**Attoclock time and exit momentum in strong-field tunnel ionization**

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Tunnel ionization belongs to the fundamental processes of atomic physics. The so-called two-step model, which describes the ionization as instantaneous tunneling at electric field maximum and classical motion afterwards, is commonly employed to describe tunnel ionization in adiabatic regimes. In this contribution, we first show by solving numerically the time-dependent Schrödinger equation in one dimension that there is a time delay between the electric field maximum and the maximum of the ionization rate. This delay is identified as the response time needed by the wavefunction to react to the field maximum. Furthermore, there is a difference between the quantum momentum and the classical momentum from the two-step model after interaction with the driving electric field. Combining both results, we conclude that the electron has an effective initial momentum at the tunneling exit. Our results imply that the two-step model needs modification. The electron’s initial momentum has to be incorporated, when tunneling times shall be determined in attoclock experiments.

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**Introduction**

In 1932 Macoll *et al.* [1] pointed out that there is a time associated with the process of a particle approaching from far away a potential barrier of a height larger than the particle’s energy and eventually tunneling through the barrier. Many efforts have been directed toward defining [2–4] and measuring [5–9] tunneling times. A related open problem is the question how long it takes to ionize by tunneling through a binding potential. Keller *et al.* have conducted experiments using the angular streaking technique aiming to measure tunneling times for ionization from a bound state, the so-called attoclock experiments [10, 11]. In the tunnel ionization case a Coulomb-bound electron is ionized by a strong electromagnetic field and a potential barrier can be defined via the electron’s binding energy and the Coulomb potential bent by the electric field’s potential, see Fig. 1. Since the attoclock experiments have been performed, many renewed efforts have been directed toward defining a tunnel ionization time because a consensus on a suitable theoretical definition of tunneling time and the interpretation of experimental results is still lacking [10–17].

The attoclock experiments aim to determine when the electron leaves the barrier. The attoclock time delay is defined as the difference between the instant of the maximum ionization rate $I(t)$ and the instant of the electric field maximum $E(t)$, i.e.,

$$\tau_A = \arg \max I(t) - \arg \max E(t).$$  \hspace{1cm} (1)

The attoclock time cannot be measured directly. Instead one has to deduce the attoclock time from another observable by applying a theoretical model. For example, the attoclock time may be determined by a measurement of the electron’s asymptotic momentum. Assuming that the electron left the barrier with zero momentum one can determine the time when it left the barrier by applying classical mechanics [18].

A further definition of tunneling time, the Wigner time [19–20], is based on the comparison of classical and quantum trajectories. Here, the classical trajectories are given via the two-step model [21], where the electron leaves the barrier with zero momentum when the electric field is maximal and then follows Newton’s equations of motion. Furthermore, using the Wigner formalism [22–23] one can follow the peak of the electron’s wave-packet and define a quantum trajectory. This so-called Wigner trajectory can be written as

$$f_W(x) = \frac{\partial \phi(x, \epsilon)}{\partial \epsilon} \bigg|_{\epsilon = \epsilon_0},$$  \hspace{1cm} (2)

where $\phi(x, \epsilon)$ is the phase of the fixed-energy propagator, and $\epsilon_0$ is the energy of the bound state. Comparing the times of arrival at a far-away detector $t_W(x_d)$ and $t_c(x_d)$ of the quantum trajectory and the classical trajectory one defines the so-called (asymptotic) Wigner time delay $\tau_W$ as

$$\tau_W = t_W(x_d) - t_c(x_d),$$  \hspace{1cm} (3)

where $x_d$ is the position of the detector. Note that the Wigner formalism is valid only in the static limit of constant electric fields. For barriers of small width realized by large electric fields (near-threshold regime) the Wigner formalism predicts that the quantum particle arrives earlier than the classical particle [19–20], i.e., $\tau_W$ is negative. This implies here that the quantum particle has a larger asymptotic momentum than the classical particle.

