

PACS numbers: 42.65.Ky; 32.80.Fb
DOI: 10.1070/QE2001v031n01ABEH001891

Interference of electron trajectories and generation of high-order optical harmonics in a Coulomb system

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***Abstract*. The amplitudes of harmonics of the atomic response are determined as functions of the intensity of the pump light wave within the range of intensities of 4.9×10^{13} – 2.1×10^{14} W cm^{-2} through the numerical solution of the Schrödinger equation for a hydrogen atom in an oscillating electric field. For the amplitudes of harmonics starting from the 5th up to at least the 55th order, these dependences display a deep modulation. Generation of high-order harmonics is analysed within the framework of semiclassical theory including several factors that were ignored in earlier studies. Relatively simple formulas for the amplitudes of high-order harmonics are derived. These formulas agree well with the results of numerical simulations in the range of tunnelling ionisation and provide a satisfactory agreement with numerical simulations in the range of barrier-suppression ionisation.**

***Keywords*:** *high order harmonics, X-rays, electron trajectory interference*.

1. Introduction

High-order harmonic generation in atomic gases is widely employed in physical experiments as an efficient way of producing coherent soft X-ray radiation. Unfortunately, the efficiency of high-order harmonic generation is rather low, which is, to a considerable degree, due to the fact that it is difficult to phase-match harmonic generation within rather large interaction lengths. The results of experiments [1] and theoretical analysis performed in [2] demonstrate that phase -matched high-order harmonic generation can be implemented due to the nonmonotonic dependence of the high-frequency response of a medium on the intensity of the pump light wave. Therefore, it would of particular interest to elucidate the nature and the character of this dependence.

The above-mentioned nonmonotonic dependence is observed in calculations [2, 3] performed within the framework of single-electron quantum-mechanical theory [3, 4] based on the method of successive iterations. This theory is widely used for the calculation of the atomic response under conditions of high-order harmonic generation. Unfortunately, such calculations are very labour-consuming and cannot provide an adequate accuracy, since this theory neither allows one to go beyond the first-order approximation nor permits the extension to multielectron systems.

The semiclassical theory [5] is also widely used for a qualitative interpretation of high-order harmonic generation (as well as for some related calculations). In particular, the nonmonotonic dependence of the atomic response on the intensity can be understood in terms of this theory as a consequence of interference of different electron trajectories (see the discussion below). Since many aspects of the semiclassical theory are still to be adequately developed, this approach was never applied for atomic-response calculations. However, as will be shown below, this theory allows the development of a simple and efficient technique for many useful calculations. Apparently, the main obstacle that has prevented the development of such a technique so far was the absence of reliable experimental or some other data that could be employed to test this procedure.

Thus, the fundamental problem of the nonmonotonic intensity dependence of the atomic response and the possibility of modulation of this response should be examined with the use of more reliable methods. Numerical simulations involving detailed calculations of the atomic response through the numerical solution of the Schrödinger equation for a single-electron atom in an oscillating field seem to be the most natural way to accomplish this goal. Although such simulations are rather labour-consuming, they can be performed with a sufficiently high accuracy. Simulations of this type have been carried out earlier for a hydrogen atom and for other single-electron model systems. However, these simulations were not quite systematic and were never employed for the analysis of the intensity dependence of the atomic response.

This paper presents the results of detailed calculations performed for the high-frequency response of a hydrogen atom to the field of a linearly polarised light wave ($\lambda =$ 1.06 μm) within a broad range of intensities of this wave in the ranges of tunnelling and barrier-suppression ionisation. It will be demonstrated that harmonics of the atomic response are modulated with a large modulation depth (which is close to unity). Based on these test results, we will perform a semiclassical analysis of the problem under study including several factors that were previously ignored. Formulas derived for the amplitudes of high-order harmonics using this approach are, to some extent, empirical and relatively simple (expressions for harmonic amplitudes have been previously derived in the form of rather complicated integrals [3, 4, 6]). In the range of tunnelling ionisation, pre-

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Received 11 September 2000
Kvantovaya Elektronika **31** (1) 55 – 60 (2001)
Translated by A M Zheltikov

dictions of these formulas agree well with the results of numerical simulations.

