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Research Article

ODD-EVEN HIGH-ORDER HARMONIC GENERATION FROM HELIUM ATOM APPROACHING FROM TIME-DEPENDENT DENSITY FUNCTIONAL THEORY

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ABSTRACT

Recently, we found that the even-to-odd ratio of high-order harmonic generation (HHG) emitted from atoms or symmetric molecules in the combination of a mid-IR laser pulse and THz electric field is a universal quantity, i.e., independent of mid-IR laser's parameters and the choice of the target. However, the targets are considered within the one-electron model, and the conclusions are derived from directly numerically solving the time-dependent Schrödinger equation. In this work, we investigate the validation of the even-to-odd universality helium atom consisting of two electrons, applying the time-dependent density functional theory. The results demonstrate that the multi-electron effect manifesting through the repulsive Coulomb and exchange-correlation interactions does not considerably change the universality of the even-to-odd ratio of the helium atom.

Keywords: correlation; helium; HHG, odd-even; THz; universality

1. Introduction

High-order harmonic generation (HHG) is a non-linear optical phenomenon occurring when matter is exposed to an intense laser pulse (Ferray et al., 1988; Mcpherson et al., 1987). HHG emitted from gaseous-phase atoms and molecules can be intuitively described by the semi-classical model whose process is followed by three steps: (i) the external electric field deforms the atomic/molecular potential so electron easily tunnels out; (ii) ionized electron quasi-freely travels in the laser field and gains energy; (iii) when the laser field reverses its direction, the electron goes backward, recombines into the parent ion and converts its gained

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energy to photons called HHG (Corkum, 1993). The ratio between the energies of emitted HHG photon and the incident laser is called HHG order. HHG spectrum has a typical structure where the intensity rapidly decreases according to the perturbation regime at low harmonic orders; then, HHG intensity is almost unchanged in a broad harmonic region called the plateau. The plateau ends by the cutoff, after which the HHG intensity is dramatically suppressed.

If the laser pulse is multi-cycle, HHG spectra contain sharp peaks at integer harmonic orders. For a symmetric system consisting of an atom or nonpolar molecule and linearly-polarized multi-cycle laser pulse, HHG contains odd orders only (Ben-Tal et al., 1993). For an asymmetric laser-target system, whose symmetry-breaking is attributed to either molecular targets or laser pulses, HHG contains both odd and even orders. Clearly, odd-even HHG encodes asymmetry properties of laser-target systems; thus, finding a simple way to reversely disentangle them from measurable HHG is desirable.

One simple way to establish an asymmetric laser-target system is by adding a weak static electric field into the symmetric laser-atom system (Hong et al., 2009). However, in this way, the static electric field must be simultaneously stable and intense (~1 MV/cm), which is difficult to achieve in HHG experiments. To overcome this obstacle, it has been suggested to adopt a very long-wavelength powerful laser, such as a CO_2 laser, instead of a static electric field (Borca et al., 2000; Odžak & Milošević, 2005; Taranukhin & Shubin, 2000). Recently, intense broadband terahertz pulses with stable carrier-envelope phases have emerged as candidates to replace static electric fields in HHG studies. High-bandwidth THz radiation with peak amplitudes up to 100 MV/cm can be produced (Zhang et al., 2021). The modulation of the THz electric field is slow compared with that of a primary laser pulse; thus, THz-induced physical effects are considered as those caused by a static electric field (Hong et al., 2009).

Concerning the odd-even behavior in HHG emitted from static-field-assisted or THz-assisted laser-target systems, Wang et al. (1998) numerically showed that with increasing the static electric field (but in the weak region), the intensity of even orders initially increases, while that of the odd orders is almost unchanged. When the static field continues to enhance, the intensities of even and odd orders fluctuate irregularly. Besides, it is demonstrated numerically that the intensities of even harmonics are comparable to those of odd ones (Bao & Starace, 1996; Hong et al., 2007). In these studies, the statements are declared without detailed discussion and explanation. Therefore, it is essential to investigate the correlation between the intensities of even and odd harmonics, specifically, how their intensities respond to the additional steady electric field.

