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Improved Treatment of the Turning Point in Tunnel Ionization of Atoms in a Low-Frequency Electromagnetic Field

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Abstract—In constructing the ADK theory, the Coulomb interaction was not included as the first-order correction into the all phases, i.e., the turning point was calculated to the zero-order degree of approximation with regard to the Coulomb interaction. This was correct for fields (up to 10^{12} W/cm^2) much smaller than the atomic field (10^{16} W/cm^2). But as lately in experiments are used fields even greater than the atomic one (in this case ADK theory does not work), we decided to reconsider the influence of the Coulomb interaction on the turning point for the fields that are strong enough to make a difference and yet are smaller than the atomic fields (i.e., for fields of order of magnitude of 10^{14} W/cm^2). So, in this paper we have included the Coulomb interaction where it has been completely neglected earlier. We have shown that this more accurate approach gives somewhat different result for the ionization probability.

1. INTRODUCTION

During the last decade, it has been shown [1–4] that rare gases could be ionized relatively easily with CO_2 lasers for which Keldysh's parameter [5] $\gamma \ll 1$, this being the so-called *tunneling regime*. The tunneling regime was theoretically explained in [6], and after some time this result obtained the name ADK theory (first in paper [7], then also in papers [8–13], to mention some). Later in [14], it was shown that the set of prescriptions for calculations given in [6] is a theory, based on Landau–Dykhne adiabatic approximation [15] and Keldysh's theory [5]. As there are a lot of experimental confirmations of the ADK theory for fields up to 10^{12} W/cm^2 (see, for instance, [1–4, 7–11]), though this theory is not valid in the superstrong fields case, we felt the need to make its foundations more firm and to include into this theory the *Coulomb interaction* as the first-order correction into all phases of construction of the theory. As shall be seen, when determining the turning point, which is included into the theory through the Landau–Dykhne adiabatic approximation, the Coulomb interaction was completely neglected, which was correct for the case of fields much smaller than the atomic field 10^{16} W/cm^2, but for the fields that are of order of magnitude 10^{12}–10^{14} W/cm^2, the term previously neglected could give considerable gain to the probability for ejecting an electron from the atom in the strong laser field.

In the framework of Landau–Dykhne adiabatic approximation [15, 16], the transition amplitude between initial and final states is ($E_f > E_i$ on real axes)

$$A_{if} = \exp\left\{ i \int_{t_1}^{\tau} \omega_{if}(t)\,dt \right\}. \qquad (1)$$

Here, ω_{if} is the frequency of the transition in the presence of the external field and τ is the complex turning point in the time plane, for which

$$\omega_{if}(\tau) = 0. \qquad (2)$$

The transition rate $i \longrightarrow f$ is given by expression

$$W_{if} = |A_{if}|^2 = \exp\{-2\mathrm{Im}\int \omega_{if}(t)\,dt\}. \qquad (3)$$

The estimation of the probability of ionization based on (3) in the case of the short-range potential uses the fact that this kind of potential does not affect the energy of the final state *f* of the electron in the electromagnetic field, because the ejected electron is far enough from the nucleus (which is the essence of the Keldysh approximation [5, 6, 14, 16]).

In the case of Coulomb potential, typical for the atom ionization, its effect is accounted for by the addition of Coulomb potential as a small quantity to the energy of the final state [6].

Nevertheless, using condition (2) for defining the turning point with including the Coulomb interaction results in a shift of the position of turning point τ. This paper deals with the influence of that shift on the ionization probability of atoms in the low-frequency electromagnetic field.

