Ionization in attosecond pulses: creating atoms without nuclei?

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**Abstract.** It is shown that with one full cycle of a suitable attosecond laser pulse it is possible to detach the ground-state electrons from an atom and deposit them, with their wavefunction largely unchanged, as a wavepacket removed spatially from the nucleus and whose centre of charge is stationary with respect to the nucleus.

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1. Introduction

The development of femtosecond lasers has allowed molecular vibrations to be studied in real time and manipulated by laser-pulse shaping. It is predicted that the development of attosecond lasers will allow a similar manipulation of electronic states. With a sufficiently strong laser pulse composed of a single cycle, it is possible to ionize fully a one- or more-electron atom or

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molecule. Here, we show that with suitable choice of the pulse parameters, the initial bound electronic wavepacket can be transported away from the nuclei, to leave it localized in free space, with zero velocity with respect to the nuclei and with minimal change of shape. The achievement of this is based on two separate properties required of short laser pulses. Firstly, by ‘short’ we imply a restriction to pulse durations much shorter than the characteristic orbital time of ground-state electrons. For the hydrogen atom this is about 24 as. Secondly, the two halves of the one-cycle laser pulse must interact coherently with the electrons, i.e. the electrons’ propagation over sufficiently short times must not destroy this coherence. Indeed, under these circumstances, the ‘clinical’ removal of the nucleus from an atom could also be achieved with pulses comprising of a few complete cycles, depending upon the pulse length.

To set the electrons free in space, the atom (in the following, for simplicity, we refer to atoms but the same can be achieved with small molecules) must be completely ionized in the first half-cycle. The dynamics of ionization in a strong, short laser pulse is completely different from that in a long, weaker pulse. Here strong means an electric field comparable to or greater than the typical nuclear field experienced by a bound electron.

We use atomic units throughout the paper: 1 atomic unit (au) of electric field strength is $5.14 \times 10^9$ V cm$^{-1}$, 1 au of time is 24.2 as, 1 au of laser intensity is $3.5 \times 10^{16}$ W cm$^{-2}$. For a weak field of long duration, the perturbation theory of the photo-effect applies; one photon of fixed energy is absorbed, producing a mono-energetic photo-electron. In this process, the transfer of momentum is negligible, since for visible light it is of the order of $10^{-3}$ au. This process is described by first-order perturbation theory and corresponds to a small probability of ionization, i.e. most occupation probability remains in the initial state. This is also true when several photons are absorbed, requiring higher-order perturbation theory. When the initially-ionized electron absorbs further photons (above-threshold ionization, ATI), the photo-electrons have well-defined energy and the momentum transfer is small. Also in this case of fields of intermediate strength, most population resides in the initial state at the end of the pulse.

For a strong short pulse, the perturbation picture of photo-ionization breaks down completely. In particular, the pulse time is insufficient to lead to a well-defined energy transfer. Rather, a broad spectrum of photo-electron energies is produced. The momentum transfer is non-negligible and, for strong fields, can amount to several atomic units. This is far larger than the mean momentum of a bound electron, which for hydrogen is $1/n$ in atomic units, where $n$ is the principal quantum number. Then, as in atomic collisions, it is this transfer of momentum to the bound electron that drives ionization. In contrast to the weak-field case, this ionization probability can reach 100%, so that a non-perturbative theory is required.

In the particular case of strong half-cycle pulses (HCPs) it has been known for some time that 100% ionization probability can be achieved. This has been demonstrated explicitly for ionization of electrons from Rydberg states [1]–[3] using existing pulses and predicted for the ground state of atoms [4]–[8] when pulses of sufficient strength and duration are available. References [9, 10] contain interesting discussion of the physics of the momentum transfer picture of ionization.

