



## Research Article

# SEPARATING GERADE AND UNGERADE COMPONENTS OF TEMPORAL TRANSITION DIPOLE BY FLOQUET THEOREM

*Phan Thi Ngoc Loan*

*Ho Chi Minh City University of Education*

*Corresponding author: Phan Thi Ngoc Loan – Email: [loanptn@hcmue.edu.vn](mailto:loanptn@hcmue.edu.vn)*

*Received: February 10, 2020; Revised: March 19, 2020; Accepted: March 23, 2020*

## ABSTRACT

*Recently, odd-even high-order harmonic generation (HHG) emitted from asymmetric molecules has paid much attention since its application in extracting molecular structures and probing molecular dynamics. In which, the ratio of the even and odd harmonics in HHG spectra is an important quantity characterized the molecular asymmetry. This even-to-odd ratio has been explained by the gerade and ungerade components of the temporal transition dipole. Though, the separating procedure of the temporal transition dipole has not been published in the previous study. In this paper, we present the detailed procedure of separating the gerade and ungerade components of the temporal transition dipole using the Floquet theorem. Besides, we explain the correlation between the intensities of even and odd harmonics by the new approach, using the induced dipole acceleration.*

**Keywords:** HHG; odd-even; symmetry; transition dipole; dipole acceleration

## 1. Introduction

In recent decades, laser-matter interaction is an interesting topic attracting much attention of the community studying on the strong field physics and attosecond science (Ghimire, & Reis, 2019; Lewenstein, Balcou, Ivanov, L’Huillier, & Corkum, 1994; Li et al., 2017; McPherson et al., 1987). When atoms, molecules are exposed to an intense laser, one of the nonlinear effects is the emission of photons, whose frequency is many times greater than the irradiated laser’s one, and called the high-order harmonic generation (HHG) (Lewenstein et al., 1994). The HHG can be applied to extract the atomic/molecular structure (Itatani et al., 2004; Lein, Hay, Velotta, Marangos, & Knight, 2002), or probing the ultrafast dynamics in femtosecond or attosecond scale in molecules (Borot et al., 2012).

The HHGs from multi-electron atoms or molecules are popularly observed in laboratories (Itatani et al., 2004; McPherson et al., 1987). However, the theoretical simulation for the multi-electron system is difficult due to the limitation of the computing

---

**Cite this article as:** Phan Thi Ngoc Loan (2020). Separating gerade and ungerade components of temporal transition dipole by Floquet theorem. *Ho Chi Minh City University of Education Journal of Science*, 17(3), 433-444.

resources (Abu-Samha, & Madsen, 2010; Lein et al., 2002; Bin Zhang, Yuan, & Zhao, 2014). To overcome this difficulty, the approximation models such as the strong-field approximation (SFA) (Lewenstein et al., 1994; Zhou, Tong, Zhao, & Lin, 2005), quantitative rescattering model (Le, Lucchese, Morishita, & Lin, 2009), or quantum-orbit theory (Milošević, & Becker, 2002). Besides the approximate methods, another method is *ab initio* calculating the HHG from the multi-electron system by using the single-active electron (SAE) model (Abu-Samha, & Madsen, 2010). Accordingly, only one electron from the high-occupied molecular orbital (HOMO) interacts with an intense laser. Meanwhile, the remaining electrons are attached to the nuclei and called core-electron. The effect caused by the core-electron is called the dynamic core-electron polarization (DCeP).

The DCeP significantly affects the destructive minimum in the HHG spectra emitted from CO (Le, Hoang, Tran, & Le, 2018; Bin Zhang et al., 2014) or CO<sub>2</sub> (Le, Vu, Ngo, & Le, 2019) molecules. Besides, DCeP effects on the HHG intensity near the cutoff of the HHG from CO (Le, Hoang, Tran, & Le, 2018; Bin Zhang et al., 2014) và CO<sub>2</sub> (Le, Vu, Ngo, & Le, 2019). Recently, we have also indicated the influence of the DCeP on the correlation between the intensity of the even and odd harmonics in the HHG of CO and NO molecules (Le, & Phan, 2020; Phan, Le, Hoang, & Le, 2019). To interpret this phenomenon, we have calculated the gerade and ungerade components of the temporal transition dipole (Le, & Phan, 2020; Phan et al., 2019). Accordingly, while the odd harmonics are caused by the recombination of electrons into the gerade part, the even harmonics – into the ungerade part of HOMO of CO molecule at the recombination time. It is noted that the wavefunction of an asymmetric molecule, like CO, does not have a certain parity. Therefore, we have to separate the Floquet wavefunction into two components – gerade and ungerade ones based on the Floquet theory. It should be emphasized that the Floquet wavefunction is different from the time-dependent wavefunction by a phase factor. Meanwhile, the quantity is calculated by the numerical method is the wavefunction, not Floquet wavefunction. These facts lead to the difficulty in wavefunction separation. In (Phan et al., 2019), we have successfully separated the gerade and ungerade components of the Floquet wavefunction, and the corresponding temporal transition dipole of CO molecule, however, the separating procedure is not published.

