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Filling gap of combination of gauge and analytical method in KFR-like theory*

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Bauer recently presented a formula for the ionization rate of a hydrogen atom in a strong linearly polarized laser field [*J. Phys. B* **49** 145601 (2016)]. He started from the Keldysh probability amplitude in the length gauge and utilized Reiss's method in the velocity gauge. Instead, according to the Reiss probability amplitude in the velocity gauge and Keldysh's derivation for the length gauge, we derive a formula for the ionization rate of a ground-state hydrogen atom or a hydrogen-like atom in a strong linearly polarized laser field. We compare the numerical results of the total ionization rate and the photoelectron energy distribution calculated from our formula with the results from Keldysh, Reiss, and Bauer. We find that the apparent discrepancies in the ionization rate are caused not only by different gauges, but also by different analytical methods used to derive the ionization rate.

Keywords: velocity gauge, ionization rate, energy spectra

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1. Introduction

Keldysh–Faisal–Reiss (KFR) theory[1–3] describes nonresonant multiphoton processes such as the above-threshold detachment of ions and the above-threshold ionization of atoms in an intense electromagnetic (laser) field. The theory has provided fruitful insights into a wide range of highly nonperturbative processes in intense laser–atom physics. The two commonly used versions of KFR theory describe the same physical problem, and the main difference between them is the form of the laser–atom interaction in which the $\boldsymbol{d}\cdot\boldsymbol{E}$ form, sometimes called the length gauge (LG), was used by Keldysh[1,4,5] and the $\boldsymbol{p}\cdot\boldsymbol{A}$ form, or velocity gauge (VG), was used by Reiss and Faisal.[2,3,6,7]

KFR theory utilizes S-matrix theory, which is exact in principle. 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 the field of an electromagnetic plane-wave, we used analytical approximations to evaluate the S-matrix element for bound-free transitions. Therefore, various approximate theories could lead to different expressions of the ionization rate. The main approximations of the three versions of KFR theory are the single-active-electron (SAE) approximation,[8–10] electric dipole approximation (EDA),[11,12] and a version that neglects the interaction of the escaping electron with the long-range Coulomb potential[1–7] in the case of a neutral atom ionization. In addition to the above approximations, Keldysh applied two simplifications to the derivation of the ionization rate: (i) the saddle-point method (SPM) of approximation to perform the contour integral, and (ii) the small kinetic momentum assumption. Reiss did not face the above two limitations, and his formula for the ionization rate was expressed by generalized Bessel functions (GBFs). The description of any dynamic process in atomic physics should be gauge-invariant,[13–15] meaning that calculations by two models must yield the same results. However, apparent discrepancies have been observed between the predictions from strong field approximations in the velocity and length gauges. As is well known, the two models can yield very different and occasionally contradictory results in strong electromagnetic fields.[16–23] Recently, Bauer[24] proposed a formula for the ionization rate of a hydrogen atom in a strong linearly polarized laser field. It began from the LG, but used a GBF analytical method. The numerical results calculated with his formula were compared with the results from other models. However, it remains unclear what will happen if we derive a formula by starting from S-matrix theory in velocity gauges and using the analytical SPM at the same time. In this paper, we intend to answer this question.

This remainder of this paper is organized as follows. In Section 2, we derive a formula by using the VG and SPM. In Section 3, we present numerical results calculated from our formula, including the total ionization rates and photo-

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electron energy spectra. We then compare our results with the results from the Bauer's theory, the original theory proposed by Keldysh,[1] and the results of Reiss.[2] Finally, we draw some conclusions in Section 4. Used in this work are the atomic units (a.u.), explicitly substituting -1 for the electronic charge, and the nuclear charge Z denoting the hydrogen atom in our numerical calculations, unless otherwise stated.

2. Derivation of formula with VG and SPM

In this section, we derive a formula for the ionization rate of an atom. We use the VG and SPM to perform the contour integral, in the way that Keldysh used the LG. Then, we present a formula for the energy spectrum of a photoelectron. There ae two conditions necessary for deriving the final expressions of the ionization rate as noted by Keldysh[1,4,5] and others.[24] The first is adiabatic approximation, which is necessary to perform the integral with the SPM. The second is the small final kinetic momentum approximation.

