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Infrared laser assisted photoabsorption of Ne atoms

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Abstract. We proposed recently a theoretical method to study the infrared (IR) laser assisted photoabsorption cross sections over a broad energy range by a single calculation. We apply this method to study the IR laser assisted photoabsorption of Ne atoms near the first ionization threshold. The simulation results show that the IR field modifies the photoabsorption cross sections and the energy structures. This photoabsorption cross section is an important quantity to analyze the IR-laser assisted dynamical processes by an attosecond pulse, a pulse train or a free electron laser.

1. Introduction

Understanding and controlling natural phenomena is one of the main goals of the physical researches. Photoabsorption spectra have been used to study atomic structures and to identify the constitutes in a material for a long time [1]. As the laser technology advances, one can control even the photoabsorption of atoms in a very short time scale with the assistance of a moderately intense infrared (IR) laser field by a non-coherent light source from the synchrotron radiations [2, 3, 4] or by a coherent light source from the attosecond XUV source [5, 6]. The IR field modifies the atomic structure and the photoabsorption processes, for example, the IR field induced transparency for x rays [7, 8]. For most of the moderately intense IR field assisted processes, the IR field only modifies the energy structures of the excited or continuum states without perturbing the ground state wave function. Recently, using the IR assisted photoexcitation process, Swodoba *et al.* [9] could even investigate the IR field induced energy shift of a specified excited state.

   Stimulated by those recent developments, we developed a general theoretical method to study the photoabsorption process controlled by a periodic external field and apply it here to study the IR assisted photoabsortion process of Ne atoms. The details of the theoretical method can be found in our previous work [10]. We brief some key equations here for the completeness of the paper.

2. Theoretical Method

When an atom is placed in a periodic external field, its motion is governed by the following time-dependent Schrödinger equation (atomic units $\hbar = m = e = 1$ are used unless stated

otherwise):

$$i\frac{\partial \Psi(t)}{\partial t} = H(t)\Psi(t) \tag{1}$$

with $H(t) = H_0 + V(t)$ where H_0 is the atomic external field-free Hamiltonian and $V(t)$ is periodic in T as $V(t + T) = V(t)$. Based on the Floquet theory [11] , the solution of the above equation can be generally expressed as

$$\Psi_\alpha(t) = e^{-i\epsilon_\alpha t} \sum_{n=-\infty}^{\infty} e^{-in\omega t} \phi_{\alpha,n}, \tag{2}$$

where ϵ_α is the quasi-energy, $\phi_{\alpha,n}$ is the time-independent wave function of the nth Fourier component of the α Floquet state, and $\omega = \frac{2\pi}{T}$ is the frequency of the periodic external field. If the periodic field is strong enough to modify the structures of the excited and continuum states but weak enough not to perturb the ground state, the photoabsorption cross section from the ground state to the Floquet states can be expressed as

$$\sigma(\omega_p) = \frac{4\pi\omega_p}{c}\mathrm{Im}\sum_{\alpha,n}\frac{|\langle\Psi_g|\mathbf{d}|\phi_{\alpha n}\rangle|^2}{(\epsilon_\alpha + n\omega) - (\epsilon_g + \omega_p) - i\eta}, \tag{3}$$

where η is an infinitesimal positive number to represent adiabatical switching on of the probe light, ω_p is the frequency of the probe light, $\mathbf{d}$ is the dipole operator, Ψ_g is the ground state wave function, and ϵ_g is the ground state energy. If there is no periodic external field, there is only one non-zero Fourier component for a given Floquet state and the above equation turns to the standard one for photoabsorption without the periodic field [1]. In the traditional procedure, we obtain the time-dependent wave function $\Psi_\alpha(t)$ solving the time-independent Floquet equation. The computational load increases cubically as the number of the Floquet blocks increases and the applicability of the method to real systems is limited. If many continuum states are involved, this is the case for the IR laser assisted photoabsorption process, the problem becomes even more difficult and more complicated.