An extra momentum could be of three possible reasons. The first possibility is that the quantum particle exits before the electric field reaches its maximum allowing the free particle to accelerate for longer time in the electric field and in this
way to gain extra momentum. As a second possibility the particle exits at the instant of the field maximum with a nonzero initial momentum [20]. In this article we will demonstrate by ab initio quantum calculations that the particle actually exits the barrier with a nonzero initial momentum after the electric field has reached its maximum. This initial momentum has to be taken into account to obtain the correct attoclock time from the electron’s asymptotic momentum.

**Considered system** We analyze theoretically a system similar to the one used in experiments, a bound electron ionized by an electric field pulse. To determine the attoclock time delay we solve the time-dependent Schrödinger equation. The attoclock time delay is determined by comparing the instant of maximum probability current at the potential barrier exit and the instant of maximum electric field strength. By separating the wave function into a tunneled part and a bound part after the interaction with the laser pulse we can calculate the momentum distribution of the tunneled electron.

In experiments a Coulomb-bound electron is usually excited by a laser pulse with a wavelength much bigger than the atomic dimensions such that the laser pulse is nearly homogeneous over the size of the atom. Furthermore, relativistic effects and effects due to the magnetic field component set in only for highly charged ions [19]. Thus we will apply the electric dipole approximation. The laser pulse is modeled by a time-varying homogeneous electric field \( E(t) = E_0 \exp(-\omega^2(t - t_0)^2/2), \) where \( t_0 \) denotes the instant of the maximum field strength \( E_0 \) and \( 1/\omega \) is the time scale of the raise and decay of the electric field. The dipole approximation renders the motion of the electron one-dimensional and we are interested in general features of tunneling times. Thus, we restrict ourselves to one-dimensional systems and consider an electron bound to the soft-core potential \(-Z/\sqrt{x^2 + \alpha(Z)}\) [24–27] to model the essential features of an electron in a three-dimensional Coulomb potential. Here, \( Z \) is the atomic number and the softening parameter \( \alpha(Z) = 2Z^2 \) is chosen such that the ground state energy of the soft-core potential is \(-\hbar^2 = -Z^2/2\), which equals the ground state energy of the Coulomb potential [28]. Thus the Schrödinger equation

\[
\frac{d\psi}{dt} = \hat{H}(t)\psi = \left(-\frac{1}{2} \frac{d^2}{dx^2} - \frac{Z}{\sqrt{x^2 + \alpha(Z)}} - E(t)x\right)\psi \quad (4)
\]

(in atomic units) with the Hamiltonian \( \hat{H}(t) \) will be solved numerically [29]. The so-called Keldysh parameter \( \gamma = \omega \sqrt{2\hbar/E_0} \) [12] characterizes the ionization process as dominated by tunneling for \( \gamma \ll 1 \) and by multiphoton ionization for \( \gamma \gg 1 \). Thus, simulation parameters will be set such that \( \gamma < 1 \) in the following.

**Attoclock time delay** The attoclock time delay [1] is based on the time-dependent ionization rate. In the standard tunneling picture the electron can be considered as free after the barrier exit. Thus, we determine the ionization rate via the probability current \( j(x, t) = \langle \hat{\psi}(x, t)^* \hat{\psi}(x, t) \rangle \) at the exit \( x_{\text{exit}} \) as a function of time, where \( x_{\text{exit}} \) is defined by the maximum electric field strength \( E_0 \). Monitoring the probability current at a fixed position is justified because the tunnel probability is maximal for \( E(t) = E_0 \) and it is exponentially suppressed for lower electric fields. Furthermore, \( E(t) = E_0(1 - \Delta \tau)^2/E_0^2 + O(\Delta \tau^4/E_0^4) \) for \( \Delta \tau = t-t_0 \) with \( |\Delta \tau| < \tau_E = 2\sqrt{T_E} \). Thus the ionization barrier does not change substantially if times close to \( t_0 \) are considered. Numerically, the attoclock time delay is calculated by subtracting the instant of maximum field strength from the instant of maximum current, i.e., \( \tau_A = \arg \max_j(x_{\text{exit}}, t) - \arg \max E(t), \) which yields the positive time delay shown in Fig. 2. Note that for the parameters used in Fig. 2 \( \tau_A < \tau_E \) and thus the electric field remains almost constant for times \( |\Delta \tau| < \tau_A \) justifying our choice for \( x_{\text{exit}} \).

