PROPERTIES OF HIGH-ORDER HARMONIC GENERATION SIGNALS FROM SWITCHED-OFF AlIGNED MOLECULES

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Abstract

A quantum theory of intense-field pump-probe experiments proposed recently, which successfully described the high-order harmonic generation (HHG) signals of adiabatic and non-adiabatic aligned molecules, is applied here to investigate the HHG signals from molecules aligned by using switched-off schema. The results are presented in the two externally available control parameters: the delay time, $t_d$, between the pump and the probe pulse, and the relative angle, $\alpha$, between their polarizations. To provide more succinct and clearer information of the beats involved in the signal, the signal is also presented in the frequency domain. The results show that the HHG signals of switched-off aligned molecules mimic those of the adiabatic and non-adiabatic aligned molecules, and therefore, it can be used to determine some molecular properties, as powerful as non-adiabatic signal. In addition, the HHG signals of switched-off aligned molecules also have benefit, which is it gives a greater modulation depth.

Keywords: alignment, Fourier spectrum, HHG signal, relative polarization, switched-off

1. Introduction

In recent years, there have been much interest and progress in understanding the high-order harmonic generation (HHG) of aligned molecules, due mainly to its potential applications as a source of coherent ultraviolet light and/or for generation of ultra-short attosecond laser pulses [1], and its prospect as a tool for molecular tomographic [2,3]. The HHG signal of aligned molecules is generated in a typical intense-field pump-probe experiment. A first laser beam (known as pump pulse) is subject to molecular gas, creating molecular wave packets governing the alignment angle of the molecules. The second laser beam (known as probe-pulse) is subject to the gas jet, delayed by a finite amount delay time $t_d$, with respect to the pump-pulse. The high harmonic signal produced by the probe pulse is recorded by the detector system for each selected values of $t_d$. In addition, a polarizer can be inserted to rotate the angle of polarization of the probe pulse with respect to the polarization direction of the pump pulse at any desired angle $\alpha$. Note that both $t_d$ and $\alpha$ provide controllable parameters on the high harmonic emission process from the outside.

The HHG signals are generated when electron, due to its interaction with the intense laser pulse with frequency $\omega_p$, absorbs $n$ photon, accelerates, and recombines ith its parents ion by emitting a single photon with frequency $\Omega = n\omega_p$ where $n$ is odd number known as harmonic order [4]. Clearly, the HHG yield depends on the electron abundance, and therefore depends on the symmetry of the molecules. As molecule s are non symmetrical objects, the HHG signal can be controlled by governing molecular rotation, either by choosing the $t_d$ or $\alpha$ parameters.

Depending on the duration of the pump pulse, there are three kinds of alignments, known as adiabatic alignment, non-adiabatic alignment, and switched-off alignment [5], that give a different dynamic alignment and therefore different dynamic HHG signal. In the first case, a laser field is slowly turned on and turned off such that the molecules can adiabatically adjust to the changing potential and rotate. The criterion ‘slowly’ can be satisfied by using a pulse longer than the rotational period. Adiabatic schema can reach high alignment degree but it is lost once the pulse is turned off. The second schema is the alignment by using a ‘short’ pulse that is rapidly turned on and turned off. This alignment shows recurrence even after the pulse was turned off. Unfortunately, this method can not reach an alignment degree as high as in adiabatic alignment. The third case is a ‘mixture’ between the long pulse and the short pulse...
method: an applied pulse is slowly turned on but rapidly turned off [6]. This is similar to a long pulse that is suddenly switched off at its peak. The last case takes all the benefits of the two previous cases and provides a dynamic alignment with high alignment degree. Despite its advantages, there is no interest for understanding it.

In the previous paper [7], a fully quantum theory of intense-field non-adiabatic alignment and high harmonic generation from linear molecules has been derived and used to analyze the observed dynamical HHG signals for N₂ and O₂ molecules, which clearly explained the salient experimental results of HHG signals from both adiabatic [8-10] and non-adiabatic alignment [11,12]. The theory also explicitly discussed the effect of the relative polarization angle α and predicted the existence of the ‘magic angle’ [16], that later has been confirmed experimentally [17,18]. In this paper, the theory is used to analyze the HHG signal from switched-off aligned molecules, and to directly compare the results with ones obtained by using non adiabatic schema.

