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Research Article

Excitation and ionization of helium atom induced by intense free-electron laser pulses

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Abstract
For the first time, excitation and ionization of helium atom induced by intense free-electron laser (FEL) pulses is simulated in the present work. It is found that electrons can tunnel through the ground state of helium atom (He) and leave from the atomic region induced by subsequent FEL field. Therefore, the ionization of He can happen. Additionally, some electrons can be captured by a higher electronic state, which leads to the tunneling excitation from the ground state to a specific excited state.

Keywords: Free-electron lasers; Excitation; Tunneling ionization; Wavepacket

Free-electron lasers (FEL) are capable of generating coherent light by accelerating a beam of relativistic electrons injected into an undulator magnet [1]. FEL is, similar to synchrotron radiation, a device which can produce coherent radiation from the process of stimulated bremsstrahlung. Free-electron lasers are particularly useful because they can produce radiation with a short-wavelength, covering the 50nm to 150nm range [2,3] and working in the femtosecond or nanosecond pulse model [4,5]. Thus, we believe that FEL will become an important tool for applications in many aspects, including physics and chemistry [6-8].

In this work, the excitation and ionization of helium atom induced by FEL pulses are simulated theoretically. Particular emphasis is placed on the excitation phenomenon and mechanism of helium atom (He) in the tunneling ionization region. The interaction between FEL pulses and He are solved numerically based on one-dimensional time-dependent wavepacket method. Making use of the electric dipole-moment approximation, the one-dimensional atomic motion induced by FEL obeys:

$$i\frac{\partial}{\partial t}\Psi(x,t)=\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+V_a(x)+E(t)x\right]\Psi(x,t) \qquad (-\infty < x < +\infty)$$

Where Va (x) is atomic potential, which has the functional form:

$$V_a(x)=V(a,q,x)=-\frac{q}{\left(x^2+a\right)^{1/2}}.$$

In this formula, q and a are special parameters, which are used to mediate the depth of potential well and remove the singularity of potential function at x=0.

E(t)x is the interaction potential between electron and FEL field.Ψ(x, t) denotes the wavefunction of the investigated system at time t. The split-operate method [9] is adopted to execute the wavepacket propagation. Additionally, it is necessary to employ the absorption potential so that the time-dependent wave function can eschew boundary reflections [10].

Quantum mechanical tunneling effects have already been confirmed to happen through penetrating into the classically inaccessible potential energy barrier [11]. There are well-established ionization mechanisms of atoms, including strong-field tunneling ionization and weak-field multiphoton ionization [12]. In the tunneling ionization region, some electrons can be ionized through tunneling the barrier created by the atomic Coulomb potential and FEL field, whereas some electrons merely excite, with transitions to some excited states.

The excitation of helium atom, due to interaction with the short pulses of FEL, is particularly interesting and informative. It has been shown in Figure 1 that the excitation probability of He is one order smaller than the ionization probability, and both the excitation.

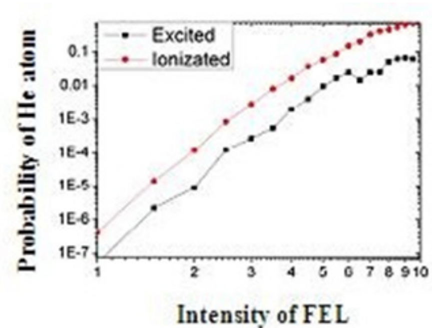

Figure 1. The probability of He atom's ionization and excitation changes with the intensity of FEL in unit of 10^{14}W/cm²

probability and ionization probability of helium atom enlarge with the increase of FEL intensity. Figure2 demonstrates the excited states, population of helium atom after radiation of FEL with 800nm wavelength and 1.3fs pulse. The excited states population of He has a single peak at n=14, under the impact of such a short FEL pulse. The evolutions of ionized and excited wavepackets of He have been shown in Figure3 and 4, with the FEL in white line. Firstly, let us have a look at the wavepacket evolution of ionized electrons in Figure3. The barrier created by the FEL field and atomic Coulomb potential becomes the lowest when the FEL field reaches the peak at $t=2.5T_0$, in which T_0 stands for the optical cycle of FEL. Therefore, electrons can tunnel through the ground state of helium atom and leave from the atomic region induced by subsequent FEL field. Thus, the ionization of He do happen eventually. However, there are also some electrons, which are trapped by the helium nucleus, undergoing the excitation process instead of ionization.

