# Simple formula for the ionization rate of diatomic molecules in an intense laser field using the velocity gauge*

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(Received 12 November 2012; revised manuscript received 21 December 2012)

We derive a general ionization rate formula for the system of diatomic molecules in the velocity gauge. A more concise expression of the photoionization rate in the tunnel region is obtained for the first time. Comparisons are made among the different versions of strong-field approximation. The numerical study shows that the ionization rate in the velocity gauge is underestimated by a few orders compared with that in the length gauge. Our simple formula of ionization rate may provide an insight into the ionization mechanism for the system of diatomic molecules.

**Keywords:** strong-field approximation, gauge invariance, tunnel ionization

**PACS:** 42.50.Hz, 33.80.Eh **DOI:** 10.1088/1674-1056/22/8/084203

## 1. Introduction

Recently, owing to the rapid advancement of laser technology, nonlinear phenomena associated with ionization of molecules in intense laser fields have aroused considerable experimental and theoretical interest. Being the same as atoms, a series of relevant strong-field processes occur in molecular systems, including above-threshold ionization and dissociation,[1–3] double and multiple ionization,[4–6] and high-order harmonic generation.[7] While, apart from the atomic photoionization, some characteristic features of the molecular ionization have been observed experimentally, such as the orientation dependence of the strong-field ionization and the suppressed molecular ionization.[8,9] To understand these phenomena, we believe that detailed studies of molecular ionization will provide an additional insight into the dynamics of ionization processes in general. Therefore, it is important to explore the molecular photoionization in more detail.

In the study of strong-field ionization of molecules, three models are widely used. First, Tong *et al.*[10] have extended the tunneling ionization model of Ammosov–Delone–Krainov (ADK) for atoms to diatomic molecules, which is referred to as the molecular tunneling theory (MO-ADK). The other two models are the velocity gauge (VG) molecular strong-field approximation (MO-SFA)[11] and the length gauge (LG) molecular strong-field approximation (MO-SFA).[12] The latter two theories are an extension of the velocity gauge version and length gauge version of the Keldysh–Faisal–Reiss (KFR) atomic theories[13–15] appropriately modified to the molecular case. Analogously, the MO-SFA theory is also based on an *S*-matrix formulation where the interaction Hamiltonian between the laser field and the ionized outgoing electron is $\boldsymbol{p}\cdot\boldsymbol{A}$ or $\boldsymbol{d}\cdot\boldsymbol{E}$ under the dipole approximation, and one also considers the direct transition between the electric ground state and the Volkov continuum state, supposing that the initial state is not dressed by the laser field and the final state is taken to be noninteracting.

Since an electromagnetic interaction is gauge-invariant, one would expect that calculations which use different gauges should produce the same results. While in the last several decades the strong-field approximations (SFAs) in the velocity gauge and the length gauge differ and apparently constitute two distinct models. The discrepancy between the KFR theories in the two gauges has caused extensive controversy about which gauge is more appropriate for the SFA.[16] In the meantime, many authors have performed studies, attempting to theoretically prove that the gauge invariant is still valid for photoionization amplitude.[17–22] However, all of them are achievable within any gauge as long as a proper partition of the Hamiltonian is performed. The case is not so optimistic in that as long as one expands the SFA to molecular systems[23,24] in any gauge, similar or even more pronounced gauge dependencies will appear. For example, the orientation behavior of the $N_2$ ionization rate was found to be quite different, if calculated in the velocity gauge version of the MO-SFA approach, from that suggested by the length gauge.[11,25] Even when the molecular axis is aligned along the laser field polarization direction, the ionization rates of $N_2$ calculated in different gauges have discrepancies by a few orders of magnitude.[26] Furthermore, the velocity gauge MO-SFA predicts very well the phenomenon observed in the experiment[27–29] about the suppression of the ionization rate for low energies for $O_2$ molecule ($\pi$ symmetry), and no suppression for $N_2$ molecule

*Project supported by the National Natural Science Foundation of China (Grant No. 11274149) and the Natural Science Foundation of Liaoning Province, China (Grant No. 20121032).

