# Keldysh theory of tunnel ionization of an atom in a few-cycle laser pulse field

Aleksei S. Kornev* and Boris A. Zon†
*Voronezh State University, Voronezh, Russia*
(Received 12 December 2011; published 7 March 2012)

We propose a simple modification of the Keldysh theory of ionization of an atom in a few-cycle laser pulse field. The results obtained agree well with the *ab initio* simulations carried out by Rohringer and Santra [Phys. Rev. A **79**, 053402 (2009)] for the Ne atom and the $Ne^+$ ion, both in the ground state and in the excited state. This is a confirmation of the model of the inelastic tunnel effect that is one of the major many-body effects in tunnel ionization theory.

DOI: 10.1103/PhysRevA.85.035402 PACS number(s): 32.80.Rm, 32.10.Fn

Various physical phenomena arising in an ultrashort laser pulse field are under active study lately [1–3]. In Refs. [4–8] the multichannel coherence of ground and excited states of an ion in the ionization of an atom by a short light pulse was investigated. In these references the probability of atom ionization in the short electromagnetic pulse field was obtained by the numerical solution of the time-dependent Schrödinger equation. Multichannel coherence in molecules is investigated in Refs. [9,10].

For a description of atom ionization in a strong light field, the duration of which significantly exceeds the optical cycle, there exists the Keldysh theory [11]. In the tunneling limit this theory is often referred to as the Ammosov-Delone-Krainov (ADK) theory [12], which has been verified experimentally many times. The numerical verification of the Keldysh theory has also been carried out many times (see, e.g., Refs. [13,14]). However in Ref. [4] the case of ionization is considered when the ion can be created in two states, the ground and the excited states. Therefore, the numerical results presented in Ref. [4] allow one to generalize the Keldysh theory to the case of ultrashort light pulses and also to verify the inelastic tunnel effect theory developed in Refs. [15–20] which quantitatively explains a substantial number of experimental data [21–23]. It should be noted that the influence of excited states on tunnel ionization of molecules has also been investigated both for simple molecules, e.g., $D_2$ [24], and for complex molecules, such as $C_{60}$ [25].

The rate of electron tunneling emission from a potential with the Coulomb asymptotic form in a dc electric field $F$ is given by the Smirnov-Chibisov formula [26],

$$W_{\nu lm}^{(\text{S-Ch})}(F) = \frac{\hbar Z^2}{a^2 m_e \nu^2} C_{\nu l}^2 \frac{(2l+1)(l+|m|)!}{2^{|m|+1}|m|!(l-|m|)!} \times \left(\frac{2F_a}{F}\right)^{2\nu-|m|-1} \exp\left(-\frac{2F_a}{3F}\right). \quad (1)$$

Here, $a$ is the Bohr radius, $m_e$ is the electron mass, $l$ and $m$ are the orbital and magnetic quantum numbers of the tunneling electron, respectively, and $Z$ is the residual ion charge. The effective principal quantum number $\nu$ is connected with the ionization potential $E_i$ by the relation

$$E_i = \frac{Z^2}{2\nu^2}\frac{e^2}{a},$$

where $e$ is the elementary charge. The dimensionless constant $C_{\nu l}$ is determined by the asymptotic behavior of the valence electron wave function in the absence of an external field,

$$\Psi(\mathbf{r}) \approx C_{\nu l}\, q^{3/2}(qr)^{\nu-1}e^{-qr}Y_{lm}(\mathbf{r}/r),$$

where $q = Z/(a\nu)$. The parameter $F_a = e/(a^2\nu^3)$ can be regarded as the electric field strength at a distance from the nucleus equal to the Bohr radius.

In an ac field, the tunnel ionization mode occurs, if the Keldysh parameter $\gamma$ is small,

$$\gamma^2 = 2m_e E_i \omega^2/(e\tilde{F})^2 < 1.$$

Here $\omega$ is the laser radiation frequency, and $\tilde{F}$ is the electric field strength amplitude,

$$F(t) = \tilde{F}\sin\omega t. \quad (2)$$

The replacement of $F$ by $F(t)$ in Eq. (1) and averaging over an optical cycle $T = 2\pi/\omega$ [27,28] result in the ADK formulas, giving the tunnel effect rate. The replacement $F \to F(t)$ assumes that the laser radiation is linearly polarized and the laser optical cycle $T$ is much longer than the typical atomic time $T_a$ so that the adiabatic approximation can be used.

