

Tunneling time, what is its meaning?

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Abstract. The tunnel time ionization dynamics for bound systems in laser fields are investigated. Numerical analysis for a step function switch-on of the field allows for the tunnel time to be defined as the time it takes the ground state to develop the under-barrier wavefunction components necessary to achieve the static field ionization rate. A relation between the tunnel time and the Keldysh time is established. The definition of the tunnel time is extended to time varying fields and experimental possibilities for measuring the tunnel time are discussed.

1. Introduction

With the development of quantum mechanics in the first few decades of the 20th century came many phenomena that possessed no classical analogue. The most ubiquitous of these is the phenomenon of tunneling [1] — the ability for a particle to surmount a potential barrier that it would otherwise be prevented from overcoming classically. Tunneling is now described in most introductory quantum mechanics texts [2, 3] and is relevant in many areas of pure and applied science, such as tunnel diodes [4], scanning tunneling microscopy [5] and, in the last few decades, attosecond science [6–9].

In his seminal work, Keldysh developed a dynamical theory of optical field ionization of atoms for a time varying laser field [10]. Ionization was characterized as either multiphoton or tunnel ionization. The regime to which ionization belonged was determined by the Keldysh parameter γ — multiphoton ionization for $\gamma \gg 1$ and tunnel ionization for $\gamma \ll 1$. The Keldysh parameter can be defined as the ratio of the Keldysh tunnel time $\tau_k = l/|v|$ and the laser oscillation period $T_0 = 2\pi/\omega$ for a laser with frequency ω . Here the tunnel time can be interpreted as the time it takes an electron with velocity $v = i\sqrt{2E_0}$ to cross a barrier of width $l = E_0/F$, where E_0 is the electron binding energy and F is the laser electric field. The velocity v is imaginary due to the fact the electron is classically forbidden from travel underneath the barrier. Nonetheless, τ_k displays the characteristics that are expected of a tunnel time. When the laser field changes too fast for the electron to escape under the barrier, tunneling is restricted.

Recent attosecond angular streaking experiments were done to measure the tunnel response time [11]. The measured time was much shorter than those predicted by most theoretical definitions, such as the Büttiker-Landauer or Keldysh times. These experiments raise the question as to the meaning of the tunnel time for ionization from bound systems. So far a more detailed theory of tunnel time for bound electrons is needed to clarify the meaning of the tunnel time.

To answer this question we examine 1D quantum systems subjected to an instantaneous switch-on of a static electric field. When the field is switched on, the ground state transforms into a dynamic resonance state decaying with a time-dependent ionization rate $w(t)$. When the

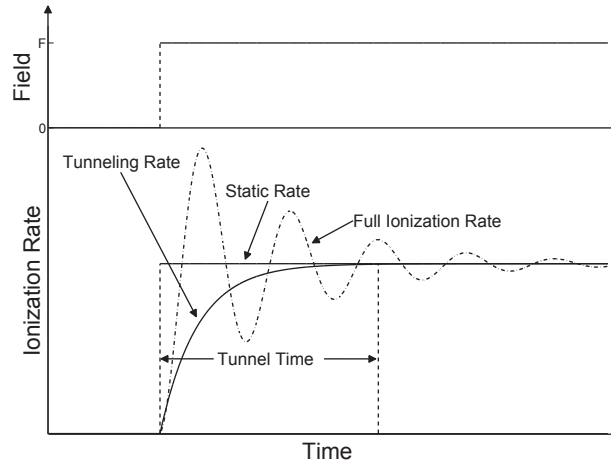


Figure 1. Schematic of the tunneling process for a step function switch-on. The dotted line represents the full ionization rate $w(t)$. The filtered ionization rate (labeled “Tunneling Rate”) is represented by the solid curve. The constant line is the static ionization rate $w(F)$.

wavefunction in and around the bound region approaches the static resonance, determined by the solution of the time-independent Schrödinger equation for constant field F , the ionization rate takes on a constant value $w(F)$.

For an unambiguous definition of the tunnel time of bound systems two obstacles must be overcome. First, tunnel ionization is usually measured by the outgoing current at some reference point. However, when this is done the temporal evolution of the ionization rate depends on the reference point. Second, the tunneling signal from the ground state is masked by a contribution due to the sudden switch-on resulting in population and ionization of excited states. The first obstacle can be overcome by using a time-dependent generalization of Fano-resonance theory. The ionization rate is determined by the imaginary part of the resonance making this method reference point free. The second obstacle is overcome by pairing this generalized Fano approach with a spectral filtering method that removes the contributions from the excited states. The tunnel time can then be defined as the response time it takes the part of the wavefunction tunneling directly from the ground state to reach the static ionization rate. A schematic of this process is depicted in Fig. 1.