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($\sigma$ symmetry). But the symmetry dependence of the suppression is not so clear in the length gauge MO-SFA. However, in view of the results of Ref. [25], the length gauge MO-SFA gives the most reliable predictions. To summarize, the current state of the art in strong-field ionization theory seems to be still far from a sufficiently clear insight due to numerous controversial results obtained with different gauges, therefore revising and improving them are needed.

In order to understand the discrepancy between the velocity gauge and the length gauge, Ma *et al.*[30] have derived a Keldysh-like formula of atom ionization in an intense laser field using the velocity gauge. The formula is as simple as Keldysh's formula, which may provide a more insightful guide to ascertaining the long standing discrepancy in the strong-field ionization theory. Furthermore, Mishima *et al.*[31] have improved the derivation of photoionization rate formula for one-electron atoms, proposed by Keldysh,[13] and generalized it to the photoionization rate of randomly oriented diatomic molecules in the length gauge. To investigate the gauge dependencies of molecular photoionization, in this paper, we derive the diatomic molecule ionization rate formula using the velocity gauge in the tunnel region, for which the value of Keldysh parameter $\gamma \ll 1$. The saddle point approximation is used to perform the contour integral, and we assume that the kinetic momentum of the freed electron is small and satisfies the condition $p^2 \ll 2E_\mathrm{b}$. It is important to note that the Keldysh parameter $\gamma$ in the case of the molecules can be defined in the same way as in the atomic system.

In addition, the $S$-matrix formalism of conventional SFA we used here is supplemented by the standard linear combination of atomic orbital and molecular orbital method utilized for the approximate analytical reproduction of the one-electron wave function of an initial molecular bound state.[11] As an appropriate example mentioned here is the problem of strong-field ionization of $N_2$ molecules, which recently received a special consideration within both gauges.[25,26] Our attention is directed to the highest occupied molecular orbitals (HOMOs) corresponding to the outermost molecular valence shell with $N_\mathrm{e}$ identical electrons. For the HOMO of gerade and bonding symmetry in $N_2$ molecules under consideration, the corresponding approximate two-centred single-electron molecular initial bound wave function can be expressed as an appropriate linear combination of hydrogenlike $2p_z$ atomic orbitals. We will focus on the photoionization pathway to remove the $\sigma_\mathrm{g}2p$ electron of the $N_2$ molecule and to produce $N_2^+$ in its ground electronic state $X^2\Sigma_\mathrm{g}^+$.[32,33] A closed-form formula for the tunnel ionization rate is derived, which, to the best of our knowledge, has not been published so far. This formula is as simple as Keldysh's formula for the atomic case, and may provide an insight into the dynamics of ionization processes for molecular photoionization. Throughout the paper, the atomic units ($|e| = m = h = 1$) are used, substituting explicitly $-1$ for the electronic charge.

## 2. Ionization rate formula

In this section, our aim is to derive a more exact ionization rate formula for a diatomic molecule which is subjected to an intense laser field. We choose the $N_2$ molecules as an example. Particularly, we consider the case of the molecular photoionization from the $\sigma 2p_z$ orbital of the $N_2$ molecules. In this case, the initial molecular state can be given by[31]

$$\phi_\mathrm{i}(\boldsymbol{r}) = N_{2p}[(\phi_{2p_z})_1 + (\phi_{2p_z})_2], \tag{1}$$

where $(\phi_{2p_z})_1$ and $(\phi_{2p_z})_2$ represent the atomic orbitals, $N_{2p}$ denotes the normalization constant , and

$$\phi_{2p_z}(\boldsymbol{r}) = \sqrt{\frac{1}{\pi a^5}} z \exp\left(-\frac{r}{a}\right), \quad a = \frac{2a_0}{Z}, \tag{2}$$

with $a_0$ being the Bohr radius, and $Z$ the effective nuclear charge.

