Ionization in an intense field considering Coulomb correction*

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We derive a simple ionization rate formula for the ground state of a hydrogen atom in the velocity gauge under the conditions: $\omega \ll 1$ a.u. (a.u. is short for atomic unit) and $\gamma \ll 1$ (ω is the laser frequency and γ is the Keldysh parameter). Comparisons are made among the different versions of the Keldysh–Faisal–Reiss (KFR) theory. The numerical study shows that with considering the quasi-classical (WKB) Coulomb correction in the final state of the ionized electron, the photoionization rate is enhanced compared with without considering the Coulomb correction, and the Reiss theory with the WKB Coulomb correction gives the correct result in the tunneling regime. Our concise formula of the ionization rate may provide an insight into the ionization mechanism for the ground state of a hydrogen atom.

Keywords: strong field approximation, ionization rate, Coulomb potential

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1. Introduction

With the advent of powerful laser sources of intensities well over 10^{14} W/cm^2, nonresonant multiphoton processes such as above-threshold detachment (ATD) of ions and above-threshold ionization of atoms and molecules (ATI) in an intense laser field have been the subject of many theoretical and experimental investigations.[1–3] In order to understand the photoionization processes of complicated atoms and molecules, it is necessary to investigate the photoionization mechanism of a hydrogen atom in more detail.

The strong field ionization processes can be described with the help of the Keldysh–Faisal–Reiss (KFR)[4–6] theories. The KFR theories are also called the strong field approximation theories (SFA).[7] The KFR theories start from the S-matrix element, which is widely considered to be exact in principle. Nevertheless, due to the fact that the Schrödinger equation for a charged particle interacting with both the field of an attractive Coulomb center and a strong laser field cannot be solved analytically, analytical approximations are used to evaluate the S-matrix element for bound-free transitions. All three versions of the KFR theory describe the same physical problem, and the main difference between them lies in the form of the laser-electron interaction. Under the dipole approximation, the laser-electron interaction Hamiltonians can be expressed as $\boldsymbol{r}\cdot\boldsymbol{E}$ and $\boldsymbol{p}\cdot\boldsymbol{A}$, respectively. The $\boldsymbol{r}\cdot\boldsymbol{E}$ form is usually called the length gauge (LG) SFA, which has been used by Keldysh. The $\boldsymbol{p}\cdot\boldsymbol{A}$ form is usually called the velocity gauge (VG), which has been used by Faisal[5] and Reiss.[6] Tang *et al.*[8] have derived a Keldysh-like formula of atom ionization in an intense laser field by using the velocity gauge. The formula is as simple as Keldysh's formula. Therefore, various approximate theories may lead to different expressions for the ionization rate. Although the expressions are different, the ionization rate should be the same due to gauge invariance. For example, Bauer[9] has calculated the ionization rate of a 1s hydrogen atom in an intense laser field by using both the length and the velocity gauge formulation of the SFA in the tunnel regime, and the differences between the results was at least one order of magnitude. The discrepancy between the two gauges has caused extensive controversy about which gauge is more appropriate for the strong field approximation.[10,11]

In the KFR theory, one presumes that the influence of the Coulomb potential on the final state of the outgoing electron is neglected. This is quite a good approximation for photodetachment of a negative hydrogen ion,[6] because the binding potential is certainly of finite range, in view of the neutrality of the residual atom after photodetachment. Photoionization of the initially neutral hydrogen atom does not really suit the validity conditions given by Reiss, because of the long range of the Coulomb interaction between the ionized outgoing electron and the remaining positively charged ion. The real potential exerts a long-range Coulomb force between the residual core and the ionizing electron, so the theoretical predictions would not accord with experimental results very well. In the high-intensity limit of the laser field, the electromagnetic field effects on the electron become dominant and good agreement can be expected. In practical calculation, the Volkov[8]