2. Solution of the time-dependent Schrödinger equation

Consider a 1D quantum system initially in its ground state. At time $t = 0$, a static field of strength F is switched on instantaneously. The Hamiltonian in dipole approximation and length gauge is given by,

$$H = \begin{cases} H_0 & \text{for } t < 0 \\ H_0 - Fx & \text{for } t \geq 0 \end{cases} \quad (1)$$

where $H_0 = T + V$ with T the kinetic energy and V the potential. Unless otherwise indicated, atomic units are used throughout. We then express the wavefunction as,

$$|\Psi(t)\rangle = a(t)|0\rangle + |\phi(t)\rangle \quad (2)$$

where $|0\rangle$ is the unperturbed ground state and $a(t) = \langle 0|\Psi(t)\rangle$. The last term in Eq. (2) is the part of the wavefunction that develops in response to the external field for which $\langle 0|\phi(t)\rangle = 0$ is

enforced; it is zero in the absence of the external field. Inserting Eq. (2) into the time-dependent Schrödinger equation (TDSE) with the Hamiltonian given in Eq. (1) and projecting $\langle 0|$, yields an equation of motion for $a(t)$,

$$i\dot{a}(t) = E_0 a(t) + \langle 0|H_0 - Fx|\phi(t)\rangle, \quad (3)$$

where $E_0 = \langle 0|H|0\rangle$. Choosing the *ansatz* $|\phi(t)\rangle = a(t)|\varphi(t)\rangle$ we arrive at the expression

$$\Delta E(t) = i \frac{\dot{a}(t)}{a(t)} - E_0 \quad (4)$$

where $\Delta E(t) \equiv \langle 0|H|\varphi(t)\rangle$. The rate at which probability leaves the ground state and escapes into the continuum is given by $w(t) = -2\text{Im}\{\Delta E(t)\}$. To completely determine $|\Psi\rangle$, a corresponding equation for the time evolution of $\phi(t)$ can be obtained by projecting $1 - |0\rangle\langle 0|$ on the TDSE. The resulting equation is not given, as it is not used here. Eq. (4) is the time-dependent generalization of Fano resonance theory [12]. By using the time-independent instead of the time-dependent Schrödinger equation in our derivation, the regular Fano resonance theory would be obtained yielding the static tunneling rate for ΔE .

The above equations were developed for diagnostic purposes. Time propagation is handled by expanding the total wavefunction on the eigenstates of the field-dressed Hamiltonian. This spectral method is more advantageous as it will allow for the separation of the tunneling contribution from the rest of the wavefunction. For more details about the expansion see Ref. [13].

3. Results for the instantaneous switch-on

We begin by solving the TDSE for the 1D quantum dot (QD) potential

$$V(x) = \begin{cases} \frac{1}{2}\alpha^2 x^2 - \beta & \text{for } |x| < \sqrt{2\beta}/\alpha \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

with $\alpha = 1/2$ and $\beta = 3/4$. This system contains only the ground state and a first excited state at the continuum threshold. Initially the system is in the state $|0\rangle$; at $t = 0$ the static field is switched on.

Fig. 2 shows the spectral density as a function of energy for the system at $F = 0.08$. We display the results for this field strength as they are representative of the results for all field strengths investigated. Note that the laser field turns discrete bound states into mixed bound-continuum resonance states with a finite spectral width. The spectrum has a minimum at around an energy of -0.35 , which separates two distinct features of the step response: (i) The sharp peak to the left represents tunnel ionization from the ground state directly. (ii) The broad peak to the right corresponds to photon absorption and ionization via the excited state resonance — due to the infinite bandwidth of the step function, photon absorption is dominated by single photon transitions. Both channels (i) and (ii) coexist in near infrared laser pulses as well. However, as a single photon cannot reach excited states or the continuum directly, channel (ii) occurs via multi-photon transitions. As long as the minimum is outside the spectral widths of both features, tunneling and excited state channels can be separated by multiplying a spectral filter on the probability amplitudes; see the (red) dashed line in Fig. 2. The choice of the filter function is discussed in the supplemental material of Ref. [13].