Evidently, under the same adiabatic limit

$$T \gg T_a, \quad (3)$$

but without averaging over the optical cycle, we can obtain the tunnel effect rate in a few-cycle laser pulse field,

$$W_{\nu lm}(F,t) = \frac{\hbar Z^2}{a^2 m_e \nu^2} C_{\nu l}^2 \frac{(2l+1)(l+|m|)!}{2^{|m|+1}|m|!(l-|m|)!} \times \left(\frac{2F_a}{F|\sin\omega t|}\right)^{2\nu-|m|-1} \exp\left(-\frac{2F_a}{3F|\sin\omega t|}\right). \quad (4)$$

In Eq. (4) and hereafter the tilde above the field $F$ is omitted for the sake of convenience of comparison of the obtained formulas with those usually used in the literature. Thus, $F$ in Eq. (4) and hereafter means the laser-wave electric field amplitude. Ionization of an atom by an ultrashort laser pulse

*a-kornev@yandex.ru
†zon@niif.vsu.ru

 

was also investigated in Ref. [29] by the imaginary-time method.

Expression (4) must be multiplied by the squared overlap integral of the wave functions of the atomic core in the initial and finite states if the ionized atom is not alkali-metal-like (one electron in addition to filled shells). Let us consider an atom of a rare gas, the outer shell of which has the configuration $p^6$. A single-charged ion of the atom has the configuration $p^5$ and can be found in states with the total angular momentum either $J = \frac{3}{2}$ (the ground term) or $J = \frac{1}{2}$ (the excited term). Let $M$ be the projection of the atomic-core total angular momentum onto the laser-wave electric field direction. Then the overlap integral is expressed by the Clebsch-Gordan coefficient (see the details in [16]),

$$Q_{JMm} = C^{00}_{1\,-m\;1m} C^{00}_{1/2\,M+m\;1/2\,-(M+m)} C^{JM}_{1\,-m\;1/2\,M+m}, \qquad (5)$$

where $m$ is the projection of the orbital momentum of the tunneling electron onto the same direction.

In addition to the reconfiguration of the spin-angular functions, the overlap integral can be affected by a change of the core-electron radial functions because these functions in a neutral atom and in an ion, generally speaking, are different. Neglect of this difference is known as the frozen-core approximation. Taking this difference into account means a transition to the concept of Dyson orbitals. Numerical analysis in the Hartree-Fock approximation shows, however, that the Dyson orbitals change the result by no more than by 3%. It should be noted that the Dyson orbitals are very significant for tunnel ionization of molecules [30].

As has been said already, the ion with $p^5$ configuration can be found in the ground state $^2P_{3/2}$ as well as in the excited state $^2P_{1/2}$, with the value of the fine splitting $\Delta_{3/2,1/2}$. Within the framework of the Carlson-Zon model of the inelastic tunnel effect [15,31], in the ground and excited states, respectively, in Eq. (4) we must set

$$\nu_{\rm g} = e[2aE_i]^{-1/2}, \quad \nu_{\rm ex} = e[2a(E_i + \Delta_{3/2,1/2})]^{-1/2}. \qquad (6)$$

In particular, for the neutral neon atom, $E_i = 21.565$ eV, $\Delta_{3/2,1/2} = 0.0968$ eV, and $C_{\nu 1} = 1.30$ [32].

As the tunnel effect rate (4) depends on time, the population of ionic states $P_j$ is given by the formula

$$P_j(t) = \int_{-\infty}^{t} dt'\, W_j(F,t') \times \exp\left[-\sum_{j'} \int_{-\infty}^{t'} W_{j'}(F,t'')\,dt''\right]. \qquad (7)$$

Here, the indices $j$ and $j'$ enumerate the $Ne^+$ ion states corresponding to all possible values of $J$ and $M$ for the $p^5$ configuration: $j,j' = (J = \frac{3}{2}; M = \pm\frac{1}{2}, \pm\frac{3}{2}),(J = \frac{1}{2}; M = \pm\frac{1}{2})$. The functions $W_j(F,t)$ differ from (4) in that they are multiplied by the squared overlap integral (5). The effective principal quantum number of the tunneling electron $\nu$ is given by Eqs. (6), which depend on the core angular momentum $J$. The semiclassical formula (7) is the solution to the appropriate kinetic equations. This expression takes into account the decrease of the population of the neutral Ne atom population in time.

