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Research article

On the cutoff law of laser induced high harmonic spectra

Dong-Sheng Guo[1,2,*], **Chao Yu**[1], **Jingtao Zhang**[3], **Ju Gao**[4], **Zhi-Wei Sun**[5], **Zhenrong Sun**[1,†]

[1] *State Key Laboratory of Precision Spectroscopy, Department of Physics, East China Normal University, Shanghai 200062, China*
[2] *School of Physics, Peking University, Beijing 100871, China*
[3] *State Key Laboratory of High-field Laser Physics, Shanghai Institute of Optical and Fine Mechanics, Chinese Academy of Sciences, Shanghai 201800, China*
[4] *Jingpin Opto-Electronic Co., Jiangsu FOHO Science Park, Fenhu Town, Wujiang 215211, China*
[5] *Key Laboratory of Microgravity, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China*

Corresponding authors. E-mail: [*] *dsguophd@163.com;* [†] *zrsun@phy.ecnu.edu.cn*

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The currently well accepted cutoff law for laser induced high harmonic spectra predicts the cutoff energy as a linear combination of two interaction energies, the ponderomotive energy U_p and the atomic biding energy I_p, with coefficients 3.17 and 1.32, respectively. Even though, this law has been there for twenty years or so, the background information for these two constants, such as how they relate to fundamental physics and mathematics constants, is still unknown. This simple fact, keeps this cutoff law remaining as an empirical one. Based on the cutoff property of Bessel functions and the Einstein photoelectric law in the multiphoton case, we show these two coefficients are algebraic constants, $9-4\sqrt{2}\approx 3.34$ and $2\sqrt{2}-1\approx 1.83$, respectively. A recent spectra calculation and an experimental measurement support the new cutoff law.

Keywords high harmonic generation, cutoff law, strong laser physics, nonperturbative quantum electrodynamics, Bessel functions, Einstein photoelectric effect.

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1 Introduction

High harmonic generation (HHG) is one of the most important phenomena in strong laser physics. Holding great promises on new types of stimulated emission of short wavelengths, it has attracted many experimental and theoretical attentions. Spectra of high harmonics show common features such as plateau and cutoff frequency. To describe the width of the plateau of harmonic energy spectra and the frequency or the energy of the highest valuable harmonic, a cutoff law $q_c\hbar\omega = 3U_p + I_p$, as an empirical one, was initially suggested by Krause *et al.* [1], where ω is the incident laser frequency, q_c the cutoff order of high harmonics, U_p the ponderomotive energy, and I_p the ionization potential energy. Since then, many discussions have been devoted to the cutoff law. A commonly accepted version of the cutoff law is $q_c\hbar\omega = 3.17U_p + I_p$ [2], which was derived as a three-step process: a semiclassical ionization, a classical trajectory motion, and an electron recombination process. There are also some improved versions of the cutoff law, such as $q_c\hbar\omega = 3.17U_p + 1.32I_p$ [3].

Even though this law is well accepted, it still remains as an empirical law from the point of physics. The reason is as follows. In this law, there are two distinct physical constants, 3.17 and 1.32, as the coefficients of the ponderomotive energy U_p and the atomic binding energy I_p, respectively. The background information about these two physical constants is unclear. As long as these two constants remain unclear, the empirical nature of the cutoff law also remains. When these two constants were given, some questions naturally arose. Such as, **Q.1.** Are they fundamental physics constants independent from other fundamental physics constants? **A.1.** No, they cannot. Because HHG is of the electric-magnetic interaction, the relevant fundamental physics constants can only be few, such as the Planck constant $\hbar$, the Bohr radius a_0, the fine structure constant α, the speed of light c, the rest mass of electron m_e, and the electron charge e. These fundamental ones rule out the possibility for other physics constants to be independent. For example, the electron classical radius $r_0 = a_0\alpha^2$ is not an independent one. **Q.2.** If the two coefficients are not fundamental physics constants, how do they relate to the fundamental physics constants, or do not relate at all? **Q.3.** Are they mathematical constants? The makers of the original cutoff law did not provide the answers to these questions. If these questions cannot be theoretically answered, the physical mechanism underneath the HHG phenomena still needs to be discovered.

Recent developments in laser techniques allowed experimentalists to observe ultrahigh harmonics up to orders greater than 5 000 [4]. The currently accepted cutoff law and its improved version do not quite predict the harmonics of orders as that high. Pursuing better interpretation to the experimental result, also trying to answer above basic addressed physics questions, we intend to rederive the cutoff law from fundamental theories with less assumptions.