Besides, in the works (Hu, Li, Liu, Li, & Xu, 2017), Hu *et al.* have claimed that when a CO molecule is subjected to a laser whose polarization vector is perpendicular to the molecular axis, the HHG component parallel to the electric vector contains only odd harmonics. On the contrary, the HHG component whose polarization perpendicular to the laser electric-vector consists of only even harmonics. The authors have explained that the pure odd and pure even HHG spectra based on the gerade and ungerade of the induced dipole acceleration. So the question is that, besides the approach of using temporal transition dipole as in (Le, & Phan, 2020; Phan et al., 2019), is it possible to use induced

dipole acceleration to explain the correlation between the intensity of odd and even harmonics in HHG?

In this paper, we present the detailed procedure for separation of the gerade and ungerade temporal transition dipole when electron recombines into the HOMO of CO molecule based on the Floquet theory. This explicit representation is meaningful in the explanation of the property of HHG spectra from asymmetric molecules. After that, we interpret the correlation between the intensity of the even and odd harmonics from CO molecules when considering and neglecting the DCeP effect by using the induced dipole acceleration. To calculate the HHG spectra, we employ the method of solving the Schrödinger equation (TDSE) in the framework of SAE approximation.

## 2. Theoretical background

In this section, we briefly present the model of CO molecule interacting with the laser, and the TDSE method to obtain the HHG spectra. Then, we recall the basis of the theory of strong-field approximation and the calculation method of the transition dipole. Finally, the Floquet theorem for the temporal-spatial periodic system is presented.

### 2.1. Molecular model and TDSE method

Hamiltonian of the laser-molecular system in the atomic unit has the following form

$$\hat{H} = \hat{H}_0(\mathbf{r}) + \hat{H}_i(\mathbf{r}, t), \quad (1)$$

where  $\hat{H}_0(\mathbf{r}) = -\frac{\nabla^2}{2} + V_{SAE}(\mathbf{r})$ , and  $V_{SAE}(\mathbf{r})$  is the molecular potential constructed by the SAE model (see details in (C.-T. Le et al., 2018; Phan et al., 2019)). The parameters are chosen so that the HOMO energy of CO ( $5\sigma$ ) reaches  $-0.51$  a.u.

The Hamiltonian characterized the laser-molecular coupling is separated into to components

$$\hat{H}_i(\mathbf{r}, t) = V_L(\mathbf{r}, t) + V_p(\mathbf{r}, t), \quad (2)$$

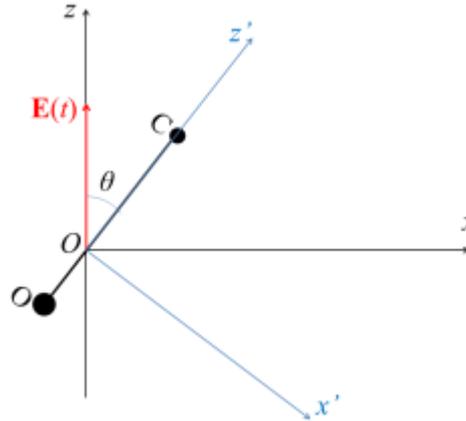
where  $V_L(\mathbf{r}, t) = \mathbf{r} \cdot \mathbf{E}(t)$  describes the interaction between the active electron and the laser electric field;  $V_p(\mathbf{r}, t) = -\frac{\mathbf{E}(t)\hat{\alpha}_c\mathbf{r}}{r^3}$  is the polarization potential considering the influence of the core-electron polarization;  $\hat{\alpha}_c$  is the polarization tensor. The tensor values are presented in (Phan et al., 2019).

The magnitude of the laser has the following form

$$E(t) = E_0 f(t) \sin \omega_0 t, \quad (3)$$

where  $E_0, \omega_0$  are the maximum amplitude and the carrier frequency of laser;  $f(t)$  is the laser envelope. In this study, we use a laser pulse with a duration of 10 optical cycles, and the laser envelope has the trapezoidal form with one-cycle turn-on, one-cycle turn-off, and eight cycles in the flat part. The laser intensity is  $1.5 \times 10^{14}$  W/cm<sup>2</sup>. The polarization vector

of the laser is aligned with the  $Oz$  axis. The CO model is present in Fig. 1. The molecular axis makes with the  $Oz$  an angle  $\theta$  – called alignment angle.



