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Formula for the ionisation rate of an atom or ion in a strong electromagnetic field for numerical simulation

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Abstract. **A formula is proposed for calculating the rate of field ionisation of an atom or ion, taking into account both tunnel ionisation and barrier suppression ionisation. Compared with the previous formula proposed in 2018, it more accurately describes the transition region between both ionisations and is determined mainly by two parameters: the ionisation potential of an atom or ion and the amplitude of an external electric field. This makes the presented formula suitable for use in numerical packages simulating the interaction of high-power laser radiation with matter by the particle-in-cell (PIC) method.**

Keywords: *field ionisation, atoms, ions, tunnel ionisation, barrier suppression ionisation, particle-in-cell method.*

Ionisation of atoms and ions is one of the key processes that accompany the interaction of high-power laser radiation with matter. The ionisation-induced mechanisms play an important role in many phenomena and applications, such as generation of high harmonics [1, 2], generation of terahertz radiation [3–5], ionisation injection in laser-plasma accelerators [6–8], initiation of quantum electrodynamic cascades by seed electrons generated during ionisation of atoms with large charge number [9, 10], etc. Ionisation in laser plasma can result from the collision of atoms with energetic particles (impact ionisation) or from the action of a strong electromagnetic field (field ionisation). In a monochromatic electromagnetic wave with arbitrary polarisation, field ionisation can occur in three different regimes depending on the amplitude of the electric field and the radiation frequency: in the multiphoton ionisation (MPI) regime, $E_{\rm max} \ll E_{\rm K}$; in the tunnel ionisation (TI) regime, $E_{\rm K} \ll E_{\rm max} \ll E_{\rm cr}$; and in the barrier suppression ionisation (BSI) regime, $E_{\rm max} \geqslant E_{\rm cr}$ (Fig. 1), where $E_{\rm max}$ is the electromagnetic field amplitude; $E_{\rm K} = \omega_{\rm las}(2m_{\rm e}I_{\rm i})^{1/2}/e$ is the threshold field related to the Keldysh parameter $\gamma_{\rm K} = \omega_{\rm las}(2m_{\rm e}I_{\rm i})^{1/2}/eE_{\rm max} = E_{\rm K}/E_{\rm max}$; $E_{\rm cr}$ is the critical field above which the atomic potential barrier is suppressed (quantified below); $I_{\rm i}$ is the ionisation potential of an atom (ion); $\omega_{\rm las}$ is the laser radiation frequency; c is the speed of light; $m_{\rm e}$ is the mass of the electron; and $e > 0$ is the elementary charge.

