Low-frequency-high-intensity limit of the Keldysh-Faisal-Reiss theory

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When a frequency of the circularly polarized laser field approaches zero the above threshold ionization rate should approach the well-known static-field limit of tunneling ionization. In the high-intensity limit of the laser field the Keldysh-Faisal-Reiss (KFR) theory is expected to be valid. For the ground state of a hydrogen atom we study various forms of the KFR theory when both conditions: $\omega \ll 1$ a.u. and $\gamma \ll 1$ (ω is the frequency and γ the Keldysh parameter) are satisfied. For the circularly polarized laser field ionization rate in the Keldysh theory [which utilizes the length gauge ($\vec{d} \cdot \vec{E}$) form of the matrix element] is calculated analytically. We show numerically that if the WKB Coulomb correction in the final state of the ionized electron is included, the Keldysh theory gives the correct result in the tunneling domain. In the barrier-suppression regime the Keldysh theory without this correction gives ionization rates close to the exact static-field results. The Reiss theory [which utilizes the velocity gauge ($\vec{p} \cdot \vec{A}$) form of the matrix element] leads to too small ionization rates in the limit $\omega \rightarrow 0$, $\gamma \rightarrow 0$.

DOI: 10.1103/PhysRevA.73.023421

PACS number(s): 32.80.Rm

I. INTRODUCTION

For many years nonresonant multiphoton processes such as above-threshold detachment (ATD) of ions and abovethreshold ionization (ATI) of atoms (see Refs. [1,2] for the earliest experiments, and for reviews see, for example, Refs. [3–5]) in an intense electromagnetic (laser) field have been described with the help of the Keldysh-Faisal-Reiss (KFR) theories [6-8]. Initially they were applied to weakly bound systems-for example, to the outer electron of a negative hydrogen ion [8]—but later also to different atoms. In the latter case (photoionization) the description is more difficult due to the long-range Coulomb potential effect on the final state of the ionized outgoing electron. From the physical point of view using linear polarization of the laser field is more interesting, because one can experimentally observe such phenomena like rescattering [9] effects in the energy spectra of outgoing electrons and nonsequential double [10] or multiple ionization. In the above-mentioned pioneering KFR papers [6-8] these phenomena were not treated, because only the so-called direct electrons were considered. The direct electron, initially in the bound state of an atom or an ion, makes only a single transition to its final free state. We believe that this simple picture of ATD and ATI is enough to correctly predict rates of single detachment or ionization for any polarization of incident laser field. In this paper we limit ourselves to photoionization of the ground state of a hydrogen atom (or a hydrogenic positive ion), but it is quite likely that our conclusions hold also for the excited states of many-electron atoms and maybe even for nonsequential double ionization.

The KFR theories utilize the *S*-matrix theory, which is in principle exact. However, since there is no general analytical solution to the Schrödinger equation for a charged particle interacting with both the field of an attractive Coulomb center and an electromagnetic plane-wave field, one has to use analytical approximations to evaluate the S-matrix element for bound-free transitions. Therefore various approximate theories may lead to different expressions for the ionization rate. All three versions of the KFR theory describe the same physical problem, and the main difference between them is in the form of the laser-atom interaction. Whereas the $d \cdot E$ form (sometimes called the length gauge) was used by Keldysh [6], the $\vec{p} \cdot A$ form (sometimes called the velocity gauge) was used by Reiss [8]. Both theories start from the time-reversed S-matrix element. The Faisal theory [7] starts from the direct-time S-matrix element in velocity gauge, but after some further approximations it ends up with an ionization rate formula identical with that of Reiss, at least for the 1s hydrogen atom [7,11]. The Reiss version of the KFR theory is also known as the strong-field approximation (SFA). In the KFR theory one assumes that the laser field is strong enough that one can neglect the influence of the Coulomb potential on the final state of the outgoing electron. This is quite a good approximation for photodetachment of a negative hydrogen ion, because the total electric charge of the remaining atom is zero. Otherwise, in the atom photoionization process (for example, hydrogen or alkaline-earth atoms), the escaping electron interacts with the long-range Coulomb potential of the remaining positively charged ion. Therefore one has to include somehow Coulomb corrections in the final state of the ionized electron (see, e.g., Ref. [12] for references therein). The KFR theory for atoms works better for circularly polarized radiation because due to selection rules, the average kinetic energy of an outgoing electron (equivalently the average number of photons absorbed) is much larger than in the case of linear polarization for the same radiation intensity [3].

Our paper is organized as follows. In Sec. II we review expressions for static-field ionization rates. In Sec. III we review the basis of the KFR theory and we define parameters important in strong-field ionization, etc. (This section may be omitted by the readers familiar with the KFR theory.) The

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ionization rate formula in the Keldysh theory for the circularly polarized laser field is derived in Sec. IV. The WKB Coulomb corrections in the final state of ionized electron are discussed in Sec. V. The numerical results and conclusions are given in Sec. VI, where we compare various KFR ionization rates for $\omega \ll 1$ a.u. and $\gamma \ll 1$ with the static-field ionization rates. The comparison has been made also with the exact static field ionization rates of Scrinzi *et al.* [13] up to F=1 a.u. (*F* is the electric field). There is also an appendix containing details of some analytical calculations. In what follows we consistently use atomic units $\hbar = e = m_e = 1$, substituting explicitly -1 for the electronic charge. We keep any nuclear charge *Z* in all the equations given below, but finally, in the numerical calculations, we put Z=1 for a hydrogen atom.