In the nonperturbative quantum electrodynamics (NPQED) theory [5], the electron transition amplitudes due to photon fields are expressed as Bessel functions with the index denoting the photon number emitted during the transition. In our previous work, the transition rate formulas for above-threshold ionization [5, 6], Kapitza–Dirac effect [7, 8], Freeman resonance [9, 10], and HHG [11–13], are all expressed in terms of Bessel functions and wave functions of initial atomic bound state. If a physical effect is not specially related to the wave function of the atomic bound state, it must be entirely determined by the property of Bessel functions. We showed that the photoelectron angular distributions (PADs) were so [14–16].

In this paper, without using the whole NPQED theory and any HHG rate calculation, we provide a self-contained theoretical proof of the cutoff frequency of high harmonic spectra. In this proof, we only use the cutoff property of Bessel functions and the Einstein photoelectric law in the multiphoton case. Since the Einstein photoelectric law is the energy conservation law and we have exact photo-number counting in the derivations, the phase-matching processes caused by the energy-momentum and photon number changes are taken care of automatically. From a direct inspection, we find that Bessel functions for a fixed argument do have a cutoff order. The example in Fig. 1 is made with the argument $x = 1472.88$, while the cutoff order $n_c \approx x$ and $n_c < x$, as expected. A natural question arising here is: Can one determine the cutoff order of HHG only from that of Bessel functions and the dynamic condition specified by the Einstein photoelectric law in the multiphoton case? To answer this question, we have to define what is cutoff order for Bessel functions. The cutoff order of Bessel functions, at a fixed argument, is defined as the order after that the value of the Bessel functions is monotonically decreasing as the order goes to the positive infinity. The reasonability and rigorous description of the definition are presented in Appendix 1.

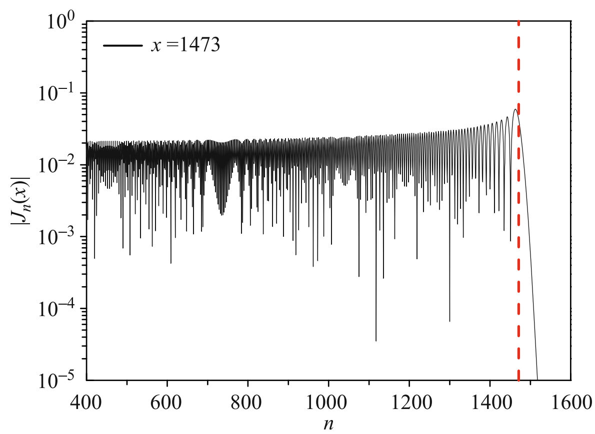

Fig. 1 For a fixed argument, the value of Bessel functions $J_n(x)$ is a function of the index n. The argument x is set as $x = 1473$, equal to the u_p in Ref. [4]. The vertical axis shows the absolute value of Bessel functions. The vertical broken line denotes the position of the cutoff order

2 The dynamic condition to limit the transferred photon numbers

In the NPQED theory, HHG is derived as a two-step process [17]. The first process is the ionization process during which the bound atomic electron ionizes into real Volkov states by absorbing j photons. The second process is the recombination process during which Volkov electrons absorb extra photons then transit back to the original bound state with an emission of a large photon of energy $q\hbar\omega$. The dynamics condition governing the first process is

$$\frac{\boldsymbol{P}^2}{2m_e} = \hbar\omega(j - u_p - e_b) \tag{1}$$

which is the Einstein photoelectric law in the multiphoton case, where $u_p \equiv U_p/(\hbar\omega)$ and $e_b \equiv I_p/(\hbar\omega)$. The Bessel functions which describe the amplitude of the electron transition induced by absorbing j photons look $J_{-j}(x)$, where

$$x = \sqrt{8u_p(j - u_p - e_b)} \tag{2}$$

as the maximized argument, is derived when the photoelectron emits in the polarization direction. In Fig. 2, the entire square-root line $x = \pm\sqrt{8u_p(j - u_p - e_b)}$ describes the dynamics condition specified by the Einstein photoelectric law in the multiphoton case, say Eq. (1). The line x_1 intersects with the positive square-root line at two points which are the cutoff orders of Bessel

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functions of positive and negative even indices. The line x_3 intersects with the negative square-root line at two points which show the cutoff orders of Bessel functions of negative odd indices, without any extra photon absorption. The lowest line x_4 denotes the maximum photon absorption due to ionization and the extra photon absorption. The line x_2 denotes the relation between the argument of the Bessel function as a function of positive index $-j+q$, which gives the maximum photon number q_c converted to the harmonic photon; since the index is positive, the argument-index relation has to satisfy the same condition for x_1 and the dynamic condition specified by the square root curve. The maximum photon conversion number q_c, i.e., the cutoff high-harmonic order, is the distance between the intersects of line x_4 and line x_2 with the vertical axis.