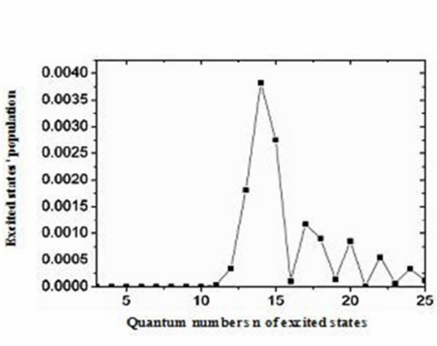

Figure 2. Population of different excited states of He atom irradiated by FEL

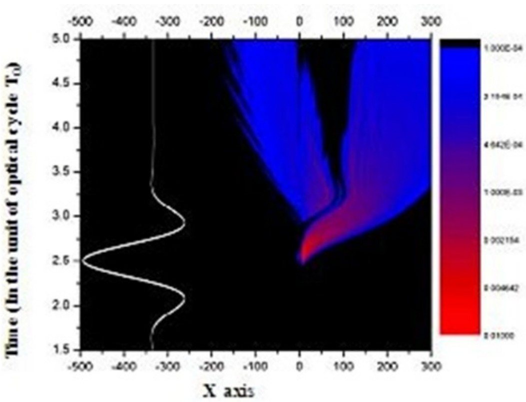

Figure 3. Wavepacket evolution of ionized electrons, with the white line standing for FEL

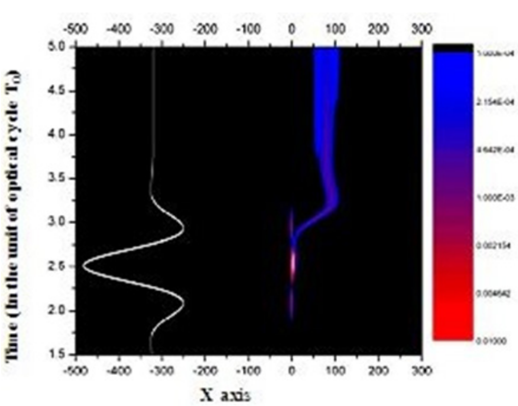

Figure 4. Wavepacket evolution of excited state, with the white line denoting FEL

Now let us talk about the wavepacket evolution of excited state, as is illustrated in Figure 4. The velocity of electrons, which tunnel the barrier along the positive side of x axis, is reduced near $t=2.8T_0$ due to the negative force of the electric field. The wavepacket velocity of excited state is 0 when the FEL field becomes zero at $t=3.2T_0$, which means that electrons cannot penetrate into the potential barrier. Since there are no tunneling electrons through the barrier when the FEL pulse is over, the wavepacket of excited state stay still at the neighborhood of x=80. Meanwhile, these electrons can be captured by a highly electronic state, which thus accomplishes the tunneling excitation from the ground state to a specific excited state.

Based on these scenarios discussed above, we can have a clear understanding of the excitation mechanism of helium atom irradiated by FEL pulses. The reason why there is a single peak for the population of excited states in Figure 2, which dominates at n=14 under the impact of intense FEL with short pulses, can thus be explained fairly well. With the rapid development of future techniques, groups equipped with FEL might be able to perform such experiments at the required wavelength and pulse duration in the present work. Therefore, a comparison between experimental data and theoretical results can be made.

Acknowledgements

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Conflict of interest

The author declares no conflict of interest.

Data statement

Original data are available from the corresponding author upon request.

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