The MO-SFA theory is based on an $S$-matrix formulation where one considers the transition from a field-free initial state to a Volkov final state directly. According to Reiss,[15] the $S$-matrix can be written as

$$(S-1)_\mathrm{fi} = -\mathrm{i}\int_{-\infty}^{\infty} \mathrm{d}t\,(\psi_\mathrm{f}, H_A\varphi_\mathrm{i})_t, \tag{3}$$

where $\psi_\mathrm{f}$ represents the state vector of the final continuum state, i.e., the Volkov state and $\varphi_\mathrm{i}$ represents the initial state of the unperturbed system in the absence of field. $H_A$ is interaction Hamitonian between laser field and outgoing electron, which is treated in velocity gauge and expressed as

$$H_A(t) = \boldsymbol{A}(t)\cdot(-\mathrm{i}\nabla) + \frac{1}{2}\boldsymbol{A}^2(t). \tag{4}$$

In the dipole approximation the linearly polarized laser field can be described by the vector potential $\boldsymbol{A}(t) = A\boldsymbol{\varepsilon}\cos\omega t$, where $\boldsymbol{\varepsilon}$ represents the unit vector in the direction of polarization, $\omega$ is the frequency of the laser field, and $A$ is amplitude of the vector potential. The corresponding electric field is obtained as $\boldsymbol{F}(t) = -\partial_t\boldsymbol{A}(t) = F\boldsymbol{\varepsilon}\sin\omega t$, where $F = A\omega$ is amplitude of the electric field. The Volkov state in the velocity gauge is

$$\psi_\mathrm{f} = \frac{1}{\sqrt{V}}\exp\left[\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r} - \frac{\mathrm{i}}{2}p^2 t - \mathrm{i}\int_{-\infty}^{t}\mathrm{d}\tau H_A(\boldsymbol{p},\tau)\right], \tag{5}$$

where $H_A(\boldsymbol{p},\tau)$ is given by Eq. (4) with the $-\mathrm{i}\nabla$ operator replaced by the eigenvalue $\boldsymbol{p}$, and $V$ is a normalization volume. The initial state wave function $\varphi_\mathrm{i}$ in Eq. (3) is a stationary bound state

$$\varphi_\mathrm{i}(\boldsymbol{r},t) = \phi_\mathrm{i}(\boldsymbol{r})\,\mathrm{e}^{-\mathrm{i}E_\mathrm{i}t}. \tag{6}$$

Substituting Eqs. (5) and (6) into Eq. (3) and noting that $\psi_\mathrm{f}$ is an eigenfunction of the $H_A(t)$ operator, the result is

$$(S-1)_\mathrm{fi} = \frac{\mathrm{i}}{\sqrt{V}}\phi_\mathrm{i}(\boldsymbol{p})\left(\frac{p^2}{2} + E_\mathrm{b}\right)$$

$$\times \int_{-\infty}^{\infty} \mathrm{d}t \exp\left[\mathrm{i}\left(\frac{p^2}{2}+E_\mathrm{b}+U_p\right)t - \mathrm{i}\xi\sin\omega t + \mathrm{i}\frac{z'}{2}\sin 2\omega t\right], \quad (7)$$

where $\xi = -(1/\omega)\boldsymbol{p}\cdot\boldsymbol{A}$, $z' = A^2/4\omega$, $E_\mathrm{b} = -E_\mathrm{i}$ is the binding energy of the molecules, $U_p = A^2/4$ is the ponderomotive potential, and $\phi_\mathrm{i}(\boldsymbol{p}) = \int \mathrm{d}^3\boldsymbol{r}\,\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\phi_\mathrm{i}(\boldsymbol{r})$ is the Fourier transform of the wave function $\phi_\mathrm{i}(\boldsymbol{r})$. Using the generalized Bessel function

$$\exp\left[-\mathrm{i}\xi\sin(\omega t)+\mathrm{i}\frac{z'}{2}\sin(2\omega t)\right] = \sum_{n=-\infty}^{\infty}\mathrm{J}_n\left(\xi,-\frac{z'}{2}\right)\mathrm{e}^{-\mathrm{i}n\omega t} \quad (8)$$