Here, we consider first, in section 2, the impulsive ionization of a one-electron atom, using the hydrogen atom for simplicity. Then in section 3 the theory is generalized to many-electron atoms and multiple ionization, where the added complication of electron–electron interaction must be taken into account. Here, we consider, as example, the complete ionization of the negative hydrogen ion. In section 4, we discuss the prospects for experimental realization of the ionization phenomena with attosecond pulses which are proposed here.
2. One-electron atoms

The theory of ionization by short, linearly polarized pulses is extraordinarily simple and can be described by the first Magnus approximation (FMA) [11, 12]. In the FMA, ionization is caused by an impulsive transfer of momentum \( q \) from the field to the atom as explained above. This momentum transfer is simply the total change of vector potential given as the time integral over the classical electric field \( F(t) \) of the laser, i.e.

\[
q(t) = \int_{0}^{t} F(t') \, dt'.
\]  

(1)

Then \( q(\tau) \), where \( \tau \) is the half-cycle time, is the total momentum transferred to the atom and is simply the total area under the pulse. It is clear that \( q \) is independent of the pulse shape and that a HCP can be represented simply as a \( \delta \)-function at the peak of the half cycle, i.e.

\[
F(t) = q \delta(t - \tau/2).
\]  

(2)

The transition amplitude \( a_{fi} \) from an initial state \( \Phi_i \) to any final state \( \Phi_f \) is given by the ‘momentum boost’ matrix element

\[
a_{fi} = \langle \Phi_f | \exp(-i q \cdot r) | \Phi_i \rangle.
\]  

(3)

The two equations (1) and (3) constitute the FMA which is the lowest-order term in a series representation of the exact time propagator [11, 12]. The FMA has as its condition of validity that the total pulse time is short compared to the electron orbital time in the initial state. Since the mean momentum in this state is of the order \( Z_{\text{eff}} = \sqrt{-2E_i} \), where \( E_i \) is the eigenenergy, it is easy to see that a momentum ‘kick’ with \( q > Z_{\text{eff}} \), i.e. \( \frac{1}{2} q^2 > -E_i \) will be sufficient to transfer the electron to the continuum. For \( q \gg Z_{\text{eff}} \) the electron will be transferred with 100% probability to the continuum. That this is indeed the case has been demonstrated for a HCP [7, 8] and the validity of the FMA confirmed by comparison with the exact numerical solution. For the hydrogen ground state with \( Z_{\text{eff}} = Z = 1 \) complete ionization occurs for \( q > 3 \) au. We will also show that after a HCP, the initial momentum space wavefunction remains unchanged in shape but is shifted to be centred around a mean momentum \(-q\). If the pulse ended after a half-cycle, then this initial state wavepacket would move quickly away from the nucleus. Unfortunately, a pure HCP is extremely difficult to produce and therefore here we concentrate on the subsequent manipulation of the ionized wavepacket on the second half cycle of a one-cycle pulse.

Clearly from equation (1), for one complete cycle the total momentum transfer is zero and, according to the FMA, the electron remains in its initial state after the pulse, even though it oscillates back and forth between initial (at full cycle) and ionized (at half cycle) states. However, the numerical results [7, 8] show that this is not so; for \( q \gg Z_{\text{eff}} \) an electron, fully ionized after the first HCP, has zero probability to return to the initial state following a second HCP. From equation (2) a full-cycle pulse (FCP) can be represented by two \( \delta \)-functions of opposite sign, separated by a time \( \tau \). This is shown in figure 1. Between these two momentum kicks the field is effectively switched off so that the electron propagates in the field of the atomic nucleus alone. It is this propagation that is neglected in the FMA. Inclusion of this propagation leads to the modified Magnus approximation (MMA) with, for one complete cycle, a transition probability amplitude

\[
a_{fi} = \langle \Phi_f | \exp(i q \cdot r) \exp(-i H_0 \tau) \exp(-i q \cdot r) | \Phi_i \rangle,
\]  

(4)
where $H_0$ is the atomic Hamiltonian. In [7, 8], it was shown that the MMA gives good agreement with transition probabilities obtained from converged fully-numerical calculations of the time-dependent wavefunction. Indeed, for the large $q$ values considered here, the influence of the nuclear field during propagation between the two $\delta$-functions can be ignored, i.e. the wavepacket is taken to propagate freely [13].

