



CORRECTION OF PARAMETERS USED FOR EMPIRICAL FORMULA DESCRIBING THE IONIZATION RATE IN OVER-THE-BARRIER REGIME

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ABSTRACT

Recently, an empirical formula used for describing the ionization rate of atom in the over-the-barrier regime induced by static electric field has been proposed [Q. Zhang et al., Phys. Rev. A 90, 043410(2014)] and is valid up to $4.5F_b$ where F_b is the barrier-suppression strength. However, by providing the accurately numerical calculation of ionization rate and compare to the formula of Zhang et al., we figure out that the provided associating parameters in their formula are inappropriate. Therefore, this paper gives the correction of these vital parameters based on the proposed formula.

Keywords: ionization rate, over-the-barrier regime, empirical formula, static electric field.

TÓM TẮT

Hiệu chỉnh các tham số được sử dụng trong công thức bán thực nghiệm mô tả tốc độ ion hóa trong vùng vượt rào

Gần đây, một công thức bán thực nghiệm dùng để mô tả tốc độ ion hóa của nguyên tử trong vùng vượt rào gây ra bởi điện trường tĩnh được đề xuất bởi [Q. Zhang et al., Phys. Rev. A 90, 043410(2014)] và có thể áp dụng đến $4.5F_b$ trong đó F_b là giá trị cường độ điện trường gây ra sự suy giảm đáng kể của rào thế. Tuy nhiên, bằng tính toán giải số chính xác tốc độ ion hóa và so sánh với công thức này, chúng tôi nhận ra các tham số liên quan là không phù hợp. Do đó bài báo này cung cấp sự hiệu chỉnh các tham số quan trọng này dựa trên công thức đã được đề xuất.

Từ khóa: tốc độ ion hóa, vùng vượt rào, công thức bán thực nghiệm, điện trường tĩnh.

1. Introduction

In the context of strong-field physics, the ionization process has been considered as one of the most important problems since it triggers several non-linear dynamic phenomena in current interests such as the generation of high-order harmonics [8], above

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threshold ionization [1], and non-sequential double or multiple ionizations [3]. Thus it is obvious that the accurate evaluation of the ionization rate induced by laser field is highly desired in order to quantitatively understand these phenomena. Theoretically, there exist two primary approaches for calculating the ionization rate, the numerical and the analytical consideration. The former is able to provide accurate data of ionization rate for an arbitrarily strong electric field [7,9]; however, it is time consuming and somehow demands large resource of computation. Despite the fact that the approximately analytical method is only valid up to critical field strength, it is extremely important to help physicists easily picking out the essentially physical problems for the sake of experimental aspect. Therefore there has been several attempts to analytically describe the ionization rate of atomic and molecular systems induced by the electric field [2,10-13]. Historically, the most comprehensive and earliest theory devoting this problem is the well-known ADK theory [2] which can be applied for atomic systems. Another theory used for molecular systems was also proposed and is well-known as the MO-ADK theory [11]. In addition, a theory based on rigorously mathematical derivation has been proposed and known as weak-field asymptotic theory (WFAT) [10]. These theories work well in the deep tunneling regime where the strength of electric field is sufficiently weak and fail quantitatively as the field strength increases to the boundary between the tunneling and over-the-barrier regimes F_b . Meanwhile the currently available laser pulses have the maximum amplitude far exceed F_b . Thus several works seeking the solution to extend the applicability of these analytical formulae have been introduced based on empirical techniques up to around $2F_b$ [12] and to $4.5F_b$ for the newest work of Q. Zhang *et al.* [13]. However, we are aware that the implementing parameters given in table 6 by [13] are inappropriate while comparing to our numerical calculation obtained by Siegert state method [9]. Hence in this paper, we provide the accurately numerical calculations and use these data for fitting procedure to derive the correction parameters associating with the modified empirical formula proposed by [13].

The paper is organized as follows. In section 2, we briefly introduce several analytical formulae to describe the ionization rate. Here we focus on atomic systems, as well as numerical procedure based on Siegert state approach. Note that both analytical models and numerical method are developed for single-active-electron (SAE) potential. The Siegert state method has been thoroughly presented in our previous papers [3,9], thus in this work we only maintain several vital equations. In section 3, we present the correction parameters for calculating the ionization rate of hydrogen and several noble gas atoms such as He, Ne, Ar, Kr and Xe. We use data from accurately numerical calculation as a benchmark to validate the applicability of our new set of parameters. Section 4 concludes the paper.