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function was used as the final state of the photoionized electron. This normal Volkov function is an exact solution of the quantum-mechanical equations of motion for a free electron in a plane-wave electromagnetic field. However, in the presence of an atomic potential among particles, the Volkov function is not an exact description of the motion of the photoionizing electron. Therefore, one has to include somehow Coulomb corrections in the final state of the ionized electron. There have been many efforts made to incorporate appropriately the effect of the atomic potential into the Volkov function so far.[9,12–17] In short, there are mainly two modes. First, Reiss and Krainov[18] found a simple analytical approximation for the wave function of an electron simultaneously exposed to a strong circularly polarized laser field and an atomic Coulomb potential. This wavefunction is the Volkov state with a first-order Coulomb correction coming from some perturbative expansion of the potential in the Kramers–Henneberger reference frame. Later, according to the development of Reiss and Krainov, Mishima *et al.*[19] improved the Volkov function by including the second-order term in the perturbative expansion of the atomic potential in a linearly polarized laser field. The revised Volkov function mentioned above is usually called the Coulomb–Volkov function. Whereas, in the tunneling regime, Bauer[9] has checked that the ionization rates with and without the Coulomb–Volkov corrections are nearly identical. Second, in the tunneling domain, when $\omega \ll 1$ and $\gamma \ll 1$, the quasiclassical (WKB) approximation may be applied. Krainov and Shokri[20] have shown that for the ground state of a hydrogen atom the Volkov wave should be multiplied by the factor $2Z^2/Fr$. After this work, they generalized the results to the case of arbitrary atoms or atomic ions by using the quantum defect method. The Coulomb correction is also given in the frame of quasi-classical perturbation theory with respect to the Coulomb potential $U=-Z/r$ by the factor $(2Z^2/n^2Fr)^n$ in the Volkov wave function,[21] in which n is the effective quantum number of the initial atomic or ionic state. Bauer[9,14] pointed out that if the WKB Coulomb correction in the final state of the ionized electron is included, the KFR theory gives the correct result in the tunneling domain.

In this paper, we derive a closed-form formula for the tunnel ionization rate in the velocity gauge including the WKB Coulomb correction, which, to the best of our knowledge, has not been published so far. This formula is as simple as Keldysh's formula, and provides an insight into the ionization mechanism of atoms subjected to an intense laser field. In accordance with arguments made by Keldysh, we assume that for a linearly polarized laser field the contributions to the ionization rate mainly come from small kinetic momentum $\boldsymbol{p}$, satisfying the condition $\boldsymbol{p}^2 \ll 2E_\mathrm{b}$. Throughout the paper, the atomic units $e=m=\hbar=1$ are used, substituting explicitly -1 for the electronic charge.

2. Ionization rate formula

To be specific, we consider a hydrogen atom in the presence of a strong laser field. The rate of photoionization for direct transition from the ground bound state to the continuum state is given by

$$W=\lim_{t\to\infty}\frac{V}{t}\frac{1}{(2\pi)^3}\int \mathrm{d}^3\boldsymbol{p}\left|(S-1)_{\mathrm{fi}}^{\mathrm{WKB}}\right|^2. \tag{1}$$

According to Bauer,[14] the approximate S-matrix element describing the probability amplitude of ionization in the velocity gauge is

$$\begin{aligned}(S-1)_{\mathrm{fi}}^{\mathrm{WKB}} &= -\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}t\int \mathrm{d}^3r\frac{2}{Fr}\left(H_A\psi_\mathrm{f}\right)^*\Phi_i \\ &\quad -\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}t\int \mathrm{d}^3r\left(\psi_\mathrm{f}\right)^*\Phi_i\mathrm{i}\boldsymbol{A}(t)\cdot\nabla\frac{2}{Fr}.\end{aligned} \tag{2}$$