The origin of the attoclock time delay can be understood by considering the time-energy uncertainty principle and following its interpretation given by Mandelstam and Tamm [14, 30–32]. As a consequence of the time-energy uncertainty principle the time, which a wavefunction \( \psi \) of a system with a time-independent Hamiltonian \( \hat{H} \) needs to change significantly, is bounded from below by \( 1/(2\sigma_H^2) \), where \( \sigma_H = \sqrt{\langle \psi|\hat{H}^2|\psi \rangle - \langle \psi|\hat{H}|\psi \rangle^2} \). As outlined in the previous section the Hamiltonian in \( \hat{H} \) can be considered as time-independent for times \( |\Delta \tau| < \tau_E \). This allows us to define the Mandelstam-Tamm time

\[
\tau_{MT} = \left(2\left(\sqrt{\langle \psi(t_0)|\hat{H}(t_0)^2|\psi(t_0) \rangle} - \langle \psi(t_0)|\hat{H}(t_0)|\psi(t_0) \rangle\right)^{-1}
\]

which is indeed a lower bound to the attoclock time as indicated in Fig. 2. The attoclock time \( \tau_A \) is close to its lower bound \( \tau_{MT} \), which indicates that the attoclock time is a consequence of the wavefunction’s inertia, i.e., its ability to adopt instantaneously to the field. The attoclock time \( \tau_A \) decreases as \( E_0 \) increases at fixed Keldysh parameter \( \gamma \) and matches approximately \( \tau_{MT} \) when the regime of over-the-barrier ionization is approached, which is for \( E_0/Z^2 \approx 0.06 \text{ a.u.} \).

The observed decrease of the attoclock time with growing electric field strength (but constant \( \gamma \)) is consistent with calculations for the case of a sudden turn-on of the electric field,
which show that the time for the wavefunction to adopt to the electric field is proportional to the Keldysh time \( \tau_K = \sqrt{2T_p/E_0} \) \cite{14,32}. For a fixed maximum electric field strength \( E_0 \) but increasing \( \gamma \) the attoclock time \( \tau_A \) increases. As \( \gamma \) increases the pulse duration decreases, granting the wavefunction less time to penetrate the tunneling barrier much earlier. Thus, the wavefunction has less time to develop the necessary components for tunneling and thus needs more time to reach the maximum ionization rate.

Using the Wigner formalism and employing the constant-field model, we can calculate the time delay

\[
\tau_{\text{sub}} = t_W(x_{\text{exit}}) - t_c(x_{\text{exit}}),
\]

where the Wigner and the classical trajectories \( t_W(x) \) and \( t_c(x) \) are determined such that both coincide at the entry point \( x_{\text{in}} \). The time \( \tau_{\text{sub}} \) may be interpreted as the time spent under the barrier, since the relation \( t_c(x_{\text{in}}) = t_c(x_{\text{exit}}) \) holds in the two-step model. Also the attoclock time is often understood as the time under the barrier \cite{13}. In fact, our numerical results show that \( \tau_{\text{sub}} \) is close to the attoclock time \( \tau_A \), as shown in the Fig. 2 where \( \tau_{\text{sub}} \) is calculated for the one-dimensional Coulomb potential. Although \( \tau_{\text{sub}} \) and \( \tau_A \) agree well, it is not clear if \( \tau_A \) should be interpreted as time spent under the barrier or just as a response time \cite{14,32}, because the interpretation as under-the-barrier time is based on the assumption that tunneling starts at the instant of maximal electric field but the wavefunction starts to penetrate the tunneling barrier much earlier.