II. STATIC-FIELD IONIZATION RATES

The following formula [14–16] describes the ionization rate for the hydrogen 1s atom in an external static electric field F, provided that $F \ll 1$ a.u.:

$$\Gamma_{\text{stat}} = \frac{4Z^5}{F} \exp\left(-\frac{2Z^3}{3F}\right). \tag{1}$$

This expression is approximately valid also for the circularly polarized laser field when $\omega \ll 1$ a.u. and $\gamma \ll 1$. If we assume that the field changes periodically in time, $F(t)=F\sin(\omega t + \phi_0)$, we can average Γ_{stat} over the field period $T=2\pi/\omega$ and obtain the formula, which is approximately valid for the linearly polarized laser field (if $\omega \ll 1$ a.u. and $\gamma \ll 1$),

$$\Gamma_{\text{stat}}^{\text{av}} = \frac{8Z^5}{\pi F} K_0 \left(\frac{2Z^3}{3F}\right) \cong 4\sqrt{\frac{3Z^7}{\pi F}} \exp\left(-\frac{2Z^3}{3F}\right), \qquad (2)$$

where we have used the following integral representation of the modified Bessel function $K_0(x)$:

$$K_0(x) = \int_0^\infty dy \, \exp(-x \cosh y),$$

and its asymptotic form for $x \to \infty$, $K_0(x) \cong (\pi/2x)^{1/2} e^{-x}$. Note that the result in Eq. (2) does not depend on the frequency of the laser field. The expressions from Eqs. (1) and (2) are special cases of the well-known Ammosov-Delone-Krainov (ADK) [17,16] tunneling ionization rates, which were confirmed experimentally very well (see, for example, Refs. [18,19]). Other more accurate theoretical calculations [20,21,13] confirmed validity of Eq. (1) in the asymptotic limit $F/F_{cr} \rightarrow 0$. $F_{cr} \approx 0.15$ a.u. is the critical-field strength for the ground-state hydrogen atom [22]. The static-field limit in multiphoton ionization of this atom was investigated with the help of the Floquet method [22]. For the circularly polarized laser field the Floquet ionization rates approach Eq. (1) smoothly with decreasing frequency. For the linearly polarized laser field the Floquet ionization rates show intermediate resonances, which are absent in Eq. (2). However, it was stated quite generally, for the Floquet method, that for arbitrary polarization ionization rates approach the cycleaveraged static-field ionization rates as the frequency decreases.

III. BASIS OF THE KFR THEORY

The probability amplitude that a one-electron state $\Psi_i^{(+)}$, which has evolved under the combined effects of the Coulomb and the laser field from an initial undisturbed bound state Φ_i into some other laser-field-free final state Φ_f , is given by the overlap

$$S_{fi} = \lim_{t \to \infty} (\Phi_f, \Psi_i^{(+)}) = \lim_{t \to -\infty} (\Psi_f^{(-)}, \Phi_i),$$
(3)

where $\Psi_f^{(-)}$ is the final one-electron out-state containing the complete effects of laser and Coulomb potentials. There are two equivalent forms, the direct time and the reversed time ones, of the exact *S*-matrix in Eq. (3). There are advantages of the latter form [8,11], which are utilized in the Keldysh and Reiss theories. The following time-dependent Schrödinger equations are satisfied:

$$i\frac{\partial}{\partial t}\Phi = H_0\Phi, \quad i\frac{\partial}{\partial t}\Psi = H\Psi,$$
 (4)

where $H_0 = \vec{p}^2/2 - Z/r$ is the atomic Hamiltonian $(\hat{\vec{p}} = -i\vec{\nabla})$, $H = H_0 + H_I$, and

$$H_I = \frac{1}{c}\vec{A}(t) \cdot \vec{p} + \frac{1}{2c^2}\vec{A}(t)^2$$
(5)

is the Hamiltonian describing the interaction with the laser field in velocity gauge. The latter Hamiltonian is given here in the dipole approximation, which is roughly valid, if the wavelength of the incident radiation is much larger than the atomic size. In the present paper we disregard the effect of magnetic field component [23] of the laser field and relativistic effects. Thus the laser field inside the atom is a function of time only. $\vec{A}(t)$ is the vector potential for the circularly or linearly polarized electromagnetic plane-wave field of frequency ω in radiation gauge, with the boundary condition $\lim_{t\to\pm\infty} \vec{A}(t) = \vec{0}$. The vector potential of the laser field is given by

$$\vec{A}(t) = \frac{a}{\sqrt{2}} [\hat{e}_x \cos(\omega t + \varphi_0) \pm \hat{e}_y \sin(\omega t + \varphi_0)],$$

for circular polarization, (6a)

and

$$A(t) = a\hat{e}_z \cos(\omega t + \phi_0)$$
, for linear polarization, (6b)

where the upper and lower signs refer to the right and left circular polarization, respectively, \hat{e}_x , \hat{e}_y , and \hat{e}_z , are real unit vectors, and φ_0 is an arbitrary initial phase. In the case of circular polarization the electromagnetic plane wave propagates along the *z* axis and in the case of linear polarization along the *x* axis. This choice gives the greatest simplicity of analytical calculations. Equations (6) correspond to the same radiation intensity for both polarizations (for the same *a*, which is constant in time). Following Reiss [8], let us introduce the intensity parameter *z* such that LOW-FREQUENCY-HIGH-INTENSITY LIMIT OF THE...