2. Theoretical Method

According to intense-field theory of HHG [7],which is derived based on the IMST [19], the HHG signals of aligned N₂ is given

\[ S^{(n)}(t_d; \alpha) = C_f^{(n)} + c_{\gamma}^{(n)} \left\langle \langle \cos^2 \Theta \rangle \right\rangle (t_d) + \]

\[ + c_{\delta}^{(n)} \left\langle \langle \cos^2 2\Theta \rangle \right\rangle (t_d) + \]

\[ + c_{\epsilon}^{(n)} \left\langle \langle \cos^4 \Theta \rangle \right\rangle (t_d) + \ldots \ldots \]  

(1)

where \( C = (2\pi)^2 (\hbar / c)^3 \). Above, \( c_{i}^{(n)} \) is the coefficient for the \( i \)th term of \( n \)th harmonic order that depends on both the pump and probe pulses parameters. \( \left\langle \langle f(\Theta) \rangle \right\rangle (t_d) = \sum_{J_oM_0} \rho(J_o) \left\langle \Phi(t_d, \Theta) \right| f(\Theta) \left| \Phi(t_d, \Theta) \right\rangle \) is the quantum measurement of dynamical alignment of a rotating molecule, which is the expectation value of the \( f(\Theta) \) with \( \Theta \) is the angle between the molecular axis and the probe polarization direction; the double angular brackets stand for the expectation value with respect to the wavepacket states (inner brackets) and the statistical average with respect to the Boltzmann distribution (outer brackets) of the initially occupied rotational states. The explicit form of \( f(\Theta) \) depends on the molecular symmetry.

\[ \left| \Phi(t_d, \Theta) \right\rangle = \sum_{JM} C_{JM}^{(0)} (t) \left| JM \right\rangle e^{iEMt} \]  

is the rotational wave packets obtained by solving time dependent Schrödinger equation

\[ i \frac{\partial}{\partial t} \left| \Phi_{JM} (t) \right\rangle = \left( H_N + V_{N-L} (t) \right) \left| \Phi_{JM} (t) \right\rangle \]  

(2)

with initial state \( \left\langle J_0 M_0 \right| \) [7]. Above, \( V_{N-L} (t) \) is the interaction due to the pump pulse \( L_1 \) with the nuclear motion, at a time \( t \). In practice, the fundamental set of solutions \( \left\langle J_0 M_0 \right| \) is obtained by numerical integration, using the well-known Runge-Kutta method [20].

In Eq. (1), \( \left\langle \langle f(\Theta) \rangle \right\rangle \) is the expectation value of a function \( f(\Theta) \) given in the probe frame, but evaluated with respect to the rotational wavepackets defined in the pump frame. Here \( \Theta = \Theta(0, \alpha) \), where \( \Theta \) is the angle between molecular axis and pump polarization, whereas \( \alpha \) is the angle between two polarizations. Before evaluating \( \left\langle \langle f(\Theta) \rangle \right\rangle \), it is convenient, therefore, to transform \( f(\Theta) \) from the variables \( (\Theta, \alpha') \) to the angles \( (\theta, \alpha) \) in the pump-frame (i.e. with the \( z \) along the pump polarization). This can be done by the simple transformation

\[ \cos \theta' = \cos \theta \cos \alpha + \sin \theta \sin \alpha \cos \varphi, \]  

(3)

where \( \varphi \) is the angle between the plane containing the molecular axis and the pump polarization and the plane containing the pump and the probe polarization directions. Thus, the term \( \left\langle \langle \cos^2 \Theta \rangle \right\rangle \) in Eq. (1) reads:

\[ \left\langle \langle \cos^2 \Theta \rangle \right\rangle = \left[ \left( \cos^2 \varphi \right) + \frac{1}{2} \sin^2 \alpha \right] + \frac{1}{2} \sin^2 \alpha \left( \sin^2 2\Theta e^{i2\varphi} + cc \right) \]  

(4)

where \( cc \) stands for complex conjugate. Above, \( \sin \theta \cos \theta e^{i2\varphi} \) couples the \( J \) states with \( \Delta J = 0, \pm 2 \) and \( \Delta M = \pm 1 \), whereas \( \sin^2 \theta e^{i2\varphi} \) couples the \( J \) states with \( \Delta J = 0, \pm 2 \) and \( \Delta M = \pm 2 \). For the linearly polarized pump pulse of the present interest, the interaction Hamiltonian is proportional to \( \cos^2 \theta \), which is independent of \( M \) in the space fixed pump-frame. Thus the \( M \)-quantum number of the rotational wave-packet remains constant, or \( M'=M_0 \) throughout the evolution. Hence, the expectation values of \( \sin \theta \cos \theta e^{i2\varphi} \) and \( \sin^2 \theta e^{i2\varphi} \) vanish and Eq. (4) reads
\[ \langle \cos^2 \theta \rangle = \frac{1}{2} (\beta \cos^2 \alpha - 1) \langle \cos^2 \theta \rangle + \frac{1}{2} \sin^2 \alpha \]  