**Initial and final momenta** Applying the Wigner formalism to ionization from a zero-range potential by a static electric field it has been shown that the momentum of the tunnel-ionized electron at a far-away detector differs from the prediction of the two-step model in the so-called near-threshold-tunneling regime \cite{20}. Our numerical solution of the time-dependent Schrödinger equation allows us now to study the final momentum by going beyond the static-field approximation.

Propagating the wavefunction till some final time \( t_f \) such that \( t_f - t_0 \gg 1/\omega \) we can separate the tunnelled part from the bound part of the wavefunction. The tunnelled wavefunction \( \psi_{\text{free}}(t_f) \) is determined by projecting out all bound eigenstates of \( \hat{H} \) in Eq. (4) for \( E(t) = 0 \) from \( \psi(t) \). The resulting probability densities of \( \psi_{\text{free}}(t_f) \) and its momentum-space representation

\[
\tilde{\psi}_{\text{free}}(t_f) \text{ are shown in Fig. 3. Note that the momentum distribution of the tunnelled electron is relatively sharp whereas the position distribution is very widely spread. From } \tilde{\psi}_{\text{free}}(t_f) \text{ the most probable momentum } p_{t_f,\gamma} \text{ can be inferred by the position where } |\tilde{\psi}_{\text{free}}(t_f)|^2 \text{ is maximal.}
\]

For the same parameters of the above quantum simulations we also calculated the final momentum \( p_{t_f} \) of the tunnelled electron as predicted by the two-step model. This is accomplished by solving Newton’s equations of motion till time \( t_f \) for the initial position \( x(t_0) = x_{\text{exit}} \) and the initial momentum \( p(t_0) = 0 \). The difference between the final quantum and classical momenta \( \Delta p_f = p_{t_f,\gamma} - p_{t_f} \) is indicated in Fig. 4 by squares. Similarly, one can benchmark the final momentum given by the Wigner formalism, here for a one-dimensional Coulomb potential, against the prediction of the classical two-step model and calculate the difference of the predicted final momenta. This difference is indicated by the solid green line in Fig. 4 and agrees qualitatively with \( \Delta p_f \) for our numerical simulations. In particular, the solution of the time-dependent Schrödinger equation as well as the Wigner formalism \cite{20} yield a final momentum that differs from the prediction of the two-step model more the stronger the external electric field \( E_0 \) is.

**Modified two-step model** Our numerical quantum mechanical calculations point out two problems of the two-step model. The electron leaves the tunneling barrier after the instant of maximal electric field strength and, furthermore, there is a difference between the final momenta from the quantum theory and from the two-step model. Therefore, we suggest a modified two-step model, which allows for a nonzero initial momentum and takes into account the time delay \( \tau_A \). In this modified two-step model the initial conditions are specified at the instant of the maximal ionization rate. The initial position equals \( x(t_0 + \tau_A) = x_{\text{exit}} \) and the initial momentum is

\[
\tilde{\psi}_{\text{free}}(t_f) \text{ are shown in Fig. 3. Note that the momentum distribution of the tunnelled electron is relatively sharp whereas the position distribution is very widely spread. From } \tilde{\psi}_{\text{free}}(t_f) \text{ the most probable momentum } p_{t_f,\gamma} \text{ can be inferred by the position where } |\tilde{\psi}_{\text{free}}(t_f)|^2 \text{ is maximal.}
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**Initial and final momenta** Applying the Wigner formalism to ionization from a zero-range potential by a static electric field it has been shown that the momentum of the tunnel-ionized electron at a far-away detector differs from the prediction of the two-step model in the so-called near-threshold-tunneling regime \cite{20}. Our numerical solution of the time-dependent Schrödinger equation allows us now to study the final momentum by going beyond the static-field approximation.