2. DEFINING OF COMPLEX TURNING POINT τ

The method for calculating the probability of tunnel ionization using the Landau–Dykhne adiabatic approximation is given in book [16]. It begins with the equation (2), i.e.,

$$E_f(\tau) = E_i(\tau), \qquad (4)$$

where $E_i(\tau)$, $E_f(\tau)$ are the initial and final energy, respectively, in the external electromagnetic field, and τ is the complex time, related to the turning point. As the external field F is much smaller than the atomic ($F \ll F_{at}$) it is possible, following Keldysh [5], to consider its influence only on the final state, taking the initial state to be nonperturbated, so one has $E_i(\tau) = -E_i$, where E_i is the ionization potential of the atomic electron, or (in atomic units $e = m_e = \hbar = 1$, which will be used throughout this paper)

$$\frac{1}{2}\left(p - \frac{F}{\omega}\sin\omega\tau\right)^2 - \frac{Z}{\eta(\tau)} = -E_i. \tag{5}$$

The Coulomb term in equation (5) is small compared to the other terms, and we will be using iteration. So, for calculating classically coordinate $\eta(\tau)$ (here we are using parabolic coordinates, see [15]), it is necessary, in the zero order of approximation, to take into account only the external electric field

$$\frac{d^2z}{dt^2} = -F\cos\omega\tau. \tag{6}$$

Integrating equation (6), taking into account that $z \approx \frac{\eta}{2}$ [15], one obtains, for turning point τ,

$$\eta(\tau) = -2i\sqrt{2E_t}\tau - (2F/\omega^2)(1 - \cos\omega\tau). \tag{7}$$

The first term in (7) was chosen so that at the initial time $t = 0$ energy of the electron equals the atomic energy $-E_i$. In zero-order approximation one has $\eta(\tau_0) = -2i\sqrt{2E_i}\,\tau_0$, the expression which was used earlier in the ADK theory [6], τ_0 being the turning point in the zero-order approximation,

$$\tau_0 = \frac{p + i\sqrt{2E_i}}{F}. \tag{8}$$

Then from (5) one obtains (for $\mathrm{Re}(\omega\tau) \ll 1$)

$$p - F\tau = -\sqrt{-2E_i + \frac{Z}{\eta(\tau)/2}}. \tag{9}$$

When cosine in expression (7) for $\eta(\tau)$ is written in power series, this expression goes over to

$$\frac{\eta(\tau)}{2} = -i\sqrt{2E_i}\tau + \frac{F\tau^2}{2}.$$

Now, if we, iterating, put τ_0 instead of τ, we have

$$\frac{\eta(\tau_0)}{2} = \frac{E_i + p^2/2}{F}. \tag{10}$$

As the Coulomb correction under the root of expression (9) is very small compared to the ionization potential E_i, it is possible to expand this expression into the power series. So iterating, i.e., using (10), one obtains for the turning point

$$\tau = \frac{p}{F} + \frac{i\sqrt{2E_i}}{F}\left[1 - \frac{ZF}{(2E_i)(2E_i + p^2)}\right], \tag{11}$$

and, finally,

$$\tau = \frac{p + i\sqrt{2E_i}}{F} - \frac{iZ}{\sqrt{2E_i}(2E_i + p^2)}. \tag{12}$$

We will use expression (12) for the turning point, instead of expression (8), which was used in earlier variant of the theory [6, 16, 17]. Let us begin with calculating of the time-dependent part of the action S, which will give us the transition rate in the case of tunnel ionization (see [16]),

$$W = e^{-2\,\mathrm{Im}\,S}, \tag{13}$$

where

$$\mathrm{Im}\,S = \mathrm{Im}\int_0^\tau \left[\frac{1}{2}\left(p - \frac{F}{\omega}\sin\omega\tau\right)^2 + E_i\right]dt. \tag{14}$$

Writing sine in power series and keeping only the first term, one obtains

$$\mathrm{Im}\,S = \mathrm{Im}\int_0^\tau \left[\frac{1}{2}(p - Ft)^2 + E_i\right]dt. \tag{15}$$

