Channel-closing effects in high-order above-threshold ionization and high-order harmonic generation

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Abstract

The strong-field approximation, amended so as to allow for rescattering, is used to calculate high-order above-threshold ionization (ATI) spectra. The single-active-electron binding potential is modelled by a zero-range potential. The emphasis is on enhancements of groups of ATI peaks that occur for sharply defined laser intensities. The enhancements are traced to multiphoton resonance with the ponderomotively upshifted continuum threshold. Good agreement both with experimental data and with numerical simulations using the three-dimensional time-dependent Schrödinger equation for an optimized one-electron binding potential is observed. The physical reason for the close agreement of the results of the two, apparently so different, models is discussed. For quantitative agreement with the experimentally observed positions of the resonances, an ‘effective’ continuum threshold has to be introduced. The effects of focal averaging are evaluated and discussed. Resonant enhancement of high-order harmonic generation is also considered.

1. Introduction

The envelopes of electron spectra recorded in above-threshold ionization (ATI) \cite{1} by a linearly polarized laser field typically consist of two plateaux, one having a cutoff near \(2U_p\) and the other one near \(10U_p\) \cite{2,3}. Electrons contributing to the first plateau are often referred to as direct electrons since they leave the laser focus without further interaction with their parent ion. The second plateau, whose yield is lower by several orders of magnitude, is attributed to electrons that do undergo significant additional interaction, such as rescattering at the time when the laser field makes them return to their parent ion. This can be formalized in a classical
picture, which indeed predicts a maximal energy of $10U_P$ for an electron that backscatters around the time when the electric field of the laser goes through zero [4].

However, in addition to its cutoff, the second plateau displays a lot of structure which is beyond the reach of classical considerations. In particular, both experimental data [5, 6] and theoretical calculations [7–9] show occasional order-of-magnitude enhancements of groups of peaks, which occur upon a change of the laser intensity by just a few per cent. Also, model calculations for high laser intensity produce a plateau that consists of an irregular sequence of tops and sharp dips [10–12].

The theoretical calculations of Muller et al [7–9] are in the framework of the one-electron Schrödinger equation, employing an optimized binding potential. They produce spectra in remarkable agreement [13] with the experimental data. The agreement is excellent for the low-energy ATI peaks, but less so within the rescattering plateau. This allows one to draw the important conclusion that ATI is governed by one-electron dynamics, at least on the logarithmic scale on which both theory and data are usually presented. Scrutinizing the temporal evolution of the wavefunction of the atom in the laser field, Muller suggested that the aforementioned enhancements are related to multiphoton resonances with ponderomotively upshifted Rydberg states [8]. In some cases, in particular for the enhancements concerning the yields of electrons with rather low energy, one particular Rydberg state could be unambiguously identified as responsible [14]. In others, notably for the strong enhancement that for appropriate intensities dominates the middle of the plateau, this was not possible [14].

In this paper, we will advocate an alternative and—apparently—almost orthogonal explanation of the enhancements, which is conceptually much simpler. Namely, we will employ a binding potential of zero range and explore the consequences of ‘channel closings’. By a detailed comparison between Muller’s calculations involving an optimized one-particle potential comprised of a soft core plus the Coulomb tail and calculations employing a zero-range potential, we will conclude that, surprisingly, the latter closely simulates the former. Please note that a zero-range potential supports only one single bound state and no resonances in the continuum. Semiquantitative agreement between the two calculations can be achieved if the binding energy of the zero-range potential is slightly lowered so as to define an ‘effective onset’ of the continuum. Even though our zero-range calculations evaluate $S$-matrix elements, the formalism of ‘quantum orbits’ [15,16] allows us to investigate temporal aspects. Unexpectedly, this temporal behaviour shows many parallels to the evolution of Muller’s wavefunction. In a previous paper [17], we compared zero-range calculations to experimental spectra recorded for short laser pulses of about 50 fs. In this domain, individual Rydberg states have little significance, and the simple zero-range picture turned out to be perfectly suitable.