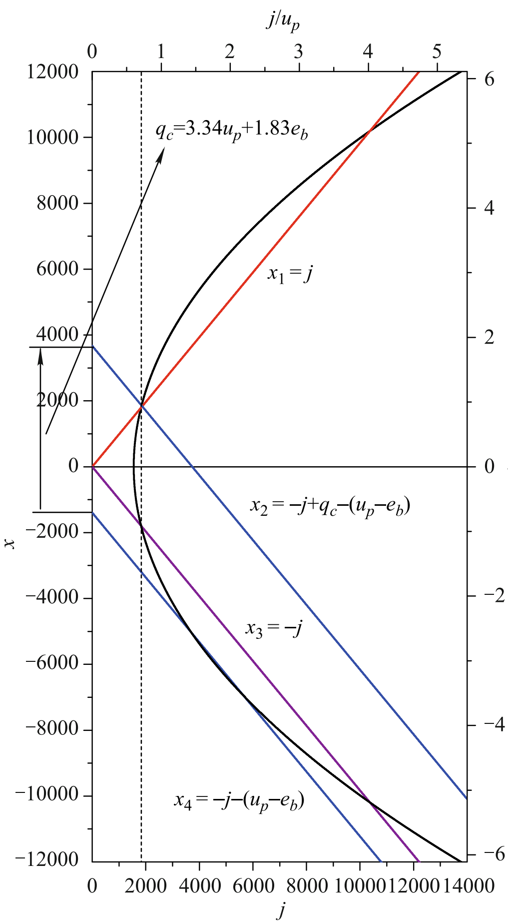

Fig. 2 Geometric method to get the cutoff order of harmonics. The horizontal axis denotes the orders of Bessel functions. The positive vertical axis shows the value of the argument of Bessel functions of positive and negative even indices. The negative vertical axis shows the negative value of the argument of Bessel functions of negative odd indices. To illustrate the recent experimental result, $u_p = 1473$ and $e_b = 77.34$ are selected.

3 The cutoff order of high harmonics

The complete lengthy mathematical proof is presented in the Appendix. The exact expression of the cutoff law in the $U_p > I_p$ case reads

$$q_c = 2(4u_p - 2\sqrt{2u_p^2 - 2u_p e_b}) + u_p - e_b. \tag{3}$$

In the limit of $U_p \gg I_p$, i.e., $u_p \gg e_b$, we obtain the following version of the cutoff law

$$q_c = (9 - 4\sqrt{2})u_p + (2\sqrt{2} - 1)e_b$$
$$\approx 3.3431457u_p + 1.8284271e_b. \tag{4}$$

In the recent experiment [4], ultrahigh harmonics in keV X-ray regime from mid-infrared femtosecond lasers were observed. The orders of these harmonics are greater than 5000. The data from this experiment can be used to test different cutoff laws. In this experiment, one of the gas media used was helium. The laser wavelength was 3900nm, beam intensity was 3.3×10^{14} W/cm^2, the highest harmonics observed were of photon energy 1.6 keV $= 5033\hbar\omega$. With $I_p = 24.587\,41$ eV, $U_p = 468.30$ eV, and $\hbar\omega = 0.3179$ eV, we have $u_p = 1472.88$, $e_b = 77.3432$. With the laser photon energy 0.3179 eV, the cutoff order converted from the experimental cutoff energy 1.6 keV is 5033. The cutoff order predicted by the 3.17 law is $q_c = 3.17u_p + e_b = 4746$. The cutoff order predicted by the improved 3.17 law is $q_c = 3.17u_p + 1.32e_b = 4771$. The cutoff order predicted by this theory is $q_c = 3.34u_p + 1.83e_b = 5060$, which is very closed to the photon number 5033 observed by the experiment, also consistent with our earlier declaration as the upper bound of the cutoff order of high harmonics. The geometric relation between the cutoff order q_c and other parameters can be seen in Fig. 2, where both the horizontal axis and the vertical axis are labeled according to the experimental conditions. The exact cutoff order can also be obtained from Fig. 2. Indeed the graphical method provides an alternative proof to the cutoff order, in addition to the regular mathematical proof presented in Appendix 1.