The tunnel ionization peak in Fig. 2 reveals the spectral signature of the tunnel ionization dynamics. An exponential decay in time corresponds to a Lorentzian spectrum, the width of which determines the tunnel ionization rate. Our spectrum is Lorentzian with a small

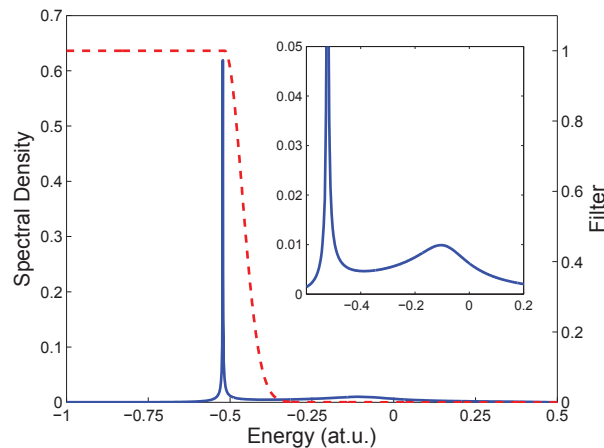


Figure 2. Spectral density (solid blue line) for the 1D quantum dot potential at $F = 0.08$. The spectral filter is shown by the red dashed line. A magnified section of the spectral density is shown in the inset.

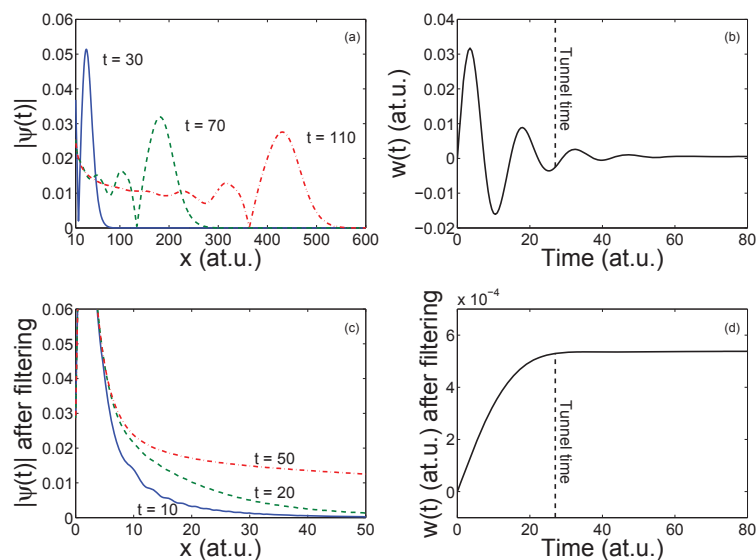


Figure 3. (a) Magnitude of $\Psi(x)$ for $t = 30$ (solid blue), $t = 70$ (dash green) and $t = 110$ (dash-dot red); to illustrate the outgoing wave, the bound region is not shown. (b) Ionization rate $w(t)$ corresponding to (a). (c) Magnitude of the filtered wavefunction (ground state resonance only) for $t = 10$ (solid blue), $t = 20$ (dash green) and $t = 50$ (dash-dot red); filter is given in Fig. 1. (d) $w(t)$ corresponding to (c). 1D quantum dot potential and $F = 0.08$ for (a)-(d).

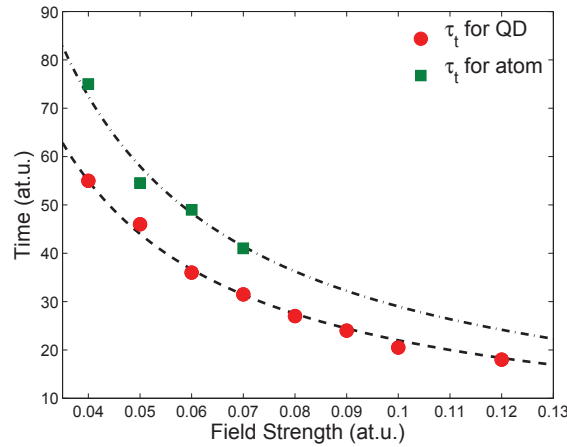


Figure 4. Calculated τ_t for the QD (●) and atomic (■) potentials. The lines in the plot represent the Keldysh time multiplied by a constant to match τ_t .

asymmetric distortion and a phase, which are responsible for the switch-on of the tunneling process. As the functional form of the spectral distortion is unknown, extraction of the tunneling time is easier in the time domain.