Here, $H_\mathrm{A}(t)=\boldsymbol{A}(t)\cdot(-\mathrm{i}\nabla)+\frac{1}{2}\boldsymbol{A}^2(t)$ is the Hamiltonian interaction between the laser field and the outgoing electron. In the dipole approximation the linearly polarized laser field may be described by the vector potential $\boldsymbol{A}(t)=A\varepsilon\cos\omega t$, where ε represents the unit vector in the direction of polarization, ω is the frequency of the laser field, and A is the amplitude of the vector potential. The corresponding electric field is obtained as $\boldsymbol{F}(t)=-\partial_t\boldsymbol{A}(t)=F\varepsilon\sin\omega t$, where $F=A\omega$ is the amplitude of the electric field. $2/Fr$ is the WKB Coulomb correction factor for a hydrogen atom. ψ_f is the Volkov state, and Φ_i is a stationary bound state. According to Krainov,[21] we have

$$(S-1)_1^{\mathrm{WKB}}=-\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}t\int \mathrm{d}^3r\frac{2}{Fr}\left(H_\mathrm{A}\psi_\mathrm{f}\right)^*\Phi_i. \tag{3}$$

$$(S-1)_2^{\mathrm{WKB}}=-\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}t\int \mathrm{d}^3r\left(\psi_\mathrm{f}\right)^*\Phi_i\mathrm{i}\boldsymbol{A}(t)\cdot\nabla\frac{2}{Fr}. \tag{4}$$

The factor $2/Fr$ changes the ground state of a hydrogen atom into the wave function of an electron in a potential of zero radius. In practical calculation, we include this factor into the initial-state wave function. Using the method which is similar to Reiss's, we obtain

$$\begin{aligned}(S-1)_1^{\mathrm{WKB}} &= \frac{\mathrm{i}}{\sqrt{V}}\frac{2}{F}\varphi^1_{i(\boldsymbol{p})}\left(\frac{p^2}{2}+E_\mathrm{b}\right)\int_{-\infty}^{\infty}\mathrm{d}t \\ &\quad\times\exp\left[\mathrm{i}\left(\frac{p^2}{2}+E_\mathrm{b}+U_\mathrm{p}\right)t\right. \\ &\quad\left.-\mathrm{i}\xi\sin\omega t+\mathrm{i}\frac{z}{2}\sin 2\omega t\right],\end{aligned} \tag{5}$$

$$\begin{aligned}(S-1)_2^{\mathrm{WKB}} &= \frac{2}{w\sqrt{V}}\varphi^2_{i(\boldsymbol{p})}\int_{-\infty}^{\infty}\mathrm{d}t \\ &\quad\times\exp\left[\mathrm{i}\left(\frac{p^2}{2}+E_\mathrm{b}+U_\mathrm{p}\right)t\right. \\ &\quad\left.-\mathrm{i}\xi\sin\omega t+\mathrm{i}\frac{z}{2}\sin 2\omega t\right],\end{aligned} \tag{6}$$

where $\xi = -(1/\omega)\boldsymbol{p}\cdot\boldsymbol{A}$, $z = A^2/4\omega$, E_b is the binding energy, and $U_\mathrm{p} = A^2/4$ is the ponderomotive potential (the energy of oscillating motion of a free electron driven by incident laser field). In addition, the Reiss parameter $z_1 = 2U_\mathrm{p}/E_\mathrm{b}$ and the Keldysh parameter γ are related by the Reiss parameter $z_1 = 1/\gamma^2$ for linear polarization. $\varphi^1_{i(\boldsymbol{p})}$ and $\varphi^2_{i(\boldsymbol{p})}$ are the Fourier transform of the initial-state wave function,

$$\varphi_i^1(\boldsymbol{p}) = \frac{2\pi}{\sqrt{\pi a^3}}\frac{1}{p^2/2+E_\mathrm{b}}, \tag{7}$$

$$\varphi_i^2(\boldsymbol{p}) = \frac{4\pi}{p\sqrt{\pi a^3}}\arctan(ap), \tag{8}$$

where $a = 2a_0/Z$, with a_0 being the Bohr radius.