**Figure 1.** CO molecule in the molecular frame  $Ox'z'$  and laboratory frame  $Oxz$

To solve the Schrödinger equation for time-dependent Hamiltonian (1), we use the method presented in (Le et al., 2018; Phan et al., 2019). After obtaining the time-dependent wavefunction  $\psi(\mathbf{r}, t)$ , the induced moment dipole parallel to the electric field is defined as

$$D_z(t) = \langle \psi(\mathbf{r}, t) | z | \psi(\mathbf{r}, t) \rangle. \tag{4}$$

In this article, we present the results for the HHG with the parallel polarization. For perpendicular HHG, the procedure is similar (Phan et al., 2019). The HHG spectra are calculated as the square of the Fourier transform of the acceleration of the transition moment (4). For solving TDSE, we use the computational parameters as presented in (Phan et al., 2019).

### 2.2. Transition dipole

The TDSE method gives the result with high precision (Le et al., 2018, 2019; Phan et al., 2019), while the approaches using the model provide the intuitive picture to explain the physical mechanism. In which, the SFA model interprets the HHG by the three steps (Lewenstein et al., 1994; Zhou et al., 2005). First, the electron tunnels into a continuum then accelerates in the electric field; finally, when the electric field changes its directions, the electron returns to the parent ion. The HHG is emitted at the last step.

According to SFA, the HHG intensity is proportional to the square of the transition dipole from the continuum into the bound states, which characterizes the third step in the three-step model (Itatani et al., 2004). Therefore, to clarify the feature and property of HHG, the transition dipole is considered. For simplicity, the continuum wave functions are assumed as plane waves. The transition dipole has the following form

$$d_z(\omega) = \langle \psi(\mathbf{r}) | z | e^{i\mathbf{k}(\omega)\mathbf{r}} \rangle, \tag{5}$$

where  $\omega$  is the harmonic frequency;  $\mathbf{k}(\omega)$  is the wavenumber satisfied the dispersion

formula  $|\mathbf{k}(\omega)| = \sqrt{2\omega}$ . In most works (Itatani et al., 2004; Bing Zhang, Chen, Jiang, & Sun, 2013), the authors have claimed that the molecular HOMO is not deformed while interacting with the laser; therefore, the wavefunction  $\psi(\mathbf{r})$  is the initial wavefunction, i.e., when the molecule has not yet interacted with the laser.

However, to interpret the dynamic properties of a molecule, the temporal transition dipole is used (Bin Zhang et al., 2014). Its expression is written as

$$d_z(\omega, t) = \langle \psi(\mathbf{r}, t) | z | e^{i\mathbf{k}(\omega)\mathbf{r}} \rangle. \quad (6)$$

### 2.3. Floquet theorem

The Floquet theorem describes the property of the wavefunction of a temporal-spatial periodic potential. This theorem has been presented in detail in many references (Bavli & Metiu, 1993; Tal, Moiseyev, & Beswick, 1993). Here, we summarise some main equations.

Consider a system described by a Hamiltonian satisfied the periodic condition

$$\hat{H}(\mathbf{r}, t) = \hat{H}(-\mathbf{r}, t + T_0 / 2), \quad (7)$$

where  $T_0$  - an optical cycle. For this system, the time-dependent wavefunction obeys the Floquet theorem, i.e., the wavefunction is presented as a product of an exponential factor and Floquet wavefunction

$$\psi(\mathbf{r}, t) = e^{-i\varepsilon t} \varphi(\mathbf{r}, t), \quad (8)$$

where  $\varepsilon$  is the Floquet quasi-energy, and  $\varphi(\mathbf{r}, t)$  is the Floquet wavefunction satisfied the symmetry condition

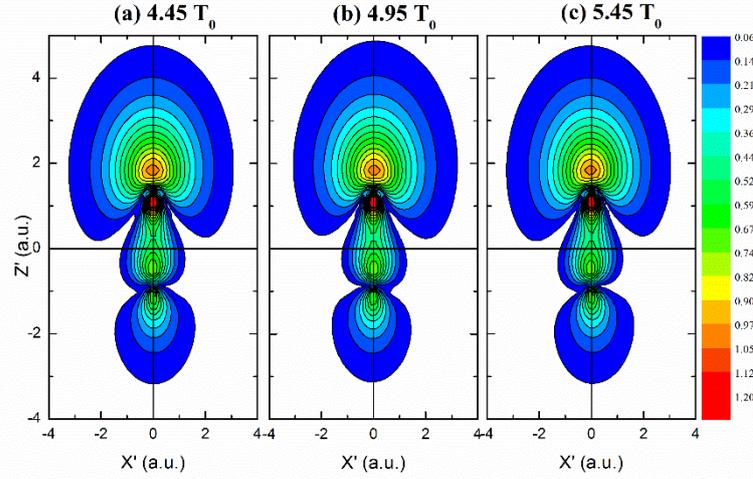
$$\varphi(\mathbf{r}, t) = \pm \varphi(-\mathbf{r}, t + T_0 / 2). \quad (9)$$