Considering hydrogen atoms in the bound state in a linearly polarized laser field, the S-matrix element describing the probability of direct transition from a bound state to a free state can be expressed as

$$(S-1)_{\rm fi} = -{\rm i}\int {\rm d}t(\psi_{\rm f}, H_{\rm I}\phi_i), \tag{1}$$

where $\phi_{\rm i}(\boldsymbol{r})$ is a stationary, initial bound state wave function and $\psi_{\rm f}$ is the Volkov state.

The Hamiltonian interaction between the laser field and the outgoing electron in the VG can be written as

$$H_{\rm I}(t) = \boldsymbol{A}\cdot(-{\rm i}\nabla) + \frac{1}{2}\boldsymbol{A}^2, \tag{2}$$

where $\boldsymbol{A}$ is the vector potential and $\boldsymbol{A} = \boldsymbol{A}(t)$ in the dipole approximation.

According to the strong field approximation, the influence of the interaction of the remaining atom in the final state with the escaping electron is entirely neglected. 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. The Volkov state can be written as

$$\psi_{\rm f} = \frac{1}{\sqrt{V}}\exp\left\{{\rm i}\boldsymbol{p}\cdot\boldsymbol{r} - \frac{\rm i}{2}\boldsymbol{p}^2 t - {\rm i}\int_{-\infty}^{t}{\rm d}\tau H_{\rm I}(\boldsymbol{p},t)\right\}, \tag{3}$$

where V represents a normalization constant. In the dipole approximation, $\psi_{\rm f}$ is an eigenfunction of the $H_{\rm I}$ operator, and thus

$$H_{\rm I}\psi_{\rm f} = H_{\rm I}(\boldsymbol{p},t)\psi_{\rm f}. \tag{4}$$

Using an approach similar to that of Reiss,[2] substituting the initial state $\phi_{\rm i}(\boldsymbol{r})$, the final state wave function $\psi_{\rm f}$, and the interaction Hamilton $H_{\rm I}$ into Eq. (1), and then partially integrating the resulting equation over t, the S-matrix can be expressed as follows:

$$(S-1)_{\rm fi} = \frac{\rm i}{\sqrt{V}}\bar{\phi}(\boldsymbol{p})\left(\frac{\boldsymbol{p}^2}{2}+E_{\rm b}\right)L(\boldsymbol{p},t), \tag{5}$$

where $E_{\rm b}$ is the binding energy and $E_{\rm b} = -E_{\rm i}$, $\bar{\phi}(\boldsymbol{p})$ is the Fourier transform of

$$\bar{\phi}(\boldsymbol{p}) = (\mathrm{e}^{{\rm i}\boldsymbol{p}\cdot\boldsymbol{r}}, \phi_{\rm i}(\boldsymbol{r})), \tag{6}$$

$$L(\boldsymbol{p},t) = \int_{-\infty}^{\infty}{\rm d}t\exp\left\{{\rm i}\left(\frac{\boldsymbol{p}^2}{2}+E_{\rm b}\right)t + {\rm i}\int_0^t\left(\boldsymbol{A}\cdot\boldsymbol{p}+\frac{\boldsymbol{A}^2}{2}\right){\rm d}\tau\right\}. \tag{7}$$

The vector potential for a monochromatic linearly polarized plane wave is

$$\boldsymbol{A}(t) = A\boldsymbol{\varepsilon}\cos\omega t, \tag{8}$$

where $\boldsymbol{\varepsilon}$ represents the unit vector in the direction of polarization, ω is the frequency of the laser field, and $\boldsymbol{A}$ is the amplitude of the vector potential. The corresponding electric field is

$$\boldsymbol{F}(t) = -\frac{\partial}{\partial t}\boldsymbol{A} = F\boldsymbol{\varepsilon}\sin\omega t, \tag{9}$$

where $\boldsymbol{F} = \boldsymbol{A}\omega$ is the amplitude of the electric field.

An integration can now be carried out over τ in Eq. (7),

$$L(\boldsymbol{p},t) = \int_{-\infty}^{\infty}{\rm d}t\exp\left\{{\rm i}\left[\left(\frac{p^2}{2}+E_{\rm b}+U_{\rm p}\right)t - \zeta\sin\omega t + \frac{z}{2}\sin 2\omega t\right]\right\}, \tag{10}$$

where $z = A^2/4\omega = U_{\rm p}$ and $\zeta = A(\boldsymbol{p}\cdot\boldsymbol{\varepsilon})/\omega = Ap\cos\theta/\omega$.