2. Numerical procedure and results of simulations

The Schrödinger equation was integrated in the coordinate representation in cylindrical coordinates. The z axis was directed along the electric field vector of the light wave. The Coulomb potential in these simulations was replaced by a potential $V(r) = -1/(r^2 + 0.01)^{1/2}$ (in atomic units). This potential corresponds to a binding energy $I \approx 0.98$Ry, where Ry is the Rydberg constant. The distance from the centre of the simulation grid to its boundaries along the z axis was equal to $3eE_0/m\omega^2$ (where E_0 and ω are the amplitude and the frequency of the field and m is the electron mass). The distance to the side boundary was 25 au. A layer with a smoothly varying absorption was placed near the grid boundaries to suppress the reflection of the wave packet.

The electric field was defined as a field of a pulse with a super-Gaussian front. The peak intensity was varied from 0.0014 up to 0.006 au (from 4.9×10^{13} up to 2.1×10^{14} W cm^{-2}) with a step of 0.0001 au. A fragment of this pulse is shown in Fig. 1 along with the results of calculations performed for the intensity of 0.004 au, which lies on the boundary separating the ranges of tunnelling and barrier-suppression ionisation.

Fig. 1 displays the probability $N_s = \langle\psi(t)|\psi(t)\rangle$ that an electron does not escape from the simulation grid by the moment of time t, the normalised population $N_0 = |\langle\psi_0|\psi(t)\rangle|^2$ of the ground state ψ_0, the average force $f(t) = -E - \langle\psi(t)|\partial V/\partial z|\psi(t)\rangle$ acting on the electron, and the strength E of the electric field in the light wave.

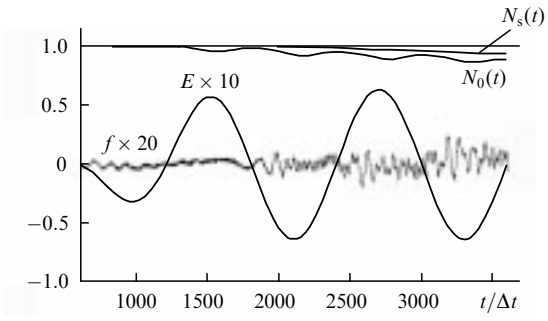

Figure 1. Time dependences of the electric field strength E (in atomic units), N_s (in arbitrary units), normalised population N_0 (in arbitrary units), and the average force f (in atomic units) acting on an electron (Δt is the time step in calculations).

Fig. 2 presents the amplitudes of odd harmonics of the force g_n calculated within two half-cycles on the plateau of the pump pulse for the intensity $u = 0.0039$ au. We should note an apparent irregularity of the spectral structure. The dependences of $|g_n|^2$ on the intensity u for several harmonics are presented in Fig. 3.

All the dependences $|g_n(u)|^2$ for harmonics up to at least the 55th order display a deep, nearly 100 %, modulation. Interestingly, low-order harmonics with the energies of quanta lower than the ionisation energy of the atom are also modulated (only the third harmonic displays virtually

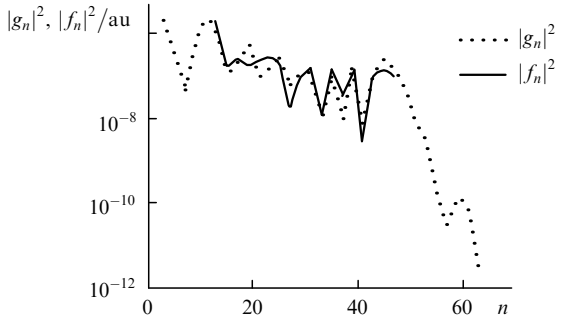

Figure 2. Amplitudes of odd-order harmonics simulated numerically (g_n) and calculated analytically (f_n) as functions of the harmonic number.