and its inverse Fourier transformation

$$\mathrm{J}_n\left(\xi,-\frac{z'}{2}\right) = \frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}x\exp\left[\mathrm{i}\left(nx-\xi\sin x+\frac{z'}{2}\sin 2x\right)\right], \quad (9)$$

equation (7) can be written as

$$(S-1)_\mathrm{fi} = \frac{\mathrm{i}}{\sqrt{V}}\phi_\mathrm{i}(\boldsymbol{p})\left(\frac{p^2}{2}+E_\mathrm{b}\right)\sum_{n=n_0}^{\infty}\int_{-\pi}^{\pi}\mathrm{d}x\exp\left[\mathrm{i}S_p(x)\right] \times\delta\left[\frac{p^2}{2}+E_\mathrm{b}+\left(z'-n\right)\omega\right], \quad (10)$$

where $x=\omega t$ and 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, the $\delta$ function reflects the conservation of the total energy after ionization, the explicit form of $S_p(x)$ in Eq. (10) is

$$S_p(x) = nx - \xi\sin x + \frac{z'}{2}\sin 2x. \quad (11)$$

The exponent in Eq. (10) contains a rapidly oscillating component, which means that the integral over $x=\omega t$ can be calculated using the saddle point method. Introducing a complex variable $u=\cos x$, results in

$$S_p(u) = f(u)\left(n\cos^{-1}u - \xi\sqrt{1-u^2}+z'u\sqrt{1-u^2}\right), \quad (12)$$

where $f(u)=\pm 1$. The positions of the saddle points are given by $\mathrm{d}S_p(u)/\mathrm{d}u = 0$, which yields

$$2z'u_\upsilon^2 - \xi u_\upsilon + n - z' = 0. \quad (13)$$

From Eq. (13) we obtain the saddle points

$$u_\upsilon = \gamma\left[-\frac{p\cos\theta}{k} \pm \mathrm{i}\left(1+\frac{p^2\sin^2\theta}{2k^2}\right)\right], \quad (14)$$

where $\upsilon = 1,2$, $k=\sqrt{2E_\mathrm{b}}$, $\gamma = \omega\sqrt{2E_\mathrm{b}}/F$ is the Keldysh parameter, which is connected to the Reiss parameter $z_1$ for linear polarization: $z_1 = 1/\gamma^2$, $\theta$ is the angle between $\boldsymbol{p}$ and the polarization direction of the field. Then we can change Eq. (10) into a contour integral in the complex plain

$$(S-1)_\mathrm{fi} = \frac{\mathrm{i}}{\sqrt{V}}\phi_\mathrm{i}(\boldsymbol{p})\left(\frac{p^2}{2}+E_\mathrm{b}\right) \times\sum_{n=n_0}^{\infty}\int_c\frac{-\mathrm{d}u}{f(u)\sqrt{1-u^2}}\exp\left[\mathrm{i}S_p(u)\right] \times\delta\left[\frac{p^2}{2}+E_\mathrm{b}+\left(z'-n\right)\omega\right]. \quad (15)$$

Using the method which is similar to that given by Gribakin and Kuchiev,[34] we perform the above contour integration and obtain

$$(S-1)_\mathrm{fi} = \frac{\mathrm{i}}{\sqrt{V}}\phi_\mathrm{i}(\boldsymbol{p})\left(\frac{p^2}{2}+E_\mathrm{b}\right) \times\sum_{n=n_0}^{\infty}\sum_{\upsilon=1}^{2}\frac{-1}{f(u)\sqrt{1-u_\upsilon}}\left[\frac{2\pi}{-\mathrm{i}S_p''(u_\upsilon)}\right]^{1/2}\exp\left[\mathrm{i}S_p(u_\upsilon)\right] \times\delta\left[\frac{p^2}{2}+E_\mathrm{b}+\left(z'-n\right)\omega\right]. \quad (16)$$