Since for large $q$ the initial state is depleted after one cycle and the electron does not return to the initial state, the question arises; where does the electron go? Here, we show that there is complete ionization on the first half-cycle, the electron then propagates freely until the second momentum kick, reversing the first, results, for appropriate choice of pulse parameters, in the reconstruction of the initial bound state wavefunction. This is separated spatially from the nucleus and stationary with respect to the nucleus. We use the word ‘stationary’ to indicate that the momentum expectation value is equal to zero after the interaction with the one-cycle pulse. That is, the nucleus has been removed clinically from the atom, without disturbing the initial-state distribution essentially. Of course one cannot neglect the spreading of the wavepacket between the two half-pulses. However, we show that by suitably choosing the pulse parameters and propagation time in the continuum, this wavefunction spreading can be suppressed, apart from initial $s$-state wavefunctions which are finite at the nucleus. This is because the high momentum components which spread most, are dominant in deciding the wavefunction at the origin in configuration space. Even for $s$-states, however, the probability distribution in configuration and in momentum space hardly changes during the short propagation time.

How the ionized wavepacket can be manipulated is simply understood with reference to figure 1 where we have calculated the electron wavefunction beginning in the hydrogen ground state and following successive time steps according to the transition matrix element equation (4) read from right to left. In figure 1, the real parts of the momentum space wavefunctions are shown, plotted as a function of $p_z = \mathbf{p} \cdot \hat{\mathbf{q}}$. The initial state is shown at time point A, before the...
Figure 2. The real part of the momentum wavefunction at time point D, defined in figure 1, taken with its final spatial position as the origin of space coordinates. The pulse duration corresponds to $\tau = 0.3$ au. The dashed curve is the initial wavefunction.

The first HCP, in figure 1(a) and has wavefunction $\langle p | \Phi_1 \rangle_i \equiv \langle p | \Phi_i \rangle_A$, where the subscript on the ket denotes the time point. At time point B, just after the first HCP, the wavefunction is unchanged in shape but shifted by the momentum transfer $-q$ to become $\langle p | \Phi_i \rangle_B = \langle p + q | \Phi_i \rangle_A$. Then, in the approximation of [13], there is free propagation until time point C, where the momentum space wavefunction becomes

$$\langle p | \Phi_i \rangle_C = \langle p | \exp(-iH_0\tau) \exp(-iq \cdot r) | \Phi_i \rangle_A \approx \exp \left(-i\frac{p^2}{2}\tau\right) \langle p + q | \Phi_i \rangle_A$$

(5)

In the above equation the phase acquired due to propagation from B to C has been decomposed into three terms: a constant phase $\exp(-iq^2/2)$, independent of $p$, which is omitted in the plots in the time points C and D, not only in figure 1 but also in figures 3–5; the energy phase $\exp(-i|p + q|^2\tau/2)$, which accounts for the spreading of a free wavepacket centred at momentum $p = -q$; the phase $\exp(i(p + q) \cdot q \tau)$ which corresponds to the shifting of the wavepacket in configuration space by $\Delta r = q \tau$. The dominant contribution comes from this last term. It is this phase that accounts for the oscillation seen in figure 1(c).

The second momentum kick $-q$ simply stops the propagation, i.e. the wavepacket becomes stationary in space (figure 1(d)) and the momentum space wavefunction at time point D becomes

$$\langle p | \Phi_i \rangle_D = \exp \left(-i\frac{q^2}{2}\tau\right) \exp \left(-i\frac{p^2}{2}\tau\right) \exp(i p \cdot q \tau) \langle p | \Phi_i \rangle_A.$$  

(6)

The phase translational factors are now those of a wavepacket centred at momentum $p = 0$. That is, up to the phases due to propagation, the momentum space wavefunction is unchanged by the FCP. This is illustrated in more detail in figure 2 where the real part of the momentum...
wavefunction at time point D is plotted without the oscillatory factor \( \exp(i \mathbf{p} \cdot \mathbf{q} \tau) \) due to spatial propagation and on a log plot. For small \( p \) this wavefunction is identical with the initial one, shown by the dashed line. However, for large \( p \) the wavefunction oscillates. This is simply due to the phase \( \exp(-i p^2/2 \tau) \) arising from the time propagation and clearly it is the high momentum components (the ‘fast’ electrons) which cause most spreading of the configuration space wavefunction.

