I. INTRODUCTION

In the last two decades multiphoton processes have been studied intensively, experimentally as well as theoretically. The inherent time-dependent nature of an atomic or molecular excitation process induced by a short laser pulse renders a theoretical description problematic in two respects. Firstly, a full quantum calculation in three dimensions requires a large computational effort. For this reason, quantum calculations have been restricted to one active electron in most cases \[1,2\]. Secondly, an intuitive understanding for an explicitly time dependent process seems to be notoriously difficult, exemplified by pertinent discussions about stabilization in intense laser fields \[3,4\]. Many studies have been carried out to gain an intuitive understanding of the two most prominent strong field phenomena, namely High Harmonic Generation (HHG) and Above Threshold Ionization (ATI). In the well established early analytical formulation by Keldysh, Faisal and Reiss the atomic potential is treated as a perturbation for the motion of the electron in a strong laser field \[5\].

This picture is still used in more recent models, where the classical dynamics of the electron in the laser field is explicitly considered, e.g. in Corkum’s rescattering model which can explain the cutoff observed in HHG for linearly polarized laser light in one spatial dimension \[6\]. The corresponding Hamiltonian reads \[7\].

\[
H = H_0 + E_0 f(t) x \sin(\omega_0 t + \delta), \tag{1}
\]

where \(H_0 = \frac{1}{2} p^2 + V(x)\) is the atomic Hamiltonian, \(f(t)\) is the time-profile of the laser pulse with maximum amplitude \(E_0\), and \(\omega_0\) is the laser frequency. The interaction of the electron with the atom is specified by the potential \(V\).

Lewenstein et al. extended Corkum’s rescattering idea to a quasiclassical model which contains one (relevant) bound state not influenced by the laser field on the one hand side and electrons which only feel the laser field on the other side \[8\]. This simple model explains qualitatively the features of HHG well. The same is also true for an alternative model, where the electron is bound by a zero-range potential \[9\]. However, the basic question if and to which extent these multiphoton processes can be understood semiclassically, i.e., by interference of classical trajectories alone, remains unanswered. It is astonishing that no direct semiclassical investigation of the Hamiltonian Eq. \(1\) has been performed while a number of classical as well as quantum calculations for Eq. \(1\) have been published. However, only recently, a semiclassical propagation method has been formulated which can be implemented with reasonable numerical effort. This is very important for the seemingly simple Hamiltonian Eq. \(1\) whose classical dynamics is mixed and in some phase space regions highly chaotic which requires efficient computation to achieve convergence. Equipped with these semiclassical tools we have studied multiphoton phenomena semiclassically in the framework of Eq. \(1\). In comparison to the exact quantum solution we will work out those features of the intense field dynamics that can be understood in terms of interference of classical trajectories.

The plan of the paper is as follows. In section II we provide the tools for the calculation of a semiclassical, time-dependent wavefunction. In section III we discuss Above-Threshold-Ionization (ATI) and work out the classical quantities which structure semiclassically the relevant observables. In section IV we use this knowledge for the description of Higher-Harmonic-Generation (HHG). Section V concludes the paper with a comparison of HHG and ATI from a semiclassical perspective and a short summary.
II. CALCULATION OF THE SEMICLASSICAL WAVE FUNCTION

A (multi-dimensional) wave function $\Psi_\beta(x,t)$ can be expressed as

$$\Psi(x,t) = \int_0^t dx' K(x,x',t) \Psi(x'). \tag{2}$$

Here, $\Psi(x')$ is the initial wave function at $t = 0$ and $K(x,x',t)$ denotes the propagator. We will not use the well-known semiclassical Van Vleck-Gutzwiller (VVG) propagator which is inconvenient for several reasons. Firstly, one has to deal with caustics, i.e. singularities of the propagator, and secondly, it is originally formulated as a boundary value problem. For numerical applications much better suited (and for analytical considerations not worse) is the so called Herman-Kluk (HK) propagator

$$K^{HK}(x,x',t) = \frac{1}{(2\pi \hbar)^n} \int dp dq C_{qp}(t) e^{i S_{qp}(t)/\hbar} g_\gamma(x;q(t),p(t)) g_\beta^*(x';q,p) \tag{3}$$

with

$$g_\gamma(x;q,p) = \left(\frac{\gamma}{\pi}\right)^{n/4} \exp\left(-\frac{\gamma}{2}(x-q)^2 + \frac{i}{\hbar} p (x-q)\right) \tag{4}$$

and

$$C_{qp}(t) = \left| \frac{1}{2} \left( Q_q + P_p - i \hbar \gamma Q_p - \frac{1}{i \hbar \gamma} P_q \right) \right|^2 \tag{5}$$

Each phase space point $(q,p)$ in the integrand of Eq. (3) is the starting point of a classical trajectory with action $S_{qp}(t)$. The terms $X_q$ in the weight factor $C_{qp}(t)$ are the four elements of the monodromy matrix, $X_q = \partial x_q/\partial y_i$. The square root in Eq. (3) has to be calculated in such a manner that $C_{qp}(t)$ is a continuous function of $t$. The integrand in Eq. (3) is – depending on the system – highly oscillatory. Although we restrict ourselves to one spatial dimension (see Eq. (3)) the number of trajectories necessary for numerical convergence can reach $10^7$. We note in passing that an integration by stationary phase approximation over momentum and coordinate variables reduces the HK-propagator to the VVG-propagator [3].