The total transition probability from the molecular ground bound state to the Volkov state is

$$W = \frac{1}{3}\lim_{t\to\infty}\frac{V}{t}\frac{1}{(2\pi)^3}\int\mathrm{d}^3\boldsymbol{p}\left|(S-1)_\mathrm{fi}\right|^2. \quad (17)$$

Substituting the $S$-matrix [Eq. (16)] into Eq. (17) and integrating with respect to $\boldsymbol{p}$ lead to

$$W = \frac{32}{3\pi\sqrt{E_\mathrm{b}}Fa^7\omega^2\sqrt{1+\gamma^2}}S(\gamma,F,E_\mathrm{b}) \times\exp\left[-\frac{4\sqrt{2}E_\mathrm{b}^{3/2}}{3F}\left(1-\frac{\gamma^2}{10}\right)\right], \quad (18)$$

where

$$S(\gamma,F,E_\mathrm{b}) = \frac{1}{\sqrt{\bar{C}}}\sum_{n=n_0}^{\infty}\frac{2\omega\left[n-(U_p+E_\mathrm{b})/\omega\right]}{(n-z')^4} \times\exp\left[-\bar{B}\left(n-\frac{U_p+E_\mathrm{b}}{\omega}\right)\right]\Phi(\xi_n), \quad (19)$$

and

$$\bar{B} = \frac{2\gamma^3}{3}(1-B), \quad (20)$$

$$\bar{C} = \frac{\sqrt{E_\mathrm{b}}}{\sqrt{2}F\sqrt{1+\gamma^2}}(1+C), \quad (21)$$

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

$$\Phi(\xi_n) = \int_0^{\xi_n}\exp\left(y^2-\xi_n^2\right)\mathrm{d}y \quad (22)$$

with

$$\xi_n = \left[4\omega\bar{C}\left(n-\frac{U_p+E_\mathrm{b}}{\omega}\right)\right]^{1/2}. \quad (23)$$

In this paper, $B$ and $C$ are equal to $3F/4\sqrt{2}E_b^{3/2}\left(1+\gamma^2\right)^2$ and $F\left(1+4\gamma^2\right)/4\sqrt{2}E_b^{3/2}\left(1+\gamma^2\right)^{3/2}$, respectively. In the tunneling domain, i.e., in the tunneling limit case: $\omega \ll 1$ and $\gamma \ll 1$, we look for a version of MO-SFA, which leads to a proper ionization rate. For this case, the minimal number of photons absorbed $n_0 \gg 1$, the sum over $n$ can be replaced by an integral over the parameter $\beta = (n-n_0)/n_0$, and the main contribution in Eq. (19) is made by large $n$. Consequently, carry out the integral over $\beta$, then we will obtain

$$S(\gamma,F,E_b) = \frac{\pi\omega^3}{32\bar{C}E_b^{5/2}} \exp\left(\frac{2\sqrt{2}E_b^{3/2}}{3F}\gamma^2\right). \tag{24}$$

As a result, the total photoionization rate for the system of molecules is described by the formula

$$W = \frac{\sqrt{2}\omega}{3a^7E_b^{7/2}(1+C)} \exp\left[-\frac{4\sqrt{2}E_b^{3/2}}{3F}\left(1-\frac{3}{5}\gamma^2\right)\right]. \tag{25}$$

This is the main result of this paper, i.e., a formula for the ionization rate of diatomic molecule which is as simple as that of an atom in the atomic case derived by Keldysh[13] using the length gauge. Such a simple formula is first provided for the molecular case in the velocity gauge.