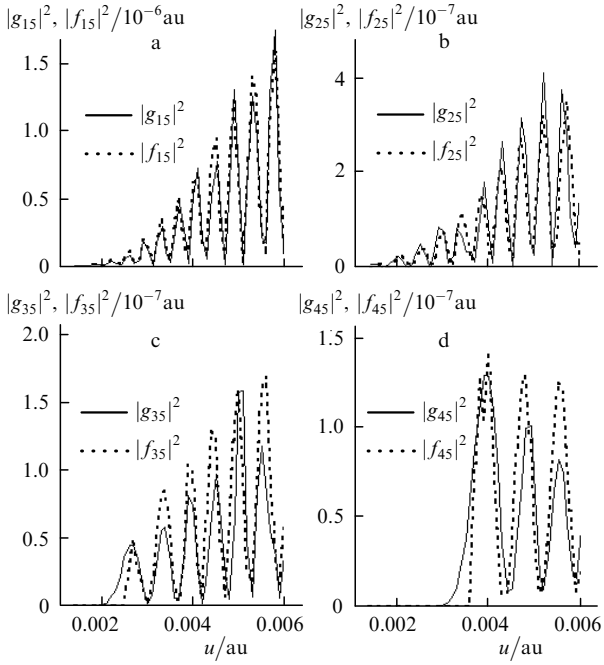

Figure 3. Amplitudes of odd-order harmonics simulated numerically (g_n) and calculated analytically (f_n) as functions of the intensity of pump radiation for $n = 25$ and 35.

no modulation), although the modulation depth is much less in this case. The modulation frequency slowly changes as a function of the harmonic number, remaining virtually independent of the intensity in the range of tunnelling ionisation. Hence, it is clear that, with $u \sim \exp(-r^2)$, the dependence $|g_n(r)|^2$ quite adequately describes the interference of two axially symmetric light beams with different divergences and comparable intensities. This circumstance is very useful for the prediction of the spatial structure of the field of harmonics generated in a macroscopic medium. Interpretation of this effect is a problem of fundamental importance for the microscopic theory of the phenomenon under study.

Comparison of the results of simulations with the predictions obtained by means of successive iterations using analytical expressions presented in [6] shows that the formulas of [6] satisfactorily describe the structure of the dependences $|g_n(u)|^2$ for high-order harmonics (approximately, starting with the 25th harmonic). A satisfactory agreement is observed not only in the range of tunnelling ionisation, but also in the domain of barrier-suppression ionisation. The absolute values of the amplitudes predicted by the analytical formulas are considerably (roughly, by an order

of magnitude) underestimated. For $n \geqslant 25$, these discrepancies decrease with the growth in the harmonic number. The fact that the analytical approach considerably underestimates harmonic intensities as compared with the experimental data was pointed out several times before and was attributed to the multielectron nature of harmonic-generating atoms. In fact, this discrepancy may arise because of a rather rough first-order approximation employed in the analytical approach. This approximation substantially overestimates the spreading rate of the wave packet after ionisation (since the initial sizes of the wave packet are underestimated, while the influence of Coulomb forces on this packet is ignored). The behaviour of the dependences presented in Fig. 1 [in particular, the fact that the curve $N_s(t)$ lags behind the curve $N_0(t)$] indicates that, in reality, the spreading rate of the wave packet is not very high.

In practical terms, the phenomenological approach based on the semiclassical approximation is more flexible, allowing formulas for amplitudes to be 'constructed' from separate elements including various aspects of the phenomenon under study. In what follows, we will construct such formulas using the results well known from the semiclassical theory of high-order harmonic generation [4, 6] and taking into consideration the oscillatory behaviour of dependences $f(t)$ (see Fig. 1). Variations in the amplitude of these oscillations within a half-cycle are unexpectedly slow. Changes in the amplitude from half-cycle to a half-cycle correlate with the ionisation probability at the preceding moments of time (separated from the current moment of time by approximately three quarters of a cycle). The oscillation frequency reaches its maximum around the nodes of the field, i.e., at the points close to those predicted by the semiclassical theory. Within the initial section of the plateau in harmonic spectra, harmonic amplitudes considerably exceed harmonic amplitudes around the cut-off. In the regime of tunnelling ionisation, the plateau width increases in accordance with predictions of the semiclassical theory. Subsequently, this growth in the plateau width becomes somewhat slower.

The main method of testing the constructed formulas involves the comparison of the predictions of these formulas with the results of simulations presented in Fig. 3.