In all calculations presented here we have used a Gaussian wave packet as initial wave function,

$$\Psi_\beta(x') = \left(\frac{\beta}{\pi}\right)^{1/4} \exp\left(\frac{\beta}{2}(x' - q\beta)^2\right). \tag{6}$$

With this choice, the overlap

$$f_{\gamma\beta}(q,p) = \int g_\gamma^*(x';q,p) \Psi_\beta(x') dx' \tag{7}$$

can be calculated analytically and Eq. (3) reads together with Eq. (6)

$$\Psi^{HK}_\beta(x,t) = \left(\frac{4\gamma\beta}{\alpha^2}\right)^{1/4} \frac{1}{2\pi \hbar} \int dp dq e^{i S_{qp}(t)/\hbar} C_{qp}(t) g_\gamma(x;q(t),p(t)) f_{\gamma\beta}(q,p) \tag{8}$$

with $\alpha = \gamma + \beta$. For all results presented here we have taken $\gamma = \beta$.

For comparison with our semiclassical calculations we determined the quantum mechanical wave function using standard Fast Fourier Transform split operator methods [4].

III. ABOVE THRESHOLD IONIZATION

We start from Eq. (1) with $\delta = 0$ and use a rectangular pulse shape $f(t)$ which lasts for 4.25 optical cycles. This setting is very similar to the one used in [11].

The energy spectrum of the electrons can be expressed by the Fourier transform of the autocorrelation function after the pulse, i.e. for times $t > t_f$,

$$\sigma(\omega) = \text{Re} \int_{t_f}^\infty e^{i \omega t} \langle \Psi(t) | \Psi_f \rangle dt, \tag{9}$$

where $\Psi_f = \Psi(t_f)$ is the wave function after the pulse and correspondingly

$$|\Psi(t)\rangle = e^{i H_0(t-t_f)/\hbar} |\Psi_f\rangle \tag{10}$$

is calculated by propagating $\Psi_f$ for some time with the atomic Hamiltonian $H_0$ only after the laser has been switched off.

A. Quantum mechanical and semiclassical spectra for ATI

We will present results for two types of potentials to elucidate the dependence of the semiclassical approximation on the form of the potential.

1. Softcore potential

First we apply the widely used softcore potential [15,16]

$$V(x) = -\frac{1}{\sqrt{x^2 + a}} \tag{11}$$

with $a = 1$ and with an ionization potential $I_p = 0.670$ a.u.. We have checked that the correlation function differs little if calculated with the exact ground state or with the ground state wave function approximated
by the Gaussian of Eq. (8) where \( \beta = 0.431 \) a.u. and \( q_\beta = 0 \). However, the semiclassical calculation is considerably simplified with a Gaussian as initial state as can be seen from Eqs. (8-11). Therefore we use this initial state and obtain the propagated semiclassical wavefunction in the closed form Eq. (12). In Fig. 1 the quantum and semiclassical results at a frequency \( \omega_0 = 0.148 \) a.u. and a field strength \( E_0 = 0.15 \) a.u. are compared. The Keldysh parameter has the value 1.14. The quantum mechanical calculation (dotted line) shows a typical ATI spectrum. Intensity maxima with a separation in energy of \( \hbar \omega_0 \) are clearly visible. The first maximum has the highest intensity while the second maximum is suppressed.

![Intesity maxima with separation in energy of \( \hbar \omega_0 \)](image)

FIG. 1. Quantum mechanical (dotted line) and semiclassical (solid line) ATI spectra for the Hamiltonian of Eq. (1) with \( E_0 = 0.15 \) a.u., \( \omega_0 = 0.148 \) a.u. and the softcore potential Eq. (11).

The semiclassical result (solid line) is ambiguous: On the one hand there are clear ATI maxima with a separation of \( \hbar \omega_0 \). All peaks but the first one have roughly the correct magnitude. Again the second maximum is missing. On the other hand we see a constant shift (about 0.02 a.u.) of the spectrum towards higher energies. Therefore, a quantitative semiclassical description is impossible, at least with the present parameters and the softcore potential. Next, we will clarify whether the shift in the spectrum is an inherent problem of a semiclassical ATI calculation or if it can be attributed to properties of the softcore potential.

2. Gaussian potential

To this end we take a potential which has been used to model the “single bound state” situation mentioned in the introduction [17]. It is of Gaussian form

\[ V(x) = -V_0 \exp (-\sigma x^2) \]  \( (12) \)

With our choice of parameters \( V_0 = 0.6 \) a.u. and \( \sigma = 0.025 \) a.u., the potential contains six bound states and can be approximated, at least in the lower energy part, by a harmonic potential for which semiclassical calculations are exact. Hence, the semiclassical ATI spectrum with this potential should be more accurate if the discrepancies in Fig. 1 are due to the potential and not due to the laser interaction. The ground state wave function itself is again well approximated by the Gaussian Eq. (1) with \( \beta = 0.154 \) a.u. and \( q_\beta = 0 \). The laser has a frequency \( \omega_0 = 0.09 \) a.u., a field strength \( E_0 = 0.049 \) a.u., and a pulse duration of 4.25 cycles. The Keldysh parameter has the value 1.87.