2. Theoretical models and Siegert state method for calculating of ionization rate

Table 1. Value of asymptotic parameter C_ℓ [11]

	H ($1s$)	He ($2s$)	Ne ($2p$)	Ar ($3p$)	Kr ($4p$)	Xe ($5p$)
C_ℓ	2.00	3.13	2.10	2.44	2.49	2.57

The ionization rate in the ADK theory for atomic system for states with the angular momentum ℓ and magnetic quantum number m is expressed as [2] (unless otherwise stated, atomic units are used throughout this paper)

$$\Gamma_{\text{ADK}}(F) = \frac{C_\ell^2}{2^{|m|}|m|!} \frac{(2\ell+1)(\ell+|m|)!}{2(\ell-|m|)!} \frac{1}{\kappa^{2Z_C/\kappa-1}} \left(\frac{2\kappa^3}{F}\right)^{2Z_C/\kappa-|m|-1} \exp\left(\frac{-2\kappa^3}{3F}\right), \quad (1)$$

where Z_C is the charge of ion under investigation, $\kappa = \sqrt{2I_p}$ with I_p is the ionization potential of considered state and C_ℓ is the coefficient describing the wave function in the asymptotic region given in table 1 for several concerned atoms. Note that for all cases of consideration, the magnetic quantum number m is always equal to 0. We also note that for hydrogen atom in ground state, i.e. $1s$ state, taking into account the value of C_ℓ from table 1, equation (1) can be rewritten in form of

$$\Gamma_{\text{H-1s}}(F) = \frac{4}{F} \exp\left(\frac{-2}{3F}\right), \quad (2)$$

which coincides with a well-known result of [6]. ADK theory works well only in deep tunneling regime where the electric field strength is sufficiently weak. For extending the applicability of the analytical formula describing the ionization rate while keeping the simplicity of the formula, empirical method has been considered as one of the most efficient approaches [12,13]. One of them was proposed in 2005 by X. M. Tong and C. D. Lin and having the form of [12]

$$\Gamma_{\text{TL}}(F) = \exp\left(-\alpha \frac{Z_C^2}{I_p} \frac{F}{\kappa^3}\right) \Gamma_{\text{ADK}}, \quad (3)$$

and is able to cover the ionization rate up to $2F_b$ where F_b is the critical barrier-suppression field strength

$$F_b = \frac{I_b^2}{4Z_C}. \quad (4)$$

Equation (3) consist of only one free parameter α which can be straightforwardly derived by least-square fitting procedure and its values of particular atoms are presented in table 2 in [12]. Note that the accurately numerical data is used as benchmarked for fitting

process. The second empirical formula has been introduced recently in 2014 by Q. Zhang *et al.* as [13]

$$\Gamma_Q(F) = \exp \left[- \left(a_1 \frac{F^2}{F_b^2} + a_2 \frac{F}{F_b} + a_3 \right) \right] \Gamma_{ADK} . \quad (5)$$

Here, fitting procedure using quadratic function forthrightly provides values of three free parameters a_1 , a_2 , and a_3 as in table 2 for concerned atoms in this work by Q. Zhang *et al.*

Table 2. Value of associating parameters in equation (5) by Q. Zhang *et al.* [13]

	H (1s)	He (2s)	Ne (2p)	Ar (3p)	Kr (4p)	Xe (5p)
a_1	0.11714	0.13550	0.10061	0.16178	0.14640	0.21080
a_2	-0.90933	-0.86210	-1.04832	-1.50441	-1.36533	-1.88482
a_3	-0.06034	0.02156	-0.07542	0.32127	0.02055	0.57428

Table 3. Corresponding parameters of the SAE potential model used by Tong and Lin in equation (8) [12]

	H (1s)	He (2s)	Ne (2p)	Ar (3p)	Xe (5p)
Z_c	1.0	1.0	1.0	1.0	1.0
b_1	0.000	1.231	8.069	16.039	51.356
b_2	0.000	0.662	2.148	2.007	2.112
b_3	0.000	-1.325	-3.570	-25.543	-99.927
b_4	0.000	1.236	1.986	4.525	3.737
b_5	0.000	-0.231	0.931	0.961	1.644
b_6	0.000	0.480	0.602	0.443	0.431