Using GBFs,

$$\exp\left\{-{\rm i}\zeta\sin\omega t + {\rm i}\frac{z}{2}\sin 2\omega t\right\} = \sum_{n=-\infty}^{\infty}J_n\left(\zeta,-\frac{z}{2}\right)\mathrm{e}^{-{\rm i}n\omega t}, \tag{11}$$

and the inverse function

$$J_n\left(\zeta,-\frac{z}{2}\right) = \frac{1}{2\pi}\int_{-\pi}^{\pi}{\rm d}x\exp\left\{{\rm i}\left(-\zeta\sin x+\frac{z}{2}\sin 2x+nx\right)\right\}. \tag{12}$$

Utilizing the method of Keldysh in the LG and substituting Eqs. (11) and (12) into Eq. (10), we obtain

$$L(\boldsymbol{p},t) = \sum_{n=-\infty}^{\infty}\int_{-\pi}^{\pi}{\rm d}x\exp[{\rm i}S_{\rm p}(x)] \times\delta\left(\frac{p^2}{2}+E_{\rm b}+U_{\rm p}-n\omega\right), \tag{13}$$

where $S_{\rm p}(x) = nx - \zeta\sin x + (z/2)\sin 2x$.

The saddle point integral method is used to integrate over $x = \omega t$, and the position of the saddle point is determined by $\mathrm{d}S_\mathrm{p}/\mathrm{d}x = 0$. Equations (6) and (13) are substituted into Eq. (5). The approximate S-matrix element describing the probability amplitude of ionization can be written as follows:

$$\begin{aligned}(S-1)_\mathrm{fi} &= \frac{2\pi\mathrm{i}}{\sqrt{V}}\sqrt{\frac{2\omega}{kAa^5}}\sum_{n=n_0}^{\infty}\frac{(1-u_1^2)^{-1/4}}{(n-z)}\left(1+\frac{p^2\sin^2\theta}{2k^2}\right)^{-1/2}\\ &\times\exp[\mathrm{i}S_\mathrm{p}(u_1)]\delta\left[E_\mathrm{b}+\frac{p^2}{2}+(z-n)\omega\right],\end{aligned}\tag{14}$$

where $k=\sqrt{2E_\mathrm{b}}$,

$$u_1=\gamma\left[\frac{p\cos\theta}{k}-\mathrm{i}\left(1+\frac{p^2\sin^2\theta}{2k^2}\right)\right],$$

and $\gamma=\omega\sqrt{2E_\mathrm{b}}/F$ is the Keldysh parameter, θ is the angle between the momentum and the polarization direction of the field.

According to the method of Lin *et al.*,[25] pre-exponent factors can be represented approximatively in the exponent forms. Equation (14) is then expressed as follows:

$$\begin{aligned}(S-1)_\mathrm{fi} &= \frac{2\pi}{\sqrt{V}}\sqrt{\frac{2\omega}{kAa^5}}(1+\gamma^2)^{-1/4}\sum_{n=n_0}^{\infty}\frac{\exp\{\mathrm{i}S_\mathrm{p}(u_1)+\Delta S_\mathrm{p}\}}{(n-z)}\\ &\times\delta\left[E_\mathrm{b}+\frac{p^2}{2}+(z-n)\omega\right],\end{aligned}\tag{15}$$

where ΔS_p can be written as

$$\begin{aligned}\Delta S_\mathrm{p} &= -\mathrm{i}\frac{p\cos\theta\gamma^2}{2k(1+\gamma^2)}-\frac{p^2\gamma^2}{2k(1+\gamma^2)}\\ &+\frac{p^2\cos^2\theta(4-\gamma^2)}{8k^2(1+\gamma^2)^2}-\frac{p^2}{4k^2}+\frac{p^2\cos^2\theta}{4k^2}.\end{aligned}\tag{16}$$

Then, the square of the complex modulus of the S-matrix that is the probability amplitude of ionization is written as

$$\begin{aligned}|(S-1)_\mathrm{fi}|^2 &= \frac{4\pi^2}{V}\frac{2\omega}{kAa^5}\frac{\sum\limits_{n=n_0}^{\infty}\exp(-2\mathrm{Im}[S_\mathrm{p}(u_1)]+2\mathrm{Re}[\Delta S_\mathrm{p}])}{\sqrt{1+\gamma^2}(E_\mathrm{b}+p^2/2)}\\ &\times\delta\left[E_\mathrm{b}+\frac{p^2}{2}+(z-n)\omega\right],\end{aligned}\tag{17}$$