## 3. Results

In this section, first, we present the detailed procedure for separating the gerade and ungerade components of temporal transition dipole. Then, this procedure is applied to explain the correlation between the intensity of even and odd harmonics. Finally, we interpret the ratio between the intensity of even and odd harmonics (referred to the even-to-odd ratio) by the induced dipole acceleration.

### 3.1. Procedure for separating gerade and ungerade components of temporal transition dipole

Usually, to investigate the intensity correlation between even and odd harmonics, the gerade and ungerade components of transition dipole (5) are considered (Bing Zhang et al., 2013). The work (Bing Zhang et al., 2013) has shown that the recombination of the electron into the gerade wavefunction results in odd harmonic generation. On the contrary, the recombination into the ungerade HOMO leads to the emission of the even harmonics.



**Figure 2.** The HOMO of CO molecule in the molecular frame  $Ox'z'$  at the instances  $4.45T_0$  (a),  $4.95T_0$  (b), and  $5.45T_0$  (c) when neglecting the DCEP effect. The alignment angle is  $45^\circ$

However, to investigate the influence of the DCEP on the HHG intensity correlation between the even and odd orders, the temporal transition dipole (6) is needed since the DCEP distorts the HOMO during the interaction (Phan et al., 2019; Bin Zhang et al., 2013), results in changing the wavefunction parity. Therefore, we have to consider the temporal wavefunction.

For atoms or symmetric molecules, the potential  $V_{SAE}(\mathbf{r})$  is inversion symmetry, i.e., their time-dependent Hamiltonian satisfies the symmetry condition (7). As a consequence, the time-dependent wavefunction obeys the Floquet condition (8), (9) (Tal et al., 1993). However, for asymmetric molecules, such as CO, the potential is not inversion symmetric (see Fig. 2), that the Floquet wavefunction does not satisfy the symmetric condition (9), i.e., it does not possess a certain parity. However, we can theoretically separate the unsymmetric Floquet wave function into the symmetric  $\varphi^g(\mathbf{r}, t)$  and antisymmetric  $\varphi^u(\mathbf{r}, t)$  ones

$$\varphi^{g(u)}(\mathbf{r}, t) = \frac{\varphi(\mathbf{r}, t) \pm \varphi(-\mathbf{r}, t + T_0 / 2)}{2}. \quad (10)$$

The time-dependent wavefunction also can be separated into two corresponding components  $\psi^{g(u)}(\mathbf{r}, t) = e^{-i\epsilon t} \varphi^{g(u)}(\mathbf{r}, t)$ . The corresponding temporal transition dipoles

$$d_z^{g(u)}(\omega, t) = \langle \psi^{g(u)}(\mathbf{r}, t) | z | e^{i\mathbf{k}(\omega)\cdot\mathbf{r}} \rangle. \quad (11)$$

These components are responsible for generating the odd and even harmonics, respectively (Phan et al., 2019).

However, in practice, the separating of the Floquet wavefunction (10) faces difficulty since the solution from the TDSE is the time-dependent wavefunction, not Floquet

wavefunction and Floquet quasi-energy. Fortunately, looking insight the Hamiltonian (1), we realize that although it is not symmetric through the transformation  $P: \mathbf{r} \rightarrow -\mathbf{r}, t \rightarrow t + T_0 / 2$ , but it is symmetric through  $P': \mathbf{r} \rightarrow \mathbf{r}, t \rightarrow t + T_0$ . This fact can be illustrated in Fig. 2 for HOMO of CO molecule at the instances  $4.45T_0, 4.95T_0, \text{ và } 5.45T_0$ . This HOMO is not symmetric through half-cycle translation but is repeated after each optical cycle. Therefore, the Floquet wavefunction satisfies