Recently, we have investigated the odd-even HHG emitted from atoms and symmetric molecules in the combination of mid-infrared (mid-IR) and THz laser pulses (Trieu et al., 2023). We have found out that the dimensionless even-to-odd ratio, i.e., the ratio between the intensities of the even order and the average of the two adjacent odd orders, is a universal quantity. Particularly, the even-to-odd ratio is independent of the parameters of both the mid-IR laser pulse and target. Besides confirming numerically, we also analytically derived a simple relation describing this universality.

This universality has been confirmed for various atoms and symmetric molecules; however, within single-active electron (SAE) approximation, i.e., the outermost electron actively interacts with the laser electric field while other electrons are frozen, accompanying nuclei. Further confirmation of the even-to-odd ratio universality for multielectron targets, such as helium atoms, is desirable. Moreover, in Ref. (Trieu et al., 2023), since the targets are treated within one-electron models, directly solving the time-dependent Schrödinger equation (TDSE) is employed. However, applying the TDSE method for multielectron systems is especially challenging because of the multi-variable problem. For including the multielectron effects, time-dependent configuration interaction (Klamroth, 2003) or time-dependent density functional theory (TDDFT) (Marques & Gross, 2004) are promising alternatives.

In this work, we examine the universality of the even-to-odd ratio of HHG emitted from helium atoms in the combination of mid-IR laser and THz pulses. The helium atom is chosen since it is the simplest multielectron atom with two electrons. The multielectron effect is embedded in (i) Hartree potential describing electron-electron Coulomb repulsion and (ii) exchange-correlation potential. To realize this purpose, we adopt the TDDFT method where the time-dependent Hamiltonian is presented as a function of electron density (Huix-Rotllant et al., 2021; Marques & Gross, 2004; Runge & Gross, 1984). The TDDFT is embedded in the open-source code Octopus (Marques et al., 2003). To examine the Coulomb and exchange-correlation effects, we respectively apply the exact-exchange (EXX) and local-density approximation (LDA) functionals, which are available on Libxc – a library of exchange-correlation functionals for density functional theory (DFT) (Marques et al., 2012).

2. Theoretical background

In this section, we first present the TDDFT method for simulating HHG (Marques & Gross, 2004). Then, we briefly summarize the analytical formula of the universal rule of the harmonic even-to-odd ratio found by Trieu et al. (2023).

2.1. Time-dependent density functional theory for simulating HHG

The main idea of the TDDFT method is based on the Runge-Gross theorem (which is similar to the Hohenberg-Kohn theorem for DFT), stating that there is a unique mapping between the time-dependent external potential of an electronic system and its time-

dependent density. As a consequence, the physical quantities of the system can be determined as a function of time-dependent electron density alone. Thereby, the Schrödinger equation of an *N*-electron system with 3*N* spatial variables reduces to a three-variable Kohn-Sham (KS) equation in terms of system electron density. In this framework, the time propagation of a real interacting system is substituted by the propagation of a system of non-interacting electrons, called the KS system. For more detail, see Huix-Rotllant et al. (2021), Marques and Gross (2004), and Runge and Gross (1984). Here, we briefly present its spirit and main formulae.

Since the objective is HHG emitted from helium in the combination of co-linearly polarized mid-IR and THz pulses, the electron wavepacket mostly evolves in the polarization direction. Therefore, one-dimensional (1D) is implemented to simplify and save computational costs. The 1D time-dependent Kohn-Sham equation is written within the atomic units as the following

$$\mathrm{i}\frac{\partial}{\partial t}\psi_j(x,t)=\left[-\frac{1}{2}\nabla^2+V_{\mathrm{KS}}[\rho](x,t)\right]\psi_j(x,t), \quad (1)$$

where, $\psi_j(x,t)$ with $j=1,2,..N$ stands for the wavefunction of KS orbital j. The variable x is the position of the electron. The KS potential V_{KS}, as a functional of electron density $\rho(x,t)=\sum_{j=1}^{N/2}\mu_j\left|\psi_j(x,t)\right|^2$ with μ_j is the occupation of each KS orbital, is given by

$$V_{\mathrm{KS}}[\rho](x,t)=V_0(x)+V_{\mathrm{H}}[\rho](x,t)+V_{\mathrm{XC}}[\rho](x,t)+V_{\mathrm{I}}(x,t). \quad (2)$$

