Identification of the Keldysh time as a lower limit for the tunneling time

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By using first-principles arguments, based on the time-energy uncertainty principle in the form given by Mandelstam and Tamm, we show that the Keldysh time represents a lower limit for the tunnel time. We use the definition of the tunnel time as identified in a recent numerical investigation [C. R. McDonald *et al.*, Phys. Rev. Lett. **111**, 090405 (2013)]; it is the time it takes for the unperturbed initial ground-state wave function to evolve into the field-perturbed final eigenstate which is the quasistatic field dressed resonance.

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In a seminal paper, Keldysh gave the first theoretical description of laser-driven ionization of atoms with ionization potential $|E_0|$ [1–3]; the strong laser field is characterized by field strength F and frequency ω. A semiclassical integration of the Schrödinger equation revealed that ionization can be characterized by the Keldysh parameter γ_k as multiphoton or as tunnel ionization [4,5] in the limits of $\gamma_k > 1$ and $\gamma_k \ll 1$, respectively. The Keldysh parameter is defined as the ratio of the Keldysh time τ_k and the laser oscillation period $T_0 = 2\pi/\omega$ and is given by $\gamma_k = 2\pi\tau_k/T_0$. To fully appreciate the meaning of the γ_k parameter, a physically satisfactory interpretation of τ_k is required.

The Keldysh time can be written as $\tau_k = l/|v|$, where $l = |E_0|/F$ is the barrier width and $v = i\sqrt{|E_0|/2}$ is the average speed of an electron under the *static* barrier [6,7]. This definition offers the following interpretation: the Keldysh time is the time it takes a classical electron with average velocity v to cross the static barrier of length l. For this reason τ_k is sometimes referred to as the Keldysh tunnel time. The electron velocity is imaginary because classically the electron is not allowed to enter the barrier. As a result, this interpretation, although intuitive, is unsatisfactory. The lack of understanding of the Keldysh time has been highlighted by the discrepancy between recent measurements of the tunnel time [8] and various theoretical definitions [1,9].

The goal of this Brief Report is to derive τ_k from basic principles of quantum mechanics without the need to rely on a semiclassical approximation. As a result, the meaning of the Keldysh time is revealed as presenting a lower limit to the tunnel time. Our work builds on the tunnel time as identified in a recent paper [10], through a numerical analysis of one-dimensional (1D) model atoms perturbed by an external electric field F that is suddenly switched on. A schematic of the dynamical processes is presented in Fig. 1. In regular quasistatic ionization theory, the bound system would start ionizing with the full static ionization rate [11]. In reality, the bound system builds up ionization via two channels, the tunnel (horizontal) ionization channel and the single- or multiphoton (vertical) channel. The ionization buildup ends when the quasistatic resonance with static ionization rate $w(F)$ is realized. The dash-dotted line represents the total ionization rate as would be obtained by a complete numerical solution of the Schrödinger equation; it contains both ionization channels. In Ref. [10] it was shown how the vertical channel can be filtered out to isolate the tunneling dynamics alone, which is represented by the solid line in Fig. 1. Both the tunnel ionization rate and the full ionization rate reach the same static ionization rate $w(F)$, but over different response times τ_t and τ_f, respectively. The response time τ_t was defined as the tunnel time in Ref. [10]; it is the time it takes for the bound state to develop the underbarrier tunneling components of the final quasiresonance state, so that full tunnel ionization with rate $w(F)$ occurs.

The tunnel time τ_t was found numerically to be proportional to and longer than the Keldysh time τ_k. Furthermore, τ_t was generally shorter than τ_f, the response time of the full ionization rate. As a result, the Keldysh time τ_k was found to be the shortest time over which the system can respond. In this sense, the numerical analysis suggested that the Keldysh time presents a lower limit to the tunnel time. The purpose of our Brief Report is to prove this conjecture by first-principles arguments and to explore its consequences.

The following derivation relies exclusively on the time-energy uncertainty principle, as established by Mandelstam and Tamm [12–14]. This allows us not only to put the numerical findings of Ref. [10] on a more rigorous theoretical footing, but also to generalize the definition of the tunnel time to three-dimensional (3D) atomic systems. Most of the papers that have dealt so far with the tunneling problem have investigated reduced-dimensionality (1D) systems with the notable exception of Ref. [15], where the lateral spreading of the tunneling wave function has been used as a quantum clock to measure the tunnel time. The use of a realistic 3D model is important because it facilitates the comparison between theoretical and experimental results. Finally, our analysis does not rely on the semiclassical approximation commonly used in the analysis of the tunnel time.