Figure 3 shows how the system responds to the instantaneous switch-on of the field for both the total (unfiltered) and filtered wavefunction. Figure 3(a) shows that for the total wavefunction an outward propagating wave is created from the excited state ionization channel. In its wake this wave leaves a steady flow of probability from the ground state into the continuum representing the static resonance with constant tunneling rate. The corresponding ionization rate in Fig. 3(b) shows strong oscillations that mask the tunneling signal. Eventually the oscillations decrease and the ionization rate reaches the static rate.

When the filter is applied, the initial outgoing wave ceases to exist and the wavefunction monotonically rises towards a steady-state; see Fig. 3(c). The corresponding ionization rate in Fig. 3(d) shows the resulting tunneling rate rise monotonically and approaches the steady state value. It is this rise time that we define as the electron tunneling time τ_t . For times much shorter than the tunneling time, the wavefunction components under the barrier that are necessary for tunneling cannot be developed and tunnel ionization does not occur. For all investigated field strengths, the tunnel time is considerably shorter than the time it takes for the excited state ionization signal to subside. Therefore, filtering is indispensable for extracting the tunnel time.

The tunneling time τ_t is calculated by using $w(t)$ after filtering and determining when the ionization is within 1% of the static value. Results for the QD potential and for a 1D softened Coulomb potential $V(x) = 1/\sqrt{x^2 + b^2}$ are shown in Fig. 4. The shielding parameter b is chosen so that the ionization potential is ≈ 0.5 (the same as the QD potential). The spectral features for the Coulomb potential are similar to those of the QD except that the two peaks merge at lower field strength — around $F = 0.07$ — than for the QD. The results of our calculations show that the tunnel time scales with the Keldysh time as $\tau_t \approx 2.2\tau_k$ for the QD and as $\tau_t \approx 2.9\tau_k$ for the Coulomb potential. In addition to this scaling, it has been shown that the Keldysh time is in fact a lower limit for the tunneling time [14].

4. Sinusoidal switch-on

Up to this point the tunnel time has been defined for a step-function response. In this section the definition for the tunnel time will be generalized to time varying fields. To define the duration of

any physical process, it is necessary to have an initial and final reference point. So far we have used the ground state and the static resonance between which the tunnel time can be measured. Tunneling cannot manifest for $t \ll \tau_t$ and maximum tunneling with the static ionization rate is reached for $t \gtrsim \tau_t$.

To extend the definition of τ_t to time varying fields, consider an initially bound electron interacting with a monochromatic, linearly polarized laser field $F = F_0 \sin(\omega t)$ where F_0 is the peak strength and ω the frequency.

To understand what happens in a sinusoidal laser field, first decompose it into small step functions. The field changes from F to $F + \Delta F$ and remains constant over a time Δt ; the step size $\Delta F \propto \omega \Delta t$. In the tunneling regime, $\gamma \lesssim 1$, the initial state at F is no longer the unperturbed ground state, but a state that has already developed tunneling components. The dynamics that takes place during Δt is the wavefunction attempting to develop components to realize the static resonance state for $F + \Delta F$. The time needed for realizing the static resonance for one step can be viewed as a local tunnel response time that will vary throughout the laser cycle. However, a meaningful tunnel time cannot be defined, as both initial and final states are tunnel ionizing.

For a sinusoidal field with peak value F_0 and period T_0 , a natural way to generalize the tunnel time is to use a quarter cycle; this resembles a softened switch-on function. In contrast to the step function the time of measurement is not free but determined by $T_0/4$; it can only be varied by changing ω . Initial and final reference states are taken at the field minimum and its subsequent maximum. This applies to linearly as well as elliptically polarized fields. It is assumed that the initial state at the field minimum is close to the ground state where tunnel ionization is negligible compared to the field maximum. As a result, the tunnel time is determined by the quarter oscillation period for which the ground state transforms into the static resonance for F_0 .

5. Considerations for experimental measurement of the tunnel time

From our analysis it is clear that experiments based on the notion of a tunnel time required for a particle to cross the barrier with fail. There are no time dynamics visible in the wavefunction that indicate such a behaviour. Instead, the tunnel time must be seen as the time required to establish a tunnel through the potential by which the particle can escape. This is achieved by the wavefunction developing the under-the-barrier components of the (quasi-static) resonance.

For a sinusoidal laser field the tunnel time cannot be measured directly because the field changes. However, it is possible to measure it indirectly. In the tunneling limit, for laser frequencies for which $\gamma \leq 1$, tunnel ionization is fully established and will be maximum at and around the peak of an optical half cycle. In the transition regime, tunnel ionization at the peak will decrease as a function of increasing laser frequency. In the multi-photon regime, tunnel ionization is expected to be negligible. As a result, by measuring tunnel ionization at the peak of the laser half-cycle as a function of laser frequency ω , we expect the tunneling yield to increase with decreasing frequency until it saturates when $\gamma \leq 1$ is reached.