![Quantum mechanical and semiclassical spectra for the Hamiltonian of Eq. (1)](image)

FIG. 2. Quantum mechanical (dotted line) and semiclassical (solid line) ATI spectra for the Hamiltonian of Eq. (1) with \( E_0 = 0.049 \) a.u., \( \omega_0 = 0.09 \) a.u. and the Gaussian potential Eq. (11).

We obtain a quantum mechanical ATI spectrum (dotted line in Fig. 3) with six distinct maxima. The semiclassical spectrum (solid line) is not shifted, the location of the maxima agrees with quantum mechanics. Hence, one can conclude that the softcore potential is responsible for the shift. The height of the third maximum is clearly underestimated and the details of the spectrum are exaggerated by the semiclassical calculation. Apart from these deviations the agreement is good enough to use this type of calculation as a basis for a semiclassical understanding of ATI.

B. Semiclassical interpretation of the ATI spectrum

1. Classification and coherence of trajectories

With the chosen parameters most of the trajectories ionize during the pulse (~92%). We consider a trajectory as ionized if the energy of the atom

\[ \epsilon(t) = p(t)^2/2 + V(q(t)) \]  \( (13) \)

becomes positive at some time \( t_n \) and remains positive, i.e. \( \epsilon(t) > 0 \) for \( t > t_n \). Typically, the trajectories ionize around an extremum of the laser field. Tunnelling can not be very important, otherwise the agreement between quantum mechanics and semiclassics would be much worse. The Keldysh parameter of 1.87 suggests
that we are in between the tunnelling and the multiphoton regime. Interestingly, the semiclassical description is successful although we are way below energies of the classically allowed over the barrier regime.

An obvious criterion for the classification of the trajectories is the time interval of the laser cycle into which their individual ionization time \( t_n \) falls, see Fig. 3. Typically ionization of trajectory happens around \( t_n = (2n-1)T/4 \) when the force induced by the laser reaches a maximum. Hence, the ionized trajectories can be attached to time intervals \( I_n = [(n-1)T/2, nT/2] \). In Fig. 3 we have plotted four trajectories from the intervals \( I_1 \) to \( I_4 \) which end up with an energy \( E = 0.36 \text{ a.u.} \). After ionization each trajectory shows a quiver motion around a mean momentum \( p_f \). One can distinguish two groups of intervals, namely those with trajectories ionized with positive momentum \( p_f \) (the intervals \( I_{2k-1} \)) and those with trajectories with negative \( p_f \) (the intervals \( I_{2k} \)). These two groups contribute separately and incoherently to the energy spectrum as one might expect since the electrons are easily distinguishable. One can see this directly from the definition Eq. (13) of the electron energy spectrum. For relative high energies \( \hbar \omega \) the (short-range) potential energy may be neglected in the Hamiltonian \( H_0 \) and we get

\[
\sigma(\omega) = \text{Re} \int_{t_f}^{\infty} e^{i\omega t} \langle \Psi_f | e^{-iH_0(t-t_f)} | \Psi_f \rangle \, dt
\]

\[
\approx \text{Re} \int_{0}^{\infty} e^{i\omega t} \langle \Psi_f | e^{-i\frac{p^2}{2\hbar}t} | \Psi_f \rangle \, dt
\]

\[
= \int_{-\infty}^{\infty} \delta (\omega - \frac{p^2}{2\hbar}) |\Psi_f(p)|^2 \, dp
\]

\[
= \left( |\Psi_f(-\sqrt{2\hbar\omega})|^2 + |\Psi_f(\sqrt{2\hbar\omega})|^2 \right) (\hbar/2\omega)^{1/2}
\]

\[
\equiv \sigma-(\omega) + \sigma+(\omega).
\]

Hence, to this approximation, the ATI spectrum is indeed given by the incoherent sum of two terms belonging to different signs of the momenta of electrons ionized in different time intervals as described above.

Figure Fig. 4(a) shows that Eq. (14) is a good approximation.

Only for small \( \omega \) the spectra do not agree, where the kinetic energy is comparable with the (neglected) potential energy.

Quantum mechanically, all contributions from trajectories which lead to the same momentum \( p_f \) of the electron are indistinguishable and must be summed coherently. To double check that the interference from different intervals \( I_n \) is responsible for the ATI peaks, we can artificially create a spectrum by an incoherent superposition \( \tilde{\sigma}_+ = \sigma_+ + \sigma_0 + \sigma_8 + \sigma_8 \) of contributions from trajectories ionized in the intervals \( I_2 \). This artificially incoherent sum (Fig. 4(b)) shows similarity neither with \( \sigma_+(\omega) \) nor with any kind of ATI spectrum.