$$\varphi(\mathbf{r}, t) = \pm \varphi(\mathbf{r}, t + T_0), \tag{12}$$

and the time-dependent wavefunction obeys

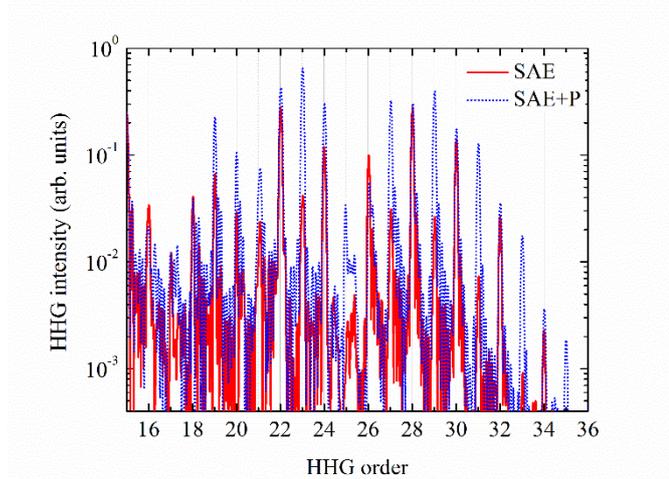
$$\psi(\mathbf{r}, t + T_0) = \pm e^{i\varepsilon T_0} \psi(\mathbf{r}, t). \tag{13}$$

By the Eq. (13) we can calculate the phase factor  $e^{i\varepsilon T_0}$  from the time-dependent wavefunction calculated by the TDSE method. After getting the phase factor, or Floquet quasi-energy, the symmetric and antisymmetric components  $\psi^{g(u)}(\mathbf{r}, t)$  of the time-dependent wavefunction is calculated as

$$\begin{aligned} \psi^{g(u)}(\mathbf{r}, t) &\equiv e^{-i\varepsilon t} \varphi^{g(u)}(\mathbf{r}, t) = \frac{e^{-i\varepsilon t} \varphi(\mathbf{r}, t) \pm e^{-i\varepsilon t} \varphi(-\mathbf{r}, t + T_0 / 2)}{2} \\ &= \frac{e^{-i\varepsilon t} \varphi(\mathbf{r}, t) \pm e^{i\varepsilon T_0 / 2} e^{-i\varepsilon(t + T_0 / 2)} \varphi(-\mathbf{r}, t + T_0 / 2)}{2} \tag{14} \\ &= \frac{\psi(\mathbf{r}, t) \pm e^{i\varepsilon T_0 / 2} \psi(-\mathbf{r}, t + T_0 / 2)}{2}. \end{aligned}$$

From these components, the grade and ungrade temporal transition dipoles are calculated by Eq. (11).

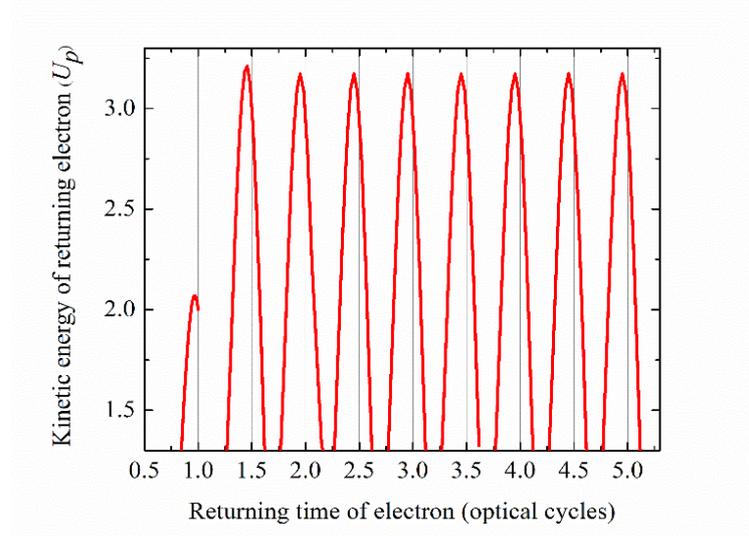
### 3.2. Application to explain the intensity correlation between even and odd harmonics



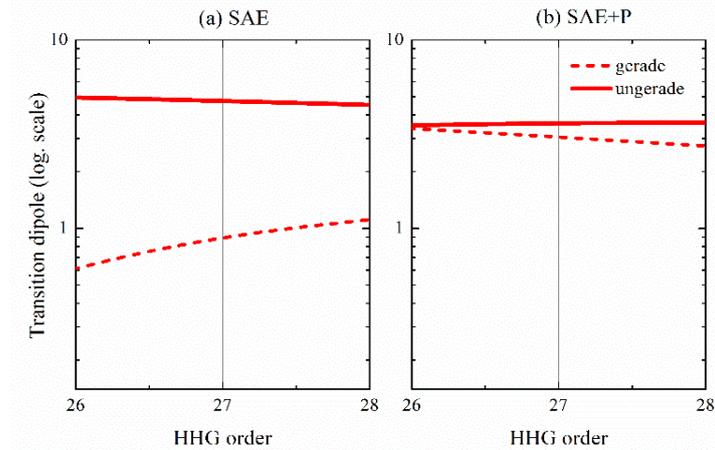
**Figure 3.** The parallel HHG emitted from CO molecule with alignment angle  $45^\circ$  when including (SAE+P) and ignoring (SAE) DCeP effect