3. Theoretical analysis

The semiclassical theory treats harmonic emission as a complicated periodic process, which involves ionisation, the stage of a free motion of an electron in the field of a light wave, and radiative recombination with a return of the electron to the initial state. This approach assumes that ionisation and recombination are instantaneous processes, the electron velocity immediately after ionisation is equal to zero, and the trajectory of a free electron starts and ends at a point $r = r_1$ around a nucleus (usually this point is chosen in such a way that $r_1 = 0$) and is governed by classical equations of motion ignoring the Coulomb forces. Within the framework of this approach, the energy of the emitted quantum (the sum of the ionisation energy I and the kinetic energy ε acquired by an electron at the stage of free motion) is unambiguously determined by the phase of the field at the moment of ionisation. A discrete spectrum of harmonics is emitted due to the periodicity of this process. Only odd harmonics are generated under these conditions.

An electron returns to the initial point r_1 after the stage of free motion if the ionisation moment t_i falls within the interval $(NT/2, NT/2 + T/4)$, where N is an integer and T is the field cycle (we assume that the field oscillates as $\cos \omega t$). In what follows, we set $N = 0$. The moment t_i, the recombination moment t_r, and the kinetic energy ε of a recombining electron are related to the time τ of free motion of this electron by the following formulas [6]:

$$\omega t_i(\tau) = \arctan \frac{1 - \cos \omega\tau}{\omega\tau - \sin \omega\tau}, \tag{1}$$

$$t_r(\tau) = t_i(\tau) + \tau, \tag{2}$$

$$\varepsilon(\tau) = \mathrm{U} \frac{(2 - 2\cos \omega\tau - \omega\tau \sin \omega\tau)^2}{1 - \cos \omega\tau - \omega\tau \sin \omega\tau + \omega^2\tau^2/2}, \tag{3}$$

where U is the ponderomotive energy of the electron. The function $\varepsilon(\tau)$ reaches its maximum at the point $\tau_{max} \approx 4.1/\omega$ and takes a value of about $3.17U$ at this point. Importantly, if the energy $n\hbar\omega$ falls within the interval between the ionisation potential I and the maximum value $I + \varepsilon(\tau)$, then the equation

$$n\hbar\omega = I + \varepsilon(\tau) \tag{4}$$

has two roots, $\tau_a(n)$ and $\tau_b(n)$, within the segment $(0, T)$. These two roots lie within the intervals $(T/4, \tau_{max})$ and (τ_{max}, T). The values of t_i and t_r corresponding to these roots will be denoted as t_{ia}, t_{ib} and t_{ra}, t_{rb}. Eqn (4) may also have roots falling beyond the segment $(0, T)$, but these roots are less important. Electrons undergoing ionisation within the time interval $(0, T/4)$ mainly emit harmonics within the interval $(T/2, T)$.

Thus, two trajectories correspond to the emission of the quantum of an nth harmonic. The fields emitted by an electron moving along these trajectories interfere with each other. This interference is usually referred to as the interference of trajectories. Correspondingly, the amplitude of the nth harmonic of the nuclear field acting on an electron can be represented as a sum

$$f_n = a_n + b_n, \tag{5}$$

where the terms are related to the electron trajectories corresponding to the roots τ_a and τ_b. Indeed, in accordance with a concept of the semiclassical theory of high-order harmonic generation, the time dependence $f(t)$ can be represented as

$$\begin{aligned} f(t) &= f^-(t) + \text{c.c.}, \\ f^-(t) &= F(t) \exp\left(-\mathrm{i} \int \Omega \mathrm{d}t\right) = \sum_n f_n \exp(-\mathrm{i}n\omega t), \end{aligned} \tag{6}$$

where $F(t)$ is the slowly varying amplitude (which reverses its sign at extremal points of the field) and $\Omega(t) = [I + \varepsilon(\tau(t))]/\hbar$; $\tau(t)$ is the function inverse of $t_r(\tau)$ [see Eqs (1) and (2)]. The explicit form of the function $\Omega(t)$ is of no importance for our analysis. It is important only that this function takes the value $n\omega$ twice per each half-cycle [at the points $t_{ra}(n)$ and $t_{rb}(n)$]. The neighbourhoods of these points provide the main contribution to the Fourier amplitude f_n. A straightforward analysis based on integration with the

use of the stationary-phase method shows that the first term in Eqn (5) is given by

$$a_n = f^{-}(t_{ra}) \exp(\mathrm{i}n\omega t_{ra})\omega[2/(\pi|\dot{\Omega}(t_{ra})|)]^{1/2}. \tag{7}$$

at least for harmonics whose frequencies lie far from $I/\hbar$ and $(I+\varepsilon_{\max})/\hbar$.