(5)

In a similar way, it is easy to obtain the expectation value for the higher order moments

\[ \langle \cos^2 \theta \rangle^2 = \frac{1}{4} (\beta \cos^2 \alpha - 1)^2 \langle \cos^2 \theta \rangle^2 + \frac{1}{4} \sin^4 \alpha \]

\[ + \frac{1}{2} (3 \cos^2 \alpha - 1) \sin^2 \alpha \langle \cos^2 \theta \rangle \]  

(6)

and

\[ \langle \cos^4 \theta \rangle = \frac{1}{8} (35 \cos^4 \alpha - 30 \cos^2 \alpha - 3 \langle \cos^4 \theta \rangle)

\[ + \frac{3}{8} (10 \cos^4 \alpha + 12 \cos^2 \alpha - 2 \langle \cos^2 \theta \rangle) \]

\[ + \frac{3}{8} \sin^4 \alpha \]  

(7)

The method of calculating the expectation values can be found in references [5, 21, 22].

3. Results and Discussion

Signals in the time domain. Now, the formula (Eq. 1) is applied to analyze the HHG signals from switched-off aligned diatomic molecules \( N_2 \). To do this, a long pulse satisfying \( \frac{B_{\text{long pulse}}}{\hbar} > \tau \) [23], with \( B \) is rotational periods of the molecules, is used. The quantity \( \frac{\pi h}{B} \) is known as the rotational period. For \( N_2 \) with \( B = 1.98958 \text{ cm}^{-1} \) [24], we have \( \frac{\pi h}{B} = 2.65747 \text{ ps} \). In this calculation, a pump pulse of intensity \( I_{\text{pump}} = 1.8 \times 10^{14} \text{ W/cm}^2 \), turn-on duration of \( \tau_{\text{on}} = 2.65747 \text{ ps} \) and turn-off duration \( \tau_{\text{off}} = 40 \text{ fs} \), is first subject to an ensemble of \( N_2 \) to set it into free rotation. The HHG signals were detected by monitoring the emission due to a second femtosecond probe pulse of intensity \( I_{\text{probe}} = 1.7 \times 10^{14} \text{ W/cm}^2 \), the central wavelength \( \lambda = 800 \text{ nm} \), and pulse duration \( \tau = 40 \text{ fs} \), that was delayed with respect to the first by successively increasing the time intervals, \( t_d \), in the picosecond domain, between them.

Fig. 1 (panel a), shows the calculated HHG signals as a function of \( t_d \) for \( N_2 \), obtained for the 19th order harmonic, with the effective ensemble temperature was taken to be \( T = 200 \text{ K} \). It can be seen from the figure that the calculated data for \( N_2 \) show the ‘revival’ phenomenon with a full revival period \( T_{\text{rev}} = 8.4 \text{ ps} \) (which is consistent with the rotational constant of \( N_2 \)) as well as a half and a fourth fractional-revival. As a comparison, Fig. 1 (panel b) shows the calculated ‘degree of alignment’, \( \langle \cos^2 \theta \rangle \), obtained by the similar parameters.

To understand the properties of the HHG signal of \( N_2 \), one can use Eq. (1). The first term gives a constant background. The second term \( \langle \cos^2 \theta \rangle \) is the dominant dynamic term and makes the signal to mimic its ‘degree of alignment’, as shown in Fig. 1. The third term \( \langle \cos^2 \theta \rangle^2 \) gives unequal maxima and minima, i.e. the difference between the maximum signal and the average signal is greater than the difference between the average signal and the minimum signal.

In Fig. 2, the HHG signal from switched-off aligned molecules (panel a) is directly compared with the calculated HHG signal obtained by using non-adiabatic schema (panel b), with the similar parameters (except that \( \tau_{\text{off}} = \tau_{\text{on}} = 40 \text{ fs} \) for non-adiabatic alignment). As shown in the figures, both signals still recur, even after the pulse was turned off. The signals also have same revival period \( T_{\text{rev}} \). As \( T_{\text{rev}} \) depends on the rotational periods of the molecules [7], the results enable us to predict the unknown molecule from its HHG signal. However, the switched-off schema has advantage that it produces a stronger top signal and a weaker anti-top signal, and therefore gives us a greater modulation depth. This benefit is valuable for producing a stronger attosecond signal.