Why the cutoff orders predicted by the expression $q_c = 3.34u_p + 1.83e_b$ are greater than those predicted by the classical-field or semiclassical-field theories? The reason is as follows. In the Bessel function method, the laser photons to participate the photon-mode up-conversion are not only those ionization photons which show up in the Einstein's photoelectric law, but also some non-ionization photons. In a full quantum mechanical treatment, all possible transition channels must occur if they are not ruled out by mathematical restrictions which embody all kinds of conservation laws in physics. The process for absorbing non-ionization photons to participate the photon-mode up-conversion may be called accompanying Raman effect. The absorbed laser photons to participate the photon-mode up-conversion are from the both, photoelectric effect and accompanying Raman effect.

4 Conclusion

The cutoff order for laser induced high harmonics can be completely determined by the Einstein photoelectric law in the multiphoton case and the properties of Bessel functions of first kind. The new cutoff law

$$q_c\hbar\omega = (9-4\sqrt{2})U_p + (2\sqrt{2}-1)I_p$$

extends the cutoff orders predicted by the traditional one and offers a new reference to future experimental measurements of cutoff orders. It also answers the questions addressed in the Introduction section. The two coefficients in the cutoff law do not depend on any fundamental physics constants which are already contained in the two interaction energies, U_p and I_p. The two coefficients are of algebraic constants. To the new cutoff law, the current paper offers two different theoretical proofs, the graphical method and the mathematical deduction method; the calculation using the formulas derived from the NPQED theory of HHG [17] provides a fine numerical test; and the recent experimental measurement [4] shows a good agreement with. The four independent methods constitute a firm basis of the new cutoff law.

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Appendix 1: Mathematical proof to the cutoff law

To study the cutoff property of Bessel functions, we start from the following recurrence relations

$$J_{n-1}(x) - J_{n+1}(x) = 2J_n'(x) \tag{5}$$

$$J_{n-1}(x) - \frac{n}{x}J_n(x) = J_n'(x) \tag{6}$$

$$\frac{n}{x}J_n(x) - J_{n+1}(x) = J_n'(x) \tag{7}$$

With these identities, we prove the following lemmas.

Lemma 1 *At and only at the extremum points $x_i (i = 1, 2, 3, \cdots)$ of the Bessel function $J_n(x)$, where $x > 0$ and $n = 1, 2, 3, \cdots$, $J_{n-1}(x)$ and $J_{n+1}(x)$ intersect.*

Proof: Bessel functions have no stationary points other than extremum points. This lemma is an obvious consequence of Eq. (5). (Q.E.D.)

Note: $x_i \quad (i = 1, 2, 3, \cdots)$ are functions of n, e.g., $x_1(n)$ means the first extremum point of $J_n(x)$, which is, indeed, a maximum.

Lemma 2 *At and only at the maximum points $x_i (i = 1, 3, 5, \cdots)$ of the Bessel function $J_n(x)$, the relation $J_{n-1}(x) > J_{n+1}(x)$ turns into $J_{n-1}(x) < J_{n+1}(x)$; at and only at the minimum points x_i $(i = 2, 4, 6, \cdots)$ of the Bessel function $J_n(x)$, the relation $J_{n-1}(x) < J_{n+1}(x)$ turns into $J_{n-1}(x) > J_{n+1}(x)$.*

Proof: At x_i $(i = 1, 3, 5, \cdots)$, the Bessel function $J_n(x)$ has maximum and $J_n(x)' = 0$. When $x < x_i$, since $J_n(x)' > 0$, according to Eq. (5), $J_{n-1}(x) > J_{n+1}(x)$. For the same reason, when $x > x_i$, since $J_n(x)' < 0$, then $J_{n-1}(x) < J_{n+1}(x)$. The relation $J_{n-1}(x) > J_{n+1}(x)$ turns into $J_{n-1}(x) < J_{n+1}(x)$. The proof for the other part $(i = 2, 4, 6, \cdots)$ of the lemma is similar to this proof. (Q.E.D.)

With the understanding of the mathematical phenomenon described by Lemma 2, we can define the cutoff order of Bessel functions for a fixed argument such that after this order, none of Bessel functions have the first maximum $x_1 \leqslant x$.

Definition *The cutoff order n_c of the set of Bessel functions $\{J_j(x)\}$ $(j = 0, 1, 2, \cdots, n_c, \cdots)$ for a fixed positive x is defined such that the first extremum (maximum) point of $J_{n_c}(x)$ satisfies*

$$x_1(n_c) \leqslant x, \quad x_1(n_c+1) > x \tag{8}$$

In other words, we say $n_c = Max\{n \mid x_1(n) \leqslant x\}$ and $n_c + 1 = Min\{n \mid x_1(n) > x\}$.