For validating the empirical formula introduced by Q. Zhang *et al.* as in equation (5) with parameters given in table 2, we numerical solve the static Schrödinger equation

$$\left[-\frac{1}{2} \Delta + V(\mathbf{r}) + Fz - E \right] \psi(\mathbf{r}) = 0 . \quad (6)$$

Here $V(\mathbf{r})$ is the interaction potential between nuclei and electron in the SAE approximation. Note that there are several SAE models widely used in consideration of ionization process and the deviation between numerical calculations using these models are not noticeable [13]. Thus in accordance with [13], we adapt the Green, Sellin, and Zachor (GSZ) model [4]

$$V(r) = -\frac{\frac{(Z-Z_c)}{H(e^{r/d}-1)+1} + Z_c}{r}, \quad (7)$$

for Kr with $Z_c = 1$, $H = 5.507$, and $d = 1.055$. For other atomic systems, the SAE model of [12] is used

$$V(r) = -\frac{Z_c + b_1 e^{-b_2 r} + b_3 r e^{-b_4 r} + b_5 e^{-b_6 r}}{r}, \quad (8)$$

with corresponding parameters are shown in table 3. Note that in asymptotic region, all SAE models approach a much simpler form of hydrogenic system

$$V(r) \Big|_{r \rightarrow \infty} = -\frac{Z_c}{r}. \quad (9)$$

The Schrödinger equation (1) is solved in parabolic coordinated defined by [6] since both asymptotic Coulomb tail of the atomic potential and the interaction part with the field allow separation of variables. The asymptotic form of nuclei- electron interaction also accords to the outgoing-wave boundary conditions of equation (1) (equation (18) in [3]). The Siegert states are represented by the solutions to equations (1) satisfying the outgoing-wave boundary condition in the asymptotic region. Such solutions exist only for a discrete set of generally complex values of E . The real and imaginary parts of the Siegert state eigenvalue E define the energy ε and the ionization rate Γ of the state, respectively

$$E = \varepsilon - \frac{i}{2}\Gamma \quad (10)$$

The calculation using numerical program based on Siegert state method are considered to be highly accurate and converged at least six-digits for noble-gas atomic systems [3,9]. For the sake of brevity, we refer the data from accurately numerical calculation, from empirical formula (5) using corresponding parameters in table 2 by Q. Zhang *et al.*, and from our correction parameters in table 4 as “exact”, “Q. Zhang”, and “modified” ones, respectively.

3. Results and discussion

For deriving parameters associating with formula (5), we follow the procedure proposed by Q. Zhang *et al.* with minor modification by defining the natural logarithmic ratio between exact and ADK ionization rates as

$$R(F) = \ln \left(\frac{\Gamma_{\text{ex}}}{\Gamma_{\text{ADK}}} \right). \quad (11)$$

In figure 1, we present $R(F)$ as a function of electric field for hydrogen and several noble gas atoms in unit of F_b as solid black curve. We note that the curve is not continued to smaller F due to a fundamental limitation of numerical procedure in calculating very low ionization rates, our calculations with double precision fail in case of $\Gamma_{\text{ex}} \leq 10^{-10}$ a.u. Taking into account equation (5), the fitting function is sought in form of

$$y(F) = - \left(a_1 \frac{F^2}{F_b^2} + a_2 \frac{F}{F_b} + a_3 \right), \quad (12)$$

and is also presented in figure 1 (red dashed lines) for corresponding parameters provided by Q. Zhang *et al.* in table 2. Obviously, the Q. Zhang's fitting curve is totally diverged from the exact curve. Another interesting feature can be observed from figure 1 is the non-zero values of fitting function $y(F)$ as F goes to 0 in cases of He, Ne, Kr, and Xe which is inappropriate. Since for the limit of F goes to 0, the results from numerical calculation and ADK theory well coincide, thus the ratio $\Gamma_{\text{ex}} / \Gamma_{\text{ADK}}$ goes to unity, then $R(F)$ has to approach 0. Detailed investigation and the suggestion for modified empirical formula which smoothly covers the $R(F)$ for $F \rightarrow 0$ as well as extends the validity up to $10F_b$ is deferred to our next work.