The expression for the amplitude b_n can be written in a similar form. (Such a representation is the most adequate way to describe the initial section of the 'experimental' dependence $f(t)$ shown in Fig. 1. In the course of time, this dependence becomes somewhat more complicated, since, for some t_i, an electron returns to the atomic residue at least twice. Such electrons are characterised by a low energy and introduce low-frequency 'distortions' into the dependence $f(t)$, having a weak influence on harmonic amplitudes.)

The following key assumption will be used to determine a_n in Eqn (7). At the moments of time close to $t_{ra}(n)$, the wave function of an electron around a nucleus can be approximated with a superposition of the ground state and a plane wave packet:

$$\psi_n \approx N_0^{1/2}\psi_0 \exp\left(\frac{\mathrm{i}It}{\hbar}\right) + \left(\frac{K_n N_{an}}{S_{an}L_{an}}\right)^{1/2} \times \exp\left[\frac{\mathrm{i}s_{an}(t,z)}{\hbar}\right], \tag{8}$$

where S_{an} and L_{an} are the cross section and the length of the wave packet resulting from ionisation within the time interval $(t_{ia}(n-1), t_{ia}(n+1))$ and evolving in a free space up to the moment of time $t_{ra}(n)$. Here, N_{an} is the number of electrons in this wave packet, K_n is the dimensionless correction factor including the compression of the packet due to the Coulomb forces, s_{an} is the action defined as

$$s_{an}(t,z) = It_{ia} - \int_{t_{ia}}^{t} \frac{1}{2m}\left(p + \frac{e}{c}A\right)^2 \mathrm{d}t' + \left(p + \frac{e}{c}A\right)(z - z_{an}),$$

A is the vector potential, $p = -(e/c)A(t_{ia})$ is the canonical momentum, and

$$z_{an} = \frac{I}{2eE(t_{ia})} + \left\{\left[\frac{I}{2eE(t_{ia})}\right]^2 - \frac{e}{E(t_{ia})}\right\}^{1/2}$$

is the coordinate of the point corresponding to the location of an electron after tunnelling at the moment of time t_{ia} and after free motion and return at the moment of time t_{ra}. The action $s_{an}(t, z)$ is defined in such a way that, for $t = t_{ia}$, the phase of a free wave packet at the point $z = z_{an}$ coincides with the phase of the bound state.

Calculating the mean value of the force $-e^2z/r^3$ in the state defined by Eqn (8) and using Eqs (6) and (7), we can express the amplitude a_n in terms of the parameters of the state (8) and the derivative $\dot{\Omega}(t_{ra})$. The denominator of the resulting expression involves the quantity $(|\dot{\Omega}(t_{ra})|L_{an})^{1/2}$. To eliminate this quantity, we assume that the frequency Ω changes from $(n-1)\omega$ up to $(n+1)\omega$ within the time interval equal to $L_{an}m/p_n$, where $p_n = [2m(n\hbar\omega - I)]^{1/2}$. Then, we derive

$$a_n = \exp[\mathrm{i}\phi_a(n)]F_n\left(\frac{K_n N_0 N_{an}\pi r_0^2}{S_{an}}\right)^{1/2}, \tag{9}$$

where r_0 is the Bohr radius,

$$\phi_{an} = -2\frac{U}{\hbar}\int_{t_{ia}}^{t_{ra}} (\sin\omega t - \sin\omega t_{ia})^2 \mathrm{d}t + n_0\omega(t_{ia} - t_{ra}) + n\omega t_{ra} + \frac{p_n z_{an}}{\hbar}; \tag{10}$$

$$n_0 = \frac{I}{\hbar\omega};$$

$$F_n = -\left(\frac{m\omega}{\pi^2 r_0^2 p_n}\right)^{1/2}\left\langle\psi_0\left|\frac{e^2 z}{r^3}\right|\exp\left(-\mathrm{i}\frac{p_n z}{\hbar}\right)\right\rangle$$

is a quantity having dimensions of a force and depending only on the harmonic number and the field frequency. For a hydrogen atom, we have

$$F_n = \mathrm{i}\frac{e^2}{r_0^2}\left(\frac{8}{\pi n_0}\right)^{1/2}\left(\frac{n_0}{n-n_0}\right)^{5/4} \times \left[\left(\frac{n-n_0}{n_0}\right)^{1/2} - \arctan\left(\frac{n-n_0}{n_0}\right)^{1/2}\right]. \tag{11}$$

For small $n - n_0$, the force given by Eqn (11) is proportional to $(n-n_0)^{1/4}$.