2. Ponderomotive energy and channel closings

In the presence of a sufficiently long laser pulse, the effective continuum threshold is raised by the so-called ponderomotive energy, which is the cycle-averaged wiggling energy of an otherwise free electron in the field of the laser with vector potential $A(t)$ and frequency $\omega$, that is

$$U_P = \frac{e^2 \langle A^2(t) \rangle_t}{2m} = \frac{e^2 \langle E^2(t) \rangle_t}{2mo^2}$$

(1)

where $\langle \cdots \rangle_t$ denotes the temporal average over one cycle. The physical reason for this raised threshold is simply that the state of lowest energy for an electron in the laser field is the one where it performs just this wiggling motion without additional drift momentum $p$ (the drift momentum is the one measured at the detector outside the laser field). Therefore, the ATI electron spectrum exhibits peaks at
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\[ E_n = \frac{p^2}{2m} = n\hbar \omega - U_P - |E_0| \] (2)

where \( E_0 \) is the ground-state energy of the atom whose Stark shift can be safely neglected. The high-lying Rydberg states, in most cases, are also upshifted approximately by the ponderomotive energy [18], provided the amplitude of the wiggling motion is smaller than the spatial extent of the Rydberg state in the absence of the laser field. Short-range and zero-range potentials have no Rydberg series below the continuum threshold.

According to equation (2), with increasing intensity, more and more photons are required for ionization. When the intensity has reached the precise magnitude where \( k \) photons are no longer sufficient and \( k + 1 \) photons are needed, that is when

\[ |E_0| + U_P = k\hbar \omega \] (3)

one speaks of the \( k \)-photon channel having closed. Near a channel closing, in view of equations (2) and (3), electrons can be released with very low drift momenta \( p \) (for \( n = k \)). This aspect will turn out to be crucial below.

Exactly at a channel closing, in view of equations (2) and (3), the electron spectrum has peaks at the energies

\[ E_n = \frac{p^2}{2m} = s\hbar \omega \] (4)

for integer \( s \), regardless of the intensity. In numerical simulations, Faisal and Scanzano [19] observed spikes at these energies in power-broadened ATI spectra for the direct electrons.

For a short-range binding potential, Wigner’s threshold law [20, 21] states that the cross section of a particular channel behaves like \( E^{l+1/2} \), when the excess energy \( E \) above the channel closing goes to zero (\( l \) denotes the angular momentum of the respective channel). Multiphoton channel closings have been observed for negative ions [22]. For \( l = 0 \), according to Wigner’s threshold law the respective channel closes with a vertical tangent. Via unitarity, such an abrupt channel closing must have implications for other channels as well [19, 23]. Indeed, calculations of high-order harmonic generation spectra as a function of the (fixed) laser intensity have demonstrated such effects. Experimentally, this is difficult to see since most experiments imply some average over the laser intensity.

3. Effects of channel closings

3.1. ATI spectra

In this section, we present calculated ATI spectra for a linearly polarized laser field, with the position of the detector in the direction of the laser’s electric field. All calculations employ a modified version of the strong-field approximation (SFA) such that one act of rescattering is accounted for. The SFA neglects the effect of the laser field on the initial bound state and the effect of the binding potential on the final state as well as the state in between ionization and rescattering [24]. Under these assumptions, the matrix element for ionization into a state with drift momentum \( p \) is given by [10]

\[ M_p = \int_{-\infty}^{\infty} dt_f \int_{-\infty}^{t_f} dt_i \langle \psi_p^{(Vv)}(t_f) | V U^{(Vv)}(t_f, t_i) V | \psi_0(t_i) \rangle. \] (5)

The atomic binding potential is denoted by \( V \), \( U^{(Vv)}(t, t') \) represents the Volkov propagator, \( |\psi_p^{(Vv)}(t)\rangle \) and \( |\psi_0(t)\rangle \) designate the final Volkov state and the initial field-free bound state, respectively. The physical significance of the integration variables \( t_f \) and \( t_i \) is discussed below.
in connection with the approximation of the matrix element (5) in terms of quantum orbits. Obviously, the calculations are significantly facilitated if the (regularized) zero-range potential is used as the binding potential as we will do throughout this paper. For this case, explicit evaluations of the matrix element (5) are given elsewhere \[10, 25\]. Comparison of the results based on the zero-range potential with more realistic calculations and experimental data sheds light on the physical origin of the phenomena that are and those that are not reproduced by using the zero-range potential.

The use of a zero-range potential to model the interaction of intense laser fields with negative ions dates back to the work of Berson \[26\] and Manakov and Rapoport \[27\] for circular polarization and of Manakov and Fainstein \[28\] for linear polarization, who concentrated on the quasi-energy of the ground state; see also \[29–32\]. Above-threshold detachment spectra for a finite pulse were calculated by Faisal \textit{et al} \[33\] and Filipowicz \textit{et al} \[34\]. However, they do not reach into the rescattering plateau, which is of central concern to this paper. A recent survey of the interaction of a negatively charged ion, modelled by the three-dimensional zero-range potential, with a laser field plus a static electric field was given by Manakov \textit{et al} \[35\].