Table 4. Similar to table 2 but for our fitting correction

	H (<i>1s</i>)	He (<i>2s</i>)	Ne (<i>2p</i>)	Ar (<i>3p</i>)	Kr (<i>4p</i>)	Xe (<i>5p</i>)
a_1	-0.14802	-0.11730	-0.09739	-0.14318	-0.15150	-0.18659
a_2	1.09025	0.81081	1.03390	1.36228	1.35273	1.73556
a_3	-0.16715	0.11778	0.08354	-0.08263	0.35530	-0.32581

Now using $R(F)$ as benchmark, we straightforwardly obtain associating parameters of equation (11) by least-square fitting method and present our correction ones in table 4 as well as figure 1 (dash-dotted curves). Conspicuously, our correction is in good agreement with $R(F)$ for all considered systems in the range of electric field under consideration up to $5F_b$.

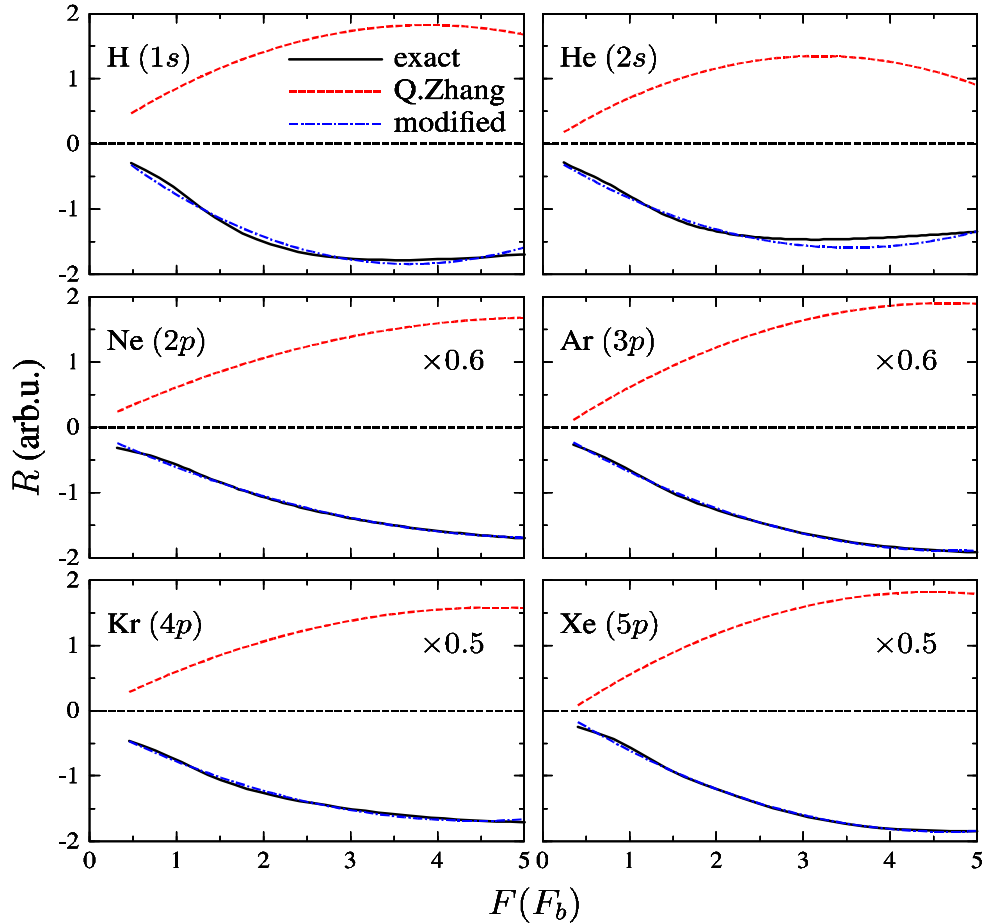


Figure 1. The natural logarithmic ratio between exact and ADK ionization rate $R(F)$ (solid black curve). Parabolic fitting curves in equation (12) using corresponding parameters of Q. Zhang et al. in table 2 (dashed red curve) and our corrections in table 4 (dash-dotted green curve) are also presented. All data sets for Ne, Ar, Kr, and Xe are scaled to fix the general vertical scale.