Only the upper limit influences quantity (15), as the lower limit is real, so

$$\mathrm{Im}\,S = \mathrm{Im}\left[\left(E_i + \frac{p^2}{2}\right)\tau - \frac{pF}{2}\tau^2 + \frac{F^2}{6}\tau^3\right]. \tag{16}$$

Now, putting expression (12) into equation (16), and turning to the approximation used earlier [6], one gets

$$\mathrm{Im}\,S = \frac{(2E_i)^{3/2}}{3F} + \frac{1}{2} \times\left[-\frac{Z}{\sqrt{2E_i}} + \frac{p^2F}{(\vec{p}^2 + 2E_i)\sqrt{2E_i}} + \frac{Z\sqrt{2E_i}}{(p^2 + 2E_i)}\right]. \tag{17}$$

In equation (17), we have kept only the first-order terms of the Coulomb interaction. Expression in the parentheses on the right-hand side of equation (17) is identically equal to zero, so one obtains

$$\mathrm{Im}\,S = \frac{1}{3}\frac{(2E_i)^{3/2}}{F} \tag{18}$$

or, using equation (13),

$$W = \exp\left[-\frac{2}{3}\frac{(2E_i)^{3/2}}{F}\right], \tag{19}$$

which is exactly the well-known expression for the probability in the tunneling case. So, including Coulomb interaction to the first order of approximation does not change this part of the tunneling formula.

3. INFLUENCE OF THE COULOMB INTERACTION ON THE ESTIMATING OF THE PRE-EXPONENT IN THE RATE OF TUNNELING IONIZATION

It is necessary here to examine the influence of the turning point, given by equation (12), on the pre-exponent obtained in the ADK theory.

As it is already known [6], the pre-exponent was obtained by including Coulomb interaction into the calculation of the time-dependent part of the action (Coulomb interaction was expressed in parabolic coordinates, and, in fact, this method was developed in [17], so the ADK theory only used this result). In this theory, the energy of final state with defined parabolic quantum numbers (n, n_1, n_2, m) is, for $m = 0$, given by

$$E_f(t) = \frac{1}{2}(p - Ft)^2 - \frac{(2n_2 + 1)}{n^*\eta(t)}. \tag{20}$$

Here, $n^* = (2E_i)^{-1/2}Z$ is the effective principal quantum number, defined by the ionization potential of the atomic electron E_i, and

$$\eta(t) \approx -2i\sqrt{2E_i} + Ft^2. \tag{21}$$

We are working in the limit $\omega \longrightarrow 0$ for the electromagnetic field, and with classical perturbation theory for including Coulomb interaction.

And so, Coulomb interaction gives the following part of the action:

$$\delta S_c = -\int_0^\tau \frac{(2n_2 + 1)\sqrt{2E_i}}{2\eta(t)Z}dt. \tag{22}$$

Here, we have used the well-known relation between parabolic coordinates: $-\xi \ll \eta$, as ξ is of the order of magnitude of atomic distances, and η is much larger [15], then, to complex turning point $\eta(\tau)$, and, finally, to arbitrary point $\eta_a = 2r_a$, at which the field of atomic residue is already small and the external field could be yet neglected ($E_i \gg F\eta_a \gg \frac{Z}{\eta_a}$). Expression (20) is true for $t > t_a$ (t_a being the time related to coordinate η_a), i.e., when the electron is under the barrier, and the atomic potential is negligible.

It should be stressed once again that regions $\eta < \eta_a$, corresponding to the time $t < t_a$, and $\eta > \eta_a$, connected with the time $t > t_a$, respectively, are essentially different. Indeed, in region $\eta < \eta_a$ quantum effects are very strong, and this region should be treated in a completely different manner than the region $\eta > \eta_a$.

So we should divide integral (22) into two parts,

$$\delta S_c = \delta S_0 + \delta S_a = \int_0^{t_a} + \int_{t_a}^{\tau}, \tag{23}$$

where by writing symbolic expression (23) we have defined new quantities δS_0 and δS_a.