Typical ATI spectra calculated from equation (5) for randomly chosen parameters all look very similar: at the end of the first plateau around $2U_P$, the yield drops steeply by several orders of magnitude down to the second plateau, viz the rescattering plateau. This consists of a sequence of well-developed broad round tops, which are separated by sharp dips. It terminates with one particularly noticeable top, usually the highest of all, near $10U_P$, after which the yields quickly drop. The higher the intensity of the laser field, the better developed are these features. They are caused by successively constructive and destructive interference of the contributing quantum orbits \[16, 25\].

A calculated spectrum typical of moderate laser intensity is displayed in figure 1. For various closely spaced intensities around $U_P = 2.526\hbar\omega$ (corresponding to an intensity of $I = 6.6 \times 10^{13}$ W cm$^{-2}$ and a Keldysh parameter $\gamma \equiv \sqrt{\langle E_0 \rangle/(2U_P)} = 1.37$), it shows the rescattering plateau of the ATI spectrum. The intensities are characterized by the dimensionless parameter $\eta = U_P/(\hbar\omega)$. The most eye-catching feature of the figure is the group of ATI peaks between 20 and 35 eV at its centre whose yields rise and fall by almost one order of magnitude, while the laser intensity changes by no more than 15%. This intensity range spans the $k = 12$ channel closing (as defined by equation (3)). Clearly, what is represented in figure 1 has the appearance of a resonance. At the same time, the low-energy part of the spectrum (the ‘direct’ electrons in the upper left) depends much more smoothly on the intensity; roughly, its yields just increase according to the lowest-order perturbation theory (LOPT) multiphoton order of 10. The part of the spectrum preceding the cutoff again displays a remarkable dependence on the intensity. Away from channel closings, the final maximum of the spectrum occurs at the energy $10U_P$, to an excellent approximation. For the five intensities considered in figure 1, we have $10U_P$ [eV] = 36.1, 37.6, 39.2, 40.7, 42.3, respectively. In contrast, inspection of the figure shows that the final maximum of the spectrum actually is located at 36.0, 38.3, 43.5, 42.1, 43.1 eV, respectively, as marked by the arrows. For $\eta \leq 2.3$ and again for $\eta > 2.8$, this maximum agrees with $10U_P$. In between, right at the channel-closing intensity, it performs a jump to higher energy. Such a jump has been observed in the experimental data too \[17\]. Also, for this intensity the yield is significantly lower than for adjacent intensities. All of these features are typical of even-order channel closings, irrespective of the binding energy and the laser frequency.

In figure 2 we investigate the consequences of the six channel closings ($k = 11, \ldots, 16$) in the ATI spectrum on a linear scale over a large range of intensities. Each trace corresponds to one particular ATI peak, and the order $n$ (as defined by equation (2)) is indicated on its left-hand side. The figure includes the $k = 12$ channel closing explored in figure 1. This is
Figure 1. Calculated ATI spectrum in the forward direction for a binding energy of \( E_0 = -0.54 \) au, \( \omega = 0.057 \) au, and various intensities characterized by \( \eta = U_p/\omega \) on either side of the \( k = 12 \) channel closing at \( \eta = 2.526 \). Arrows located at the final maximum of the spectrum identify the cutoff of the plateau. The calculation produces discrete peaks, marked by the full symbols. The full curves show the envelopes. For the two intermediate intensities corresponding to \( \eta = 2.426 \) and 2.626, only the envelopes are displayed.