Since the time τ_a of free motion is usually large, it would be natural to define the cross section S_{an} by the relation $S_{an} = \pi(p_r^2/m^2)\tau_a^2(n)$, where p_r^2 is the mean square of the transverse component of the momentum after ionisation. As shown in [7], in the tunnelling regime, we have $p_r^2 = p_0^2 E/E_0$, where $p_0^2 = 2mI$ and $E_0 = (I/\mathrm{Ry})^{1/2}e/r_0^2$ (the coefficient $(I/\mathrm{Ry})^{1/2}$ is given here for the sake of generality). Finally, we arrive at

$$S_{an} = \pi r_0^2 E(t_{ia})\left[\frac{p_0\tau_a(n)}{m}\right]^2 \frac{(\mathrm{Ry}/I)^{1/2}}{e}. \tag{12}$$

Note that the ratio $S_{an}/\pi r_0^2$ is always large, i.e., a free wave packet is subject to a substantial spreading. It would be natural to assume that, due to Coulomb forces, the wave packet is contracted toward the axis. This contraction, which is not necessarily uniform, becomes especially noticeable for small p_n when the packet slowly passes through the area around the force centre. Contraction of this type can be considered as scattering by a Coulomb centre. Therefore, the correction factor K_{an} should be related to the relevant scattering cross section. It would be natural to represent this factor in the following form:

$$K_{an} = 1 + \frac{S_{sc}(p_n)}{\pi r_0^2}\kappa, \tag{13}$$

where

$$S_{sc}(p_n) = 4\pi r_0^2\left(\frac{n_0}{n-n_0}\right)^2$$

is the cross section of scattering of a classical electron with a momentum p_n by an angle exceeding $\pi/2$. The constant κ is close, in accordance with our assumption, to unity and

can be determined from an appropriate fitting procedure (see the discussion below).

The number of electrons in the packet is given by

$$N_{an} = N_0(t_{ia}(n))w_a(E(t_{ia}(n)))|t_{ia}(n+1) - t_{ia}(n-1)|, \quad (14)$$

where $w_a(E)$ is the ionisation rate, which is considered as an instantaneous function of the field strength. Naturally, this approximation inevitably gives rise to some difficulties. We assume that the ionisation rate adiabatically follows the field strength only around the maximum of the field strength. Correspondingly, at the moments of time t_{ib}, which always lie around the maximum of the field strength, the rate $w_a(E)$ can be estimated from the well-known formula [8] for the ionisation rate of a hydrogen atom in a dc field: $w_0(E) = (2I/\hbar)(4E_0/E)\exp(-2E_0/3E)$. (This formula becomes inapplicable only for high intensities in the regime of barrier-suppression ionisation.) On the other hand, the trajectories corresponding to the root τ_a display the following specific feature: the higher is the intensity and the lower is the harmonic number, the less is the field strength $E(t_{ia})$ at the moment of time corresponding to ionisation (and the faster is the variation of this field strength). In the case of harmonics whose numbers are close to n_0, any estimate for $w_a(E(t_{ia}))$ obtained with the use of the formula presented above or any other approximate formula assuming that ionisation is an instantaneous process inevitably leads to underestimation. Keeping this circumstance in mind, we assume below that

$$w_a(E(t_{ia})) = w_0(E(t_{ia} - \delta t)), \quad (15)$$

where δt is the fitting parameter (in what follows, we set $\delta t = \hbar/I$).

We will also assume that the amplitude b_n in Eqn (5) is defined by formulas that can be derived from Eqs (9)–(15) with a replacement $a \to b$. The parameter δt (with the chosen value of this parameter) has virtually no influence on the amplitudes b_n.