In configuration space, the initial state at time point A is centred on the nucleus, at \( r = 0 \) of course. Figure 3(a) shows the hydrogen 1s wavefunction as a function of \( z = r \cdot \hat{q} \). After the initial momentum kick with \( q \gg Z_{\text{eff}} \) (equal to 1 for hydrogen) an oscillatory wavefunction \( \exp(-i \mathbf{q} \cdot \mathbf{r}) \Phi_1(\mathbf{r}) \) still centred on the nucleus (figure 3(b)) is produced (time point B after the first \( \delta \)-function pulse). Then comes a propagation of the wavepacket for a time \( \tau \) with momentum \( -\mathbf{q} \) to the time point C, just before the second HCP. The wavepacket then is centred at a point \( r = -\mathbf{q} \tau \). As remarked above, in [7, 8, 13] it was shown that for large \( q \) the nuclear potential can be neglected in this propagation, i.e. to good approximation the motion of the wavepacket is free. The configuration space wavefunction spreads a little during this time as can be seen in figure 3(c). The second HCP, in which the wavefunction is multiplied by \( \exp(i \mathbf{q} \cdot \mathbf{r}) \), acts coherently to remove the oscillations and, at time point D, after the second HCP, a wavepacket approximating the initial 1s wavefunction is obtained, see figure 3(d). The effect of spreading is to damp the wavefunction at the origin in configuration space, where a maximum occurs for an s-state. This is to be expected since the momentum space wavefunction is only altered for large momenta, see figure 2. However, when one plots the probability density, as in figure 3(e), which gives zero weight to the origin, one sees that the effect of wavepacket spreading is not so large.
That the effect of spreading affects the wavefunction only near the origin is illustrated in figures 3(f)–(j). Here, we consider an initial 2p wavefunction, which has a zero at the origin (as do all wavefunctions other than those of s-symmetry). One sees that during free propagation between time points B and C there is no perceptible change of the wavefunction. Then the second HCP faithfully reconstructs the initial wavefunction but now centred at \( r = -q \tau \), i.e. separated spatially from the nucleus and with mean momentum zero, i.e. the wavepacket becomes stationary in space. Hence, the net result at the end of the FCP (time point D in figure 3(i)) is a bare nucleus with the electron, in its initial wavefunction state, simply removed from it. The atom has been ‘filleted’ of its nucleus. This simple result is readily explained if the spreading of the wavepacket is ignorable, as appears to be the case for a 2p wavefunction. This is equivalent to making a ‘peaking’ approximation in which it is assumed that in the \( r \)-space integral in equation (4) only continuum states with momentum \( p = -q \) are important in the integrand. Then one can derive a remarkably simple form for the transition amplitude of equation (4). In this approximation \[14\] one has,

\[
a_{fi} = \int d^3r \Phi_1^* f(r) \Phi_1 (r + q \tau).
\] (7)

The peaking approximation is good when \( q \) is much greater than the momentum width of the wavepacket. Since this width is \( Z_{\text{eff}} \) one has again the condition \( q \gg Z_{\text{eff}} \).