Figure 2 explores the effects of the channel closings for high intensities. We take the example of helium, which we describe by a binding energy of 0.881 au. The laser frequency of \( \omega = 0.057 \) again corresponds to a Ti:Sa laser. According to equations (2) and (3), channel closings occur for \( \eta = k - 15.46 \). In figure 3, we investigate \( k = 36, 37 \) and 38. The Keldysh parameter (\( \gamma = 0.60 \) for \( \eta = 21.54 \)) definitely assigns this case to the tunnelling regime. The plateau displays a dramatic intensity dependence. A change of the intensity by 1% may cause a change of the yield of individual peaks by one order of magnitude, occasionally even more. For the two even-order channel closings, we observe enhancements that are very pronounced throughout the lower half of the plateau (between 100 and 200 eV) and less well developed between 260 and 290 eV. In the odd-order case, there is a marked enhancement between 100 and 160 eV, and no regular pattern elsewhere. There is hardly any effect of the channel closings
Figure 2. Left-hand panel: ATI peaks \( n = 23, \ldots, 37 \) (with \( n \) as defined in equation (2)) as a function of the field strength \( F \) in atomic units. Each ATI peak is represented by one trace (with its order \( n \) given on the ordinate) and plotted on a linear scale. In order to make this possible, the strong growth of the peaks with intensity was compensated by dividing their yields by the common factor \( \exp\left(-0.622/F-8.27\right) \). Vertical broken lines identify the channel closings with \( k = 11, 12, 13, 14, 15, 16 \) from left to right. The \( k = 12 \) channel closing is the one investigated in figure 1. The classical cutoff at \( E_n \approx 10U_p \) is visible in the pronounced humps in the left-hand (low-field) parts of the traces. It follows the parabola \( n = 11F^2/(4\omega^3) + |E_0|/\omega \). Right-hand panel: the full curve represents the total ATI yield (the sum over all peaks) in the direction of the laser field. The two broken curves are two different analytical fits to this curve, as indicated at the bottom. The (upper) broken curve is the fit used by Muller in figure 3 of [8] in a plot otherwise analogous to the left-hand panel. The (lower) chain curve is the fit that was used to normalize the peaks as presented in the left-hand panel. This fit underestimates the yields for high fields, and this shows by their strong growth in the upper right part of the left-hand panel. It was employed to provide a good representation of the low-field part of the spectrum.

on the spectrum for the direct electrons below about 70 eV (except for the ponderomotive shift of the individual peaks, which is hardly visible on the scale of the figure) and in the part of the spectrum preceding the cutoff (above about 300 eV, corresponding to energies larger than \( 8.5U_p \)). The suppression of the yield around the cutoff at the channel-closing intensities is no longer existent for the high intensities of figure 3.
Figure 3. Envelopes of ATI spectra in the direction of the laser field for $E_0 = -0.881$ au (corresponding to helium) and $\omega_0 = 0.057$ au. Three channel closings are explored: $k = 36$ (lower panel), 37 (middle panel), and 38 (upper panel). Each panel presents the spectrum for the channel-closing intensity (shaded in medium gray), and for one intensity below the former (light gray), and one above (dark gray). The intensities are identified by the corresponding values of $\eta$. $\eta = 21.54$ corresponds to $5.6 \times 10^{14}$ W cm$^{-2}$. This figure should be compared to figure 1 of [9].

3.2. Quantum orbits

For the convenience of the reader, first we want to summarize the gist of the quantum orbit description [15, 36] of ATI. The SFA $S$-matrix element (5) can be evaluated analytically up to one quadrature, which has to be carried out numerically. This procedure underlies figures 1–3. It takes less than a second per peak on a standard workstation. However, it is much more illuminating to evaluate it by means of the method of steepest descent. To this end, we introduce the expansion

$$U^{(V)}(t_f, t_i) = \int d^3k |\psi_k^{(V)}(t_f)\rangle\langle\psi_k^{(V)}(t_i)|$$

of the Volov propagator in terms of the Volkov states $|\psi_k^{(V)}(t)\rangle$. The resulting five-dimensional integral is over the time $t_i$ when the electron is ionized, the later time $t_f$ when it rescatters, and the drift momentum $k$ of its orbit in between these two times. We then determine those values of $t_f, t_i, k$ that render the entire phase of the integrand of equation (5) stationary. In general, there will be many solutions, which we number by $t_{fs}, t_{is}, k_s (s = 1, 2, \ldots)$. In terms of these solutions, the matrix element (5) can be expanded as
The quantity \( S_p(t_{fs}, t_{is}, k_s) \) in the exponent is the aforementioned phase. It is the classical action calculated along the electronic orbit specified by the parameters \( t_{fs}, t_{is} \) and \( k_s \). The coefficients \( a_s \) need not concern us here. The method is explained in detail in [16]. It is analogous to the approach used extensively in the analysis of high-order harmonic generation in the Lewenstein model [24]. The solutions \( t_{fs}, t_{is}, k_s \) are complex as a consequence of the electron’s tunnelling into the continuum. They can be classified according to the lengths \( \tau_s \equiv \text{Re}(t_{fs} - t_{is}) \) of their travel times. For each half period of the laser field, there is a pair of solutions such that \( sT/2 \leq \tau_s \leq (s + 1)T/2 \) (\( s = 1, 2, \ldots \)). The important point now is that in most cases the matrix element \( M_p \) is very well approximated by the four or six trajectories with the shortest travel times, shorter than two periods of the laser field [16]. However, this is not so near a channel closing.