$$U_P = z\omega = \left\langle \frac{\vec{A}(t)^2}{2c^2} \right\rangle = \frac{a^2}{4c^2} = \frac{I}{4\omega^2},$$
 (7)

where U_P stands for the ponderomotive potential [the timeaveraged kinetic energy $\langle E_k(t) \rangle$ of a classical free charge oscillating in an electromagnetic plane-wave field] and *I* stands for the radiation intensity in atomic units (1 a.u. $\cong 3.51 \times 10^{16} \text{ W/cm}^2$; for circular polarization $I=2F^2$ and for linear polarization $I=F^2$, where *F* is the electric-field vector amplitude). The second expression from Eq. (3), Eqs. (4), and the boundary condition $\lim_{t\to\infty} \Psi_f^{(-)} = \Phi_f$ lead to the exact timereversed *S*-matrix element [8,11,24]

$$(S-1)_{fi} = -i \int_{-\infty}^{\infty} dt (\Psi_f^{(-)}, H_I \Phi_i).$$
(8)

The initial state Φ_i is the initial state of an atom or an ion. The KFR theory is based on replacing the exact wave function $\Psi_f^{(-)}$ by the Volkov (or Gordon-Volkov) state [25] describing the electron freely oscillating in the electromagnetic plane-wave field. Thus the influence of the remaining atom or ion on the final state of the escaping electron is entirely neglected in the KFR theory [6–8]. The Volkov state and the equation it obeys are given as

$$\Psi^{V}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \exp\left[i\vec{p}\cdot\vec{r} - \frac{i}{2}\int_{-\infty}^{t} \left(\vec{p} + \frac{1}{c}\vec{A}(\tau)\right)^{2}d\tau\right],$$
(9a)

$$i\frac{\partial}{\partial t}\Psi(\vec{r},t) = \frac{1}{2}\left(-i\vec{\nabla} + \frac{1}{c}\vec{A}(t)\right)^2\Psi(\vec{r},t). \tag{9b}$$

This approximation is supposed to be valid for a very intense field, when the oscillation energy of the detached electron in the laser field dominates the atomic binding energy. When Eqs. (5) and (9a) are employed in Eq. (8) one obtains the Reiss theory, which improves as the laser field becomes stronger. Two conditions usually determine the lower and upper applicability limits of the KFR theory:

$$z_{1} \equiv \frac{2U_{P}}{E_{B}} = \frac{I}{2\omega^{2}E_{B}} \gg 1, \quad z_{f} \equiv \frac{2U_{P}}{c^{2}} = \frac{I}{2\omega^{2}c^{2}} \ll 1.$$
(10)

Equations (10) say that the ponderomotive potential of the outgoing electron should be much larger than the electron binding energy $E_B = Z^2/2$ (in the atom or in the ion) and much less than the electron rest energy. The latter condition is due to nonrelativistic description of the process. The Keldysh parameter γ is connected with the Reiss parameter z_1 : $z_1=1/\gamma^2$ for linear polarization and $z_1=2/\gamma^2$ for circular polarization. In the length gauge the laser-atom interaction Hamiltonian is

$$H_I^{dE} = \vec{r} \cdot \vec{F}(t), \quad \text{with } \vec{F}(t) = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t}$$
(11)

being the electric field vector, and the Volkov state in this gauge is

$$\Psi^{V,dE}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \exp\left[i\left(\vec{p} + \frac{1}{c}\vec{A}(t)\right) \cdot \vec{r} - \frac{i}{2} \int_{-\infty}^{t} \left(\vec{p} + \frac{1}{c}\vec{A}(\tau)\right)^{2} d\tau\right].$$
 (12)

The time-dependent Schrödinger equation for the atom in velocity gauge, in the dipole approximation [the second equation of Eqs. (4) with Eq. (5)] can be transformed by applying the unitary operator (with β being arbitrary number)

$$\hat{U}(\beta) = \exp\left[i\frac{\beta}{c}\vec{A}(t)\cdot\vec{r}\right].$$
(13)

The wave function and operators change in accordance with the rules $\Psi' = \hat{U}\Psi$, and $\hat{O}' = \hat{U}\hat{O}\hat{U}^{-1}$. We note that for $\beta=0$ this transformation becomes an identity. With the help of the Baker-Cambell-Hausdorff formula one easily finds that the transformed operators are

$$\left(\frac{\partial}{\partial t}\right)' = \frac{\partial}{\partial t} - i\frac{\beta}{c}\vec{r} \cdot \frac{\partial\vec{A}(t)}{\partial t}, \quad (\hat{\vec{p}})' = \hat{\vec{p}} - \frac{\beta}{c}\vec{A}(t), \quad (\vec{r})' = \vec{r},$$
(14)

and using Eq. (11) one obtains the transformed timedependent Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi'(\vec{r},t) = \left[\frac{1}{2}\left(\hat{\vec{p}} - \frac{\beta}{c}\vec{A}(t) + \frac{1}{c}\vec{A}(t)\right)^2 + \beta\vec{r}\cdot\vec{F}(t) - \frac{Z}{r}\right]\Psi'(\vec{r},t).$$
(15)

In this equation both scalar and vector potentials describe the interaction of the atom with the laser field. For $\beta=0$, Eq. (15) is in velocity gauge, and for $\beta=1$, it is in length gauge, but for any other β it is in some "intermediate" gauge. In each case both potentials describe the same magnetic \vec{B} and electric \vec{E} fields of the plane wave in the dipole approximation:

$$\vec{B} = \vec{\nabla} \times (1 - \beta)\vec{A}(t) = \vec{0},$$
$$\vec{E} = -\frac{1}{c}\frac{\partial}{\partial t}(1 - \beta)\vec{A}(t) - \vec{\nabla}(\beta\vec{r}\cdot\vec{F}(t)) = \vec{F}(t).$$
(16)

We will return to the problem of choice of β in Sec. VI.