The choice of the parameter κ in Eqn (13) is alleviated by the fact that, within the range where $n \approx n_{\max}$, the parameter δt has virtually no influence on the amplitudes a_n. Thus, κ remains the only free parameter determining the amplitudes. A good agreement between the quantities $|f_n|^2$ calculated with the use of the formulas presented above and the results of numerical solution of the Schrödinger equation can be achieved by setting $\kappa = 2$. The influence of this coefficient increases with a decrease in the harmonic number and becomes noticeable, roughly, with $n = 45$. If this coefficient is set equal to zero, then the quantities $|f_n|^2$ with smallest numbers ($n = 13$, 15) are underestimated by 1–1.5 orders of magnitude. The quantity κ has no influence on the structure of intensity dependences of $|f_n|^2$.

By contrast, the parameter δt in Eqn (15) determines the structure of these dependences. If this parameter is set equal to zero, then the amplitudes a_n in the range where $n \leqslant 31$ are underestimated with respect to the amplitudes b_n. As it follows from Eqs. (5) and (9), oscillations in intensity dependences of $|f_n|^2$ become less pronounced in this case, nearly vanishing for n close to n_0. The value $\delta t = \hbar/I$ (which seems quite reasonable) corresponds to a deep modulation of the considered dependences up to $n = 13$ (the first harmonic with $n > n_0$), exerting virtually no influence on the form of the dependences under study for $n > 31$.

Closing this discussion, we should note that the conclusions of the above analysis are not quite applicable in the case of the highest order harmonic within the plateau. A more detailed analysis shows that, if Eqn (4) has the $(n+1)$th root, then $t_{ia}(n+1)$ should be replaced by $t_{ia}(n)$ in Eqn (14) for this harmonic. If such a root does not exist, then, in addition to the above-specified replacement, the amplitude f_n should be multiplied by $0.5^{1/2}$.

In the range of barrier-suppression ionisation, the formulas derived above become inapplicable. However, in what follows, we will also employ these formulas in the range of barrier-suppression ionisation. If this approach gives a complex coordinate z_{an} (z_{bn}), then such a coordinate is replaced by the coordinate $[e/E(t_{ia})]^{1/2}$ ($[e/E(t_{ib})]^{1/2}$).

Thus, our approach to the calculation of the amplitude of the nth harmonic involves two steps. First, we search for the roots τ_a and τ_b of the transcendental Eqn (4) within the interval $(0, T)$ and employ Eqs (1) and (2) to find the quantities t_{ia}, t_{ib}, t_{ra}, and t_{rb}. Then, we use Eqs (5) and (9)–(15), as well as similar formulas for the amplitude b_n. The results obtained with this approach will be referred to as analytical results.

4. Discussion of the results

In the range of tunnelling ionisation ($u < 0.004$ au), the analytic intensity dependences of $|f_n|^2$ derived above agree well with the results of numerical simulations for all the harmonics. Oscillation frequencies in these dependences coincide with an error of the order of 1 %, while the amplitudes differ by a factor not exceeding 1.5. Note that we calculate the phases (10) without any fitting parameters using formulas that are more reliable than expressions for the absolute values of amplitudes (the latter depend, in particular, on the ionisation probability, which is usually determined with a sufficiently large uncertainty).

In the range of barrier-suppression ionisation, the depth and the amplitude of oscillations in analytical dependences also agree fairly well with the results of numerical simulations. The frequency of oscillations is overestimated in this range. To achieve an agreement between analytical dependences and the results of numerical simulations in this range, we multiplied the phase difference $\phi_{an} - \phi_{bn}$ by a quantity $\alpha_n(u)$, deviating from unity for $u > 0.004$ au. Fig. 3 displays the dependences thus obtained for harmonics with the numbers $n = 15$, 25, 35, and 45 along with the numerically simulated dependences $|g_n(u)|^2$. The relation $\alpha_n(u) = 1 - 2.4n(u - 0.004)\Phi(u - 0.004)$, where Φ is the Heaviside step function, was used for $n = 15$, 25, and 35; $\alpha_{45}(u) = 0.62$. Fig. 2 presents the spectra of the force simulated numerically and calculated with the use of analytical formulas for the intensity of 0.0039 au.