For three of the intensities considered in figure 1—above, at, and below the channel closing at \( \eta = 2.526 \)—figure 4 shows several approximations to the calculated ATI spectrum of figure 1, such that the sum (7) extends over the trajectories of the first pair, the first three pairs and the first twenty pairs. The latter include travel times of up to ten periods of the field. In each case, the results of the exact integration of equation (5) are marked by full symbols. Off the channel closings, the first three pairs essentially reproduce the exact result5. At the channel closing, however, the approximation that incorporates three pairs is still off by half an order of magnitude. Note that the contribution of the pair with the shortest travel times displays no pronounced intensity dependence. The physical implication is that the contributions from orbits with longer and longer travel times conspire to add coherently at and only at the channel closings. For the closely related case of high-order harmonic generation, the slow convergence at the channel closings of the integration over the travel time in the analogous matrix element was noticed earlier [23]. The situation is much the same here: inspection of the integral (5) reveals that for even-order channel closings the first derivative of this integral with respect to either \( E_0 \) or \( U_P \) becomes divergent. For odd orders, this does not happen before the second derivative.

The expansion of the amplitude in terms of quantum orbits immediately explains why strong enhancements do not occur in the upper plateau: energies exceeding 8.7\( U_p \) can only be generated by the pair of orbits with the shortest two travel times. Their interference creates the well-developed final two humps of the spectrum. Each pair of quantum orbits has a simple and smooth intensity dependence and, consequently, when \( U_P \) increases by \( \Delta U_P \) this whole pattern just moves towards higher electron energy by 10\( \Delta U_P \). Sufficiently many orbits for an efficient constructive interference are only available below about 7\( U_P \) [16].

3.3. Comparison to numerical experiments

In this subsection we will compare the ATI spectra discussed above to those calculated by Muller [7–9] from a numerical solution of the three-dimensional time-dependent Schrödinger equation (3D TDSE) for a single active electron subject to the laser field and initially bound in a potential judiciously chosen for an optimal description of the respective atom. The latter typically includes a soft core and the long-range Coulomb potential.

5 Actually, the approximation to the exact result in terms of quantum orbits is less than satisfactory near the cutoffs, regardless of how many orbits are included. This is clearly visible near the cutoffs of the spectra displayed in figure 4. It points to a technical problem with the saddle-point approximation which is particularly noticeable for the comparatively low intensity that is considered here. This problem is discussed in [16].
Figure 4. Approximation of the spectrum of figure 1 by the first 2 (broken curve), 6 (chain curve) and 40 (full curve) quantum orbits. The full symbols denote the exact result from equation (5). The intensities include a subset of those in figure 1: above (upper frame), at (middle frame), and below the channel closing at $\eta = 2.526$.

For argon, figure 2 was set up so as to allow one an easy comparison with the right-hand panel of figure 3 of [8] which plots ATI electron spectra for the same binding energy and frequency in the same fashion. Two vertical structures dominate the middle of the latter figure which look very similar to the two channel closings for $n = 12$ and 13 in our figure 2, except for the fine structure which is absent in our results. All the same, for the intensity where the enhancement is maximal ($\eta = 2.526$), the respective group of peaks looks virtually identical to the corresponding 3D-TDSE result of Muller (figure 1 of [8]).

At this stage, an important point must be addressed. In our calculation for ‘argon’, we used $E_0 = -0.54$ au in place of the actual binding energy of argon, which is 0.58. Had we not done so, the enhanced spectrum would have looked much the same, but the enhancement would have occurred, in view of equation (3), at a different intensity. Essentially, the objective for lowering the continuum threshold is this: while the binding energy is, of course, well defined both for a Coulomb and for a zero-range potential (and, via equation (2), determines the positions of the ATI peaks), for the former a clear distinction between bound states and continuum states for practical purposes does not exist [37]. This is compounded in intense short laser pulses, where the higher Rydberg states acquire finite widths, owing both to ionization and to the short pulse length. The zero-range potential is specified by one single parameter, which usually
is adjusted so as to reproduce the binding energy of the real atom or ion in question. In the present case, in view of the above, it makes more physical sense to adjust it to a *bona fide* onset of the continuum of the real atom. The spectrum of the argon atom has a first noticeable gap at a binding energy of $-0.0397$ au. In view of this, we lowered the continuum threshold by this amount\(^6\). The price to be paid is an unphysical uniform shift in energy of all ATI peaks.