IV. KELDYSH THEORY

If we put $\beta=1$ and utilize Eqs. (11) and (12) in the matrix element (8), we will obtain the Keldysh probability amplitude of ionization:

$$(S-1)_{fi}^{\text{Keldysh}} = -i \int_{-\infty}^{\infty} dt \int d^3r \, \Psi^{V,dE}(\vec{r},t)^* \vec{r} \cdot \vec{F}(t) \Phi_i(\vec{r},t),$$
(17)

where the initial, ground state of a hydrogen atom $(E_B = Z^2/2)$ is described by the wave function

$$\Phi_i(\vec{r},t) \equiv \Phi_i(\vec{r})\exp(iE_B t) = \sqrt{\frac{Z^3}{\pi}}\exp(-Zr)\exp(iE_B t)$$
(18)

in position space or by its Fourier transform

$$\tilde{\Phi}_{i}(\vec{p}) = \int \frac{d^{3}r}{(2\pi)^{3/2}} \exp(-i\vec{p}\cdot\vec{r}) \Phi_{i}(\vec{r}) = \frac{\sqrt{8Z^{5}}}{\pi} \frac{1}{(Z^{2}+p^{2})^{2}}$$
(19)

in momentum space. In both spaces their absolute values squared are normalized to unity. Starting from Eq. (17), Keldysh [Eq. (20) of Ref. [6]] derived the following ionization rate formula for the linearly polarized laser field:

$$\Gamma_{\rm lin}^{\rm Keldysh} = \frac{\sqrt{3\,\pi ZF}}{2^{7/4}} \exp\left\{-\frac{2Z^3}{3F} \left[1 - \frac{1}{10} \left(\frac{\omega Z}{F}\right)^2\right]\right\}, \quad (20)$$

where F is the electric-field amplitude. In obtaining his result Keldysh utilized the saddle-point method and the condition that the number of photons absorbed be much larger than unity. One can avoid this condition at the cost of an additional summation in the ionization rate formula.

To the best of our knowledge, for the circularly polarized laser field, the formula analogical to Eq. (20) has not been known so far. Our derivation will be similar to that of Reiss [8]. A pretty much simplification comes from the fact that

$$\frac{\partial}{\partial t} \exp\left(-\frac{i}{c}\vec{A}(t)\cdot\vec{r}\right) = i\vec{r}\cdot\vec{F}(t)\exp\left(-\frac{i}{c}\vec{A}(t)\cdot\vec{r}\right),\quad(21)$$

where Eq. (11) has been used. After this substitution the integration by parts upon time can be done and interchanging the order of integrations we obtain

$$(S-1)_{fi}^{\text{Keldysh}} = i \int_{-\infty}^{\infty} dt \widetilde{\Phi}_i \left(\vec{p} + \frac{1}{c} \vec{A}(t) \right) \left[\frac{1}{2} \left(\vec{p} + \frac{1}{c} \vec{A}(t) \right)^2 + E_B \right]$$
$$\times \exp\left[\frac{i}{2} \int_{-\infty}^t \left(\vec{p} + \frac{1}{c} \vec{A}(\tau) \right)^2 d\tau + i E_B t \right]. \quad (22)$$

This expression is quite general and describes the Keldysh probability amplitude of ionization (or detachment) for any initial state described by $\Phi_i(\vec{r},t)$ in the laser field (of any polarization, but in the dipole approximation) given by $\vec{A}(t)$. For the 1s hydrogen atom the denominator in $\tilde{\Phi}_i(\vec{p} + (1/c)\vec{A}(t))$ is proportional to the square of the second factor in Eq. (22). Therefore the product of the first two factors in Eq. (22) is proportional to

$$\left[\frac{1}{2}\left(\vec{p}+\frac{1}{c}\vec{A}(t)\right)^2 + E_B\right]^{-1} = \sum_{k=-\infty}^{\infty} A_k(\vec{p})e^{ik(\omega t + \varphi_0 + \varphi_0)} \quad (23)$$

and can be expanded in the above Fourier series. The coefficients A_k are calculated in the Appendix. We use a spherical system of coordinates in which the z axis is parallel to the propagation direction of the incoming electromagnetic plane wave. Thus (ϑ, φ) are polar and azimuthal angles of the canonical momentum \vec{p} of the outgoing electron. Next we proceed in the standard way [7,8] using the Fourier-Bessel expansion for the exponential factor in Eq. (22):

$$e^{ix\sin\alpha} = \sum_{n=-\infty}^{\infty} J_n(x)e^{in\alpha}.$$
 (24)

From Eqs. (22), (23) and (24) we get the following expression for the Keldysh probability amplitude of ionization:

$$(S-1)_{fi}^{\text{Keldysh}} = i\sqrt{2Z^5}e^{i(\sqrt{2z}/\omega)p\sin\vartheta}\sin\vartheta\sin(\varphi_0\pm\varphi)$$
$$\times \sum_{n=-\infty}^{\infty}\sum_{k=-\infty}^{\infty}J_n\left(\sqrt{\frac{2z}{\omega}}p\sin\vartheta\right)A_k(\vec{p})e^{i(n+k)(\varphi_0\pm\varphi)}$$
$$\times\delta\left(\frac{p^2}{2} + E_B + z\omega + (n+k)\omega\right).$$
(25)

The differential ionization rate $\gamma(\vec{p})$, which is the transition probability per unit time and unit volume in the canonical momentum (\vec{p}) space, can be found from

$$\gamma(\vec{p}) = \lim_{t \to \infty} \frac{|(S-1)_{fi}|^2}{t}.$$
(26)