For both signals, the modulation depth at quarter-revivals (\( B \) and \( D \) in panel (a), and \( B' \) and \( D' \) in panel (b)) is smaller than those at half and full revivals (\( A \) and \( C \) in panel (a), and \( A' \) and \( C' \) in panel (b)). It is due to the properties of molecular wave function of even and odd \( J \), which are in phase at half revivals and in opposite phase at quarter-revivals. For \( N_2 \), both \( J \)s are
are present with ratio $J_{\text{even}}:J_{\text{odd}} = 2:1$. The amplitude at quarter-revival arises from the difference of even and odd $J$ contributions. In contrast, the amplitude at the half-revival is the sum of both $J$, and therefore is always three times greater than those at quarter revivals [7].

Despite the similarities, it is worthwhile to remark the different characters of the dynamic HHG signal from the turn-off schema, as follow; (i) Comparing to the non-adiabatic case, the switched-off schema has a benefit that it gives a greater top signal, a smaller anti-top signal, and as a consequence a greater modulation depth. (ii) In switched-off schema, the non-adiabatic changing starts when the HHG signal reaches its peak, and therefore the time-dependent signal starts with revival $A$. In the non-adiabatic schema, the changing starts when the signal at its average value, and therefore it starts with revival $A'$. It can be seen from the Fig. 2, that revival $A$ (in panel (a)) has similar shape with revival $D'$ (in panel (b)). It means that the switched-off HHG signal comes $90^\circ$ earlier than the non-adiabatic signal. The similar behaviors have been observed for switched-off aligned CO$_2$, observed by using optical Kerr effect's signal [25].

**Signals in the frequency domain.** To further compare the results with non-adiabatic case, the calculated dynamic signals are then Fourier transformed to get their spectra in the frequency domain. The results for the 19th harmonic signal for N$_2$ are shown in Fig. 3. It can be seen that the spectrum exhibits two prominent series I: ($6,14,22,30,\ldots$) $Bc$ and II: ($10,18,26,34,\ldots$) $Bc$, which are also present in the non-adiabatic spectrum [13]. They can be easily understood to arise from the F.T. of the $\langle \cos^2 \theta \rangle$ term in Eq. (1) which vanishes unless $\Delta J = 0,\pm 2$; this produces a frequency $\omega_0 = 0$ and a sequence of lines of frequency $\omega_1$ yields $(E_{J+2} - E_J)/2\pi = (4J + 6)Bc$, and gives the series I and II, for the even and the odd $J$ levels, respectively. The relative prominence of the series I over the series II seen in Fig. 3 could be understood as the 2:1 ratio of the $J$ even over $J$ odd levels, a well-known consequence of the nuclear spin statistics of N$_2$ (e.g. [26,27]). Please also note that the peak of intensity of Fourier spectrum occurs at $J_{\text{max}}=10$, whereas with the same pulse parameter (except that $\tau_{\text{off}}=\tau_{\text{on}}=40$ fs for non-adiabatic alignment), the non-adiabatic spectrum has $J_{\text{max}}=8$. This can be understood as due to the longer interaction between the molecular and pump pulse in switched-off schema, and therefore increases the mean molecular energy, as indicated by a greater $J_{\text{max}}$.

The weakly resolved series III: ($20,28,36,\ldots$) $Bc$ and series IV: ($4,8,12,16,\ldots$) $Bc$ in Fig. 3 are the unexpected series that could not be produced by the F.T. of the leading term $\langle \cos^2 \theta \rangle(t_d)$. To interpret their origin, it is reasonable to consider the two higher order terms in the signal for N$_2$, in Eq. (1), involving $\langle \cos^4 \theta \rangle(t_d)$ and $\langle \cos^2 \theta \rangle(t_d)$. Due to the squaring, the expected beat frequencies from $\langle \cos^2 \theta \rangle(t_d)$ does not only include the frequencies $\omega_0$ and $\omega_1$, but also their sum and difference of frequencies. The sum frequency $(\omega_0 + \omega_1)$ yields the $[4(J+J') + 12]Bc$ beats, whereas the difference $(\omega_0 - \omega_1)$ produces the beats $4(J-J')Bc > 0$. For integer $J$ and $J'$ they yield the series IV: ($4,8,12,16,\ldots$)$Bc$. The next term...
\[ \langle \cos^4 \theta \rangle (t_d) \] vanishes, unless \( \Delta J = 0, \pm 2, \pm 4 \), produces not only beats \( (E_{J+2} - E_J)/2\pi = (4J + 6)Bc \) but also \( (E_{J-2} - E_J)/2\pi = (8J + 20)Bc \) that generates the series III \( (20, 28, 36, \ldots) \) \( Bc \). Note that series III is identical, and overlapping, with the series IV: \( (4, 8, 12, 16, \ldots) \) \( Bc \) and adds to its signal strength. The existence of series III and IV unambiguously shows that the dynamic signal of \( N_2 \) can not be fully described in term of \( \langle \cos^2 \theta \rangle (t_d) \) only.