Propagating the wavefunction till some final time \( t_f \) such that \( t_f - t_0 \gg 1/\omega \) we can separate the tunnelled part from the bound part of the wavefunction. The tunnelled wavefunction \( \psi_{\text{free}}(t_f) \) is determined by projecting out all bound eigenstates of \( \hat{H} \) in Eq. (4) for \( E(t) = 0 \) from \( \psi(t) \). The resulting probability densities of \( \psi_{\text{free}}(t_f) \) and its momentum-space representation

\[
\tilde{\psi}_{\text{free}}(t_f) \text{ are shown in Fig. 3. Note that the momentum distribution of the tunnelled electron is relatively sharp whereas the position distribution is very widely spread. From } \tilde{\psi}_{\text{free}}(t_f) \text{ the most probable momentum } p_{t_f,\gamma} \text{ can be inferred by the position where } |\tilde{\psi}_{\text{free}}(t_f)|^2 \text{ is maximal.}
\]
\[ p(t_0 + \tau_A) = p_0 \]  
This effective initial momentum \( p_0 \) is chosen such that the final momentum \( p'_f \) predicted by this modified two-step model agrees with the final quantum momentum \( \text{fina}_f \). Our numerical results yield that the effective initial momentum is almost independent of the Keldysh parameter \( \gamma \) and the maximal electric field strength \( E_0 \) as indicated by the circles in Fig. 4. As \( p_0 \) does not depend on the parameters of the external electric field it must result from the initial quatum state, i.e., the ground state of the binding potential. In fact, the ground state of the employed soft-core potential has in momentum space a width of about \( 0.38 \times Z \), which is of the same order as \( p_0 \), see Fig. 4. The fact that \( p_0 \) scales with the width of the ground state’s momentum distribution and not with its mean (which is zero), may be interpreted as momentum components, which propagate into the ionization direction, being ionized preferably. Finally, Fig. 4 shows also the initial momentum as predicted by the Wigner formalism for the one-dimensional Coulomb potential (green-dashed curve), which reflects the same characteristic behavior as the effective initial momentum \( p_0 \).

Our results have implications for the interpretation of attoclock experiments. These experiments aim to determine the attoclock delay, i.e., the time delay between the instant of electric field maximum and the instant of tunneling. The latter is not directly accessible experimentally. Instead the final momentum of the tunneled electron is measured. Because the final momentum depends on at which moment the electron started to propagate freely in the field one can infer the instant of leaving the barrier from the final momentum. This is commonly realized by employing the two-step model assuming zero initial momentum, which yields a delay \( \tau_2 \). Since we have shown that the electron exits with an effective initial momentum, however, the instant of tunneling cannot be determined on the basis of the standard two-step model. The initial momentum has to be included. In fact, the delay \( \tau_2 \) for our model system (4) does not coincide with the looked for delay \( \tau_A \), as shown in Fig. 2. In the deep-tunneling regime the delay \( \tau_2 \) is almost zero, which may explain the results of [10, 11].

**Conclusions**  
We reexamined tunneling times in strong field ionization by an *ab initio* solution of the time-dependent Schrödinger equation. Our calculations show that there is a delay \( \tau_A \) (the attoclock time delay) between the maximum of the ionization rate and the maximum of the electric field strength. This delay can be explained as the response time needed by the wavefunction to react to the change of the driving electric field. Furthermore, there is a discrepancy between the final momentum of the ionized electron as calculated via the Schrödinger equation and as predicted by the classical two-step model. Describing the ionization, however, by a modified two-step model, where ionization happens \( \tau_A \) after the electric field has reached its maximum and which allows for a suitable initial momentum into the direction of the electric field, gives the correct final momentum. The initial momentum in this modified two-step model can be estimated by the width of the groundstate’s momentum distribution, which is \( Z \) for the three-dimensional Coulomb potential. The time \( \tau_A \) may be estimated by \( \tau_{\text{sub}} \), which is for the three-dimensional Coulomb potential \( \approx 9.0 \sqrt{1 - 9.5E_0/Z^2}/Z^2 \).

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