3. Two-electron atoms

In the above, we claim that a single-electron atomic state can be transported away from its nucleus by a single-cycle attosecond pulse. Naturally the question arises, can one do this for few-electron atoms, or even small molecules? As we now show, the answer is a qualified ‘yes’. The additional complication arising (for simplicity, let us say, for two-electron atoms) is the omnipresent electron–electron repulsion, whose strength is unchanged, even when the wavepacket is at large separation, either in configuration or momentum space, from the nucleus. Now the atomic Hamiltonian \( H_0 \) in equation (4) contains the electron–electron repulsion \( V_{12} = 1/r_{12} \), where \( r_{12} = |r_1 - r_2| \), which cannot be ignored in the propagation from point B to C. However, retaining this term but making the same peaking approximation as before, the transition amplitude to a final two-electron state can be written \[14\]

\[
a_{fi} = \int d^3r_1 \Phi_1^*(r_1, r_2) \exp \left(-i \frac{\tau}{r_{12}} \right) \Phi_1 (r_1 + q \tau, r_2 + q \tau).
\] (8)

This result is interesting in that the finite time \( \tau \) between half pulses appears as an effective strength of the interelectronic repulsion. The larger \( \tau \), the stronger the interaction, corresponding to the expectation, on simple physical grounds, that the longer the time of propagation, the more the electrons will fly apart under their mutual repulsion. Nevertheless, we show in figure 4 that for sufficiently short \( \tau \) the effect of the repulsion remains small so that the two-electron initial wavefunction can be transported away from the nucleus effectively undisturbed. Clearly nothing will change if the two electrons are initially bound to more than one nucleus, e.g. the \( H_2 \) molecule, so that one should also be able to detach the electron wavefunction from small molecules as well.

The propagation of the \( H^- \) two-electron wavepacket is shown in figures 4 and 5. A correlated two-electron wavefunction (number 2 in table 1 of \[15\]) is used for the ground state. In figures 4(a)–(d) the wavepacket is shown at the time points A, B, C and D as in figure 1.
the wavefunction has six dimensions, cuts through the wavepacket must be made. In figure 4 the axes are chosen to be $z_1$ and $z_2$, where $z_{1,2} = r_{1,2} \cdot \hat{q}$, i.e. the projection of the electron coordinates along the field direction. Then for $z_1 = z_2$ the two electrons are collinear and both are aligned in a direction along or opposite to the field direction, which maximizes their mutual repulsion. In figure 4(a), we show the initial wavepacket at time point A. Note that, since we have a total s-state, the wavefunction maximizes at $r_1 = 0$ and $r_2 = 0$. Also noteworthy is that the electron correlation leads to higher amplitude for location in opposite directions than for collinear configuration of the two electrons where they are aligned in the same direction.

As in figure 1, shifting the wavepacket in momentum space by $-q$, following the first HCP, leads to oscillations arising from the factor $\exp(-i q \cdot r)$, as shown in figure 4(b). There then follows propagation in space for a time $\tau$ to give a wavepacket centred at $-q \tau$. Now however, in contrast to the one-electron case, at time point C, shown in figure 4(c), there appears a localized diminishing of the wavefunction along the line $z_1 = z_2$. This is just the effect of the electron repulsion acting for a time $\tau$ as expressed in equation (8). As shown in figure 4(d), after the second HCP, the initial wavefunction is reconstructed, centred at $-q \tau$, apart from the

Figure 4. The real part of the two-electron wavefunction for the $H^-$ initial state at points A–D in (a)–(d), respectively. The interelectronic angle is zero. The momentum transfer $q$ is equal to 10 au and the pulse duration $\tau$ is equal to 0.3 au.
narrow strip where the electrons have repelled each other. Figure 4 has been chosen to show
the absolute maximum effect of electron repulsion. In other cuts, where the electrons are not
collinear, the effect of repulsion is negligible. This is illustrated in figure 5 where the axes are
chosen such that the interelectronic angle is fixed at $\pi/4$ (figure 5(a)) or $\pi/2$ (figure 5(b)). Here,
only a small effect of the repulsion is to be seen near the centre of the wavepacket. For an angle
of $\pi$ (back-to-back emission), there is no influence of the repulsion as can be seen by comparing
the second and fourth quadrants on figure 4(a) with the same quadrants on figure 4(d). These
two quadrants correspond to a mutual angle of $\pi$. Hence, we conclude, as in the case of one
electron, that the whole two-electron initial wavepacket can be removed, essentially unaltered,
from the nucleus and brought to rest at a distance $q\tau$ away.