It is also important to point out that the relative strengths of the lines in a calculated spectrum were found to depend sensitively on the assumed molecular temperature, which is known to be difficult to determine experimentally. This observed sensitivity suggests a useful means to estimate the temperature of the molecular ensemble of interest in the experiment, by requiring that the strongest rotational line in the Fourier spectrum of the dynamic HHG signal should correspond to the most highly occupied rotational level in the thermally distributed initial of rotational levels. Hence, the temperature of the initial Boltzmann distribution may be found by adjusting the temperature to make the level at the peak of the Boltzmann distribution to match with the highest line of the Fourier spectrum of the HHG signal observed (see, for example [3, 15]).

Interplay of polarization geometry \( \alpha \) and delay time \( t_d \). So far the applications of the theory are limited to the HHG signal for parallel geometry of the pump and probe polarizations. Now, it is the to consider the more general case when probe polarization is rotated by a given angle \( \alpha \). Fig. 4 shows the computational results of the HHG signals of \( N_2 \) as a function of \( t_d \), at various \( \alpha \). We note that the signal for \( \alpha = 90^\circ \) changes its phase by \( \pi \) with respect to the signal for \( \alpha = 0^\circ \), a phenomenon that is also observed in non-adiabatic case [17]. In contrast, the signal for \( \alpha = 45^\circ \) is seen to remain rather flat with change of \( \alpha \).

To see the essential \( \alpha \)-dependence of HHG signal of \( N_2 \), one can consider the leading term of Eq. (1) which is given by

\[
S^{(\alpha)} (t_d; \alpha) = C \left[ e^{(\alpha)} + \frac{e^{(\alpha)}}{2} \sin^2 \alpha \right. \\
+ \left. (3 \cos^2 \alpha - 1) \langle \cos^2 \theta \rangle \right] + ...
\]

(8)

Thus, the HHG signal mimics \( \langle \cos^2 \theta \rangle (t_d) \) for the parallel polarizations and mimics \( 1 - \langle \cos^2 \theta \rangle (t_d) \) for the perpendicular polarizations, which are clearly of opposite phase as a function of \( t_d \). Eq. (8) also implies that the modulation depth for \( \alpha = 90^\circ \) is smaller than the one for \( \alpha = 0^\circ \), a fact that could not be accounted for by a planar model (e.g. [11]). Eq. (1) also implies that the extrema of the signal would occur for \( \sin \alpha \cos \alpha = 0 \), which predicts that the maximum would occur at \( \alpha = 0^\circ \) and the minimum at \( \alpha = 90^\circ \); as shown in Fig. 5. Eq. (1) also predicts that there is a ‘magic’ angle \( \alpha_c \) given by \( 3 \cos^2 \alpha_c - 1 = 0 \) i.e. \( \alpha_c = \tan^{-1} \sqrt{2} \approx 54.7^\circ \), where the time dependent signals become the same for all delay \( t_d \) times. This geometry therefore can be used to generate a steady state HHG signal from \( N_2 \). The magic angle at \( \alpha = 54.7^\circ \) also appears in non-adiabatic case [7], and, in fact, it is a generic signature for the \( \sigma_g \) symmetry of the active molecular orbital. Its presence in the data therefore can be helpful to identify the symmetry of the molecular orbital involved.

4. Conclusion

To conclude, the intense-field theory of HHG signal of free rotating molecules is applied to analyze the HHG signal of switched-off aligned \( N_2 \), and to directly compare the results with ones obtained by using non-adiabatic schema. As mentioned above, both signals have similarities, that (i) their dynamic HHG signals
have similar revival periods, (ii) their Fourier spectrum exhibit the similar frequency series, and (iii) their $\alpha$-dependent signals cross at the same angle $\alpha_c = 54.7^\circ$. It means that the HHG signal of switched-off aligned molecules can be used to determine molecular type, orbital symmetry, and nuclear statistics of unknown molecule. It also can be used to predict the initial temperature of the gas jet.

In spite of some similarities, there are three different characters of the HHG signal from the switched-off schema. First, comparing to the non-adiabatic case, the switched-off schema has a benefit that it gives a stronger top signal, a weaker anti-top signal, and as a consequence a greater modulation depth. Second, the dynamic HHG signal from switched-off aligned molecules comes $90^\circ$ earlier than that of non-adiabatic schema. Third, the peak of intensity of Fourier spectrum occurs at a greater $J_{\text{max}}$. The first difference is an advantageous factor for producing attosecond pulse.

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