2. Classical signature of bound and continuum motion in the laser field

The great advantage of an ab initio semiclassical description lies in the possibility to make dynamical behavior transparent based on classical trajectories, particularly in the case of explicit time dependent problems where our intuition is not as well trained as in the case of conservative Hamiltonian systems. The classical quanti-
ties enter semiclassically mostly through the phase factor
\[ \exp(i[S_{qp}(t) - p(t)q(t)]/\hbar) \equiv \exp[i\Phi/\hbar] \] (15)
which each trajectory contributes to the wave function Eq. (8). Although the prefactor \( C_{qp}(t) \) in Eq. (8) may be complex itself, the major contribution to the phase comes from the effective action \( \Phi \) in the exponent of Eq. (15). Figure 3 shows the energy \( \varepsilon \) of the atom and the accumulated phase \( \Phi \). One can recognize a clear distinction between a quasi-free oscillation in the laser field after the ionization and the quasi-bound motion in the potential. The latter is characterized by an almost constant averaged bound energy \( \langle \varepsilon(t) \rangle \) (Fig. 3(a)) of the individual trajectory giving rise to an averaged linear increase of the phase (Fig. 3(b)). After ionization the phase decreases linearly with an oscillatory modulation superimposed by the laser field. The almost linear increase of \( \Phi \) without strong modulation of the laser field during the bound motion of the electron is remarkable, particularly looking at the laser induced modulations of the bound energy seen in Fig. 3(a). The averaged slope of the phase (positive for bound motion, negative for continuum motion) corresponds via \( d\Phi/dt = -E \) to an averaged energy. The behavior can be understood by a closer inspection of the action
\[ \Phi(t) \equiv S_{qp}(t) - p(t)q(t) = \int_{0}^{t} (2T - H - \dot{p}(\tau)q(\tau) - \dot{q}(\tau)p(\tau))d\tau - qp . \] (16)
Here, \( T = \frac{p^2(t)}{2} \) refers to the kinetic energy and \( H \) to the entire Hamiltonian of Eq. (8), the dot indicates a derivative with respect to time, and \( q \equiv q(t = 0) \). With the help of Hamilton’s equations and a little algebra \( \Phi \) from Eq. (16) can be simplified to
\[ \Phi(t) = -\int_{0}^{t} \left( \varepsilon(\tau) - \frac{q(\tau)DV}{dq} \right) d\tau \] (17)
where \( \varepsilon \) is the atomic energy Eq. (13). With Eq. (17) we can quantitatively explain the slope of \( \Phi \) in Fig. 3(b). For the low energies considered the potential Eq. (14) can be approximated harmonically,
\[ V(q) \approx -V_0 + V_0 \sigma q^2 \] (18)
Averaging \( \Phi \) over some time yields then \( \Phi(t) \approx \Phi_0 \), for any bound energy of a classical trajectory since for an oscillator averaged kinetic and potential energy are equal. Indeed, the numerical value for the positive slope in Fig. 3(b) is 0.6 a.u. in agreement with the value for \( \Phi_0 \).

For the ionized part of the trajectories we may assume that the potential vanishes. The corresponding solutions for electron momentum \( p(t) \) follows directly from Hamilton’s equation \( \dot{p} = -E_0 \sin \omega_0 t \),
\[ p(t) = \frac{E_0}{\omega_0} \cos(\omega_0 t) + p, \] (19)
where \( p \) is the mean momentum. Without potential the phase from Eq. (17) reduces to \( \Phi(t) = -\int p^2(\tau)/2 d\tau \) and we obtain with Eq. (19)
\[ \Phi_p(t) = -\frac{U_p}{2\omega_0} \sin(2\omega_0 t) - \frac{E_0 p}{\omega_0^2} \sin \omega_0 t - (U_p + p^2/2) t \] (20)
with the ponderomotive potential \( U_p = E_0^2/4\omega_0^2 \). We note in passing that Eq. (20) is identical to the time dependent phase in the Volkov state (see the appendix).

3. Semiclassical model for ATI

FIG. 5. Part (a) shows the atomic energy \( \varepsilon = p^2/2 + V(q) \) as a function of time for three trajectories from the intervals \( I_2 \) (dashed line), \( I_4 \) (dotted line) and \( I_6 \) (dashed-dotted line). Part (b) shows the corresponding phases \( \Phi(t) \).

The clear distinction between classical bound and continuum motion in the laser field as demonstrated by Fig. 3 and illuminated in the last section, allows one to derive easily the peak positions of the ATI spectrum. Moreover, this distinction also supports the so called strong field approximation (e.g. \( \Phi_{ph} \)) where electron dynamics in the laser field is modelled by one bound state and the continuum. While this is postulated in \( \Phi_{ph} \) as an approximation and justified a posteriori by the results the corresponding approximation is suggested in the present context of a semiclassical analysis by the full classical dynamics, i.e., the behavior of the trajectories, as shown in Fig. 3(b). There, we have seen that each classical bound motion leads to the characteristic linear increase of the phase. If the entire phase space corresponding to the initial (ground state) wave function is probed with many trajectories of different energy, the dominant contribution will appear at the bound state energy which implies
\[ \Phi_{bs}(t) \approx I_p t , \] (21)
where \( I_p \) is the ionization potential. The time for which a trajectory does not fall into one of the two classes, bound or continuum, is very short (Fig. 3). Hence, we can approximately compose the true phase \( \Phi = \Phi_b + \Phi_c \). However, we don’t know for an electron with mean momentum \( p \) when it was ionized. Hence, we have to sum over all trajectories with different ionization times \( \tau \) but equal final momentum \( p = p_f \) which leads to the propagated wavefunction

\[
\Psi_f(t, p) \sim \int_0^t d\tau \exp[i(\Phi_b(\tau) + \Phi_c(t) - \Phi_c(\tau))]
\]

\[
\sim \sum_{n,m} J_n \left( \frac{E_0 p}{\omega_0} \right) J_m \left( \frac{U_p}{2\omega_0} \right) \int_0^t d\tau e^{i\Delta_{mn}/\hbar}, \tag{22}
\]

where the phase \( \Delta \) is given by

\[
\Delta_{mn} = I_p + U_p + p^2/2 - (n + 2m)\hbar\omega_0. \tag{23}
\]

From Eq. (23) and Eq. (22) follows that ATI peaks appear at integer multiples \( n\hbar\omega_0 \) of the laser frequency, when

\[
\frac{p^2}{2} = n\hbar\omega_0 - I_p - U_p. \tag{24}
\]

One can also see from Eq. (22) that the ATI maxima become sharper with each optical cycle that supplies ionizing trajectories. Of course, this effect is weakened by the spreading of the wavepacket hidden in the prefactor of each trajectory contribution (see Eq. (3)) not considered here.