Applying generalized Bessel function expansion:

$$\exp\left(-\mathrm{i}\xi\sin\omega t+\mathrm{i}\frac{z}{2}\sin 2\omega t\right) = \sum_{n=0}^{\infty}\mathrm{J}_n\left(\xi,-\frac{z}{2}\right)\mathrm{e}^{-\mathrm{i}nwt}. \tag{9}$$

Inverse function

$$\begin{aligned}&\mathrm{J}\left(\xi,-\frac{z}{2}\right)\\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}x\exp\left[\mathrm{i}\left(-\xi\sin x+\frac{z}{2}\sin 2x+nx\right)\right], \qquad (10)\\ &\int_{-\infty}^{\infty}\mathrm{d}t\exp\left[\mathrm{i}\left(\frac{p^2}{2}+E_\mathrm{b}+U_\mathrm{p}\right)t-\mathrm{i}\xi\sin\omega t+\mathrm{i}\frac{z}{2}\sin 2\omega t\right]\\ &= \int_{-\pi}^{\pi}\mathrm{d}x\exp[\mathrm{i}S_{p(x)}]\delta\left(\frac{p^2}{2}+E_\mathrm{b}+U_\mathrm{p}-n\omega\right),\\ &S_{p(x)} = nx-\xi\sin x+\frac{z}{2}\sin 2x. \qquad (11)\end{aligned}$$

By using the saddle point integral and the property of the δ function, substituting the S-matrix (Eq. (5) and Eq. (6)) into Eq. (1), and integrating with respect to $\boldsymbol{p}$ lead to

$$\begin{aligned}W_1 &= \frac{8\omega^2}{F^3\pi a^3\sqrt{E_\mathrm{b}}\sqrt{1+\gamma^2}}S(\gamma,F,E_\mathrm{b})\\ &\quad\times\exp\left[-\frac{4\sqrt{2}E_\mathrm{b}^{3/2}}{3F}\left(1-\frac{\gamma^2}{10}\right)\right], \qquad (12)\\ W_2 &= \frac{8\sqrt{2}\arctan^2(ap_0)}{Fa^3\pi\sqrt{E_\mathrm{b}}\sqrt{1+\gamma^2}p_0^2}S(\gamma,F,E_\mathrm{b})\\ &\quad\times\exp\left[-\frac{4\sqrt{2}E_\mathrm{b}^{3/2}}{3F}\left(1-\frac{\gamma^2}{10}\right)\right], \qquad (13)\\ W &= W_1+W_2, \qquad (14)\end{aligned}$$

where

$$S(\gamma,F,E_\mathrm{b}) = \frac{1}{\sqrt{\bar{C}}}\sum_{n=n_0}^{\infty}\exp\left[-\bar{B}\left(n-\frac{U_\mathrm{p}+E_\mathrm{b}}{\omega}\right)\right]\Phi(\xi_n), \tag{15}$$

with

$$\bar{B} = \frac{2\gamma^3}{3}(1-B), \tag{16}$$

and

$$\bar{C} = \frac{\sqrt{E_\mathrm{b}}}{\sqrt{2}F\sqrt{1+\gamma^2}}(1+C), \tag{17}$$

$\Phi(\xi_n)$ being the Dawson's integral, defined by

$$\Phi(\xi_n) = \int_0^{\xi_n}\exp\left(y^2-\xi_n^2\right)\mathrm{d}y \tag{18}$$

with

$$\xi_n = \left[4\omega\bar{C}\left(n-\frac{U_\mathrm{p}+E_\mathrm{b}}{\omega}\right)\right]^{1/2}. \tag{19}$$

The minimal number of photons absorbed is $n_0 = \langle E_\mathrm{b}/\omega+z+1\rangle$, the symbol $\langle\cdots\rangle$ denotes the integer part of the number inside. We note that the kinetic energy of the ionized outgoing electron is $p^2/2 = n\omega-z\omega-E_\mathrm{b}$. In this paper B and C are equal to

$$\frac{3F}{4\sqrt{2}E_\mathrm{b}^{3/2}}\left(1+\gamma^2\right)^2 \quad\text{and}\quad \frac{F\left(1+4\gamma^2\right)}{4\sqrt{2}E_\mathrm{b}^{3/2}},$$

respectively. In the tunneling domain, we look for a version of SFA, which leads to a proper ionization rate. For this case, the minimal number of photons absorbed $n_0 \gg 1$ and the sum over n can be replaced by an integral over the parameter $\beta = (n-n_0)/n_0$, and the main contribution to Eq. (15) is made by large n. Consequently, carrying out the integral over β, we obtain

$$S(\gamma,F,E_\mathrm{b}) = \frac{\sqrt{\pi}}{4\bar{C}\sqrt{\omega}\sqrt{\bar{B}}}. \tag{20}$$