Now we apply the above procedure to calculate the gerade and ungerade temporal transition dipole to explain the intensity correlation between even and odd harmonics of CO molecule. Figure 3 presents the component of HHG whose polarization is parallel to the molecular axis for CO molecule at alignment angle  $45^\circ$ , when considering (SAE+P) and neglecting (SAE) the DCeP effect. The results calculated by the TDSE method show that the cutoff of the spectra is 29<sup>th</sup> order, is consistent with the predicted ones by the three-step model (Lewenstein et al., 1994). Besides, the HHG spectra contain both odd and even orders. Especially, for harmonics near the cutoff, when considering the DCeP, the intensity of the even harmonics is lower than that of the odd ones. The intensities of the even harmonics for both cases – including and neglecting the DCeP, are comparable. Meanwhile, for the odd harmonics, its intensity for the case SAE is much less than that of the SAE+P case. These results have been presented in our recent study (Phan et al., 2019).

To explain the intensity correlation between the even and odd harmonics near the cutoff, we calculate the temporal transition dipole. First, we determine the recombination time of electron resulted in harmonics near cutoff. Figure 4 shows the kinetic energy of the returning electron. The results show that, for every half cycle, there is one instance that the kinetic energy reached maximum -  $3.17U_p$ , where  $U_p$  is the ponderomotive energy. The recombination instances are  $1.45T_0, 1.95T_0, 2.45T_0, 2.95T_0, \dots$



**Figure 4.** The kinetic energy of the returning electron



**Figure 5.** The transition dipole at  $4.45T_0$  of the CO molecule with alignment angle  $45^\circ$

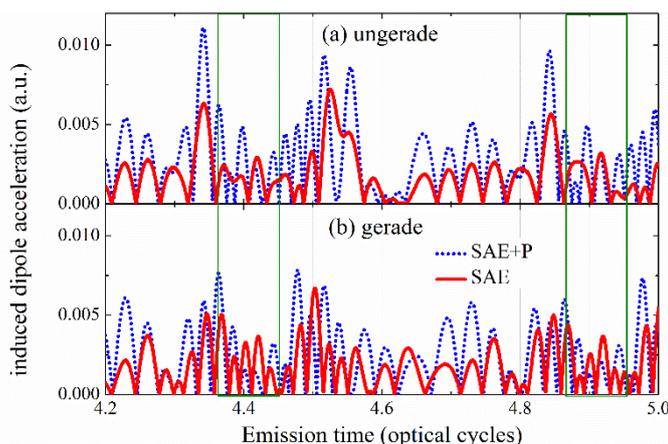
Figure 5 presents the gerade and ungerade transition dipole at the recombination time  $4.45T_0$ , corresponding to the harmonic  $27^{\text{th}}$  at the cutoff according to the three-step model. The results show that, when ignoring the DCEP effect (Fig. 5a), the ungerade transition dipole is much greater than the gerade’s one, leading to the more efficient of even harmonics compared to the odd’s one. Meanwhile, when including the DCEP (Fig. 5b), the magnitude of the two components of transition dipole is comparable, leading to the equivalence of odd and even harmonics. The correlation between the gerade and ungerade transition dipoles plays a decisive role in the intensity correlation between the odd and even harmonics in HHG spectra.

**3.3. Explanation of intensity correlation between even and odd harmonics by induced dipole acceleration**

To continue, we explain the correlation between odd and even harmonics by the approach differed from the one using in (Phan et al., 2019). Here, we use the induced dipole acceleration calculated by the second differential of induced dipole moment written by Eq.(4). Based on the nature of the Fourier transform, the odd harmonics in HHG is caused by the ungerade induced dipole acceleration through the transformation  $t \rightarrow t + T_0 / 2$ . Meanwhile, the even harmonics are raised by the gerade one. For CO molecule, the dipole acceleration does not possess a certain parity; therefore, it can be separated into

$$a^{g(u)}(t) = \frac{a(t) \pm a(t + T_0 / 2)}{2}, \tag{15}$$

where  $a^g(t)$  và  $a^u(t)$  are the gerade and ungerade components.