The first term presents ion-electron interaction. In our study, we apply the soft-Coulomb potential as used in Ref. (Castro et al., 2015)

$$V_0(x)=-\frac{2}{\sqrt{x^2+1}}. \quad (3)$$

The second term in Eq. (2) is the Hartree potential $V_{\mathrm{H}}[\rho](x,t)=\int\frac{\rho(x',t)}{|x-x'|}\mathrm{d}x'$, which describes the repulsive Coulomb interaction between the electrons. The next term $V_{\mathrm{XC}}[\rho](x,t)$ is called exchange-correlation potential between electron-electron, which includes non-trivial many-body effects. It should be noted that the major problem of DFT (and TDDFT) is that exact functionals for exchange-correlation potential are unknown, so approximations are needed. Undoubtedly, these approximations strongly govern the accuracy and reliability of the simulated results. Various types of exchange-correlation functionals are available in the Libxc library (Marques et al., 2012).

In our 1D simulation, the exchange-correlation potential consists of two separate parts – exchange potential and correlation potential. For the first part, we adopt the exact-exchange approximation (EXX) whose form for helium is $V_{\mathrm{X}}[\rho](x,t) = -\frac{1}{2}V_{\mathrm{H}}[\rho](x,t)$. For the correlation potential $V_{\mathrm{C}}[\rho](x,t)$ of 1D system, there are only two functionals named LOOS and CSC (Loos, 2012) which are constructed based on local-density approximations. We have examined and confirmed that these two density functionals give the same results, so we show the results for the case of using LOOS functional only.

The last term in Eq. (2) presents the interaction between the electron and the external field which is linearly polarized along x axis

$$V_{\mathrm{I}}(x,t) = xE(t). \tag{4}$$

Here, the field is the combination of a mid-IR and THz pulses

$$E(t) = E_0 f(t)\cos\left(\omega_0 t + \frac{\pi}{2}\right) + E_{\mathrm{T}}\cos(\omega_{\mathrm{T}} t), \tag{5}$$

where E_0, ω_0 are the peak amplitude and the central frequency of the mid-IR laser. E_{T}, ω_{T} are those for the THz field. $f(t)$ is the envelope of mid-IR pulse which has the trapezoidal form to easily attain sharp HHG peaks.

To solve Eq. (1), we first need the initial state (at $t = 0$) where the KS system is at the ground state, i.e., $\psi_j(x, t=0) = \psi_j^{\mathrm{gs}}(x)$. It is solved by the DFT method with the self-consistent procedure, which starts with the initial guess density to construct kinetic and potential functionals, followed by solving the KS equation. Then the obtained KS wavefunctions are used to calculate the electron density, and the iterative procedure is continued until the convergence condition is satisfied.

After receiving the converged initial wavefunction, its time-evolution $\psi_j(x,t)$ is treated by the approximated enforced time-reversal symmetry (AETRS) method with the time step of 0.01 a.u. Once we obtain the time-dependent wavefunction $\psi_j(x,t)$ and the electron density $\rho(x,t)$, we calculate the time-dependent dipole moment

$$D_x(t) = \int x\rho(x,t)\,\mathrm{d}x, \tag{6}$$

and HHG spectrum as

$$S_x(\omega) = \left|\int_0^{\tau} \mathrm{d}t\, e^{i\omega t}\frac{\mathrm{d}^2}{\mathrm{d}t^2}D_x(t)\right|^2, \tag{7}$$

where ω is the harmonic frequency, and τ is the mid-IR laser duration.

For the simulation, we choose a spherical box whose radius of $R = 900$ a.u. and the spatial grid step of 0.1 a.u. To avoid the reflection of the wavefunctions at the boundary of the simulation box, an absorption potential function in the form of $-i\xi \sin^2\left(\frac{\pi}{2}\frac{x-r}{R-r}\right)$ with $\xi = -0.2$ is applied beyond $r = 630$ a.u. All the simulation process is executed by the open-source code Octopus (Marques et al., 2003).