To obtain the total ionization probability per unit time, Γ , one has to integrate the differential ionization rate over all the possible final momenta of the outgoing electron. The Dirac δ function reflects the conservation of the total energy after ionization and leads to the summation over N=n+k in the final expression:

$$\Gamma_{\rm cir}^{\rm Keldysh} = \int d^3 p \, \gamma(\vec{p})$$
$$= 2Z^5 \sum_{N=N_0}^{\infty} \sqrt{2E_N} \int_0^{\pi} d\vartheta \sin \vartheta \left[\sum_{k=-\infty}^{\infty} |A_k(E_N, \vartheta)| \times J_{N+k} \left(2\sqrt{\frac{zE_N}{\omega}} \sin \vartheta \right) \right]^2, \quad (27)$$

where the minimal number of photons absorbed is $N_0 = [z + E_B/\omega] + 1$ and the kinetic energy of the ionized outgoing electron is $E_N = p_N^2/2 = N\omega - z\omega - E_B$. (The symbol [···] denotes the integer part of the (positive) number inside.) In deriving Eq. (27) we have used the following property of the Bessel functions: $J_{-n}(x) = (-1)^n J_n(x)$ and we have also used the relation $A_k(\vec{p}) = (-1)^k |A_k(\vec{p})|$ (see the Appendix). The expression analogical to Eq. (27) in the Reiss theory is very well known [8] and in our notation is given as

$$\Gamma_{\rm cir}^{\rm Reiss} = 2Z^5 \sum_{N=N_0}^{\infty} \frac{\sqrt{2E_N}}{(E_N + E_B)^2} \\ \times \int_0^{\pi} d\vartheta (\sin \vartheta) J_N^2 \left(2\sqrt{\frac{zE_N}{\omega}} \sin \vartheta \right), \quad (28)$$

with the same meaning of N_0 and E_N .

V. KELDYSH THEORY WITH THE WKB COULOMB CORRECTION

During the photoionization of neutral atom one should take into account the long-range Coulomb potential effect on

the final state of the outgoing electron. In the tunneling domain, when $\omega \ll 1$ a.u. and $\gamma \ll 1$, the quasiclassical (WKB) approximation may be applied. Krainov and Shokri [26,27] have shown that for the ground state of a hydrogen atom the Volkov wave function should be multiplied by the factor of $2Z^2/Fr$. Their expression $V(\vec{r},t) = \vec{p} \cdot A/c + A^2/2c^2$ [see, for example, Eq. (8) of Ref. [27]] suggests that calculations have been done utilizing the $\vec{p} \cdot A$ form of the S-matrix element. However, one must remember that \vec{p} in $H_I = \vec{A}(t) \cdot \vec{p}/c$ $+\tilde{A}(t)^2/2c^2$ and in this matrix element is the operator $-i\vec{\nabla}$ [see, for example, Eq. (6) of Ref. [8]]. Therefore the Volkov wave function times const/r is not an eigenfunction of H_I and one cannot proceed in further calculations following Reiss [8]. Only if one neglects an additional term in the S-matrix element, connected with acting $\vec{p} = -i\vec{\nabla}$ on the factor of const/r, one can include this factor in the initial-state wave function. In this way the factor of const/r changes the ground state of a hydrogen atom into the wave function of an electron in a potential of zero radius. The probability amplitude of ionization in the Reiss theory [the expression analogical to Eq. (22) is the following:

$$(S-1)_{fi}^{\text{Reiss}} = i \int_{-\infty}^{\infty} dt \tilde{\Phi}_i(\vec{p}) \left(\frac{p^2}{2} + E_B\right) \\ \times \exp\left[\frac{i}{2} \int_{-\infty}^t \left(\vec{p} + \frac{1}{c}\vec{A}(\tau)\right)^2 d\tau + iE_B t\right].$$
(29)

Comparing Eqs. (22) and (29) we see that when the product of the first two factors in each of these equations is a constant, both equations become identical. This is the case of the initial-state wave function (in the zero-radius potential) proportional to e^{-Zr}/r . Then the Keldysh and Reiss ionization rates are equal. This explains why our length gauge calculations given below in this section lead to a result similar to the result of Krainov. In fact, we find that Eq. (7) of Ref. [27] integrated over spherical angles gives our result, Eq. (32a), times $e^2/2\pi \approx 1.18$. (It is connected with different normalization constant of the initial-state wave function, which is given in more general and large-*r* asymptotic form in Ref. [27].)

Let us now calculate ionization rate in the Keldysh theory (when both conditions $\omega \ll 1$ a.u. and $\gamma \ll 1$ are satisfied) with the WKB Coulomb correction in the final state of the ionized electron. We start from Eq. (17), where we substitute Eqs. (18) and (11), but instead of Eq. (12) we substitute the Volkov wave function [Eq. (12)] times the factor of $2Z^2/Fr$. Since the laser-atom Hamiltonian is a number now, we can include the factor of const/r into the initial-state wave function. We proceed further likewise in Sec. IV, utilizing Eqs. (21) and (22). When the position-space wave function (normalized to unity) is given by

$$\Phi(\vec{r}) = \sqrt{\frac{Z}{2\pi}} \frac{e^{-Zr}}{r},$$
(30)

its momentum-space counterpart (also normalized to unity) is given by

$$\tilde{\Phi}(\vec{p}) = \int \frac{d^3r}{(2\pi)^{3/2}} \exp(-i\vec{p}\cdot\vec{r})\Phi(\vec{r}) = \frac{\sqrt{Z}}{\pi} \frac{1}{p^2 + Z^2}.$$
 (31)

Using also the equality $E_B = Z^2/2$, we see that $\tilde{\Phi}(\vec{p})(p^2/2 + E_B)$ is a constant indeed. We finally find ionization rates for circular and linear polarization of incident radiation, respectively:

$$\Gamma_{\rm cir}^{\rm Keldysh,WKB} = \frac{8Z^7}{F^2} \sum_{N=N_0}^{\infty} \sqrt{2E_N} \times \int_0^{\pi} d\vartheta \sin \vartheta J_N^2 \left(2\sqrt{\frac{zE_N}{\omega}} \sin \vartheta \right),$$
(32a)

$$\Gamma_{\rm lin}^{\rm Keldysh,WKB} = \frac{8Z^7}{F^2} \sum_{N=N_0}^{\infty} \sqrt{2E_N} \\ \times \int_0^{\pi} dv \sin \vartheta J_N^2 \bigg(\sqrt{\frac{8zE_N}{\omega}} \cos \vartheta, -\frac{z}{2} \bigg),$$
(32b)

with the same meaning of N_0 and E_N as before. There are generalized Bessel functions in Eq. (32b) (see, for example, Ref. [8] for their definition).