Solution of the TDSE allows one to inspect the process of photoelectron emission as a function of time. As discussed in [8], closer inspection of this time dependence reveals that electrons that will ultimately contribute to the enhanced peaks, after they have found their way into the continuum, stay close to the ion for several cycles of the field before finally moving away owing to rescattering, as if they were trapped in a resonant state in the continuum. In the zero-range SFA calculations, this is matched by the need, in the immediate vicinity of the channel closings, to include quantum orbits with exceptionally long travel times in the sum (7).

For helium, recent 3D-TDSE calculations [9, 41] at high intensity (585 TW cm\(^{-2}\)) show a resonant-like enhancement of the entire ATI plateau at intensities corresponding to the channel closings (3) with, however, $N$ replaced by approximately $N + 0.5$. As in previous calculations [7,8], the optimally chosen single-active-electron model binding potential contains both the Coulomb part and a short-range part. We now compare these calculations (specifically figure 1 of [9]) to the results of the SFA with the zero-range potential, shown in our figure 3. The two calculations share many features, such as the very existence of enhancements, and the fact that the latter are restricted to about the lower two-thirds of the plateau. There are some major discrepancies, too. Most notably, in the TDSE calculation the plateau is quite uniformly enhanced by about one order of magnitude, while the zero-range SFA exhibits a less pronounced and less uniform enhancement. Remarkably, the plateau generated by the TDSE calculation, in the resonant as well as in the nonresonant case, betrays no evidence of the interferences that are an ubiquitous feature of SFA calculations\(^7\).

As discussed before in the case of argon, another persistent and obvious discrepancy is related to where exactly the enhancements of the plateau electrons occur: precisely at the channel closings (3) in our SFA results or about halfway in between for the realistic simulation [9]. The calculations of figure 3 employed the nominal binding energy of helium. If, however, we proceed as in the case of argon we observe a first gap in the bound-state spectrum of helium at a binding energy of $-0.0154$. If we lower the continuum threshold accordingly, the channel-closing intensities move by $\Delta \eta = 0.4$, close to the intensities where they occur in the TDSE calculations.

### 4. Focal averaging

All spectra discussed thus far were made up by discrete peaks at the positions specified by equation (2). These positions depend, via the ponderomotive energy, on the laser intensity at the point in space and time where the electron is set free. Hence, averaging over the intensity distribution of the laser focus produces a continuous spectrum\(^8\). Of course, there are additional physical mechanisms that contribute to the continuous character of the spectrum, such as the finite laser pulse length. Below, we first present the technical details of carrying out a focal average and then consider the results of such calculations.

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\(^6\) Different rationales for what amount to lower the continuum threshold by were invoked in [44].

\(^7\) 3D-TDSE calculations of ATI in hydrogen at $10^{14}$ W cm\(^{-2}\) [38] show well developed interferences, too, which largely agree with the results of zero-range SFA calculations.

\(^8\) This statement does not hold for pulses that are long enough that electrons can escape on the side of the pulse [40].
4.1. Gaussian focal averages

Let \( \frac{d^4 N}{d^3 r \, dt} \equiv R(I) \) denote the number of electrons generated per volume and time at the constant intensity \( I \). Then, for a Gaussian beam with the intensity distribution

\[
I(\rho, z) = I_0 \left( \frac{w_0}{w(z)} \right)^2 \exp \left( -\frac{\rho^2}{w(z)^2} \right)
\]

(8)

where

\[
w(z) = w_0 \left[ 1 + \left( \frac{z}{z_0} \right)^2 \right]^{1/2}
\]

(9)

and \( w_0 = \sqrt{z_0/\pi} \) denotes the Rayleigh range, the rate of electrons generated within the focal volume is

\[
\frac{dN}{dt} = \int d^3r R(I(\rho, z)) = \frac{\pi w_0^2 z_0}{3} \int_0^{t_0} \frac{dI}{I^2} \sqrt{I_0 - I (2I + I_0)} R(I).
\]

(10)

This average is applicable for tight focusing. For short pulses, the average over the temporal pulse shape has to be considered, too. For a Gaussian pulse with temporal width \( \tau \), the intensity profile is

\[
I(\rho, z, t) = I(\rho, z) \exp \left( -\frac{(t - z/c)^2}{\tau^2} \right).
\]

(11)

The integrations over the Gaussian distributions can be carried out analytically, and the total number of electrons generated by the pulse is

\[
N = 2\pi \tau z_0 w_0^3 \int_0^{t_0} \frac{dI}{I} R(I) \int_0^{\zeta(I)} d\zeta (1 + \zeta^2) \left[ \ln \frac{I_0}{I(1 + \zeta^2)} \right]^{1/2}
\]

(12)

where \( \zeta(I) = \sqrt{I/I_0} - 1 \). For weak focusing, when the Rayleigh range is large compared with the diameter \( \bar{z} \) of the jet of atoms, the \( \zeta \) integration can be disposed of by putting \( \zeta = 0 \). This yields

\[
N = \pi \tau \bar{z} w_0^2 \int_0^{t_0} \frac{dI}{T} R(I) \left( \ln \frac{I_0}{I} \right)^{1/2}.
\]

(13)

Please note that the pulse length \( \tau \) only enters the result as a trivial constant of proportionality. Below, we will present examples of employing both the strong-focusing average (10) and the weak-focusing average (13).