2.2. Analytical view of even-to-odd ratio universality

Our recent work (Trieu et al., 2023) has shown the universality of the even-to-odd ratio, i.e., the ratio between intensities of even-order harmonic and the average of the two adjacent odd orders when atoms or symmetric molecules interact with a combination of mid-IR and THz laser pulse. We have also described the universality by a simple analytical formula

$$\eta = \tan^2\left(C\chi\right), \tag{8}$$

The symbols η, χ denote the even-to-odd ratio and the scaled THz electric field, respectively. We define χ by the explicit expression

$$\chi = \frac{E_0}{\omega_0^3} E_{\mathrm{T}}. \tag{9}$$

We have numerically and analytically proved that C is a constant for each harmonic energy. Specifically, for harmonic at cutoff, C is 2.558. It is emphasized that C does not contain any parameters of the mid-IR laser or target, either explicitly or implicitly. Therefore, Eq. (8) indicates the universality of even-to-odd ratio and scaled THz electric field. This analytical relation entirely matches the even-to-odd ratio numerically calculated for varied parameters of the mid-IR laser. It is also validated when various atomic targets within one-electron models are used for numerical simulation. In this paper, we verify its validation for the helium atom whose electron-electron interaction plays a crucial role.

3. Results and discussion

3.1. HHG from helium within TDDFT approach

To get a reliable even-to-odd ratio numerically, accurate HHG spectra are a prerequisite requirement. To this end, in this section, we show the HHG spectra and benchmark them with available data published previously (Castro et al., 2015; Reiff et al., 2020). Since the available data are for helium exposed to an intense laser pulse only; thus in this subsection, THz pulse is temporally not included for convenience in benchmarking. We, in turn, present the cases: including Hartree potential only, and including both Hartree and exchange-correlation potentials.

3.1.1. Considering Hartree potential only

When including Hartree potential, Eq. (2) for the KS potential is simplified as

$$V_{\mathrm{KS}}[\rho](x,t)=V_0(x)+V_{\mathrm{H}}[\rho](x,t)+V_{\mathrm{I}}(x,t). \quad (10)$$

It should be noted that the TDDFT with KS potential in this form is identical to the time-dependent Hartree-Fock equation, where only exchange interaction is included. Our simulation gives the ionization potential of the helium atom of 0.75 a.u., which is consistent with that presented in Ref. (Castro et al., 2015). To continue, we calculate the HHG from the helium atom in the infrared laser (without THz field), which has a wavelength of 800 nm, intensity of 0.31×10^{14} W/cm^2, and duration of 200 optical cycles. The resultant HHG is exhibited in Fig. 1 which reveals resolved sharp peaks at odd-order harmonics. Besides, the HHG ends at the cutoff of $17\omega_0$ which is well consistent with the cut-off law $I_p+3.17U_p$ where I_p and U_p are respectively the ionization potential and electron's ponderomotive energy accumulating during an optical cycle (Lewenstein et al., 1994). For benchmark, in Fig. 1, the HHG simulated in Castro et al. (2015) with the same laser parameters is also presented, but with a horizontally shifted half-harmonic order for clarity. The figure clearly shows its consistency both in shape and intensity with our result. Therefore, we assert that our simulated HHG is reliable.

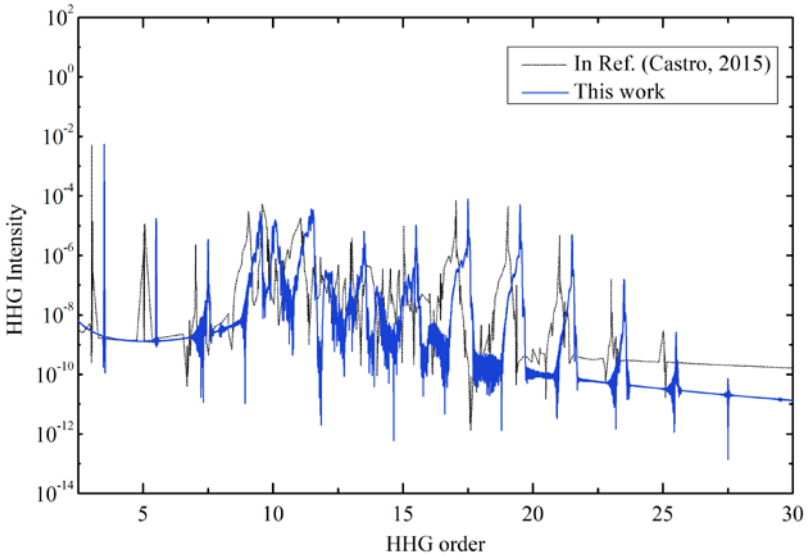

Figure 1. *The calculated HHG (solid blue curve) and the benchmark from Ref.* (Castro et al., 2015) *(black curve) when including Hartree's potential. For a clear illustration, the benchmark HHG is horizontally shifted by* $0.5\omega_0$