VI. NUMERICAL RESULTS AND CONCLUSIONS

In this section we numerically look for a version of the KFR theory, which leads to proper ionization rate in the limit $\omega \rightarrow 0, \gamma \rightarrow 0$. Small Keldysh parameters $(\gamma \rightarrow 0)$ are equivalent to large Reiss parameters $(z_1 \rightarrow \infty)$. On the ground of the well-known results from Sec. II we expect that for the circularly polarized laser field the proper KFR ionization rate should approach Eq. (1) and for the linearly polarized laser field Eq. (2). Among various versions of the KFR theory we have chosen these with no Coulomb corrections in the final state of the outgoing electron [6,8] and those of recent interest with the WKB Coulomb correction. For completeness we quote here, in our notation, the Reiss result [8] for the ground state of a hydrogen atom in the linearly polarized laser field:

$$\Gamma_{\rm lin}^{\rm Reiss} = 2Z^5 \sum_{N=N_0}^{\infty} \frac{\sqrt{2E_N}}{(E_N + E_B)^2} \int_0^{\pi} d\vartheta(\sin\vartheta) \\ \times J_N^2 \left(\sqrt{\frac{8zE_N}{\omega}}\cos\vartheta, -\frac{z}{2}\right),$$
(33)

with the same meaning of N_0 and E_N as before. Recently A. Becker *et al.* [28] extensively investigated for hydrogen, but also for other atoms like He, Ne, Ar, Kr, and Xe, the Reiss ionization rate formula (the "plane-wave KFR rate" [28]) with the Coulomb correction factor, the so-called C^2 correction factor [29]. This result is approximate (a "WKB estimate" [28]), and it is based on a simplification of the result obtained earlier by Krainov and Shokri [26,27]. In our case, for the 1*s* hydrogen atom, the C^2 correction factor is equal to



FIG. 1. Plot of the ratios of four different KFR ionization rates (for the circularly polarized laser field) to static-field (the same electric field) ionization rate against the laser frequency (see text for details). The Reiss intensity parameter is constant here: $z_1 = 100$.

 Z^6/F^2 for both polarizations. (*F* is the electric field amplitude.) Hence for circular and linear polarization we obtain, respectively,

$$\Gamma_{\rm cir}^{\rm A. \ Becker \ et \ al.} = \frac{Z^6}{F^2} \Gamma_{\rm cir}^{\rm Reiss} = \frac{2Z^6}{I} \Gamma_{\rm cir}^{\rm Reiss} = \frac{Z^6}{2z\omega^3} \Gamma_{\rm cir}^{\rm Reiss},$$
(34a)

$$\Gamma_{\rm lin}^{\rm A. \ Becker \ et \ al.} = \frac{Z^6}{F^2} \Gamma_{\rm lin}^{\rm Reiss} = \frac{Z^6}{I} \Gamma_{\rm lin}^{\rm Reiss} = \frac{Z^6}{4z\omega^3} \Gamma_{\rm lin}^{\rm Reiss},$$
(34b)

where the Reiss ionization rates are given by Eqs. (28) and (33).

We investigate the two-parameter limit $(\omega \rightarrow 0, z_1 \rightarrow \infty)$, for which an additional condition $(F \leq 1 \text{ a.u.})$, connected with the applicability of Eqs. (1) and (2), should be satisfied. Therefore it is reasonable to keep one of the parameters fixed and change the other one, and then reversely. In numerical



FIG. 2. Same as Fig. 1 (circular polarization), but against the Reiss intensity parameter z_1 . The laser frequency is constant here: $\omega = 0.01$ a.u.



FIG. 3. Same as Fig. 1, but for the linearly polarized laser field (see text for details). The Reiss intensity parameter is constant here: $z_1 = 100$.

calculations of different ionization rates we have decided to fix either the Reiss parameter at $z_1 = 100$ or the laser frequency at $\omega = 0.01$ a.u. Thereby our parameters are well in the range described by two conditions $\omega \ll 1$ a.u. and z_1 \geq 1. With the change of these parameters ionization rates change very rapidly, over several orders of magnitude. Therefore in Figs. 1-4 we do not show ionization rates themselves. Instead we show the ratios of the ionization rates of interest to the static field ionization rates [Eq. (1) or (2)] for the same electric-field amplitude. These ratios change rather slowly. There are four ratios that we plot in each of Figs. 1-4 as a function of ω or z_1 . The dotted lines concern the Reiss ionization rates [Eq. (28) or (33)]. The ionization rates of A. Becker et al. [Eq. (34a) or (34b)] correspond to dot-dashed lines. The dashed lines concern the Keldysh theory [Eq. (20)or (27)]. The Keldysh theory with the WKB Coulomb correction [Eq. (32a) or (32b)] is displayed with solid lines. Figures 1 and 2 relate to circular polarization of the incident laser field. Figure 1 shows the above-mentioned ratios of ionization rates for $z_1 = 100$ as a function of the laser frequency. Figure 2 shows the same, but for $\omega = 0.01$ a.u. as a function of the Reiss intensity parameter z_1 . Figures 3 and 4



FIG. 4. Same as Fig. 2, but for the linearly polarized laser field. The laser frequency is constant here: $\omega = 0.01 \text{ a.u.}$

are counterparts of Figs. 1 and 2 for linear polarization of the laser field.