We developed a theoretical method to study the photoabsorption process in an oscillating magnetic field for a non-degenerate system [12]. We extend the method to a general case in which both bound and continuum degenerate states are involved. For such a purpose, we define the time-dependent Hamiltonian as $H(t,\tau) = H_0 + V(t+\tau)$ with τ a time shift which corresponds to an initial phase $\delta = \frac{2\pi\tau}{T}$ and set the initial wave function $|\Psi(t=0,\tau)\rangle = \mathbf{d}|\Psi_g\rangle$. The time-dependent wave function $\Psi(t,\tau)$ is obtained from Eq. (1) using the split-operator method with the generalized pseudospectral grid in the energy representation [13] for a given $H(t,\tau)$. Defining a generalized autocorrelation function as

$$C(t) = \frac{1}{T}\int_0^T \langle\Psi(t=0,\tau)|\Psi(t,\tau)\rangle d\tau, \tag{4}$$

the photoabsorption cross section can be represented as

$$\sigma(\omega_p) = \frac{4\pi\omega_p}{c}\mathrm{Im}\int_0^\infty iC(t)e^{i(\omega_p+\epsilon_g)t-\eta t}dt. \tag{5}$$

In the practical simulation, we confine the numerical calculation in a finite space and have to filter out the wave function in the outer region using an energy dependent optical potential [14, 15]. Generally speaking, the quasi-energy ϵ_α in Eq. (2) is a complex number with the
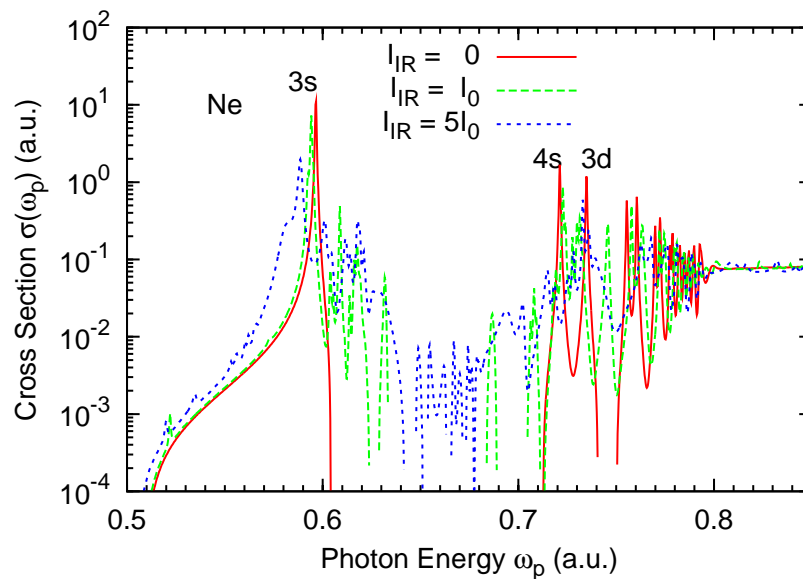
Figure 1. The IR assisted photoabsorption cross sections of Ne at three IR intensities: 0 (solid line), I_0 (dashed line) and $5I_0$ (dotted line), respectively with $I_0 = 10^{12}$ W/cm^2.

imaginary part representing the width of the Floquet state. To avoid the divergency at $t \to -\infty$ in Eq. (5), we adiabatically switch off the probe field instead of adiabatically switching it on.

The equivalence of Eqs. (3) and (5) has been proved in our previous work [10]. We focus on how to apply this general theoretical method to study the IR assisted photoabsorption cross sections of Ne atoms at different intensities for an 800 nm IR laser. The atomic Hamiltonian can be written as $H_0 = -\frac{1}{2}\nabla^2 + V_{eff}(r)$ with a model potential $V_{eff}(r)$ [16] describing the electron parent-core interaction. The interaction of the IR field with the active electron is written as $V(t) = -zE_0 \cos(\omega t + \delta)$, where z is the electron z coordinate, E_0 is the IR field strength and $\delta = \frac{2\pi\tau}{T}$ is the initial phase. We assume that both the IR laser and the probe light are linearly polarized along the z direction. Similarly to the He case [10], we propagate the wave function for 256 o.c. (o.c. denotes the IR optical cycle).