As a result, the total photoionization rate for 1s hydrogen atom is described by the formula

$$\begin{aligned}W &= \left(\frac{\arctan^2(ap_0)}{\sqrt{\omega}p_0^2}+\frac{\omega^{3/2}}{F^2}\right)\frac{2\sqrt{2}}{\sqrt{\pi}a^3E_\mathrm{b}\sqrt{\bar{B}}(1+C)}\\ &\quad\times\exp\left[-\frac{4\sqrt{2}E_\mathrm{b}^{3/2}}{3F}\left(1-\frac{\gamma^2}{10}\right)\right], \qquad (21)\end{aligned}$$

with $p_0 = \sqrt{2\omega n_0}$.

This is the main result of this paper: a formula for the ionization rate of 1s hydrogen atom which is as simple as Keldysh's formula with using the length gauge. Such a simple formula is first provided for 1s hydrogen atom including the long-range Coulomb potential effect in the velocity gauge.

3. Numerical results and discussion

In this section, we will obtain numerical results by using our analytical formula (Eq. (18))for the atomic system, and compare them with numerical results from other authors. The expression for the tunnel ionization of atoms in a linear polarized laser field is[9,22]

$$W_\mathrm{stat}^\mathrm{av} = \frac{8Z^5}{\pi F}K_0\left(\frac{2Z^3}{3F}\right), \tag{22}$$

where $K_0 = \int_0^\infty \mathrm{d}y \exp(-x\cosh y)$ and Z is the nuclear charge. According to Bauer,[9] the Keldysh result for the 1s state of a hydrogen atom in the linearly polarzed laser field with the WKB Coulomb correction is

$$W_{\mathrm{lin}}^{\mathrm{Keldysh,WKB}} = \frac{8Z^7}{F^2} \sum_{n=n_0}^{\infty} \sqrt{2E_n} \int_0^{\pi} \mathrm{d}\theta \sin\theta J_n^2 \times \left(\sqrt{\frac{8zE_n}{\omega}} \cos\theta, -\frac{z}{2} \right), \tag{23}$$

where $E_n = p^2/2 = n\omega - z\omega - E_{\mathrm{b}}$.

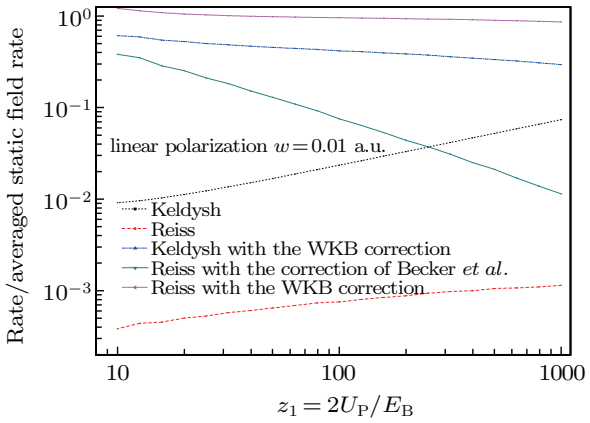


Fig. 1. (color online) Plot of various KFR ionization rates for the linearly polarized laser field or static-field ionization rate as a function of Reiss intensity parameter z_1, with the laser frequency ω fixed at 0.01 a.u.