The concept of tunnel time has been hotly debated for a long time and many possible definitions have been proposed so far [9,15–18]. Our work adds two main points. First, the Keldysh time is equal to the Mandelstam-Tamm (MT) time. The MT time is the time over which the ground state cannot respond to the external perturbation [19,20]. As a result of the equality of MT time and Keldysh time, the Keldysh time represents a lower limit for the tunnel time. Consequently, the tunnel time, independently of the exact definition, has to be larger than the Keldysh time. Second, our analysis reveals that tunnel time and Keldysh parameters emerge from the same underlying concept, as they should: the time it takes the particle wave

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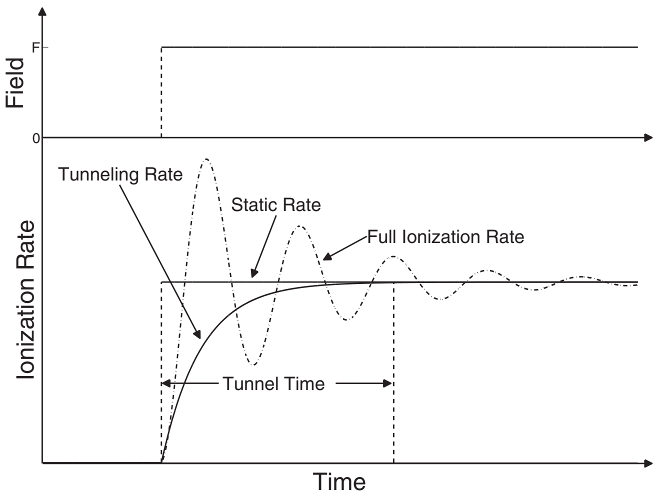

FIG. 1. Schematic of the tunneling process for a step-function switch-on. The dotted line represents the full ionization rate $w(t)$. The solid line is the filtered ionization rate (labeled "Tunneling Rate"). The constant line represents the static ionization rate $w(F)$.

function to evolve from the ground state into the quasistatic field dressed resonance. Thus, the definition of Keldysh time and the Keldysh parameter are brought in line. Finally, the identified definition of Keldysh and tunnel time can be used for a more accurate quantitative interpretation of the Keldysh parameter.

Our analysis starts from an atomic system perturbed by a laser electric field with a step-function switch-on from 0 to F. We work within the single-particle approximation; atomic units are used throughout. At $t = 0$ the atomic electron is in the ground state $|0\rangle$ of the unperturbed Hamiltonian H_0 with energy eigenvalue $E_0 < 0$. The Hamiltonian H of the system is given by

$$H = \begin{cases} H_0 & \text{for } t < 0, \\ H_0 - \mathbf{F}\cdot\mathbf{x} = H_0 - Fx & \text{for } t \geqslant 0, \end{cases} \tag{1}$$

where $H_0 = -\nabla^2/2 + V$ with V the potential energy operator, and F presents the strength of the static electric field directed along the x axis ($\mathbf{F} = F\hat{\mathbf{x}}$). The potential energy V is a general inverse-square-law function of the form $V(\mathbf{x}) = -K^2/|\mathbf{x}|^\lambda$, with $0 < \lambda < 2$ and K a numerical coupling constant. Atomic units are used throughout. Because of the presence of the perturbation, the state $|0\rangle$ has a nonzero energy uncertainty $\delta E = \sqrt{\langle H^2\rangle - \langle H\rangle^2}$ for $t > 0$. Here, all expectation values are taken with respect to $|0\rangle$; this is the case throughout the rest of this Brief Report unless otherwise stated.

It is straightforward to show the equality of MT time τ_{MT} and Keldysh time τ_{k} by using the following observations. Due to the symmetry of the potential $V(\mathbf{x})$, the initial position and momentum expectation values are $\langle\mathbf{x}\rangle = \langle\mathbf{p}\rangle = 0$, and, thus, $\langle H\rangle = E_0$ and $\langle H^2\rangle = E_0^2 + F^2\langle x^2\rangle$. This results in $\delta E = F\sqrt{\langle x^2\rangle}$.

Because of the spherical symmetry of the potential V, we have, for the position and momentum uncertainty, $\delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \delta y = \delta z$ and $\delta p_x = \sqrt{\langle p_x^2\rangle - \langle p_x\rangle^2} = \delta p_y = \delta p_z$; therefore, $\delta E = F\delta x = \alpha\frac{F}{\delta p_x} = \alpha F\sqrt{\frac{3}{2\langle T\rangle}}$. The term $\alpha = \delta x\delta p_x \geqslant 1/2$ is a numerical constant and $\langle T\rangle = \frac{1}{2}\langle\mathbf{p}^2\rangle = \frac{3}{2}\langle p_x^2\rangle = \frac{3}{2}(\delta p_x)^2$ is the average kinetic energy of the unperturbed ground state. We stress that α depends only on the form of the ground state and not on the electric field strength F.