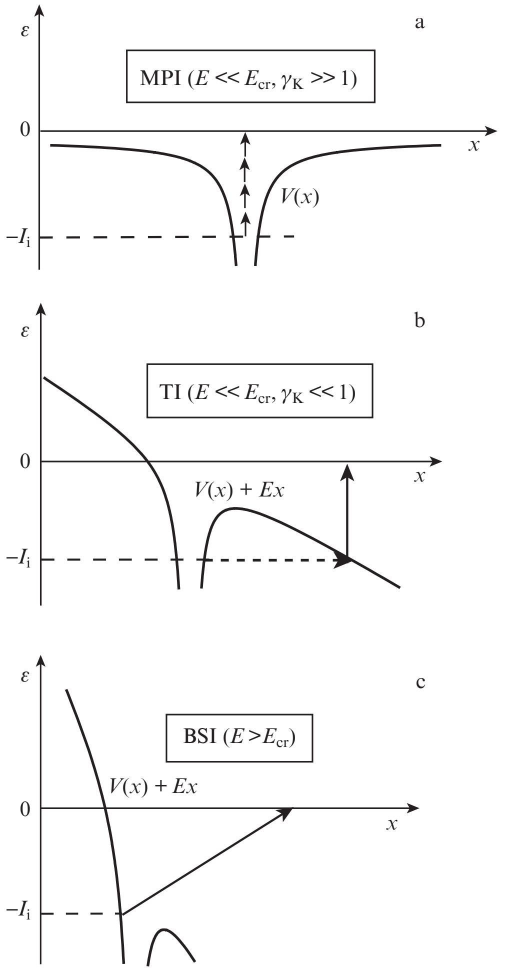

Figure 1. Schematic representations of (a) multiphoton and (b) tunnel regimes, as well as (c) the barrier suppression regime for strong-field ionisation, which are realised depending on the external field strength. The solid curves show the atomic potentials $V(x)$ or superpositions of the atomic potential and the external field potential [$V(x) + Ex$]. Arrows show an electronic transition during ionisation; ε and x are the electron energy and coordinate.

The ionisation rate in multiphoton and tunnel regimes can be calculated analytically [11–14]. While the multiphoton ionisation process requires periodic field modulation, tunnel ionisation in a strong field $\gamma_{\rm K} \ll 1$ can be calculated in the stationary field approximation. In this case, the tunnel ionisation rate has the form [14–16]

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$$w_{\rm TI}(F) = w_{\rm a} k^2 C_{kl}^2 (2l+1)\left(\frac{2}{F}\right)^{2n^*}\left(\frac{F}{2}\right)^{m+1} \times \frac{(l+m)!}{2^m m!(l-m)!}\exp\left(-\frac{2}{3F}\right), \quad (1)$$

$$C_{kl}^2 = \frac{2^{2n^*}}{n^*\Gamma(n^*+l^*+1)\Gamma(n^*-l^*)},$$

where $F = E/(k^3 E_{\rm a})$ is the instantaneous normalised electric field strength; $k^2 = I_{\rm i}/I_{\rm H}$; $n^* = Z/k$ is the effective principal quantum number of the ion; Z is the charge number of the ion; $l^* = n^* - 1$ is the effective orbital quantum number; l and m are the orbital and magnetic quantum numbers, respectively; $I_{\rm H} = m_{\rm e}e^4/(2\hbar^2) \simeq 13.6$ eV is the ionisation potential of the hydrogen atom; $E_{\rm a} = m_{\rm e}^2 e^5 \hbar^{-4} \approx 5.1\times10^9$ V cm^{-1} is the atomic electric field; $w_{\rm a} = m_{\rm e}e^4\hbar^{-3} \simeq 4.1\times10^{16}$ s^{-1} is the atomic frequency; and $\Gamma(x)$ is the gamma function [17]. To calculate the total probability of a single ionisation event, we should integrate the ionisation rate:

$$W_{\rm i}(t) = 1 - \exp\left\{-\int_{-\infty}^{t} w_{\rm i}[E(t')]{\rm d}t'\right\}, \quad (2)$$

where $w_{\rm i}$ is the ionisation rate (which can be either $w_{\rm TI}$ or another formula for the ionisation rate applicable in the case under consideration), and the instantaneous value (without averaging over the period) of the external field strength $E(t)$ should be substituted into the formula.

When the external field is so strong that the maximum of the potential barrier formed as a result of a superposition of the atomic and external fields is lower than the initial electron energy level, the field ionisation develops in the barrier suppression regime, in which the electron becomes free and can move above the barrier instead of tunnelling. In the barrier suppression regime, the amplitude of the external field exceeds $E_{\rm cr} = E_{\rm a}k^4/(16Z)$. For example, for a hydrogen atom, $E_{\rm cr} = E_{\rm a}/16 \approx 3.2\times10^8$ V cm^{-1}, which corresponds to a laser field intensity of 1.4×10^{14} W cm^{-2}.