The good agreement between our modification and $R(F)$ guarantees perfect description of the ionization rate for wide range of electric field. Indeed, figure 2 clearly shows that the deviation between our modifications and exact ones are not noticeable and lower than 5% in the whole region. While Q. Zhang's results always overestimate the exact ones. This is in contradiction to their marvelously graphic presentation (see figures 1-4 in [13]). We strongly believe that such difference only stems from the improper parameters given by Q. Zhang et al. and this is just a minor inaccuracy of those authors. We note that similar consequences can be drawn for other systems like Ar^+ , Ne^+ which are not shown in this paper.

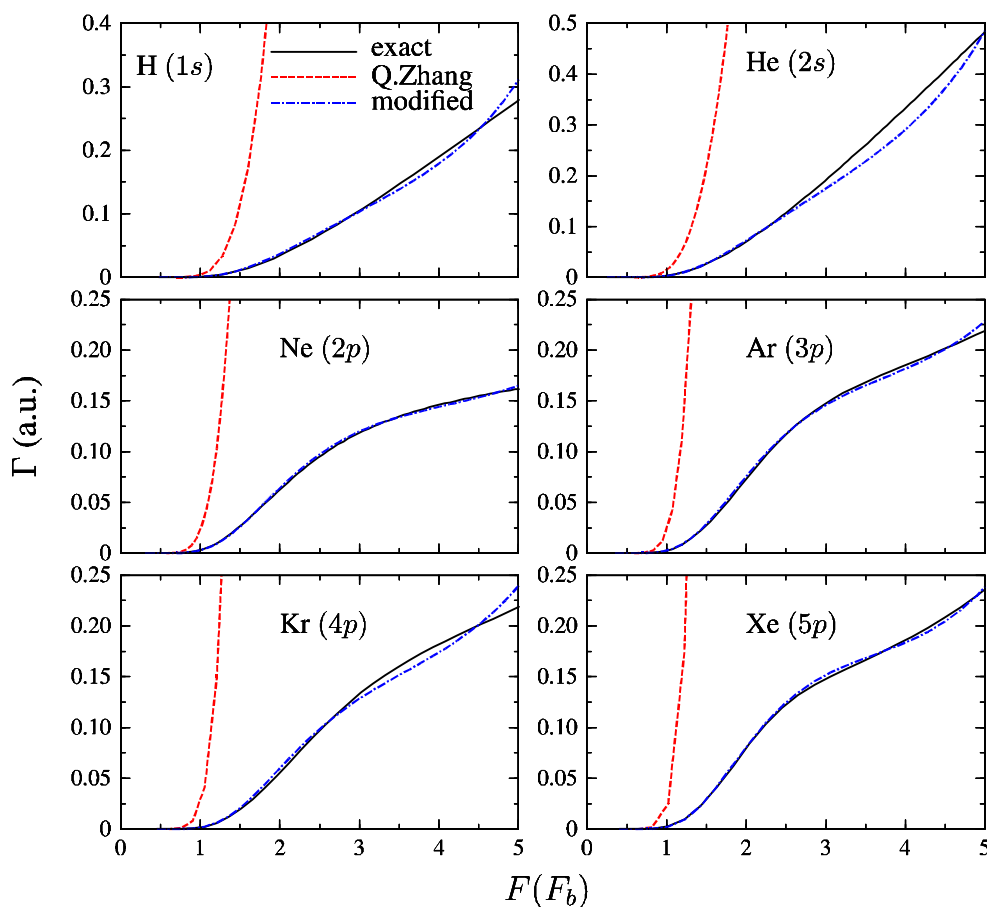


Figure 2. The ionization rate obtained from numerical calculation (solid black curve), Q. Zhang formula with parameters provided in table 2 (dashed red curve), and with our correction parameters in table 4 (dash-dotted blue curve).

4. Conclusion

In conclusion, we have shown that the parameters given by Q. Zhang *et al.* are inappropriate to describe the ionization rate using the empirical formula (5). Then we provide the correction parameters based on fitting procedure proposed in [13] and show that our modifications work well in the whole region of electric field under investigation up to $5F_b$. The extension of applicability of analytical formula in depicting the ionization rate in much deeper over-the-barrier regime is now considered.

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