Trajectories that are ionized during different laser cycles accumulate a specific mean phase difference. The phase difference depends on the number \( k \) of laser cycles passed between the two ionization processes:

\[
\Delta\Phi(p) = kT \left( I_p + \frac{p^2}{2} + U_p \right). \tag{25}
\]

The trajectories interfere constructively if

\[
\Delta\Phi(p) = 2\pi l \Rightarrow \frac{1}{2} p^2 = \frac{l}{k} \omega_0 - I_p - U_p. \tag{26}
\]

If an energy spectrum is calculated exclusively with trajectories from two intervals separated by \( k \) cycles there should be additional maxima in the ATI spectrum with a distance \( \hbar\omega_0/k \).

As a test for this semiclassical interpretation of the ATI mechanism we have calculated three spectra with trajectories where the mean time delay between ionizing events is given by \( \Delta t = T \), \( \Delta t = 2T \) and \( \Delta t = 3T \). For the spectrum Fig. 6 (a) we have used exclusively trajectories from the intervals \( I_2 \) and \( I_4 \) (\( \Delta t = T \)). One can see broad maxima separated by \( \hbar\omega_0 \) in energy. Trajectories from the intervals \( I_2 \) and \( I_6 \) (see Fig. 6 (b)) form a spectrum where the maxima are separated by \( \hbar\omega_0/2 \) – as predicted for \( \Delta t = 2T \). In analogy the separation for the ATI maxima in a spectrum with trajectories from the intervals \( I_2 \) and \( I_8 \) is given by \( \hbar\omega_0/3 \) (Fig. 6 (c)). The interference of trajectories ionized in many subsequent cycles suppresses the non-integer maxima according to Eq. (23). If the field strength is high enough the atom is completely ionized during the first cycle. The opportunity for interference gets lost and we end up with an unstructured energy spectrum.

![FIG. 6. Semiclassical spectra calculated with trajectories from the intervals \( I_2 \) and \( I_4 \) (a), \( I_2 \) and \( I_6 \) (b), and \( I_2 \) and \( I_8 \) (c).](image)

In an extreme semiclassical approximation we would have evaluated the integral in Eq. (22) by stationary phase. The condition

\[
d/d\tau[\Phi_b(\tau) - \Phi_c(\tau)] = I_p + p^2(\tau)/2 = 0 \tag{27}
\]

leads to complex ionization times \( t_n \) whose real part is periodic and allows for two ionizing events per laser cycle, close to the extrema of the laser amplitude. The derivation is simple but technical, therefore we don’t carry it out explicitly here. However, it explains the observation that ionization occurs close to the extrema of the laser field and it also makes contact with the tunnelling process often referred to in the literature since the complex time can be interpreted as tunnelling at a complex "transition" energy.

Clearly, our semiclassical analysis as described here supports the picture which has been sketched in interpreting a quantum calculation. The authors assume that wave packets are emitted every time the laser reaches an extremum. The interference of the different wave packets gives rise to the ATI peaks.

In the following we will discuss the process of higher harmonic generation (HHG) which is closely related to ATI. In fact, the separation into a bound and continuum
part of the electron description is constitutive for HHG as well, the prominent features, such as cutoff and peak locations, can be derived from the same phase properties Eq. (22) as for ATI. However, there is a characteristic difference, how these phases enter.

IV. HIGH HARMONIC GENERATION

First, we briefly recapitulate the findings of [21], where we have calculated the harmonic spectrum with the soft-core potential Eq. (11). With our choice of \( \alpha = 2 \) the ionization potential is given by \( I_p = 0.5 \text{ a.u.} \). The laser field has a strength \( E_0 = 0.1 \text{ a.u.} \), a frequency \( \omega_0 = 0.0378 \text{ a.u.} \) and a phase \( \delta = \pi/2 \). The initial wave packet with a width of \( \beta = 0.05 \text{ a.u.} \) is located at \( q_\beta = E_0/\omega_0^2 = 70 \text{ a.u.} \). Note, that the cutoff energy \( E_C \) in such a symmetric laser scattering experiment is given by

\[
E_C = I_p + 2U_p. \tag{28}
\]

From the dipole acceleration (see Fig. 7)

\[
d(t) = - \left\langle \Psi(t) \left| \frac{dV(x)}{dx} \right| \Psi(t) \right\rangle, \tag{29}
\]

follows by Fourier transform

\[
\sigma(\omega) = \int d(t) \exp(i\omega t) \, dt \tag{30}
\]

the harmonic power spectrum (see Fig. 8).

![Graph](image)

FIG. 7. Quantum (a) and semiclassical (b) dipole acceleration of higher harmonics according to Eq. (29).