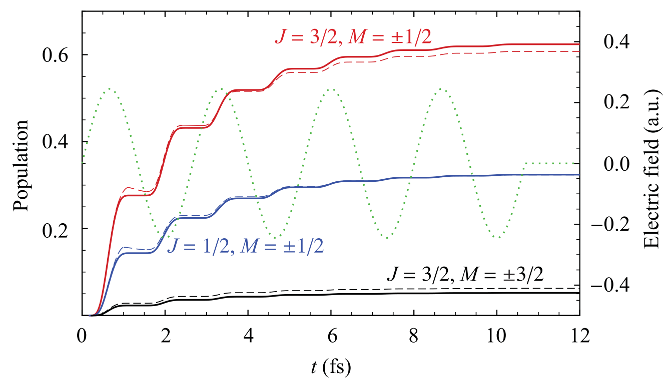


FIG. 1. (Color online) Population of the $Ne^+$ ion doublet terms depending on time. The solid lines correspond to the result of the present work; the dashed lines to the numerical simulation [4]. The dotted line shows the electric field intensity in a pulse with a rectangular envelope. See the radiation parameters in the text.

The results of calculations by formulas (4) and (7) are presented in Fig. 1 for a Ne atom and a four-cycle pulse with a rectangular envelope. The laser wavelength is 800 nm, the optical cycle is 2.67 fs, and the radiation intensity is $2.1 \times 10^{15}$ W/cm$^2$. For a pulse of such a shape the lower integration limit in Eq. (7) can be equal to zero. In Fig. 1, the results from Ref. [4] are given for comparison. As in Ref. [4], the results of our calculations of ion state populations are normalized in such a way that the population of the neutral Ne at $t = 0$ is equal to 1. As the neutral Ne atom is ionized completely by a laser pulse with the given laser parameters, the sum of the populations of the ground and excited $Ne^+$ states at $t \to +\infty$ is equal to 1. Evidently, our calculations agree well with the results obtained in Ref. [4]. The difference between formula (4) and the general Keldysh theory formulas becomes apparent in the vicinities of the field nodes, where the field is small and electron tunneling does not occur. Therefore, populations essentially do not depend on time in the vicinities of the field nodes. The small population probability for ionic states with $J = 3/2$, $M = \pm 3/2$ is explained by the fact that for the occurrence of such a core angular momentum projection it is necessary that the orbital momentum projection of the tunneling electron $m = \pm 1$. But as is apparent from Eqs. (1) and (4), the corresponding tunneling rates are suppressed compared to those with $m = 0$.

Similar calculations of the $Xe^+$ ion level population probabilities agree less well with the numerical simulations, which were also presented in [4]. This may be caused by the greater polarizability of the Xe neutral atom, exceeding the Ne polarizability by ten times ($27.08a^3$ and $2.68a^3$, respectively [32]). Therefore, the Xe electron wave functions are perturbed significantly, which must be shown in the tunnel effect rate. The perturbation of the bound atomic state wave functions due to the external field is not taken into account by the Keldysh theory. At present, an analytical perturbation theory of bound states in a few-cycle laser pulse field is lacking. Note that for formation of multiply charged ions as studied in Refs. [15–20] the perturbation of bound electron states by the field is small, as the polarizability decreases greatly with increase in the ion charge.

In conclusion, a simple modification of the Keldysh theory permits part of the results obtained in Ref. [4] to be reproduced by numerical simulation. In turn, these results confirm the theory of the inelastic tunnel effect developed in Refs. [15–20]. Although the kinetic equations are inherently semiclassical, they represent well the results of a consistent quantum description of the ionization process [4].

The authors thank V. S. Yakovlev for helpful discussions and RFBR (Grant No. 11-02-00170) for financial support.