## 3. Numerical results

In this section, we numerically present the results [Eq. (18) and Eq. (25)] for the ionization rate of $N_2$ molecules exposed to the linearly polarized laser field by using velocity gauge, and compare them with those obtained from the following two versions of MO-SFA: the formula derived by Mishima *et al.*,[31] who have utilized the length gauge,

$$W_{(\mathrm{LG})} = \frac{2^6\sqrt{2E_b\omega}}{3}\frac{\gamma^{3/2}\left(2\gamma^2+3\right)^2}{\left(1+\gamma^2\right)^{5/2}}N(\gamma,\omega,E_b) \times \exp\left[-\frac{4\sqrt{2}E_b^{3/2}}{3F}\left(1-\frac{\gamma^2}{10}\right)\right], \tag{26}$$

where

$$\begin{aligned} &N(\gamma,\omega,E_b) \\ &= \sum_{n=0}^{\infty}\exp\left[-2\left(\left\langle\frac{E_b+U_p}{\omega}+1\right\rangle-\frac{E_b+U_p}{\omega}+n\right)\right. \\ &\left.\times\left\{\sinh^{-1}\gamma-\frac{\gamma}{\sqrt{1+\gamma^2}}\right\}\right] \\ &\times\Phi\left[\left\{\frac{2\gamma}{\sqrt{1+\gamma^2}}\left(\left\langle\frac{E_b+U_p}{\omega}+1\right\rangle\right.\right.\right. \\ &\left.\left.\left.-\frac{E_b+U_p}{\omega}+n\right)\right\}^{1/2}\right], \end{aligned} \tag{27}$$

and the result obtained by Muth-Böhm *et al.*[9] and Zhang and Zhao[26] through using the velocity gauge,

$$W_{(\mathrm{VG})} = 2\pi N_e\sum_{n=n_0}^{\infty}\int \mathrm{d}\Omega\,|A_n|^2 p, \tag{28}$$

where

$$A_n = (U_p-n\omega)\,\phi_i(\boldsymbol{p})\,\mathrm{J}_{-n}\left(\frac{\boldsymbol{p}\cdot\boldsymbol{A}}{\omega},\frac{U_p}{2\omega}\right), \tag{29}$$

$\mathrm{J}_n$ is a generalized Bessel function, and $\mathrm{d}\Omega$ is the solid angle element. Equation (26) is the generalization of the Keldysh theory to the ionization rate of diatomic molecules. The expressions we obtain in this paper [Eq. (18) and Eq. (25)] are actually the generalization of Reiss theory. In order to estimate the diatomic molecular photoionization rates accurately in the same condition, we compare the predictions of two theories in the tunneling limit case: $\omega \ll 1$ and $\gamma \ll 1$. Small Keldysh parameter ($\gamma \ll 1$) is equivalent to a large Reiss parameter ($z_1 \gg 1$). In addition, for the purpose of numerical comparison with the results given by Mishima *et al.*,[31] we only consider the case $B = 0$ and $C = 0$ in the numerical calculation.

We investigate the ionization rate as a function of the parameter pair ($\omega$, $z_1$), for which the conditions $\omega \ll 1$ and $z_1 \gg 1$ should be satisfied. Therefore it is reasonable to keep one of the parameters fixed and change the other one, and then to perform the converse. In numerical calculations of molecular ionization rates, we have fixed either the Reiss parameter at $z_1 = 100$, or the laser frequency at $\omega = 0.01$ a.u. Therefore, our parameters lie well in the range described by the two conditions $\omega \ll 1$ a.u. and $z_1 \gg 1$. There are four ionization rates plotted in Fig. 1 each as a function of the Reiss intensity parameter $z_1$ for $\omega = 0.01$ a.u. The dotted–dashed line represents the length gauge ionization rate [Eq. (26)]. The ionization rate given in Refs. [9] and [26] (Eq. (28)) corresponds to double-dotted line. Our results (Eqs. (18) and (25)) are displayed with dashed line and solid line, respectively. In Fig. 2, the ionization rates are plotted each as a function of the laser frequency $\omega$ for $z_1 = 100$. These four ionization rates are shown with the same kinds of lines as the previous ones. Referring to Fig. 1, as expected, our results from Eq. (18) and Eq. (25) are in good agreement with each other. But for Fig. 2, it should be pointed out that our results do not accord with them very well when $\omega \to 1$; this can be understood by recalling that Eq. (25) is valid only for $\omega \ll 1$. It is obvious that the ionization rates are underestimated in the velocity gauge MO-SFA compared with in the length gauge MO-SFA, which is similar to the Reiss ionization rate that is usually smaller by a few orders of magnitude than it is from the Keldysh formula for the atomic case. While in the molecular case, the discrepancy between the ionization rates calculated using the different gauges is more pronounced. On the other hand, in the whole range of the figures,

our prediction accords very well with those given in Refs. [9] and [26].