where

$$\mathrm{Im}[S_\mathrm{p}(u_1)]=A_1+B_1p^2-C_1p^2c^2,\tag{18}$$

$$\mathrm{Re}(\Delta S_\mathrm{p})=\Delta B_1p^2-\Delta C_1p^2c^2,\tag{19}$$

with

$$A_1=\frac{2\sqrt{2}E^{3/2}}{3F}\left(1-\frac{\gamma^2}{10}\right),\tag{20}$$

$$B_1=-\frac{1}{2\omega}\mathrm{sh}^{-1}\gamma,\tag{21}$$

$$C_1=\frac{\gamma}{2\omega\sqrt{1+\gamma^2}},\tag{22}$$

$$\Delta B_1=-\frac{1+3\gamma^2}{4k^2(1+\gamma^2)},\tag{23}$$

$$\Delta C_1=-\frac{1}{4k^2}-\frac{\gamma^2(4-\gamma^2)}{8k^2(1+\gamma^2)^2}.\tag{24}$$

The differential ionization rate w can be found from

$$w=\lim_{t\to\infty}\frac{1}{t}\frac{V}{(2\pi)^3}|(S-1)_\mathrm{fi}|^2,\tag{25}$$

where w represents the transition probability per unit of time in canonical momentum space.

The total photoionization rate can be derived from the integral of w as follows:

$$W=\lim_{t\to\infty}\frac{1}{t}\frac{V}{(2\pi)^3}\iiint\mathrm{d}^3\boldsymbol{p}|(S-1)_\mathrm{fi}|^2.\tag{26}$$

Performing the integration of momentum $\boldsymbol{p}$, we obtain

$$W=\frac{\pi^2\omega}{\sqrt{2}a^5E_\mathrm{b}^{5/2}C}\exp\left[-\frac{4\sqrt{2}E_\mathrm{b}^{3/2}}{3F}\left(1-\frac{3\gamma^2}{5}\right)\right]\tag{27}$$

with

$$C=1+\frac{\omega}{4E_\mathrm{b}\gamma}\frac{2+8\gamma^2+\gamma^4}{(1+\gamma^2)^{3/2}}.$$

The energy distribution of photoelectrons can be written as

$$\begin{aligned}\frac{\mathrm{d}W}{\mathrm{d}E_\mathrm{p}} &= \int\mathrm{d}\Omega w\sqrt{2E_\mathrm{p}}\\ &= \frac{\mathrm{e}^{-2A_1}\exp[4(-B_1+\Delta B_1+C_1-\Delta C_1)E_\mathrm{p}]}{2\sqrt{2}\pi a^5Ak\sqrt{1+\gamma^2}(C_1-\Delta C_1)(E_\mathrm{p}+E_\mathrm{b})^2\sqrt{E_\mathrm{p}}}.\end{aligned}\tag{28}$$

Equations (27) and (28) are the main results of this paper.

3. Results and discussion

In this section, we present the numerical results calculated with our formula, and compare them with the results from the formulae given by Keldysh, Reiss, and Bauer,[1,2,24] which are obtained by using different combinations of gauges (LG or VG) and analytical methods (SPM or GBF). The formula derived by Keldysh[1,4,5,24] utilizes the LG and the analytical SPM is expressed as

$$W^\mathrm{Keldysh}=\frac{\sqrt{3\pi F}}{2^{7/4}}\exp\left\{-\frac{2}{3F}\left[1-\frac{1}{10}\left(\frac{\omega}{F}\right)^2\right]\right\}.\tag{29}$$

Reiss' ionization rate formula is derived by using the VG and the GBF analytic method[2]

$$\begin{aligned}W^\mathrm{Reiss} &= 2\sum_{n=n_0}^{\infty}\frac{\sqrt{2E_n}}{(E_\mathrm{b}+E_n)^2}\int_0^{\pi}\mathrm{d}\theta(\sin\theta)\\ &\times J_n^2\left(\sqrt{\frac{8zE_n}{\omega}}\cos\theta,-\frac{z}{2}\right).\end{aligned}\tag{30}$$

Finally, Bauer's formula is derived in LG with the help of GBFs. The derivation of Bauer's formula can be seen from

that of Eq. (15) in Ref. [24] and the obtained formula is as follows:

$$W^{\text{Bauer}} = \sum Z^5 \sqrt{8E_n} \int_0^{\pi} \mathrm{d}\theta \sin\theta \left(\sum (-1)^k A_k J(a,b) \right), \quad (31)$$

where Z is the nuclear charge and A_k is the Fourier coefficient.