The main conclusion one can draw from Figs. 1–4 is that only the Keldysh theory with the WKB Coulomb correction (solid lines) has the correct ratio-very close to unity-of the ionization rate to its respective static-field result. Of course, one could also arrive at the conclusion that this ratio is equal to unity in the limit $\omega \rightarrow 0, z_1 \rightarrow \infty$ with the help of analytical methods, using asymptotic forms of the ordinary and the generalized Bessel functions (see, for example, Refs. [8,26]). In fact, practically this is also the only way of making numerical calculations on PC for very large photon orders [30], which must exist if $\omega \ll 1$ a.u. and $z_1 \gg 1$. The course of solid lines in Figs. 1–4 is very flat around the pair of parameters: $z_1 = 100$ and $\omega = 0.01$ a.u. for both polarizations, what confirms our conclusion. The other three lines in Figs. 1-4 lie at least one order of magnitude below unity (at $z_1 = 100, \omega = 0.01 \text{ a.u.}$, so it is hard to imagine how could they approach 1 for $z_1 > 100$ and $\omega < 0.01$ a.u. The ionization rate formulas of Keldysh and of A. Becker et al. can compete with each other, the former being better especially for larger z_1 parameters and circular polarization and the latter for smaller z_1 parameters and linear polarization. This is in agreement with the applicability limits of both formulas. The result of A. Becker et al. is valid roughly for I $\ll 1$ a.u. [28,29]. In contrast, the Keldysh formula usually has a greater high-intensity limit [Eq. (10)], but it depends on the laser frequency. The Reiss ionization rates are at least a few orders of magnitude too small in the neighborhood of the point: $z_1 = 100$, $\omega = 0.01$ a.u. There have been attempts to include Coulomb corrections, connected with the parameter $\alpha_0 = F/\omega^2$ (called the quiver radius or classical displacement of the ionized electron), in the Reiss formula for both circular [31,32] and linear polarization [33]. Mishima *et al.* have investigated the similar Coulomb α_0 corrections in the Keldysh formula for linear polarization [34]. These corrections always increase ionization rate, but this growth approaches zero in the limit $\alpha_0 \rightarrow \infty$. We have checked that, in Figs. 1–4 $\alpha_0 \ge 1$ always and the Reiss ionization rates with and without these corrections are nearly identical.

Let us note that our statements about the formula of A. Becker *et al.* for a hydrogen atom do not contradict the results shown in Figs. 1–4 of Ref. [28]. While in our paper we concentrate on parameters of the laser field rather far from typical experiment, A. Becker *et al.* investigate lower intensities and higher frequencies. Moreover, the logarithmic scales applied in Figs. 1–4 of Ref. [28] would not allow distinguishing between the ionization rate of A. Becker *et al.* and that of Keldysh theory with the WKB Coulomb correction.

In Fig. 5 we release the condition $F \ll 1$ a.u. and show various ionization rates for the circularly polarized laser field of the frequency $\omega = 0.01$ a.u. as a function of the field amplitude up to F = 1 a.u. These four ionization rates are shown with the same kind of lines as before. In Fig. 5 there are also two static-field ionization rates: the analytical result of Landau [Eq. (1), double-dot-dashed line] and the exact staticfield numerical result of Scrinzi *et al.* [13] (solid circles) obtained from solving the Schrödinger equation using the complex scaling method. Of course, the Landau ionization



FIG. 5. Plot of various ionization rates for the circularly polarized laser field (for ω =0.01 a.u.) or static-field ionization rates against the electric field (see text for details).

rate becomes exact in the limit $F \rightarrow 0$. Looking at Fig. 5 one can again convince oneself that only the Keldysh theory with the WKB Coulomb correction (solid line) has the correct behavior in the limit $F \rightarrow 0$. Some small discrepancies with the Landau ionization rate below F=0.03 a.u. are due to too small a z_1 , parameter here $(z_1 < 10)$. Let us note that for theories with the WKB Coulomb corrections the Keldysh theory is always much closer to the Landau result than the Reiss theory. Since the WKB Coulomb corrections are valid for $F \ll 1$ a.u., one should not expect from the KFR ionization rates (which include these corrections) too much accuracy for F > 0.1 a.u. But even in this case the Keldysh theory seems to be much better (see the solid and dot-dashed lines in Fig. 5). One can say the same comparing the Keldysh and Reiss theories without Coulomb corrections. With increasing the field amplitude the dashed line in Fig. 5 comes along very close the exact results of Scrinzi et al. Let us recall that the S-matrix theories have another limitation connected with their formalism: namely, with a large-time limiting procedure [see the paragraph containing Eq. (49) in Ref. [8]], which leads to the condition: $\Gamma 2\pi/\omega \ll 1$. We ascribe the discrepancy between the exact results of Scrinzi et al. and the Keldysh theory, which appears on the right-hand side of Fig. 5 to not fulfilling this condition. Also the fact that $\omega = 0.01$ a.u. is finite and not equal to zero may be of some importance.