We look for a version of the KFR theory, which leads to a proper ionization rate in the low-frequency-high-intensity limit, i.e., $\omega \ll 1$ and $z_1 \gg 1$. Therefore, it is reasonable to keep one of the parameters fixed and change the other one. In numerical calculations of different ionization rates, we fix either the Reiss parameter at $z_1 = 100$, or the laser frequency at $\omega = 0.01$ a.u. Thereby our parameters lie well within the range described by the two conditions $\omega \ll 1$ a.u. and $z_1 \gg 1$. In Fig. 1, we show five different ionization rates calculated by us and other authors as a function of the Reiss intensity parameter z_1 for $\omega = 0.01$ a.u. The dotted line denotes the Keldysh ionization rate (see Eq. (20) from Ref. [7]). The dash line refers to the Reiss ionization rate (see Eq. (33) from Ref. [7]). The Keldysh theory with the WKB Coulomb correction (Eq. (23)) is displayed with a dash dotted line. The solid line represents the ionization rate of Reiss with the WKB Coulomb correction (Eq. (21)). Finally, we add one double-dotted line corresponding to the static field ionization rate for the same electric-field amplitude F. In Fig. 2, these five ionization rates are shown with the same kind of lines as the above, but for $z_1 = 100$ as a function of the laser frequency ω. The main conclusion one can draw from the two figures is that the difference between the length gauge and the velocity gauge formulation in the SFA is as large as one or two orders of magnitude. However, it is obvious that the photoionization rate in the presence of the Coulomb potential is always larger than that in its absence and the discrepancy between the two theories can also be reduced. The results of Keldysh with the WKB correction in Ref. [14] are larger than our results, which may be because in the course of calculating Bessel functions, we use the simpler Bessel functions. Our line (Reiss with the WKB correction) accords with the line(Keldysh with the WKB correction) in Ref. [14] better. Moreover, in the whole range of the figures, our result (Eq. (21)) agrees very well with the static field ionization rate. One can convince oneself that the Reiss theory with the WKB Coulomb correction (solid line) has the correct behavior in the low-frequency-high-intensity limit.

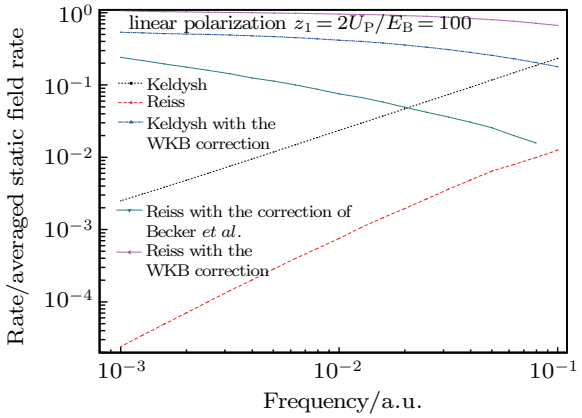


Fig. 2. (color online) Plots of various KFR ionization rates for the linearly polarized laser field or static-field ionization rate as a function of the laser frequency ω, with the Reiss intensity parameter z_1 fixed at 100.

4. Conclusions

In this work, for 1s hydrogen atom, we derive an ionization rate formula by using the velocity gauge in the tunnel region, based on the exact treatment of the WKB Coulomb correction in the continuum wave function of the ionization. Our formula is more concise than Bauer's result.[14] To the best of our knowledge, for the first time such a simple formula is obtained in the velocity gauge S-matrix theory for 1s hydrogen atom where the long-range Coulomb potential exists. An analysis of the numerical result for the ionization rate calculated via our formulas Eq. (18), as well as the combined result Eq. (20) shows that the discrepancy between the length gauge SFA and velocity gauge SFA can be reduced if one includes the WKB Coulomb correction in the final state of the ionized electron. The main conclusion one can draw is that our result is consistent with the well-known static-field limit in the tunnel region. In addition, in the tunneling domain, it should be noted that the exponential factor of the formula we obtained in this work is exactly the same as that derived by Keldysh in which the Coulomb interaction is neglected. This is consistent with the prediction made by Keldysh that if the Coulomb interaction is considered, as is well known, the power of electric laser field F in the pre-exponential expression is changed, but

the exponential itself is unchanged. This demonstrates that the ionization mechanism is essentially determined by the exponential factors.

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