In order to reveal the apparent discrepancies among the results of the four formulae, we calculate and compare the ratios of the ionization rates by using different formulae and the static field ionization rate $W_{\text{stat}} = 4\sqrt{3Z^7/\pi F}\exp(-2Z^3/3F)$ of a hydrogen atom.[26] The results are shown in Figs. 1 and 2. Since our formula and Keldysh's formula are both applicable to the case of tunneling ionization, the calculations are limited to low-frequency high-intensity region, *i.e.*, $\omega \ll 1$ and $z_1 \gg 1$.

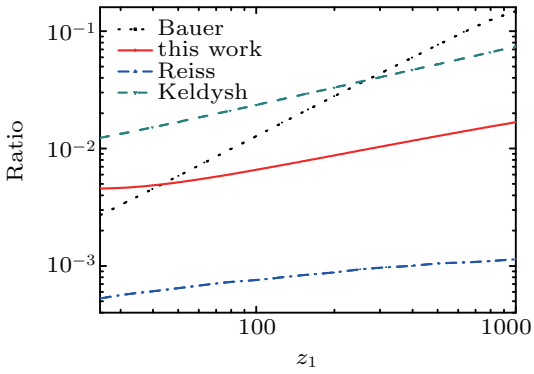


Fig. 1. Ratios of total ionization rate of H atoms *versus* Reiss intensity parameter z_1, calculated with four different models, where static-field ionization rate varies with the Reiss intensity parameter z_1 in linearly polarized laser field.

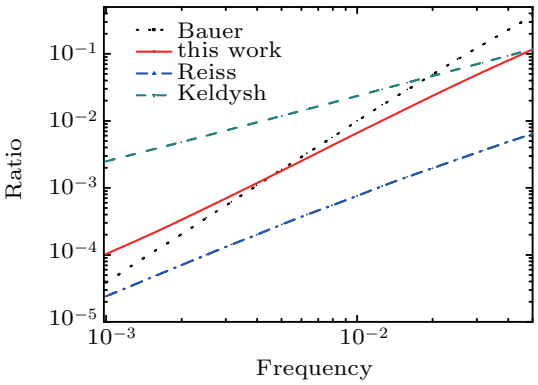


Fig. 2. Ratios of total ionization rate of H atoms *versus* frequency ω, calculated with four different models, where static-field ionization rate varies with frequency ω in linearly polarized laser field.

First, we fix the frequency $\omega = 0.01$ a.u. and the ionization rate as a function of the Reiss intensity parameter z_1. The results are shown in Fig. 1. The dashed line represents the ratio of the ionization rate according to Keldysh's formula.[1] The dash–dotted line represents the ratio of the ionization rate according to Reiss' formula.[2] The ratio of the ionization rate calculated from Eq. (27) is denoted by the solid line. The dotted line represents the ratio of the ionization rate according to Bauer's formula.[24] Second, we fix the Reiss parameter at $z_1 = 100$ and calculate the atomic ionization rate by changing the frequency ω. The results are shown in Fig. 2. In Fig. 2, these four ratios of ionization rate are shown as a function of the laser frequency ω, but where z_1 is fixed at 100, with the same denotation as before. Referring to Fig. 1, when increasing the Reiss intensity parameter z_1, the ratio derived with our formula tends to vary in a manner similar to the result from Reiss' formula. This is likely to be because the same gauge is used. However, these two ratios have different orders of magnitude in quantity. This is likely to be the consequence of different analytical methods. The ratios calculated by Keldysh's and Bauer's formula have different tendencies of change with z_1, but they both have similar magnitudes, and they use the same LG. Except for the results in Fig. 2, our results approach to Bauer's. However, we use a different gauge and analytical method. The complexity of the ionization rate changing with frequency shows an apparent discrepancy in ionization rates, due to not only the different gauges but also the different analytical methods used in the derivation of the formula.