**Figure 6.** The absolute value of the gerade and ungerade induced dipole acceleration for CO molecule with alignment angle  $45^\circ$  in two cases – ignoring (SAE) and including (SAE+) DCeP

The results of the absolute values of the gerade and ungerade dipole acceleration are presented in Fig. 6 for two cases – ignoring and including the DCeP effect. Since the dipole acceleration is periodic every optical cycle, we present in Fig. 6 only one-cycle time interval, from  $4T_0$  to  $5T_0$ . It should be noted that we are interested in the harmonics near the cutoff; therefore, we restrict the time interval inside the two green rectangles, i.e., from  $4.35T_0$  to  $4.45T_0$ ; and from  $4.86T_0$  to  $4.95T_0$ . These time intervals correspond to the short and long trajectories of the electron that converts HHG photon with energy from  $I_p + 2.5U_p$  to  $I_p + 3.17U_p$  at the recombination time (see Fig. 4), i.e., near cutoff. Figure 6a shows that in these time intervals, the value of the ungerade dipole acceleration– caused odd harmonics, in the case of neglecting DCeP is smaller than when including it. Therefore, the intensity of the odd harmonics when ignoring DCeP is less than that in the case of including it. Meanwhile, Fig. 6b shows that, on average, the absolute values of gerade dipole acceleration in two cases – ignoring and including DCeP are comparable. Thereby, the intensity of the even and odd harmonics are similar to each other. In short, by separating the gerade and ungerade components of the induced dipole acceleration, we successfully explain the intensity correlation between the even and odd harmonics in the HHG spectra of CO molecule when ignoring and including the DCeP effect.

### 3. Conclusions

In this article, we have provided a detailed procedure for separating the gerade and ungerade temporal transition dipole using the Floquet theorem. This explicit procedure will be the basis for a deeper investigation of the odd-even HHG from the asymmetric molecule. Then, we have applied the correlation between the magnitude of the gerade and ungerade transition dipole at the recombination time to explain the intensity correlation between the odd and even harmonics in HHG from CO molecule when ignoring and including the DCeP effect. Finally, we have successfully interpreted the even-odd intensity correlation by the parity of induced dipole acceleration.

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

❖ **Acknowledgement:** This work is supported by the Program of Fundamental Research of Ministry of Education and Training (Vietnam) under grant No. B2019-SPS-06. The calculation is performed by the high-performance cluster at Ho Chi Minh City University of Education, Vietnam. The author thanks Dr. Cam-Tu Le, for supporting the TDSE source code.

## REFERENCES

- Abu-Samha, M., & Madsen, L. B. (2010). Single-active-electron potentials for molecules in intense laser fields. *Physical Review A*, 81(3), 033416.
- Bavli, R., & Metiu, H. (1993). Properties of an electron in a quantum double well driven by a strong laser: Localization, low-frequency, and even-harmonic generation. *Physical Review A*, 47(4), 3299-3310.
- Borot, A., Malvache, A., Chen, X., Jullien, A., Geindre, J., Audebert, P.,... Lopez-Martens, R. (2012). Attosecond control of collective electron motion in plasmas. *Nature Physics*, 8(4), 416-421.
- Ghimire, S., & Reis, D. A. (2019). High-harmonic generation from solids. *Nature Physics*, 15(1), 10-16.
- Hu, H., Li, N., Liu, P., Li, R., & Xu, Z. (2017). Pure even Harmonic Generation from Oriented CO in Linearly Polarized Laser Fields. *Physical Review Letters*, 119(17), 173201.
- Itatani, J., Levesque, J., Zeidler, D., Niikura, H., Pépin, H., Kieffer, J. C.,... Villeneuve, D. M. (2004). Tomographic imaging of molecular orbitals. *Nature*, 432(7019), 867.
- Le, A.-T., Lucchese, R. R., Morishita, T., & Lin, C. D. (2009). Quantitative rescattering theory of high-order harmonic generation from molecules. *Physical Review A*, 80, 013401.
- Le, C.-T., Hoang, V.-H., Tran, L.-P., & Le, V.-H. (2018). Effect of the dynamic core-electron polarization of CO molecules on high-order harmonic generation. *Physical Review A*, 97(4), 043405.
- Le, C.-T., & Phan, N.-L. (2020). Odd-even harmonic generation from oriented CO and NO molecules within strong-field approximation. *Journal of Physics: Conference Series*, accepted.
- Le, C.-T., Vu, D.-D., Ngo, C., & Le, V.-H. (2019). Influence of dynamic core-electron polarization on the structural minimum in high-order harmonics of CO 2 molecules. *Physical Review A*, 100(5), 053418.
- Lein, M., Hay, N., Velotta, R., Marangos, J. P., & Knight, P. L. (2002). Interference effects in high-order harmonic generation with molecules. *Physical Review A - Atomic, Molecular, and Optical Physics*, 66(2), 023805.
- Lewenstein, M., Balcou, P., Ivanov, M. Y., L'Huillier, A., & Corkum, P. B. (1994). Theory of high-harmonic generation by low-frequency laser fields. *Physical Review A*, 49(3), 2117.
- Li, J., Ren, X., Yin, Y., Zhao, K., Chew, A., Cheng, Y.,... Chang, Z. (2017). 53-attosecond X-ray pulses reach the carbon K-edge. *Nature Communications*, 8(1), 186.