3.1.2. Considering both Hartree and exchange-correlation potentials

Now besides the Hartree potential, we add the exchange-correlation potential to calculate HHG. The general potential expressed by Eq. (2) is employed. In Fig. 2, we present

the simulated HHG of a helium atom in a 4-cycle laser pulse with the intensity of 10^{15} W/cm^2, and the wavelength of 400 nm. Our calculation shows that the exchange energy vanishes since the two electrons of the helium atom are both in the ground state.

For benchmarking, the simulated result taken from Reiff et al. (2020) is also shown in Fig. 3. It should be emphasized that in that work, the HHG spectrum is calculated within the three-dimensional TDDFT method and involves the correlation potential. For easy illustration, a vertical shift is performed. Figure 2 demonstrates good consistency between the two presented spectra despite different dimensionality. Although the 1D model leads to a discrepancy in harmonic intensity, it does not affect our interested quantity, the even-to-odd ratio, since the ratio is taken to cancel out intensity discrepancy.

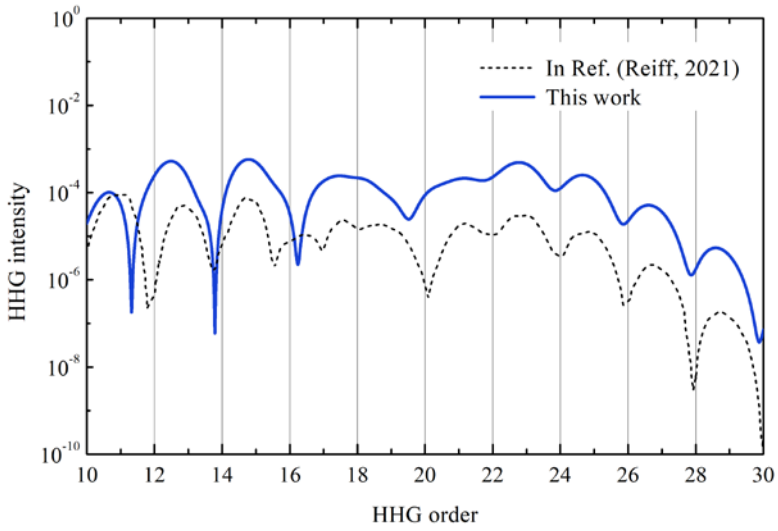

Figure 2. *The comparison between the 1D HHG (solid curve) calculated with full potential, and the 3D HHG taken from Ref.* (Reiff et al., 2020) *(dotted curve) (which is vertically shifted for clarity)*

3.2. Universality of even-to-odd ratio considering the multielectron effect

After verifying the reliability of HHG simulation for helium atom incorporating multielectron effect, we continue to investigate its even-to-odd ratio for harmonics at the cutoff as a function of scaled THz electric field χ, which is defined by Eq. (9). The adopted THz electric field has the wavelength of 231 μm which is much longer than that of mid-IR laser (Shalaby et al., 2016), and amplitude varies in the range of $(50 \div 1000)$ kV/cm. The mid-IR pulse has a duration of 10 cycles and a trapezoidal envelope with one cycle turned on, and one turned off.

In Fig. 3, we compare the even-to-odd ratio in three cases corresponding to three levels of the potential model, from the simplest to the most complicated: SAE ($V_0 + V_\mathrm{I}$), including Hartree potential only ($V_0 + V_\mathrm{H} + V_\mathrm{I}$), and both Hartree and exchange-correlation potentials (

$V_0 + V_H + V_{XC} + V_I$). The first case means the multielectron effect is neglected, and the calculation is treated within the one-electron model. The second case considers the Coulomb electron-electron repulsion, while the latest case adds the exchange-correlation interaction. The mid-IR laser with an intensity of 2.5×10^{14} W/cm^2 and wavelength of 2000 nm is used. The figure shows that for χ within the range [0.2, 1], the even-to-odd ratios are similar to each other despite the potential level. The consistency is manifested via the shape, magnitude, and position of the critical point (maximum). Moreover, the simulated even-to-odd ratios benchmark the analytical curve.