Next, we calculate and compare the photoelectron energy distributions of the different models. The results are shown in Fig. 3. As stated above, our formula and that of Keldysh's formula are both applicable to the case of tunneling ionization. The calculations are thus limited to low-frequency high-intensity region, *i.e.*, $\omega \ll 1$ and $z_1 \gg 1$. Figure 3 show photoelectron energy distribution curves. The dashed line represents the results given by Keldysh's theory, the solid line refers to the results of the proposed formula, the dashed–dotted line denotes the results of Reiss' theory, and the results given by Bauer theory are shown with the dotted line. As the laser frequency increases, the differences among these curves become more pronounced. The smaller the ω, the closer to the ω from Bauer's theory the curve obtained by us will be. Because the small final kinetic momentum approximation is utilized, only electrons with sufficiently small final kinetic energy contribute to the total ionization rate. Our results and those from Bauer theory match to each other only at lower photoelectron energy. The higher the energy, the greater the difference will be. The results from Reiss' theory are one or more orders of magnitude smaller than the results from the other three curves. As ω and F increase, discrepancies between the results from our formula and those from Keldysh's and Bauer's theory become more obvious, which come from different gauges. As the photoelectron energy increases, discrepancies between the curves of our formula and Bauer's theory become more obvious. This is obviously caused by the different analytical methods and gauges used to derive these formulae.

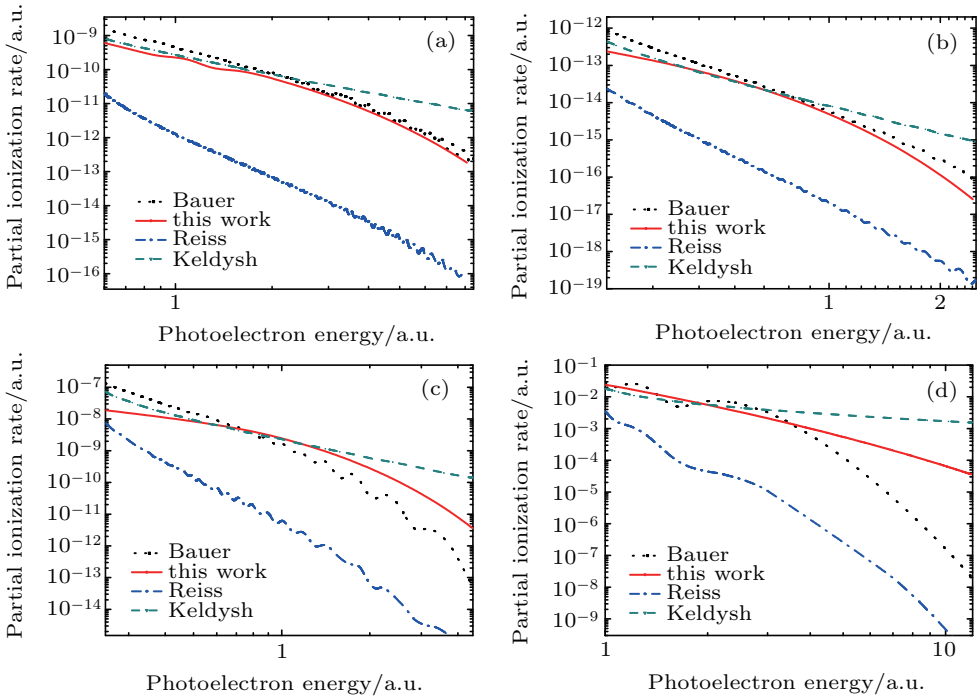


Fig. 3. Photoelectron energy spectra from Keldysh's theory, proposed formula, Reiss' theory, and Bauer's theory at (a) $\omega = 0.01$ a.u., $F = 0.05$ a.u., and $\gamma = 0.2$; (b) $\omega = 0.01$ a.u., $F = 0.03$ a.u., and $\gamma = 0.33$; (c) $\omega = 0.02$ a.u., $F = 0.06$ a.u., and $\gamma = 0.33$; (d) $\omega = 0.25$ a.u., $F = 0.75$ a.u., and $\gamma = 0.33$.

4. Conclusions

We derived the formula for the ionization rate and photoelectron energy distribution of a ground-state hydrogen atom exposed in a linearly polarized laser field by using the VG and the analytical SPM. In our numeric calculations, the laser parameters are limited in the tunnel region $\omega \ll 1$ and $z_1 \gg 1$ to satisfy the applicable condition of our formula and that of Keldysh, and the final kinetic momentum is small. The comparisons of our calculated results with the original results obtained by the Bauer, Keldysh, and Reiss theories show that our derived formula is simple and easy to understand, and that the calculated results are closer to the results of Keldysh. More importantly, our results reduce the discrepancies between the LG and the VG. This study fills a gap in the literature regarding the combination of gauges with analytical method in KFR-like theory. Discrepancies in the ionization rate are caused not only by the different gauges, but also by the different analytical methods used to derive the ionization rate. We expect that our study will help to further study the ionization mechanism of hydrogen-like atoms.

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