4.2. Focal-averaged spectra

We will be concerned with the effects of focal averaging on the spectra of figure 1. First, we concentrate on the group of peaks between 20 and 30 eV, which suffers the resonant-like enhancement, and perform the temporal and radial average (13). The results are shown in figure 5. This is for the case of weak focusing and a comparatively narrow atomic jet. As a consequence, the peaks grow very quickly as soon as the peak intensity exceeds the channel-closing intensity of \( \eta = 2.526 \) (\( I = 6.58 \times 10^{15} \) W cm\(^{-2}\)). For such intensities (the top three traces of figure 5), the peaks occur at precisely the same energies, which are given by equation (4). This absence of any ponderomotive shifts reveals that each peak receives its contributions from one particular narrow intensity region, as is the case in the Freeman resonances of the direct electrons [42, 43]. The asymmetric form of the peaks—a slope much steeper on their left-hand than on their right-hand side—can be traced to the fixed-intensity spectra of figure 1: the enhancement reduces more quickly for intensities above the channel.
Figure 5. Focal average of a group of peaks of figure 1 for several peak intensities around the $k = 12$ channel closing, 6.91, 6.78, 6.65, 6.52, and $6.39 \times 10^{13}$ W cm$^{-2}$ from top to bottom. In the figure, they are identified by the corresponding values of $\eta$. The scale of the yields is linear. The spatio-temporal average was carried out by means of equation (13) at the position $z = 0$ of the focus. The figure ought to be compared with figure 2 of [6].

closing than below. Figure 1 also shows that this is no longer so for energies of 30 eV and higher, where, indeed, the peaks of figure 5 are symmetric. Starting at an energy of about 25 eV, a second series of comparatively broad peaks becomes manifest. According to figure 1, this series is related to the $10U_p$-cutoff region for $\eta = 2.3 \ldots 2.4$. Note that for higher intensities there is a pronounced interference dip in the energy region between 30 and 40 eV. As a consequence, the broad peaks show virtually no ponderomotive shift at all, acquiring all their contributions from intensities corresponding to $\eta \leq 2.43$. Moreover, the contrast of this part of the spectrum is rather low. When two (or, for higher intensities, more) series of peaks, each generated from one particular narrow intensity region and therefore exhibiting different ponderomotive shifts, contribute to the same electron-energy region, the resulting spectrum may look quite intricate. It may simulate structured peaks as they arise from mapping the Rydberg series on the various ATI peaks [42]. Moreover, in such a case the spectrum exhibits comparably low contrast. Similar intensity-dependent variations of contrast have been reported in [39].

The spectra of [6] exhibit a characteristic intensity-dependent substructure which appears to call for an analysis in terms of three series of peaks; see figure 2 of this paper for a particularly nice example. Such a structure seems outside of the scope of a zero-range potential model. Its origin is still uncertain: it is not reproduced by the 3D TDSE simulations, either [8, 13].

Figure 6 presents focal-averaged ATI spectra over a wider range of intensities. This time, the average is carried out according to equation (10) which is applicable for tight focusing and/or a narrow atomic jet. It is clear that enhancements for well-defined fixed intensities will manifest themselves in well-defined peaks at energies corresponding to the respective
The channel-closing enhancement that is the theme of figures 1 and 5 is developing in the two traces with the highest peak intensities. The uppermost trace displays three series of peaks, each characterized by its particular ponderomotive shift: one is the ‘resonant’ group around 25 eV discussed above, the other two correspond to the constructive interferences near the 10U/p threshold. One of them (around 42 eV) starts with η = 2.626 (cf figure 1) while the other one (around 35 eV) collects contributions up to η = 2.425. The fact that these two series are separated is due to the massive destructive interference between these two values, which affects the energy range between 30 and 40 eV. In general, the contrast of the spectra (that is, the normalized difference between the peaks and the valleys in between [39]) decreases as the intensity increases. The reason is that more than one series contributes such that the peaks of one series tend to fill the valleys of the other [39]. Channel closings play a prominent role in this process, but so do destructive interferences, whose occurrence is hard to predict.