To continue, we confirm the universality of the even-to-odd ratio's validity by examining its dependence on the mid-IR laser's parameters, whose intensity and wavelength are respectively varied in the range of $(1.3 \div 3.9) I_0$ and $1600 \div 2700$ nm, where $I_0 = 10^{14}$ W/cm^2. The mid-IR laser parameters are governed so that the Keldysh parameter $\gamma = \sqrt{I_p / 2U_p}$ is kept at 0.33 to ensure the tunneling ionization regime (Keldysh, 1965).

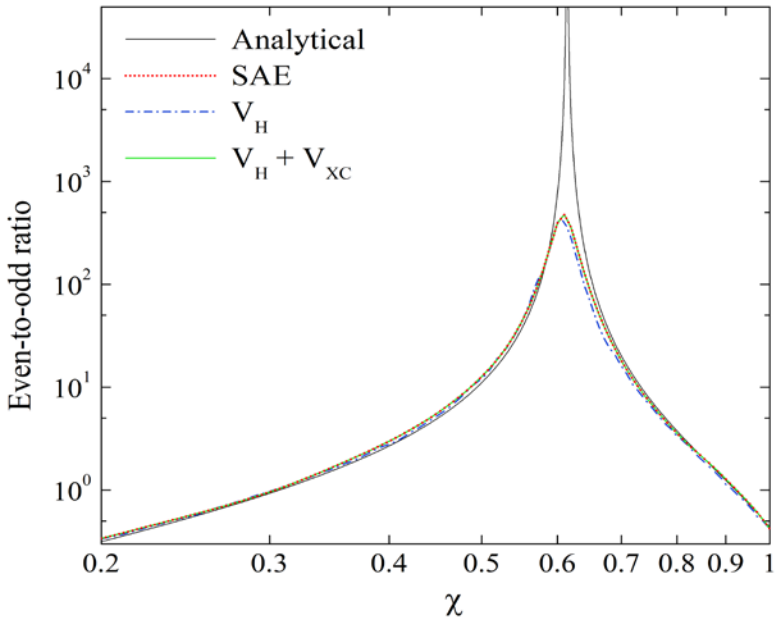

Figure 3. *The even-to-odd ratio of helium atom within SAE potential (SAE), including Hartree potential (V_H) and both Hartree and exchange-correlation potentials (V_H + V_{XC}). A 10-cycle trapezoidal primary laser pulse with the intensity of 2.5×10^{14} W/cm^2 and wavelength of 2000 nm is used. The analytical curve is plotted for the benchmark*