It follows from the estimates [18] that for focused short subpetawatt laser pulses, full ionisation can be achieved at $E \gtrsim E_{\rm cr}$, when the formulae for multiphoton and tunnel ionisations are not applicable. For field ionization at $E \gtrsim E_{\rm cr}$, many empirical formulae have been proposed [19–22], but most of them do not provide the proper asymptotic behaviour in the high-field limit corresponding to the barrier suppression regime. Moreover, they are applicable only to a limited set of atoms and ions. At the same time, previous theoretical calculations of the ionisation rate in the barrier suppression regime [23, 24] also yield results that do not coincide with those of numerical simulation. Field ionisation models are widely used in PIC modelling, which has become an indispensable tool for studying the interaction of laser radiation with matter. Some models take into account the energy losses associated with ionisation [25, 26], and can also be used to simulate many ionisation events within the same time step of the main PIC code cycle [10, 26–28]. Ideally, the formula for PIC codes should be simple and computationally inexpensive, while still being valid over a wide range of laser radiation intensities and applicable to many types of atoms and ions. Until recently, the field ionisation models used in PIC codes described only the tunnel ionisation regime or were based on too simple and inaccurate approaches. For example, one of the models is based on the use of the tunnel ionisation formula for $E < E_{\rm cr}$, and at $E \geqslant E_{\rm cr}$ the electron is automatically considered completely free (see, for example, [29]). This model can significantly overestimate the ionisation efficiency in the barrier suppression regime for a high-power electromagnetic field.

The ionisation rate in the barrier suppression regime was recently theoretically calculated in the classical [10] and quantum [18] approaches in the high-field ($E \gg E_{\rm cr}$) limit:

$$w_{\rm BSI}(E) \approx 0.8 w_{\rm a}\frac{E}{E_{\rm a}}\sqrt{\frac{I_{\rm H}}{I_{\rm i}}}. \quad (3)$$

In this limit, the ionisation rate linearly depends on the external field strength, while the atomic system is characterised by the ionisation potential of an atom or ion. A piecewise formula was also proposed for the ionisation rate in the tunnel regime and in the barrier suppression regime with correct asymptotic behaviour in the high-field limit [18]:

$$w_{\rm i}(E) \approx \begin{cases} w_{\rm TI}(E), & E \leqslant E_0, \\ w_{\rm BSI}(E), & E > E_0,' \end{cases} \quad (4)$$

where the value of E_0 is determined from the relation $w_{\rm TI}(E_0) = w_{\rm BSI}(E_0)$.

However, the accuracy of formula (4) is small in the transition region between both regimes and the corresponding field amplitude $E \gtrsim E_{\rm cr}$. In this paper, we propose an improved formula that includes not only the tunnel ionisation rate $E \ll E_{\rm cr}$ and the barrier suppression ionisation rate $E \gg E_{\rm cr}$ in the high-field limit, but also the transition ionisation rate $E \gtrsim E_{\rm cr}$. The ionisation rate near the critical field $E \gtrsim E_{\rm cr}$ can be estimated using the empirical formula proposed by Bauer and Mulser for the hydrogen atom [21],

$$w_{\rm BM} \approx 2.4 w_{\rm a}\left(\frac{E}{E_{\rm a}}\right)^2\left(\frac{I_{\rm H}}{I_{\rm i}}\right)^2. \quad (5)$$

In contrast to (3), $w_{\rm BM}$ depends quadratically on the laser field amplitude. The quadratic dependence of the ionisation rate on E and the transition to a linear dependence are seen in Fig. 6 in [21], which presents the results of numerical simulation of the nonstationary Schrödinger equation for the hydrogen atom. Strictly speaking, formula (5) is a verified approximation only for a hydrogen atom and hydrogen-like ions having one electron, charge number Z and ionization potential $I_{\rm i} = Z^2 I_{\rm H}$. Nevertheless, the formula can be generalised to the case of an arbitrary atom or ion by substituting the corresponding ionisation potential $I_{\rm i}$ in formula (5), and we assume that it will give a reasonable estimate for the ionisation rate even in this case. The final formula for the ionisation rate, including the tunnel regime, the barrier suppression regime and the transition regime, can be written in the form