Clearly, our semiclassical approach represents a good approximation. The dipole acceleration shows the characteristic feature that fast oscillations (which are responsible for the high harmonics in Fourier space) show only up after some time, here after \( t = T \). This is the first time where trajectories are trapped. Trapping can only occur if (i) \( t_n = nT/2 \), (ii) the trajectories reach a turning point (i.e. \( p(t_n) = 0 \)), and (iii) if at this time the electron is close to the nucleus (\( q(t_n) \approx 0 \)). The trapped trajectories constitute a partially bound state which can interfere with the main part of the wavepacket (trajectories) still bouncing back and forward over the nucleus driven by the laser. The group of briefly bound (i.e. trapped or stranded) trajectories can be clearly identified, either by their small excursion in space (Fig. 8a) or by the positive slope of their action (Fig. 8b) as it was the case for ATI (compare with Fig. 5). By artificially discarding the initial conditions in the semiclassical propagator which lead to trapped trajectories one can convincingly demonstrate that the plateau in HHG generation is a simple interference effect [21]. Here, we are interested firstly in linking ATI to HHG by using the same separation in bound and continuum parts of the dynamics already worked out for ATI. Secondly, we want to go one step further and construct a wavefunction based on this principle.

Semiclassically, we have to look first at the phases of the observable. Therefore, we define a linear combination for the wavefunction from the respective phase factors for bound and continuum motion. Considering only terms in the exponent the harmonic spectrum Eq. (30) reads simply
FIG. 9. Examples for direct (solid line), trapped (dotted line), and stranded (dashed line) trajectories, see text.

\[ \sigma(\omega) \sim \int dt \exp(i\omega t) \| \exp(i\Phi_b(t)/\hbar) + c \exp(i\Phi_c(t)/\hbar) \|^2, \quad (31) \]

where \( c \neq 0 \) is a (so far) arbitrary constant. In principle, \( c = c(t) \), however its change in time is much slower than that of the optical oscillations of the phases \( \Phi(t) \), hence we may approximate \( c \) by a constant. The bound and continuum phases, \( \Phi_b \) and \( \Phi_c \), are defined in Eq. (21) and Eq. (20), respectively. For \( \Phi_c \) we have \( p = 0 \), since this is the dominant contribution from the center of the wavepacket which was initially at rest. The result is shown in Fig. 10. Indeed, the plateau with the harmonics is generated, however, the initial exponential decrease is missing since we have neglected all prefactors of the semiclassical wavefunction which describe the dispersion of the wavepacket.

FIG. 10. Harmonic spectrum according to Eq. (31).

Consequently, one can evaluate Eq. (31) in stationary phase approximation. The integrand of Eq. (31) becomes stationary if

\[ \frac{d}{dt} [\hbar\omega t \pm (\Phi_b(t) - \Phi_c(t))] = 0 \quad (32) \]

which happens at

\[ \hbar \omega = 2U_p \sin^2(\omega t) + I_p. \quad (33) \]

From Eq. (33) we conclude the cut-off law

\[ \omega_{\max} = 2U_p + I_p, \quad (34) \]

as expected for laser assisted electron ion scattering [21]. Using the same expansion into Bessel functions as in Eq. (22) we obtain for the spectrum Eq. (31):

\[ \int dt \exp\left(\frac{i}{\hbar} \left[ \hbar\omega - U_p - I_p \right] t + \frac{U_p}{2\omega_0} \sin(2\omega_0 t) \right) \] \[ = \sum_{k=-\infty}^{\infty} \int dt e^{it(\Delta \omega - 2k\hbar\omega_0)/\hbar} J_k \left( \frac{U_p}{2\hbar\omega_0} \right). \quad (35) \]

Therefore, we see maxima in the harmonic spectrum for

\[ \hbar \omega_k = U_p + I_p - 2k\omega_0. \quad (36) \]

We can go one step further and construct a full time-dependent wavefunction from this semiclassical approximation, namely

\[ \Psi(x, t) = \Psi^{sc}(x, t) + c \Psi_0(x) \exp(itI_p/\hbar). \quad (37) \]

Here, \( \Psi_0(x) \exp(itI_p/\hbar) \) is the time dependent ground state wave function (without the laser field) and \( \Psi^{sc}(x, t) \) is a (semiclassical) wavepacket in the laser field but without potential. Calculating the dipole acceleration and the resulting harmonic spectrum with this wavefunction leads to a remarkably good approximation of the true quantum spectrum (compare Fig. 8 with Fig. 11). The dispersion of the wavepacket leads to the lower plateau compared to Fig. 10.

FIG. 11. Harmonic spectrum, generated from the wavefunction Eq. (37) with \( c = 0.025 \) and \( \beta = 0.05 \) a.u.

V. CONCLUSIONS
A. Semiclassical comparison between ATI and HHG

Clearly, the main structure such as the plateau, cutoff (HHG) and the occurrence of peaks and their separation in energy (ATI and HHG) is a property of the difference of the classical time-dependent actions $\Phi_b(t) - \Phi_c(t)$ alone.

However, the HHG power spectrum Eq. (30) is an integral over all the time for which the electron wavepacket is exposed to the laser field. In contrast, the ATI spectrum is obtained in the long-time limit $t \to \infty$ after the laser has been switched off. This difference may explain why the HHG results tend to be better than the ATI results semiclassically: Any semiclassical approximation (which is not exact) become worse for large times.