Experimentally, methods have already been developed that can measure tunnel ionization with sub-cycle resolution [11, 15]. Ionization is achieved with nearly circularly polarized laser pulses and the momentum of the ionized wavepacket is recorded. A unique relationship exists between the ionization time and the final momentum of the wavepacket. Wavepackets created at different times along an optical cycle carry different final momenta. As a result, there exists a relation between the time at which an electron wavepacket was born and its final momentum recorded in the momentum spectrum. The ionization dynamics can then be recovered with sub-cycle accuracy from the momentum spectrum.

These experiments measure the *tunnel delay time* — the time difference between the ionization maximum and the peak of the optical half cycle. The presence of a non-zero delay time indicates that tunneling does not have sufficient time to develop over a quarter cycle and

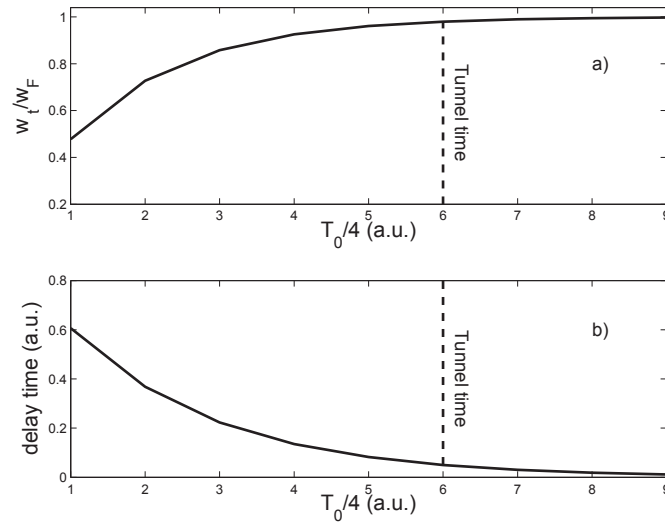


Figure 5. Schematic of tunnel time measurement. (a) Ratio w_t/w_F as a function of a quarter laser period. w_t is the tunneling rate at the half cycle peak; the field F at the half cycle peak being kept constant; w_F is the tunneling rate of the static resonance. (b) The tunnel delay time (difference between half cycle peak and maximum ionization rate) as a function of a quarter laser period. The dashed line in (a) and (b) represents the time at which the quarter cycle period is equal to the tunnel time. At this time the ionization rate reaches a chosen fraction of the static rate and correspondingly the the tunnel delay time approaches zero within some prescribed precision.

that the tunneling time is longer than the quarter cycle. Thus, the delay time obtained from experiment can be viewed as a measure of how far the wavefunction is from establishing the static resonance eigenstate at the half cycle peak. To extract the tunnel time from these experiments that is in agreement with the Keldysh tunnel time, the ionization at the half-cycle needs to be measured as a function of ω . The ionization rate saturates to a frequency independent value for $\omega < 1/\tau_t$ and correspondingly the tunnel delay time converges to zero. The tunnel time can be experimentally determined as $\tau_t^{\text{exp}} = 1/\omega_t$ with ω_t being the smallest frequency at which the ionization rate saturates and the tunnel delay time drops to zero (within some prescribed accuracy). A schematic of this idea is depicted in Fig. 5.

6. Conclusion

Nearly five decades ago Keldysh published his seminal work treating the ionization of atoms in strong laser fields. His work presents the basis on which the field of intense laser physics has been constructed. The advent of attosecond science has opened the opportunity to test and explore more deeply some of the predictions of Keldysh's original work. This has rekindled the interest in understanding the Keldysh tunnel time, and tunnel times in general, which there has remained some discrepancy.

Here we have presented a definition of the tunnel time for bound systems. In the case of an instantaneous switch-on of a field with strength F , the tunnel time is the response time for the wavefunction to develop from the ground state to the static resonance for the field value F . We presented a numerical method that allows us to remove the contributions from excited states and determine the tunnel time. It was shown that the calculated tunnel times as a function of F scale with the Keldysh time. This reveals the connection between our definition of tunnel time

and that presented by Keldysh nearly five decades ago. Finally, we have extended our definition to time varying fields and discussed how this can be applied to the experimental observation of the tunnel time.

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