4. Possibility of experimental detection

Now, we discuss under what conditions the free ground-state wavepacket might be observed.
With the aid of measurement techniques such as COLTRIMS [16] it is possible to detect several
charged particles, e.g. nuclei and electrons, in coincidence. The completely symmetric FCP is
achievable in practice but then there is a problem with the subsequent time development of the
wavepacket. Once it is brought to a standstill by the second momentum kick, it will feel the
full nuclear field which, even at a separation of a few atomic units, will lead to an attraction
and subsequent re-scattering of the wavepacket (or even capture of one electron in the case
of a two-electron wavepacket) before it can be extracted. One might question, why use a full
cycle since after a half-cycle the continuum wavepacket is created with a large velocity with
respect to the nucleus and can move away quickly? Indeed this would be an ideal method
of extracting the wavepacket. Ionization of Rydberg states by HCP has been considered but
resulting wavepackets not detected. The problem is that, strictly speaking, a propagating HCP cannot be produced \cite{17}, since the time integral under the complete pulse must be zero. Rather, a FCP with a short strong first half-cycle followed by a much weaker, much longer second half cycle to compensate, is the best that can be achieved, see for example figure 1 of \cite{1}. The precise effect of such a second HCP on the wavepacket before extraction from the interaction region would have to be calculated. Here, we suggest that a slightly asymmetric FCP with a large momentum transfer on the first half cycle and a somewhat smaller one on the second half cycle can lead to extraction of the wavepacket with minimum change in its composition. Such a second half cycle would not stop the wavepacket, only slow it down, so that it could be extracted from the nucleus. It would also satisfy the conditions of validity of the MMA, so long as the major contribution to the time integral of the second HCP is contained in an initial time interval $\tau$. A pulse of this form certainly can be realized and would require only a very long weak tail (necessary to give total area zero under the FCP) on the second half cycle, which should not disturb the wavepacket appreciably. Again, however, the precise form of the measured wavepacket would depend on the dynamics of the extraction process and the detailed experimental conditions, which question is beyond the scope of this paper.

The second question concerns the prospects for availability of suitable lasers and how to achieve the pulse strengths and durations necessary for stripping the electron wavepacket from its initial bound state. Certainly the lasers necessary to do the experiments discussed above, ionization of the H atom or of both electrons from the H$^-$ ion, are not yet available as one needs lasers with half-cycle duration of an order of 10 as and intensities of the laser pulse of the order of at least $10^{18}$ W cm$^{-2}$. However, experiments could be performed with available lasers on more weakly-bound electrons. The excitation of Rydberg states with HCP has been discussed already \cite{1} and ionization experiments suggested here are certainly feasible. In the case of two electrons, one could employ as initial wavefunction the highly doubly-excited resonant states of He or H$^-$ \cite{18} which can have lifetimes of picoseconds. Alternatively, one could bring the pulses of existing lasers into the high-field attosecond regime by using relativistic ion beams as targets. In the moving frame of the ion beam the amplitude of the field is increased by a factor $\gamma(1 + \beta)$ and the pulse time shortened by the inverse of this factor. Since storage rings achieving a $\gamma$ of the order of 30 are envisaged, the fields and pulse times to remove both electrons from H$^-$ or even ionize the He$^+$ ion are realizable.

5. Conclusions

In summary, we have shown that a half-cycle attosecond pulse of sufficient strength can bring the ground-state wavepacket of one or more electrons into the continuum with large mean momentum. Over attoseconds the spreading of this wavepacket, even under the influence of electron–electron repulsion, is small, so that a second HCP can be used to control the wavepacket motion, either to halt it completely in space (and so create atoms without nuclei) or to slow it down for extraction by detector fields. The same ionization and control of ground-state wavepackets should be feasible for small molecules when suitable attosecond lasers are developed.

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