A second point refers to the fact that the characteristic phase difference $\Phi_b(t) - \Phi_c(t)$ appears already in the wavefunction Eq. (22) for ATI, while for HHG it occurs only in the expectation value Eq. (23). However, this difference is artificial, since the expectation value, or better its Fourier transform the power spectrum, is not the observable of higher harmonic radiation. The correct expression is the dipole-dipole correlation function $R$ which can be approximated as $R \propto |\sigma(\omega)|^2$ under single atom conditions or in the case of an ensemble of independent atoms which radiate [1922]. Hence, in both cases, ATI and HHG, the peak structure appears already on the level of the quantum amplitude (or wavefunction) and is amplified in the true observable.

B. Summary

We have given a time-dependent fully semiclassical description of multiphoton processes. The prominent ATI and HHG features emerge naturally from properties of the classical trajectories whose contributions to the semiclassical wavefunction interfere semiclassically. Any effect of this semiclassical interference can be double-checked by disregarding the phases. This leads (with the same trajectories) to a classical observable. As we have seen, to a good approximation the classical action for an individual trajectory can be composed of one part $\Phi_b$ for the time the electron is bound (disregarding the laser field) and of another part $\Phi_c$ for the time the electron is in the continuum (disregarding the atomic potential). The relevant phase difference $\Phi_b - \Phi_c$ leads in both cases, ATI and HHG, to the prominent harmonic structures in terms of the laser energy $\hbar \omega_0$. Finally, we have been able to construct a simple wavefunction for higher harmonics generated in laser assisted scattering. Its key element is an explicitly time-dependent wavepacket of the electron under the influence of the laser field. Starting from an initial Gaussian distribution localized in space the wavepacket disperses in time providing the correct decrease of the intensity of the lower harmonics and in turn the correct height of the plateau.

Financial support from the DFG under the Gerhard Hess-Programm and the SFB 276 is gratefully acknowledged.

APPENDIX:

We want to calculate the semiclassical wave function of a free particle in a laser field according to Eq. (2). A particle in a laser field $V_L(x, t) = E_0 \sin(\omega t)$ moves with

\begin{align}
  p(t) &= p + \frac{E_0}{\omega} \cos(\omega t) \equiv p + \bar{p}(t) \\
  q(t) &= q + pt + \frac{E_0}{\omega^2} \sin(\omega t) \equiv q + pt + \bar{q}(t)
\end{align}

The weight factor $C_{qp}(t)$ is given by

\begin{equation}
  C_{qp}(t) = \left(1 - \frac{ih\gamma}{2} t\right)^{\frac{1}{2}}.
\end{equation}

For the phase factor $S_{qp}(t) = p(t)q(t)$ we get:

\begin{align}
  S_{qp}(t) &= - \frac{U_p}{2\omega} \sin(2\omega t) - U_p t \\
  &= - \frac{p^2}{2} \bar{q}(t) - q \bar{p} \tag{A4}
\end{align}

Evaluating Eq. (3) with the stationary phase approximation, which is exact for quadratic potentials, leads to the condition that

\begin{equation}
  f(q, p) = \frac{i}{\hbar} \left( x p(t) - \frac{p^2}{2} - \bar{q}(t) p - \frac{\gamma}{\alpha} q p - \frac{\beta}{\alpha} q p \right) \\
  - \frac{\gamma}{2} (x - q(t))^2 - \frac{\gamma \beta}{2 \alpha} (q - q_\beta)^2 - \frac{1}{2 \hbar^2 \alpha} p^2
\end{equation}

must have an extremum. With

\begin{align}
  \frac{\partial f}{\partial q} &= 0 = \gamma [x - q(t)] - \frac{\gamma \beta}{\alpha} (q - q_\beta) - \frac{i}{\hbar} \frac{\gamma}{\alpha} p \\
  \frac{\partial f}{\partial p} &= 0 = \gamma [x - q(t)] t - \frac{1}{\hbar^2 \alpha} p \\
  + \frac{i}{\hbar} \left( x - p t - \bar{q}(t) + \frac{\gamma}{\alpha} q - \frac{\beta}{\alpha} q \right)
\end{align}

we find

\begin{align}
  q_s &= \frac{x - \bar{q}(t) + \frac{i\hbar \beta t}{1 + i\hbar \beta t} q_\beta}{1 + i\hbar \beta t} \\
  p_s &= \frac{i\hbar \beta}{1 + i\hbar \beta t} (x - \bar{q}(t) - q_\beta) \tag{A9}
\end{align}
After some algebra we arrive at the stationary exponent

\[ f(q_s, p_s) = \frac{i}{\hbar} \tilde{p}(t) - \frac{\beta}{2(1 + i\hbar \beta t)} (x - \tilde{q}(t) - q_\beta)^2 \]

\[ = \frac{i}{\hbar} \tilde{p}(t) - i \frac{\hbar^2 \beta^2 t}{2 \sigma(t)} (x - \tilde{q}(t) - q_\beta)^2 \]

\[ - \frac{\beta}{2 \sigma(t)} (x - \tilde{q}(t) - q_\beta)^2, \quad (A10) \]

where \( \sigma(t) \) is given by

\[ \sigma(t) = 1 + \beta^2 \hbar^2 t^2. \quad (A11) \]