$$w_{\rm i}(E) \approx \begin{cases} w_{\rm TI}(E), & E \leqslant E_1, \\ w_{\rm BM}(E), & E_1 < E \leqslant E_2, \\ w_{\rm BSI}(E), & E > E_2, \end{cases} \quad (6)$$

where E_1 and E_2 are found from the relations $w_{\rm TI}(E_1) = w_{\rm BM}(E_1)$ and $w_{\rm BM}(E_2) = w_{\rm BSI}(E_2)$. The proposed formula is well suited for use in PIC codes, since the ionisation rate depends on the local instantaneous value of the ionising field strength, as well as on the ionisation potential.

To begin with, we compare the predictions of the proposed formula (6) for hydrogen with the numerical results obtained in [21] by solving the nonstationary Schrödinger equation (see Fig. 2a). The comparison demonstrates that the analytical and numerical results agree fairly well. The dependence in the high-field limit is indeed linear in numerical simulation, but the proportionality coefficients are different, which leads to a small discrepancy between the numerical curve and the model in Fig. 2a on a logarithmic scale. This difference may be due to inaccurate determination of the ionisation rate. In contrast to the tunnel regime, the time dependence of the total ionisation probability in the barrier suppression regime is not exponential even for a static field [18]; therefore, the ionisation rate depends not only on the instantaneous value of the field, but also on the history of its influence on the system. Thus, the introduction of the function $w_i(E)$ is an approximation used for a qualitative description of the ionisation process. Some methods for determining the numerical coefficient in this dependence, which lead to slightly different results, are discussed in [18]. In addition, the ionisation condition can be implemented in different ways in numerical simulation: through the correlation function between the wave function of an electron and the states of the discrete spectrum, through the flux of the wave function of an electron via a surface surrounding a nucleus of an atom or ion at a sufficiently large distance, etc. Different conditions may lead to slight differences in the calculated ionisation rate.

A similar comparison was made for the neutral atoms of helium, neon and argon (Figs 2b–2d). Numerical data were obtained by integrating the Schrödinger equation in the one-electron approximation and are presented in [22]. It can be seen from the comparison that formula (5) provides a fairly good approximation for the ionisation rate in the transition region, including for atoms other than the hydrogen atom. In addition, the data obtained in [22] do not extend to the high-field limit $E \gg E_{cr}$, which does not make it possible to numerically check the linear section of formula (6) corresponding to formula (3) for atoms other than the hydrogen atom. This section can be seen in the results of numerical simulations presented in [21] for the hydrogen atom. Since formula (3) is obtained from a theoretical consideration of an arbitrary atomic system, linear asymptotic behaviour in the high-field limit should be observed for an arbitrary atom or ion.

Thus, we have proposed a general formula for the ionisation rate of an atom or ion in a strong electromagnetic field, covering a wide range of laser radiation intensities from the tunnel ionisation regime to the barrier suppression regime. The formula is well suited for PIC codes because it contains dependences on the local instantaneous value of the ionising field strength, and the dependence on the type of atomic system is expressed in terms of its ionisation potential. Therefore, it is applicable for all types of atoms and ions, and also does