3. Results and Discussion

Figure 1 shows the IR assisted photoabsorption cross sections at 3 different IR intensities. Without the IR field, the photoabsorption spectra are divided into two parts, photoexcitation below the ionization threshold and photoionization above the threshold. The photoexcitation consists of many sharp resonances and the energy widths of the resonances are very narrow. For photoionization, the spectra change smoothly as a function of the photon energy and they are insensitive to the propagation time. As we switch on the IR laser, the atomic structures are described by the Floquet states and there are many sidebands for a bound state. For the photoionization far above the ionization threshold, the spectra depend on the IR intensity weakly. There are some structures above the ionization threshold and they are attributed to the sidebands of the bound states. A moderate intense IR laser does not modify the occupied orbits significantly due to the electron binding energies are much larger than the electron laser field interaction. For excited states, the binding energies are comparable to the electron laser field interaction so the excited energy structures are sensitive to the applied IR intensity. The
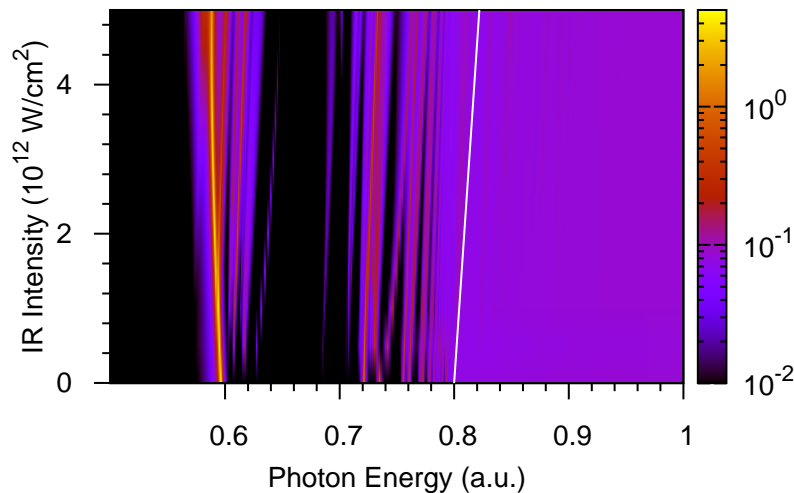
Figure 2. The IR assisted photoabsorption cross sections of Ne as a function of the IR intensity. The solid line shows the ionization threshold due to the ponderomotive shift.

strengths of the sideband contribution increase as the IR intensity increases. The ionization potential also increases as the IR intensity increases owing to the ponderomotive shift [17, 18].

Now let us focus on the bound state energy shifts, which can be seen more clearly in Fig. 2. The ionization threshold increases linearly as the IR intensity increases and it is well represented by $I_p + U_p$ with I_p atomic ionization potential and U_p the ponderomotive energy of a free electron in the laser field. The ponderomotive shift mainly affects the highly excited states and the energy shifts are well represented by the ponderomative energy. This is the reason why the above threshold ionization peaks from the highly excited states (so called Freeman resonances [19]) do not depend on the IR intensity. For the lower bound states, such as the $3s$ state, the shift moves to the opposite direction. From the energy difference, we can classify the origin of the sharp peak above the ionization threshold. As the IR intensity increases, we do not see a peak structure clearly for the highly excited states because the width of the highly excited states in the IR field is comparable to or even larger than the energy separation between the different excited states. Note that in the present non-relativistic calculation, we did not take into account the fine structure splitting. To compare with high precision experiment, we need to split the calculated spectra into two parts and shift the photon energy to fit the two ionization thresholds as we did before [20].

To summarize, we investigated the IR assisted photoabsorption processes of Ne atoms using a recently developed theoretical method. The IR field modifies the photoabsorption cross section as well as the energy structures. For the highly excited states, the IR induced energy shifts can be well explained by ponderomotive shift. For the lowest excited state, the IR induced energy shifts move to opposite direction significantly. The calculated cross sections also provide us a guide to investigate how to control the photoabsorption process by tuning the energy range of attosecond XUV source.

Acknowledgments

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