Correction to the Tunneling Theory in Atoms

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Abstract—The theory of the tunneling ionization of atoms with several outer-shell electrons is specified. Numerical calculations for the noble-gas atoms are performed.

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1. INTRODUCTION

It is known that the qualitative interpretation of tunneling was one of the triumphs of quantum mechanics. However, the development of the quantitative theory of this phenomenon for atoms and molecules appeared to be difficult. This is primarily due to the presence of the long-range Coulomb potential, which perturbs the electron motion in the continuous spectrum. Exact results were obtained only for the hydrogen atom, since the variables can be separated using the parabolic coordinate system for the Schrödinger equation of an electron that moves in the presence of the Coulomb field and a static external electric field [1, 2].

The theoretical analysis of the tunneling in atoms became topical owing to the development of laser physics and the known work [3] in which Keldysh demonstrated the tunneling ionization in the presence of an ac electric field.

Smirnov and Chibisov [4] initiated the development of the modern quantitative tunneling theory and employed the parabolic coordinates to study the free-electron motion in an arbitrary atom. For a moderate external field, the joining of the free- and bound-electron wave functions can be performed at a relatively large distance from the nucleus, where the bound-electron wave function can be considered in the approximation of the quantum-defect method (QDM). Perelomov et al. [5] generalized this result for the case of an ac electric field and demonstrated that the Keldysh tunneling ionization follows from the Smirnov–Chibisov formulas provided that the ac field is substituted in these formulas and the averaging over the field period is performed. Ammosov et al. [7] were the first to compare this theory with the experimental results from [6] and the theory became known as the ADK theory. There has been considerable recent progress in the development of the ADK theory. In particular, note the analysis of the tunneling ionization from the Rydberg [8] and low-lying [9] molecular states, the multielectron tunneling in atoms [10, 11], and the tunneling ionization of atoms with the excitation of the residual ion [12–14]. The last effect was experimentally proven in [15].

Nevertheless, the theory of the tunneling ionization of multielectron atoms is not rigorously substantiated due to the following reason. It is well known that the application of the QDM in the calculations of the oscillator strengths and the ionization widths yields an agreement with experimental data only for atoms that have one electron beyond the filled shells. The electromagnetic transitions related to this optical electron can be described using the QDM. The calculated results for atoms that have several electrons at the outer shell can differ by severalfold from the experimental results. There are doubts that the ADK tunneling ionization theory, which is based on the QDM, can be used to study multielectron atoms (in particular, noble-gas atoms). In this work, we eliminate the disadvantage of the theory.

An inaccuracy of the QDM theory has been recently demonstrated in [16–19]. Below, we briefly present the corresponding arguments.

In the QDM, the one-electron wave function of the bound state of a complicated atom is determined using the asymptotic expression represented in atomic units:

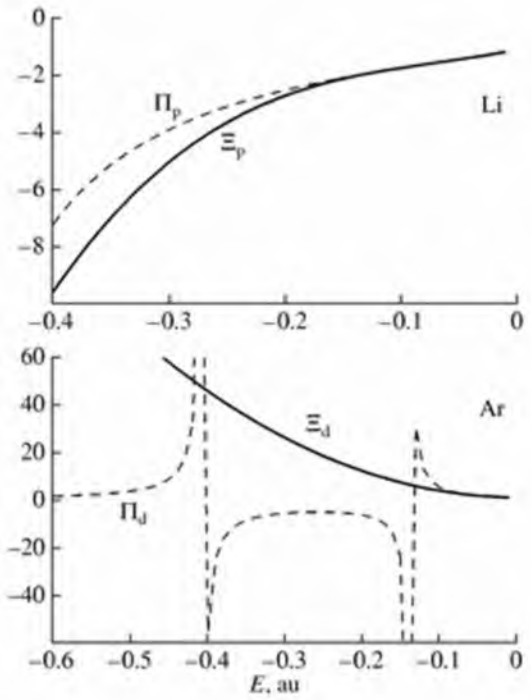
$$\Psi_{nlm}(\mathbf{r}) = C(Zr)^{\nu_{nl}-1}\exp(-Zr/\nu_{nl})Y_{lm}(\hat{\mathbf{r}}), \quad r \gg 1, \quad (1)$$

where $\hat{\mathbf{r}} = \mathbf{r}/r$, Z is the charge of residual ion, ν_{nl} is the effective principle quantum number of the electron under study, and the normalizing constant given by

$$C = \frac{Z^{1/2}}{\nu}\left[\Gamma(\nu+l+1)\Gamma(\nu-l)\left(1+\frac{\partial\mu_l(\nu)}{\partial\nu}\right)\right]^{-1/2}\Bigg|_{\nu=\nu_{nl}} \quad (2)$$

contains quantum defect $\mu_l(\nu)$.