5. High-order harmonic generation

In the semiclassical three-step model, for the two processes of high-order ATI and high-order harmonic generation the first two steps are identical. Therefore, it is suggestive that enhancements due to channel closings should also be operative in HHG. In fact, they have already been observed in calculations employing a zero-range potential [23, 45, 46].
past, any experimental observation of resonant-type enhancements was precluded by the use of Gaussian pulses, but a recent experiment in argon that employed a flat-top pulse did reveal a possibly related enhancement of the 13th harmonic [47]. This experiment was accompanied by a realistic calculation, which produced similar-looking features [47].

With this motivation, we display in figure 7 calculations of harmonic spectra in the context of the SFA and a zero-range binding potential [48,49] that illustrate the effects of channel closings. We observe a behaviour very similar to ATI: the lower half of the plateau experiences strong enhancements by up to two orders of magnitude when the intensity goes through a channel closing. The enhancements are, however, less uniform with respect to the harmonic order than in the case of ATI and may vary strongly from one order to the next. In contrast to the ATI spectra exhibited in figure 1, there is no evidence of the channel closings in the part of the spectrum before and beyond the cutoff. In contrast to the experiment, but in agreement with the calculations presented in the same paper [47], this enhancement disappears again as quickly as it sprang up, when the intensity keeps rising so that the conditions move away from the channel closing.

Since the enhancements mainly occur in the lower half of the plateau, where the Lewenstein model ceases to give a completely reliable description of high-order harmonic generation in atoms, these results cannot straightforwardly be related to experimental data. Investigations of the influence of the actual binding potential on the HHG enhancements will be reported elsewhere [50].

6. Conclusions

What is the relation between the enhancement of groups of ATI peaks for a zero-range potential that are due to channel closings and the similar-looking resonant-like structures calculated for a realistic binding potential? The similarity is puzzling since the zero-range potential, in
the absence of an applied field, does not support any excited states nor resonances in the continuum, while a potential of infinite range, owing to the presence of the Rydberg series below the continuum threshold, does not have well defined channel closings.

It appears that the element that is shared by both mechanisms is the accessibility of an intermediate state with a drift momentum near zero for certain sharply defined laser intensities which form a comb with the separation \( \Delta \eta \equiv \Delta U_p/(\hbar \omega) = 1 \). For the zero-range description, this is expressed by equation (2) which singles out the channel-closing intensities that satisfy equation (3) via a multiphoton resonance. For the more realistic Coulomb potential it is implied by the fact that highly excited Rydberg states may remain surprisingly stable in the presence of an intense laser field, just having the ponderomotive oscillation superimposed on the field-free orbit [18]. Such a state (or an appropriate superposition of such states) is preferentially populated if it is multiphoton resonant with the ground state. In either case, an electron in such a state is confronted with many recurring opportunities of rescattering. This can, but does not necessarily have to, lead to a constructive interference of many different pathways into the same final state.

The channel-closing condition (3) is of quantum-mechanical origin and cannot be rephrased in classical terms. Also, the quantum orbits discussed in section 3.2 each individually do not betray the presence of a channel closing. It is only their coherent superposition (7) that creates the sharply defined enhancements that are the object of this paper.

There are, in our opinion, two puzzles (at least) that remain unresolved. One concerns the case of helium and the very strong significance of a multiphoton resonance deep within the tunnelling regime, both in the zero-range SFA presented in this paper and in the Coulomb 3DTDSE description [9]. There is, unfortunately, no experimental evidence of resonant enhancements in the tunnelling regime; all experimental observations have been located within or at the border to the multiphoton regime. The other one is related to the general observation that a zero-range potential is able to afford such a realistic description not just of negatively charged ions in intense laser fields, but equally well of atoms. This is particularly surprising if one compares the classical orbits of electrons having tunneled out of an atom on their course back to the ion towards rescattering, in the presence or absence of the long-range Coulomb potential [51]. Coulomb refocusing caused by the latter is of decisive importance for the magnitude of the rescattering cross section while it appears to be much less significant for the shape of the electron spectrum.

The explanation in terms of channel closings projects the charm of simplicity. The quantum orbits of the zero-range potential are, in principle, accessible by analytical means while Rydberg states in the presence of an intense field are very delicate objects difficult to explore even by the most careful numerical procedures. One conclusion, however, appears to be safe: quantum mechanics plays a much more crucial role in high-order ATI than originally assumed.

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