Applying the quantum virial theorem [3,14] to the Hamiltonian H_0, we find a simple relation between $\langle T\rangle$ and the unperturbed energy, namely, $E_0 = \frac{\lambda-2}{\lambda}\langle T\rangle$. Therefore, we can rewrite the MT time as

$$\tau_{\mathrm{MT}} = \frac{1}{\alpha}\frac{\sqrt{\frac{2\lambda}{3(\lambda-2)}E_0}}{F} = \sqrt{\frac{\lambda}{3\alpha^2(2-\lambda)}}\tau_{\mathrm{k}} = c\tau_{\mathrm{k}}. \tag{2}$$

For the Coulomb interaction $\lambda = 1$, $\alpha = 1/\sqrt{3}$ [3], and, hence, the MT time is identical to the Keldysh time; that is, $\tau_{\mathrm{MT}} = \tau_{\mathrm{k}} = \frac{\sqrt{-2E_0}}{F}$. For potentials with a different λ the MT time has the same dependence on the field strength F as the Keldysh time, the only difference being the numerical coefficient in Eq. (2). As a result, the Keldysh time represents a lower limit for the tunnel time needed for the atomic ground state to develop into the quasistatic resonance and to fully develop tunnel ionization: $\tau_{\mathrm{k}} \leqslant \tau_{\mathrm{t}}$.

The MT time-energy uncertainty relation [12–14] implies that the electron wave function does not evolve significantly for $t < \tau_{\mathrm{MT}} = 1/\delta E$. In fact, Mandelstam and Tamm proved that τ_A—the time it takes for the average value $\langle 0|\hat{A}|0\rangle$ of any observable $\hat{A}$ to change significantly—must be larger than τ_{MT}, i.e., $\tau_A \geqslant \tau_{\mathrm{MT}}$. As the MT time is identical to the Keldysh time, the expectation value of any observable, and also the wave function itself, cannot evolve in a time shorter than τ_{k}. This holds important implications for the tunneling time.

In many theoretical investigations [9], the time evolution of an operator $\hat{A}_{\mathrm{clock}}$ is chosen as a possible *quantum clock* to measure the tunnel time, e.g., the spin of the tunneling particle in the gedanken Larmor clock experiment. It should be stressed that different quantum clocks may measure different tunneling times. However, by virtue of our MT analysis, the evolution (of the expectation value) of any operator $\hat{A}_{\mathrm{clock}}$ must unfold in a time longer than $\tau_{\mathrm{MT}} = \tau_k$. Consequently τ_k represents a lower limit for the tunneling time of an atomic system, as measured by any quantum clock.

The identification of the Keldysh time as a lower limit for the tunnel time is also important, as it allows a unified interpretation of the tunnel time and the Keldysh parameter γ, based on the same concept: the time it takes the ground state in the presence of a laser field to evolve into the quasistatic resonance state. Whereas the Keldysh time defines the time over which the system is too inert to respond to the external perturbation, the tunnel time sets the time over which the final quasistatic resonance state is reached.

The Keldysh parameter $\gamma_{\mathrm{k}} = \omega\tau_{\mathrm{k}} = \omega\sqrt{2|E_0|}/F$, for an atomic electron interacting with a laser field $F(t) = F\sin(\omega t)$, compares the Keldysh time with a quarter laser cycle $T_0/4 = (\pi/2)\omega \approx \omega$. When $\gamma_{\mathrm{k}} = 1$, we can conclude that the Keldysh time is of the order of a quarter cycle; consequently tunneling cannot happen, as the atom cannot respond to the laser perturbation within τ_{k}. As a result, ionization is dominated by multiphoton ionization. Alternatively, we could define a modified Keldysh parameter $\gamma_t = \omega\tau_t$. Here τ_t is the tunnel time as defined in Ref. [10] for a particle in a monochromatic laser field, i.e., the time over which the quasistatic resonance has been realized and tunnel ionization has fully developed. For this definition, $\gamma_t = 1$ means that tunneling can fully develop over a quarter cycle and that the system will dominantly ionize via tunnel ionization.

As a result, our analysis enables a more accurate quantitative interpretation of when tunnel or multiphoton ionization dominates. Multiphoton and tunnel ionization are dominant for $\gamma_k \geqslant 1$ and for $\gamma_t \leqslant 1$, respectively. The range between γ_k and γ_t defines the transition region between tunnel and multiphoton ionization.

The preceding analysis has shown that it is possible to establish the meaning of the Keldysh time τ_k as a lower limit to the tunnel time, using only basic principles of quantum mechanics. An extension of our analysis to short-range potentials is straightforward. This corroborates the conclusions drawn from numerical analysis in Ref. [10] in terms of simple, first-principles arguments.

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