Constant (2), which can be considered as the analytical function of energy, determines the one-electron Green function. It is demonstrated in [16] that this function exhibits poles corresponding to the nonphysical electron states: $1p$, $1d$, …, $2d$, $2f$, ….



The values of functions $\Xi_l(E)$ and $\Pi_l(Z/\sqrt{-2E})$ for the valence electrons in lithium and argon atoms.

To eliminate this disadvantage, one must substitute the following constant for constant C:

$$C' = B^{1/2}C, \quad B = \Xi_l(E)/\Pi_l(Z/\sqrt{-2E}). \tag{3}$$

Here,

$$\Pi_l(\nu) = \nu^{2l}\left\{\prod_{m=0}^{l-1}[m+\mu_l(\nu)+\nu][m+1-\mu_l(\nu)-\nu]\right\}^{-1}, \tag{4}$$

$\nu = \sqrt{-2E}$, and $\Xi_l(E)$ is the entire function of energy represented as

$$\Xi_l(E_n) = \Pi_l(n), \quad n \geq l+1, \tag{5}$$

where $E_n = -Z^2/(2n^2)$ are energy levels of a hydrogen-like ion.

The values of $B_l(E_{nl})$ for the valence electrons of the noble-gas atoms in the ground states with energies E_{nl}

Atom	He	Ar	Ne	Kr	Xe
$B_l(E_{nl})$	1.000	1.653	0.983	0.648	0.858

The figure demonstrates typical functions $\Xi_l(E)$ and $\Pi_l(Z/\sqrt{-2E})$ for the valence electrons in the Li ($Z = 1$ and $l = 2$) and Ar ($Z = 1$ and $l = 2$) atoms. These functions coincide at $E \longrightarrow 0$. Thus, we derive the well-known conclusion that the QDM can be used for the Rydberg states of any atoms. Note that, for the ground and low-lying excited states, functions Ξ and Π significantly differ from each other for Ar. This accounts for the poor agreement of the calculated oscillator strengths and ionization widths and the experimental results for Ar and the remaining noble gases. The energy levels of alkali atoms are similar to the atomic hydrogen spectrum. Hence, the factor is $B_l(E) \approx 1$ and the classical theory of quantum defect can be successfully employed for the alkali atoms.

The table presents the values of $B_l(E_{nl})$ for the valence electrons of the noble-gas atoms in the ground states with energies E_{nl}, where $nl = 1s, 2p, \ldots$ for He, Ne, …, respectively.

Thus, the tunneling ionization probability of the noble-gas atoms can substantially differ from the results obtained using the classical theory of a quantum defect.

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REFERENCES

1. C. Lanczos, Zs. F. Phys. **68**, 204 (1931).
2. L. D. Landau and E. M. Lifshitz, *Course of Theoretical Physics*, Vol. 3: *Quantum Mechanics: Non-Relativistic Theory*, 4th ed. (Oxford Univ. Press, Oxford, 1980).
3. L. V. Keldysh, Sov. Phys. JETP **20**, 1307 (1964).
4. B. M. Smirnov and M. I. Chibisov, Sov. Phys. JETP **22**, 585 (1965).
5. A. M. Perelomov, V. S. Popov, and M. V. Terent'ev, Sov. Phys. JETP **23**, 924 (1966).
6. F. Yergeau, S. Chin, and P. Pavigne, J. Phys. B **28**, 723 (1987).
7. M. V. Ammosov, N. B. Deloné, and V. P. Kraĭnov, Sov. Phys. JETP **64**, 1191 (1986).
8. B. A. Zon, Sov. Phys. JETP **85**, 61 (1997).
9. X. M. Tong, Z. X. Zhao, and C. D. Lin, Phys. Rev. A **66**, 033402 (2002).
10. B. A. Zon, Sov. Phys. JETP **89**, 219 (1999).