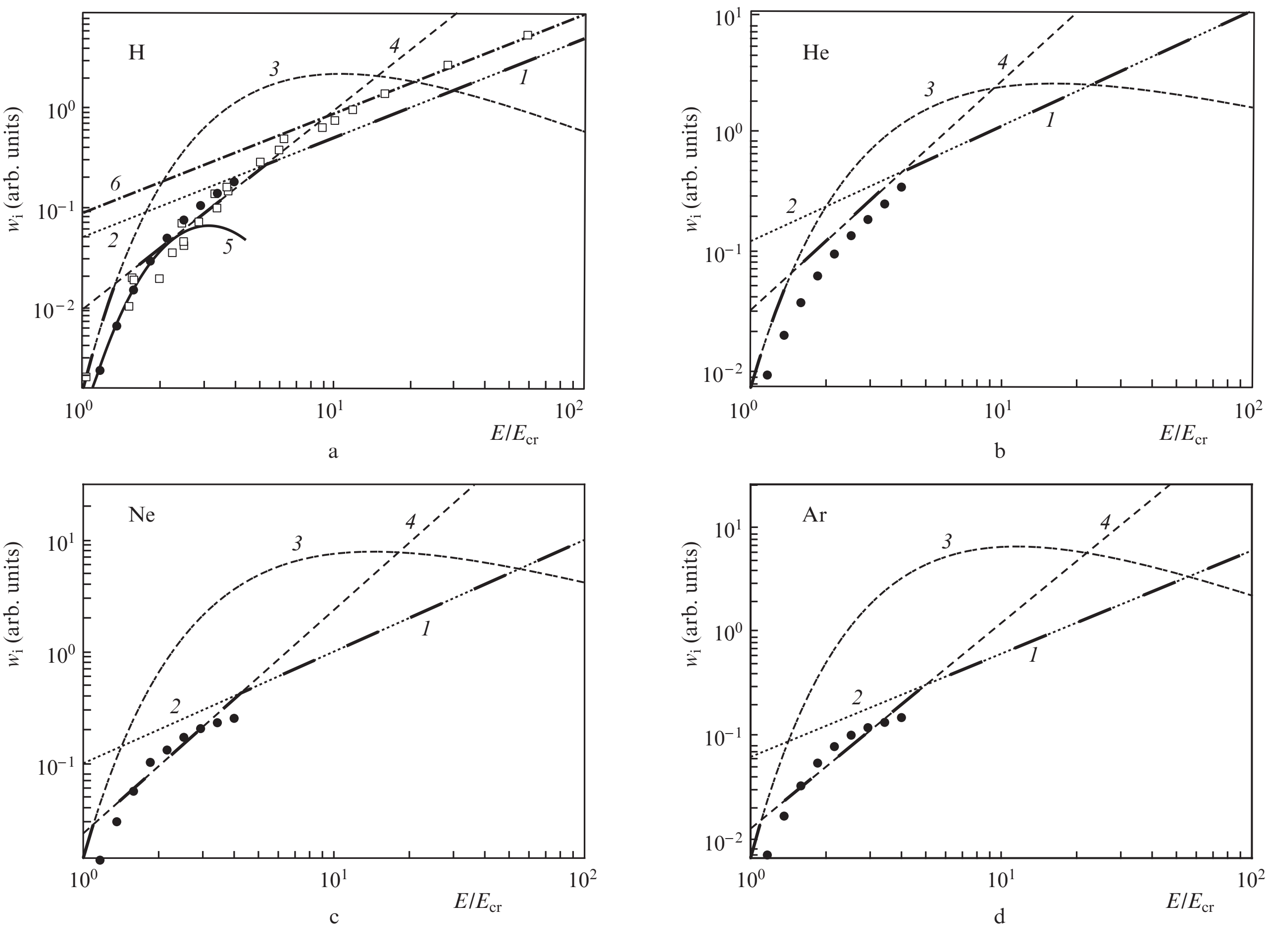

Figure 2. Dependences of the ionisation rate on the external field strength for atoms of (a) hydrogen, (b) helium, (c) neon and (d) argon in numerical calculations in (□) [21] and (•) [22], as well as dependences calculated by [curve (*1*)] equation (6), (*2*) equation (3) for ionisation in the barrier suppression regime, (*3*) equation (1) for the tunnel regime, and (*4*) equation (5); (*5*) dependence proposed in [20] and (*6*) dependence corresponding to formula (3) with a numerical coefficient of 1.4 instead of 0.8.

not require significant computational resources. The predictions of the formula are in good agreement with the results of numerical simulation of field ionisation for atoms of hydrogen, helium, neon and argon; however, additional studies are needed to verify the correctness of its use for other types of atoms and ions.

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