In Sec. III we have shown that one can consider a generalization of the KFR theory in the dipole approximation as a gauge-dependent theory, which is described by the parameter β . It was very well known a long time ago that the Keldysh (β =1) and the Reiss (β =0) theories give different results (see, for example, Refs. [35–41,11]). It is possible to repeat all the analytical calculations and to derive the ionization rate formulas for both polarizations for any β . Before starting our numerical calculations we have expected to find β (not necessary equal to 0 or 1), which leads to correct ionization rates in the limit $\omega \rightarrow 0$, $z_1 \rightarrow \infty$. This paper strongly supports the conclusion that the correct value of β is 1. Therefore the length gauge ($\vec{d} \cdot \vec{E}$) form of the matrix element should be used in Eq. (8). Similar statements about the superiority of

this matrix element over the velocity gauge $(\vec{p} \cdot \vec{A})$ form of this matrix element have recently appeared in the literature. Gribakin and Kuchiev [42] have shown that the length gauge KFR theory has the correct limit $\omega \rightarrow 0$ for short-range binding potentials and linear polarization. They stress the importance of an accurate description of the wave function in the asymptotic region, because the length gauge interaction emphasizes large distances from the ionic core. Kjeldsen and Madsen [43,44] have compared the predictions of the length and velocity gauge versions of the molecular strong-field approximation (MO-SFA). They have found different behavior in the ionization rates of the N_2 molecule in both gauges for different orientations between the polarization axis and the internuclear axis. Kjeldsen and Madsen have shown that in general the length gauge MO-SFA is in better agreement with experiments than the velocity gauge MO-SFA. Beiser et al. [45] have found a substantial discrepancy in both gauges in the kinetic energy distribution of electrons from photodetachment in a strong circularly polarized laser field. They have also shown that only the length gauge predictions are consistent with the Wigner threshold law at low energies. Chirilă and Potvliege [12] have investigated an He⁺ ion irradiated by a 400-nm linearly polarized laser pulse of 10^{16} W/cm² peak intensity. They have shown that many of the features of the ab initio photoelectron spectra (i.e., coming from the solution of the time-dependent Schrödinger equation) can be understood within the length gauge formulation of the KFR theory. Finally, for the ionization of negative ions with a ground state of odd parity in the linearly polarized laser field, D. Bauer et al. [46] have found qualitative differences in the predictions of the two gauges. They have shown that the length gauge KFR theory matches the exact numerical solution of the time-dependent Schrodinger equation. Our present paper provides us with a partial answer to the question formulated by D. Bauer et al.: which gauge is better suited for above-threshold ionization of atoms and molecules as well as nonsequential double ionization? A more general answer to this question can also be given [47].

In conclusion, we have shown that for the ground state of a hydrogen atom only the length gauge form of the KFR theory may be consistent with the static field results in the limit $\omega \rightarrow 0$, $z_1 \rightarrow \infty$. In the tunneling regime ($F \ll 1 \text{ a.u.}$) it is necessary to include the WKB Coulomb correction in the final state of the ionized electron to obtain correct ionization rate. In the barrier-suppression regime this correction should not be applied, and without it one obtains ionization rates close to the exact results of Scrinzi *et al.* It appears, contrary to the supposition formulated in Ref. [38], that the KFR theory does not have to fail for strong fields. One of the main results of this paper is also Eq. (27), the length gauge KFR formula for the ionization rate for the ground state of a hydrogen atom in the circularly polarized laser field.

ACKNOWLEDGMENTS

The author is indebted to Professor Piotr Kosiński and to Professor Kazimierz Rzążewski for useful remarks and interesting discussions concerning this paper. The author is also indebted to Professor Howard Reiss. His FORTRAN subroutines BD, GJN, and AGBD for the computation of the ordinary and the generalized Bessel functions have been utilized in this paper.

APPENDIX: FOURIER COEFFICIENTS $A_k(\vec{p})$

Let us consider the Fourier expansion of the expression $[(\vec{p} + \vec{A}(t)/c)^2/2 + E_B]^{-1}$ as a function of time for circular polarization. Multiplying both sides of Eq. (23) by $\exp[-in(\omega t + \varphi_0 \mp \varphi)]$ and integrating this equation from 0 to $T = 2\pi/\omega$, we obtain

$$A_{n}(\vec{p}) = \frac{\omega}{2\pi} \int_{0}^{T} dt \frac{\exp[-in(\omega t + \varphi_{0} \mp \varphi)]}{\frac{1}{2} \left(\vec{p} + \frac{1}{c}\vec{A}(t)\right)^{2} + E_{B}},$$
 (A1)

where the upper and lower signs refer to the right and left circular polarization, respectively. In further calculations we introduce the new parameters

$$a = \frac{p^2}{2} + \frac{Z^2}{2} + z\omega > 0, \qquad (A2)$$

$$b = \sqrt{2z\omega p} \sin \vartheta \ge 0, \tag{A3}$$

where *a* from Eq. (A2) should not be confused with *a* from Eqs. (6) and (7). One can show that b < a always and Eq. (A1) gives

$$A_{n}(\vec{p}) = \frac{1}{2\pi} \int_{\varphi_{0} \mp \varphi}^{2\pi + \varphi_{0} \mp \varphi} dx \, \frac{\exp(-inx)}{a + b \cos x}$$
$$= \frac{(-b)^{n}}{\sqrt{a^{2} - b^{2}}(\sqrt{a^{2} - b^{2}} + a)^{n}}.$$
 (A4)

In the above expression we have used a mathematical theorem about parameter-dependent integrals (which allows us to put $\varphi_0 \mp \varphi = -\pi$) and Eq. (22), p. 414, from Ref. [48]. $A_n(\vec{p})$ are real and do not depend on the initial phase φ_0 . Equation (A4) is valid for $n \ge 0$. For n < 0 we have $A_n(\vec{p}) = A_{|n|}(\vec{p})$. Equation (A4) also shows that $A_n(\vec{p}) = (-1)^n |A_n(\vec{p})|$.

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