The determinant of the second derivatives of \( f \) still has to be calculated. With

\[ \frac{\partial^2 f}{\partial q^2} = -\gamma^4 + 2\gamma \beta \frac{\partial^2 f}{\partial p^2} = -\frac{i}{\hbar} t - \gamma t^2 - \frac{1}{\hbar^2 \alpha} \]

\[ \frac{\partial^2 f}{\partial q \partial p} = -\frac{i}{\hbar} \gamma - \gamma t \quad (A12) \]

we get

\[ \det \left( \begin{array}{cc}
\frac{\partial^2 f}{\partial q^2} & \frac{\partial^2 f}{\partial q \partial p} \\
\frac{\partial^2 f}{\partial p \partial q} & \frac{\partial^2 f}{\partial p^2}
\end{array} \right) = \frac{2\gamma}{\hbar^2 \alpha} \left( 1 - i\gamma \hbar t/2 \right) \frac{\left( 1 + i\beta \hbar t \right)}{1 + \hbar \beta t}. \quad (A13) \]

The factor \( \gamma \) cancels as it should be and we are left with

\[ \Psi^{\beta}_t(x, t) = \left( \frac{\beta}{\alpha} \right)^{1/4} \sqrt{\frac{1}{1 + i\hbar \beta t}} \exp \left( \frac{i}{\hbar} \left[ \tilde{p}(t) x - U_p \sin(2\omega t) - U_p^t \right] \right) \exp \left( \frac{i \hbar^2 \beta^2 t}{2 \sigma(t)} (x - \tilde{q}(t) - q_\beta)^2 t \right) \]

\[ \exp \left( -\frac{\beta}{2 \sigma(t)} (x - \tilde{q}(t) - q_\beta)^2 \right). \quad (A14) \]

This semiclassical time dependent wavepacket is quantum mechanically exact and corresponds to a superposition of Volkov solutions according to a Gaussian distribution at time \( t = 0 \). The fact that the semiclassical wavefunction is exact is a direct consequence of the Ehrenfest theorem which implies that interactions \( V \propto x^n, n = 0, 1, 2 \) have quantum mechanically exact semiclassical solutions.

[1] K. C. Kulander, K. J. Schafer, and J. L. Krause, Adv. At. Mol. Phys. Suppl. 1 (Atoms in intense Laser Fields), 247 (1992).
[2] M. Protopapas, C. H. Keitel, and P. L. Knight, Rep. Prog. Phys. 60, 389 (1997).
[3] K. C. Kulander, K. J. Schafer, and J. L. Krause, Phys. Rev. Lett. 66, 2601 (1991).
[4] B. Sundaram and R. V. Jensen, Phys. Rev. A 47, 1415 (1993).
[5] M. Yu. Ivanov, O. V. Tikhonova, and M. V. Feodorov, Phys. Rev. A. 58, R793 (1998); O. V. Tikhonova, E. A. Volkova, A. M. Popov, and M. V. Feodorov, Phys. Rev. A. 60, R749 (1999).
[6] F. H. M. Faisal, J. Phys. B 6, L89 (1973); H. R. Reiss, Phys. Rev. A 22, 1786 (1980).
[7] P. B. Corkum, Phys. Rev. Lett. 71, 1994 (1993).
[8] M. Protopapas, D. G. Lappas, C. H. Keitel, and P. L. Knight, Phys. Rev. A. 53, R2933 (1995).
[9] M. Lewenstein, P. Balcou, M. Y. Ivanov, A. L’Huiller, and P. B. Corkum, Phys. Rev. A 49, 2117 (1994).
[10] W. Becker, S. Long, and J. K. McIver, Phys. Rev. A 50, 1540 (1994).
[11] M. F. Herman and E. Kluk, Chem. Phys. 91, 27 (1984).
[12] K. G. Kay, J. Chem. Phys. 100, 4377 (1994).
[13] F. Großmann, Comments At. Mol. Phys. 34, 141 (1999).
[14] J. A. Fleck, J. R. Morris, and M. D. Feit, App. Phys. 10, 129 (1976).
[15] J. Javanainen, J. H. Eberly, and Q. Su, Phys. Rev. A 38, 3430 (1988).
[16] D. G. Lappas, A. Sanpera, J. B. Watson, K. Burnett, P. L. Knight, R. Grobe, and J. H. Eberly, J. Phys. B 29, L619 (1996).
[17] C. Figueira de Morisson Faria, M. Dör, and W. Sandner, Phys. Rev. A 55, 3961 (1997).
[18] As already discussed in [14] it is therefore important that the calculations are stopped at times \( t_m = (2m - 1)T/4 \) so that the ionized trajectories terminate at a time where they have their mean momentum.
[19] M. Lewenstein, K. C. Kulander, K. J. Schafer, P. H. Bucksbaum, Phys. Rev. A 51, 1495 (1995).
[20] D. G. Lappas and P. L. Knight, Comments At. Mol. Phys. 33, 237 (1997).
[21] G. van de Sand and J. M. Rost, Phys. Rev. Lett. 83, 524 (1999).
[22] B. Sundaram, P. W. Milonni, Phys. Rev. A 41, 6571 (1990).
[23] S. Virito, K. T. Taylor, and J. S. Parker, J. Phys. B 32, 3015 (1999).