- McPherson, A., Gibson, G., Jara, H., Johann, U., Luk, T. S., McIntyre, I. A.,... Rhodes, C. K. (1987). Studies of multiphoton production of vacuum-ultraviolet radiation in the rare gases. *Journal of the Optical Society of America B*, 4(4), 595.
- Milošević, D. B., & Becker, W. (2002). Role of long quantum orbits in high-order harmonic generation. *Physical Review A*, 66(6), 063417.
- Phan, N. L., Le, C. T., Hoang, V. H., & Le, V. H. (2019). Odd-even harmonic generation from oriented CO molecules in linearly polarized laser fields and the influence of the dynamic core-electron polarization. *Physical Chemistry Chemical Physics*, 21(43), 24177-24186.
- Tal, N. Ben, Moiseyev, N., & Beswickf, A. (1993). The effect of hamiltonian symmetry on generation of odd and even harmonics. *Journal of Physics B*, 26(18), 3017-3024.
- Zhang, Bin, Yuan, J., & Zhao, Z. (2013). Dynamic core polarization in strong-field ionization of CO molecules. *Physical Review Letters*, 111(16), 163001.
- Zhang, Bin, Yuan, J., & Zhao, Z. (2014). Dynamic orbitals in high-order harmonic generation from CO molecules. *Physical Review A*, 90(3), 035402.
- Zhang, Bing, Chen, Y., Jiang, X., & Sun, X. (2013). Identifying the interference effect in different harmonic-emission channels from oriented asymmetric molecules. *Physical Review A*, 88(5), 053428.
- Zhou, X., Tong, X. M., Zhao, Z. X., & Lin, C. D. (2005). Alignment dependence of high-order harmonic generation from N<sub>2</sub> and O<sub>2</sub> molecules in intense laser fields. *Physical Review A*, 72(3), 033412.

---

## TÁCH PHẦN CHẴN VÀ LẼ CỦA LƯỠNG CỰC DỊCH CHUYỂN TỨC THỜI BẰNG LÝ THUYẾT FLOQUET

*Phan Thị Ngọc Loan*

*Trường Đại học Sư phạm Thành phố Hồ Chí Minh*

*Tác giả liên hệ: Phan Thị Ngọc Loan – Email: loanptn@hcmue.edu.vn*

*Ngày nhận bài: 10-02-2020; ngày nhận bài sửa: 19-3-2020; ngày duyệt đăng: 23-3-2020*

### TÓM TẮT

Gần đây, phát xạ sóng điều hòa bậc cao (HHG) có chứa cả bậc chẵn và bậc lẻ, phát ra từ phân tử bất đối xứng thu hút được nhiều sự quan tâm bởi các ứng dụng trong thu nhận thông tin cấu trúc và thăm dò động lực học phân tử. Trong đó, tỉ lệ của cường độ bậc chẵn và bậc lẻ của phổ HHG là đại lượng quan trọng thể hiện tính chất bất đối xứng của phân tử và đã được giải thích bằng hai thành phần chẵn và lẻ của lưỡng cực dịch chuyển tức thời. Mặc dù vậy, quy trình tách của lưỡng cực dịch chuyển tức thời chưa được mô tả trong các nghiên cứu trước đây. Trong bài báo này, chúng tôi sẽ trình bày chi tiết quy trình tách phần chẵn và phần lẻ của lưỡng cực dịch chuyển tức thời bằng lý thuyết Floquet. Ngoài ra, chúng tôi sẽ giải thích sự tương quan của cường độ bậc chẵn và bậc lẻ của phổ HHG bằng cách tiếp cận mới, sử dụng đại lượng gia tốc lưỡng cực cảm ứng.

**Từ khóa:** HHG; chẵn-lẻ; đối xứng; lưỡng cực dịch chuyển; gia tốc lưỡng cực