Note that high-order harmonics are generated predominantly (or exclusively, for harmonic orders starting with $n = 49$) in the range of barrier-suppression ionisation. Nevertheless, no additional correction of our formulas for the amplitudes a_n and b_n (apart from the correction of their phases) was necessary for large n up to $n = 61$. For such harmonics, the factor (13) is close to unity and the parameter δt has virtually no influence on the ionisation rate (15). Therefore, the absolute values of the amplitudes a_n and b_n are estimated with virtually no fitting. Only near the edge of the intensity range used in our simulations, the plateau width grows noticeably slower with the increase in the in-

tensity, and analytical estimates for the amplitudes with $n > 61$ are overestimated as compared with the results of numerical simulations.

Although our analysis was performed for a hydrogen atom, it allows some obvious generalisations. It is important, in this respect, that this analysis has a clear structure, and the ionisation probability is the only quantity involved in the above-derived expressions that is highly sensitive to the properties of a specific atom. The ionisation probability in the tunnelling regime was analysed in [7, 9, 10] and in several other papers (which are usually devoted to the calculation of the ionisation probability averaged over the cycle; formulas for this quantity involve an additional factor $(3E/\pi E_0)^{1/2}$). Based on the results of these studies, we can extend the theory developed above to the case of multielectron atoms. For a helium atom, the above-derived formulas hold true without any changes.

In the range of tunnelling ionisation, the accuracy of the formulas derived in this paper for the amplitudes of high-order harmonics is much higher than the accuracy of the method of successive iterations. In addition, calculations with these formulas are much simpler than the procedure of successive iterations. Therefore, the formulas presented above seem to offer much promise for the analysis of complex problems related to high-order harmonic generation in macroscopic media, which require multiple amplitude calculations. Representation of a harmonic amplitude in the form of the sum (5) is especially useful in this case. The terms of this sum can be then interpreted [6] as two independent waves with different structures of wave fronts and different divergences. These wave fronts are determined by the dependences of the phases ϕ_{an} and ϕ_{bn} on the coordinates in a macroscopic space. Examples of the dependences of the phases ϕ_{an} and ϕ_{bn} on the intensity are presented in Fig. 4.

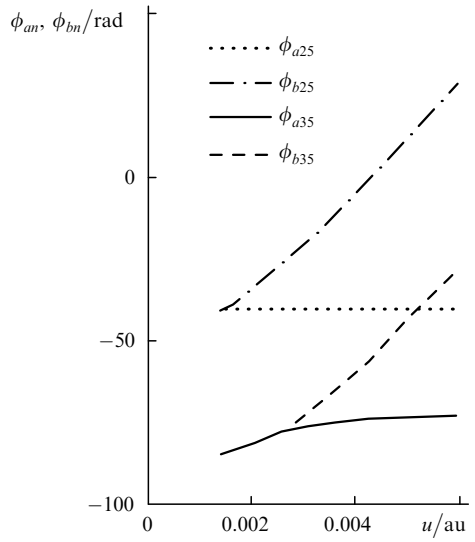

Figure 4. Phases ϕ_{an} and ϕ_{bn} calculated from Eqn (10) as functions of the pump-radiation intensity for $n = 25$ and 35.

5. Conclusions

Thus, the numerical solution of the Schrödinger equation allowed us to study the dependences of harmonics of the atomic response to the field of a light wave on the intensity of this light wave. Our analysis has shown that, in the case of pump radiation with a wavelength equal to 1.06 μm, these dependences display a deep modulation for all the harmonics starting from the 5th up to at least the 55th order (in the case of high-order harmonics, the depth of this modulation is close to 100 %).

We have performed a semiclassical analysis of high-order harmonic generation including several important additional factors. Analytical expressions derived for the amplitudes of high-order harmonics agree well with the results of numerical simulations in the range of tunnelling ionisation and provide a satisfactory agreement with numerical simulations in the range of barrier-suppression ionisation.

Acknowledgements. This work was supported by the Russian Foundation for Basic Research (Grant No. 96-15-96460, awarded to the S A Akhmanov and R V Khokhlov Scientific School on Coherent and Nonlinear Optics, and Grant No. 99-02-16489).

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