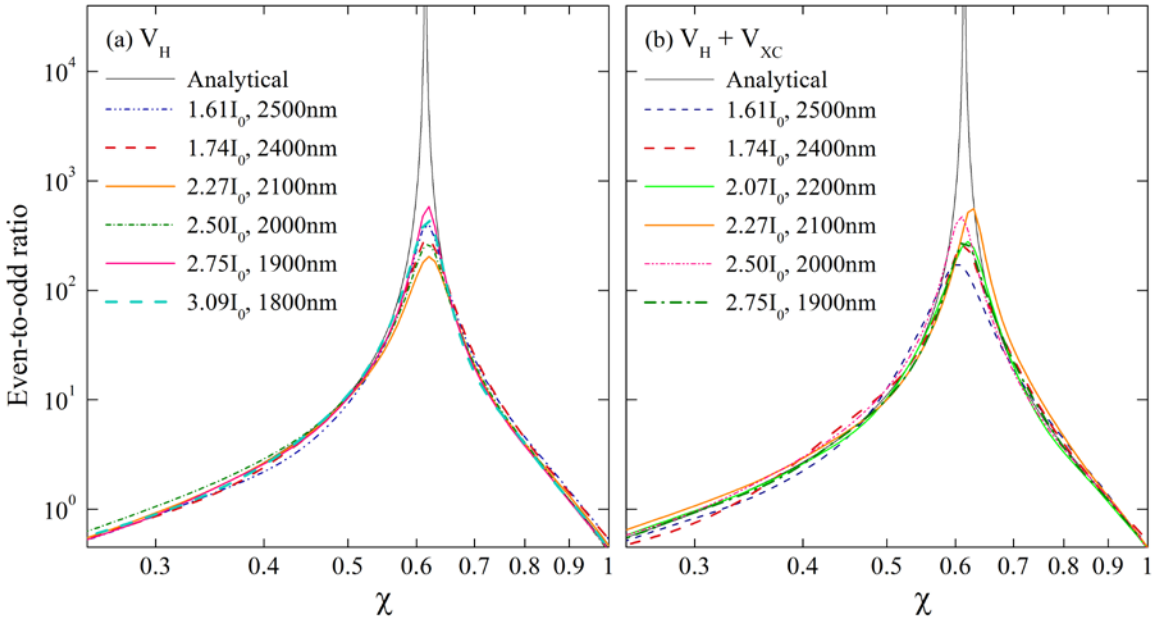

Figure 4. *The even-to-odd ratio of helium atom exposed to the combination of a primary and a THz electric fields when including (a) Hartree potential (V_H) only and (b) both Hartree and correlation potentials (V_H + V_{XC}). 10-cycle trapezoidal primary laser pulses with various intensities and wavelengths enclosed in the legends are used. The analytical curve is plotted for the benchmark*

The results are presented in Fig. 4 for two levels of considering the multielectron effect, including Hartree potential only (a) and both Hartree and exchange-correlation potentials (b). Figure 4 (a) demonstrates that although including Hartree potential, the even-to-odd ratio is considerably stable to varying laser parameters. If the exchange-correlation interaction is added [Fig. 4 (b)], the maximum position of the even-to-odd curve is slightly shifted. However, the change is insignificant. In short, we conclude that the universality of the even-to-odd ratio of helium atoms is still validated.

4. Conclusion

In this study, we have investigated the universality of the even-to-odd ratio of THz-assisted HHG emitted from helium atoms approaching from TDDFT method. We show that despite the different levels of multielectron interaction, the even-to-odd ratios are considerably consistent with each other and match the analytical prediction. Moreover, the even-to-odd ratio is also considerably independent of mid-IR laser intensity and wavelength. The results enhance the validation of the universality of even-to-odd ratio for helium atoms. However, in this study, the mid-IR is governed so that the Keldysh parameter is 0.33. Further investigation for other Keldysh parameters is established as an outlook.

❖ ***Conflict of Interest:*** *Authors have no conflict of interest to declare.*

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PHỔ PHÁT XẠ ĐIỀU HÒA BẬC CAO CHẴN-LẺ CỦA PHÂN TỬ HELI: TIẾP CẬN BẰNG LÍ THUYẾT PHIẾM HÀM MẬT ĐỘ

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TÓM TẮT

Gần đây, chúng tôi đã chỉ ra rằng tỉ số chẵn-lẻ của phổ phát xạ điều hòa bậc cao (HHG) phát ra từ nguyên tử hoặc phân tử đối xứng được đặt trong tổ hợp của điện trường laser hồng ngoại giữa và THz là đại lượng phổ quát. Đại lượng này không phụ thuộc vào thông số của laser hồng ngoại giữa, và cách chọn nguyên tử/phân tử bia. Tuy nhiên, bia nguyên tử/phân tử được sử dụng dựa trên mô hình một electron, và tính toán dựa vào giải phương trình Schrödinger phụ thuộc thời gian. Trong bài báo này, bằng lí thuyết phiếm hàm mật độ, chúng tôi mở rộng nghiên cứu tính phổ quát của tỉ số HHG chẵn-lẻ cho nguyên tử heli có hai electron. Kết quả chỉ ra rằng, hiệu ứng nhiều electron thể hiện qua tương tác Coulomb và tương tác tương quan-trao đổi đều không ảnh hưởng đến tính phổ quát của tỉ số HHG chẵn-lẻ của nguyên tử heli.

Từ khóa: tương quan; heli; HHG, chẵn-lẻ; THz; phổ quát