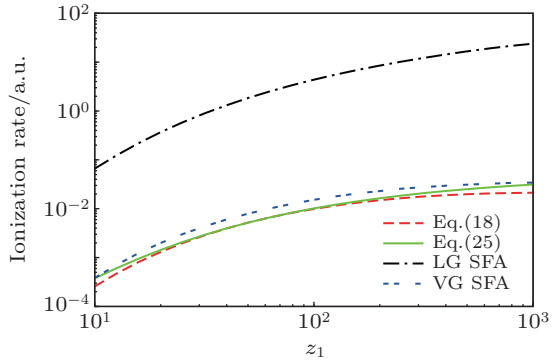



**Fig. 1.** (color online) Plots of four different molecular ionization rates for the linearly polarized laser field each as a function of the Reiss intensity parameter $z_1$, with the laser frequency $\omega$ fixed at 0.01 a.u.

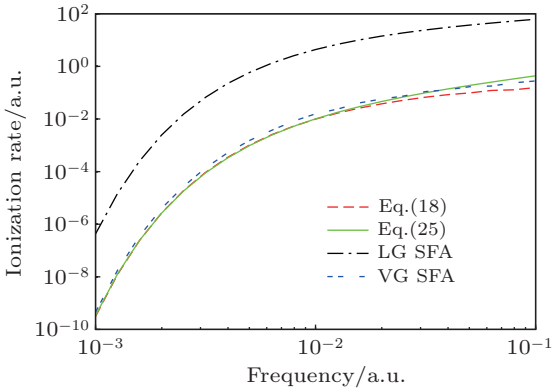



**Fig. 2.** (color online) Plots of four different molecular ionization rates for the linearly polarized laser field each as a function of the laser frequency $\omega$, with the Reiss intensity parameter $z_1$ fixed at 100.

## 4. Conclusions

In the present paper, we derived an ionization rate formula using the velocity gauge for the system of diatomic molecules in the tunnel region. Our formula is more concise than those derived by many other authors.[9,11,26] It is shown that in the low-frequency limit the ionization rate is proportional to the laser frequency $\omega$. In order to compare the photoionization rates obtained using the velocity gauge and the length gauge for the molecular case, our derivation is based on the same approximations as used by Mishima *et al.*[31] who have utilized the length-gauge in the derivation. It should be noted that if we neglect the small term of $\gamma^2$, the exponential factors of the formulas in both gauges are exactly the same as those for the atomic case.[13,30,31] This indicates that ionization mechanisms of atomic and molecular systems are essentially the same because the dominant contribution to the ionization rate is made by the exponential factor in the formula. So that the main difference between the two versions of formulas arises only from the pre-exponential factors. An analysis of the numerical results for ionization rates calculated via our formulas [Eq. (18) and Eq. (25)], and by Mishima *et al.*'s[31] formula [Eq. (26)], as well as the combined results from Ref. [26], shows that the photoionization rates of the molecular systems in the velocity gauge and the length gauge indicate similar or even more pronounced gauge dependencies and the velocity gauge MO-SFA tends to underestimate the yield by orders compared with the length gauge MO-SFA. The origin of the discrepancy between the two models of MO-SFA may have deeper implications and further studies are needed. The work in this direction is now under way. One of the main results of this paper is Eq. (25), the expression which is the velocity gauge MO-SFA formula for the ionization rate for the ground state of diatomic molecules in the linearly polarized laser field.

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