Theorem 1 *A positive number x, as a fixed argument of Bessel functions, provides an upper bound to the cutoff order of Bessel functions of positive indices, i.e.,*

$$n_c < x \tag{9}$$

Proof: In the following we adopt the notation $x_1 \equiv x_1(n_c)$. We know $x_1 \leqslant x$ from the definition.

Setting $x = x_1$ in Eq. (6) leads to $x_1J_{n_c-1}(x_1) = n_cJ_{n_c}(x_1)$. Since $J_{n_c-1}(x_1) = J_{n_c+1}(x_1) < J_{n_c}(x_1)$, noting the first extremum is a maximum and the values of the three Bessel functions are all positive at x_1, we have

$$n_c < x_1 \leqslant x \tag{10}$$

(Q.E.D.)

With Eqs. (2) and (9), we have the following inequality,

$$|j_c| \leqslant \sqrt{8u_p(j_c - u_p - e_b)} \tag{11}$$

which leads to the algebraic equation

$$j_c^2 - 8u_p j_c + 8u_p^2 + 8u_p e_b \leqslant 0 \tag{12}$$

The solutions to the above equation when taking the equal sign have two cutoff orders of the index j:

$$j_c = 4u_p \pm 2\sqrt{2u_p^2 - 2u_p e_b} \tag{13}$$

Thus we obtain:

Theorem 2 *There are two cutoff orders,* $j_{c1} = 4u_p - 2\sqrt{2u_p^2 - 2u_p e_b}$ *and* $j_{c2} = 4u_p + 2\sqrt{2u_p^2 - 2u_p e_b}$ *in the set of Bessel functions of positive orders with the dynamics condition and* $u_p \geqslant e_b$. *The orders forming the plateau are located between the two cutoff ones.*

We also obtain:

Corollary *There are two cutoff orders,* $-j_{c1}$ *and* $-j_{c2}$, *in the set of Bessel functions of negative orders with the dynamics condition and* $u_p \geqslant e_b$. *The valuable orders forming the plateau are those between the two cutoff ones.*

The two cutoff orders of Bessel functions of positive and negative even orders can be seen, in Fig. 2, as the intersects of the straight line x_1 with the square-root line of positive value, while that of negative odd orders can be seen, as the intersects of the straight line x_3 with the square-root line of negative value.

Consider Bessel functions $J_{-j-s}(x)$, where x is given in Eq. (2), with $j = 1, 2, 3, \cdots$ being the number of absorbed photons for the ionization and $s = 1, 2, 3, \cdots$ being the number of extra photon absorbed for participating only the photon-mode up-conversion, not the ionization.
Thus, we have the following theorem:

Theorem 3 *For the set of Bessel functions of negative orders with extra photon absorption,* $J_{-j-s}(x)$ *where the argument* x *subject to the dynamic condition, the extra absorbed photon number* s *has an upper bound,* $s \leqslant u_p - e_b$ *and the cutoff order is* $j_c = 3u_p + e_b$.

Proof: Combining Theorem 1 and Eq. (2), one has an equation for the cutoff j_c:

$$(j_c + s)^2 \leqslant 8u_p(j_c - u_p - e_b) \tag{14}$$

On the cutting edge, we obtain the equation

$$(j_c + s)^2 - 8u_p(j_c + s) + 8u_p^2 + 8u_p(e_b + s) = 0 \tag{15}$$

to solve for $j_c + s$. The condition for real solutions is

$$s \leqslant u_p - e_b \tag{16}$$

By selecting the equal sign $s_c = u_p - e_b$ and putting s_c into s in Eq. (15), we obtain the formula for the cutoff order,

$$j_c = 3u_p + e_b \tag{17}$$

(Q.E.D.)

Theorem 4 *The upper limit of the cutoff order of high harmonic is* $2(4u_p - 2\sqrt{2u_p^2 - 2u_p e_b}) + u_p - e_b$.

Proof: Since the photoelectron and the participating photons have to keep the energy conservation according to Eq. (1), we have $|j_c| \leqslant \sqrt{8u_p(j_c - u_p - e_b)}$, and $j_{c1,2}$ (in Theorem 2) is obtained by solving this inequality with taking the equal sign. Now we consider Bessel function $J_{-j-s+q}(x)$ where j is the ionization photons, s is the maximum possible extra photon absorbed and q denotes a harmonic order. To obtain the cutoff order for q, we need the following equation according to the Theorem 1,

$$-j_c - (u_p - e_b) + q \leqslant \sqrt{8u_p(j_c - u_p - e_b)} \tag{18}$$

With taking $j_c = j_{c1}$ and replacing the right side of above equation by j_{c1} we obtain the upper bound of the cutoff order expressed by Eq. (3). (Q.E.D.)

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