[1] F. Krausz and M. Ivanov, Rev. Mod. Phys. **81**, 163 (2009).
[2] A. Fleischer, H. J. Wörner, L. Arissian, L. R. Liu, M. Meckel, A. Rippert, R. Dörner, D. M. Villeneuve, P. B. Corkum, and A. Staudte, Phys. Rev. Lett. **107**, 113003 (2011).
[3] H. J. Wörner and P. B. Corkum, J. Phys. B **44**, 041001 (2011).
[4] N. Rohringer and R. Santra, Phys. Rev. A **79**, 053402 (2009).
[5] E. Goulielmakis, Z. H. Loh, A. Wirth, R. Santra, N. Rohringer, V. S. Yakovlev, S. Zherebtsov, Th. Pfeifer, A. M. Azzeer, M. F. Kling, S. R. Leone, and F. Krausz, Nature (London) **466**, 739 (2010).
[6] L. Greenman, P. J. Ho, S. Pabst, E. Kamarchik, D. A. Mazziotti, and R. Santra, Phys. Rev. A **82**, 023406 (2010).
[7] R. Santra, V. S. Yakovlev, Th. Pfeifer, and Z. H. Loh, Phys. Rev. A **83**, 033405 (2011).
[8] S. Pabst, L. Greenman, P. J. Ho, D. A. Mazziotti, and R. Santra, Phys. Rev. Lett. **106**, 053003 (2011).
[9] Y. Mairesse, J. Higuet, N. Dudovich, D. Shafir, B. Fabre, E. Mével, E. Constant, S. Patchkovskii, Z. Walters, M. Yu. Ivanov, and O. Smirnova, Phys. Rev. Lett. **104**, 213601 (2010).
[10] Z. B. Walters and O. Smirnova, J. Phys. B **43**, 161002 (2010).
[11] L. V. Keldysh, Sov. Phys. JETP **20**, 1307 (1965).
[12] M. V. Ammosov, N. B. Delone, and V. P. Krainov, Sov. Phys. JETP **64**, 1191 (1986).
[13] R. M. Potvliege, Comput. Phys. Commun. **117**, 42 (1998).
[14] D. Bauer and P. Koval, Comput. Phys. Commun. **174**, 396 (2006).
[15] B. A. Zon, Sov. Phys. JETP **91**, 899 (2000).
[16] A. S. Kornev, E. B. Tulenko, and B. A. Zon, Phys. Rev. A **68**, 043414 (2003).
[17] A. S. Kornev, E. B. Tulenko, and B. A. Zon, Phys. Rev. A **69**, 065401 (2004).
[18] A. S. Kornev, E. B. Tulenko, and B. A. Zon, Phys. Rev. A **79**, 063405 (2009).
[19] B. A. Zon, A. S. Kornev, and E. B. Tulenko, Sov. Phys. JETP **111**, 921 (2010).
[20] A. S. Kornev, E. B. Tulenko, and B. A. Zon, Phys. Rev. A **84**, 053424 (2011).
[21] D. N. Fittinghoff, P. R. Bolton, B. Chang, and K. C. Kulander, Phys. Rev. A **49**, 2174 (1994).
[22] K. Yamakawa, Y. Akahane, Y. Fukuda, M. Aoyama, N. Inoue, and H. Ueda, Phys. Rev. A **68**, 065403 (2003).
[23] W. A. Bryan, S. L. Stebbings, J. McKenna, E. M. L. English, M. Suresh, J. Wood, B. Srigengan, I. C. E. Turcu, J. M. Smith, E. J. Divall, C. J. Hooker, A. J. Langley, J. L. Collier, I. D. Williams, and W. R. Newell, Nat. Phys. **2**, 379 (2006).
[24] I. V. Litvinyuk, F. Legare, P. W. Dooley, D. M. Villeneuve, P. B. Corkum, J. Zanghellini, A. Pegarkov, C. Fabian, and T. Brabec, Phys. Rev. Lett. **94**, 033003 (2005).
[25] T. Brabec, M. Cote, P. Boulanger, and L. Ramunno, Phys. Rev. Lett. **95**, 073001 (2005).
[26] B. M. Smirnov and M. I. Chibisov, Sov. Phys. JETP **22**, 585 (1966).
[27] A. M. Perelomov, V. S. Popov, and M. V. Terentev, Sov. Phys. JETP **23**, 924 (1966).
[28] V. S. Popov, Phys. Usp. **47**, 855 (2004).
[29] V. S. Popov, JETP Lett. **73**, 1 (2004).
[30] R. Murray, M. Spanner, S. Patchkovskii, and M. Yu. Ivanov, Phys. Rev. Lett. **106**, 173001 (2011).
[31] T. A. Carlson, Phys. Rev. **156**, 142 (1967).
[32] A. A. Radzig and B. M. Smirnov *Reference Data on Atoms, Molecules and Ions* (Springer-Verlag, New York, 1985).