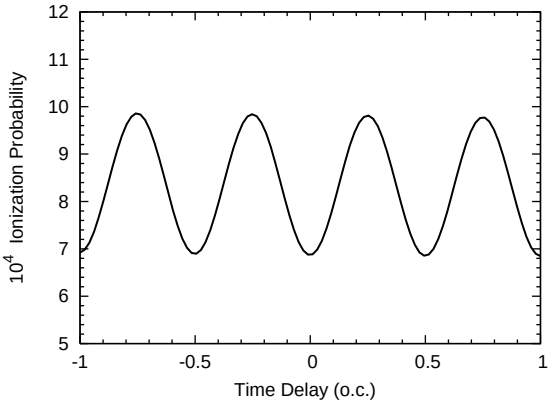

Figure 2: The Ionization probability in the overlap region.

ory, atomic structures in an IR laser field are described by Floquet states and atoms can be ionized to a Floquet state by a single AP through different Floquet components. The interference of ionization through different Floquet components results in the oscillation of the ionization yield as a function of the arriving time of the AP. Similarly, we attribute the oscillation to the interference of a Floquet state created by the transitions to different Fourier components by 13th and 15th harmonics. The time delay between the EUV pulse and IR laser pulse introduce a phase between the two transitions via different Fourier components. Based on this understanding, We can control the oscillations by either tuning the IR laser intensity or the relative field strength of the 13th and 15th harmonics. The details will be published somewhere else.

In this example, for a large time delay or long time-propagation the electron will reach the boundary and be reflected if we do not project the outer region electron into momentum space and propagate it analytically. The reflected part (unphysical part) will interfere with the electron in the inner region and ruin out the physics we are looking for. Here we gave one application of our time-dependent method. Since the method we introduced here is general we can use it to explore many other dynamical processes in the laser-atom interactions. We have extended the present method to the study of laser-molecule interactions [15]. The method can also be used to study the time-independent processes, like the antiproton collision with hydrogen atoms [16], which is difficult to be treated by the traditional method.

This work was supported by Grant-in-Aid for Scientific Research (C) from the Japan Society for the Promotion of Science. The numerical calculations have been carried out by T2K-Tsukuba System in the Center for Computational Sciences, University of Tsukuba.

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