Corresponding gain to the action of the second one of this quantities is

$$\delta S_a = \int_{t_a}^{\tau} [E_f(t) + E_i]dt. \tag{24}$$

According to relation (13), we have to calculate only the imaginary part of integral (24), which has its maximum at $n_1 = m = 0$. Taking into account that $n^* \gg 1$ we have

$$\mathrm{Im}\,\delta S_a = n^*\ln\left(\frac{Ft_a n^*}{2Z}\right) + \frac{1}{3Fn^{*3}}. \tag{25}$$

For $t < t_a$ the wave function could be treated as unperturbed atomic function

$$\psi = \left(\frac{2Zre}{n^{*2}}\right)^{n^*}\exp\left(-\frac{Zr}{n^*}\right), \tag{26}$$

where $r \approx \eta/2 \approx -i\sqrt{2E_i}\,t$ and e is logarithmic base, not to be confused with the elementary electric charge. Using semiclassical approximation, one can write $\psi(t) = \exp\{i\delta S_0(t)\}$, which gives for the imaginary part of the classical action at point t_a

$$\mathrm{Im}\,\delta S_0 = -n^*\ln\left(\frac{2Z^2 e t_a}{n^{*3}}\right). \tag{27}$$

Adding expressions (25) and (27), we get the imaginary part of the complete change of action during ionization:

$$\begin{aligned}\mathrm{Im}\,\delta S &= \mathrm{Im}\,\delta S_a + \mathrm{Im}\,\delta S_0 \\ &= \frac{1}{3Fn^{*3}} + n^*\ln\left(\frac{Fn^*}{4Z^3 e}\right).\end{aligned} \tag{28}$$

Here, the arbitrariness of point t_a becomes clear, because it does not influence expression (28), as it is ruled out of it.

So, the ionization probability is [18, 19]

$$W = \left(\frac{4Z^3 e}{Fn^{*4}}\right)^{2n^*}\exp\left(-\frac{2}{3Fn^{*3}}\right). \tag{29}$$

In order to take into account the influence of Coulomb interaction on the turning point τ, we will consider the part of the action δS_a, as this is the only

expression in these calculations where τ is explicitly figuring

$$\delta S_a = -\int_{t_a}^{\tau} \frac{(n_2+1)\sqrt{2E_i}}{-2i\sqrt{2E_i}}dt. \tag{30}$$

Here, we have used $\eta(\tau)$ from expression (7) and, taking into account that in the whole region from t_a to τ, i.e., $\eta > \eta_a$, it is $|\omega t| \ll 1$, we have used relation $(1 - \cos\omega t) \approx \omega^2 t^2/2$.

Equation (30) could be rewritten to become

$$\delta S_a = -\frac{\sqrt{2E_i}(2n_2+1)}{F}\int_{t_a}^{\tau} \frac{dt}{t^2 - (2i\sqrt{2E_i})t/F}, \tag{31}$$

and, finally,

$$\delta S_a = \frac{i(2n_2+1)}{2} \times \ln\left(\frac{\tau - (2i\sqrt{2E_i})/F}{\tau}\frac{t_a}{t_a - (2i\sqrt{2E_i})/F}\right). \tag{32}$$

Now, as $\tau \approx i\sqrt{2E_i}/F \gg t_a$, we can deduce τ given by (12)

$$\delta S_a = \frac{i(2n_2+1)}{2} \times \ln\left(\frac{p - i\sqrt{2E_i} - \dfrac{iZF}{\sqrt{2E_i}(p^2+2E_i)}}{p + i\sqrt{2E_i} - \dfrac{iZF}{\sqrt{2E_i}(p^2+2E_i)}}\frac{t_a}{(-2i\sqrt{2E_i})/F}\right) \tag{33}$$

or

$$\delta S_a = \frac{i(2n_2+1)}{2} \times \ln\left(\frac{p - i\sqrt{2E_i}}{p + i\sqrt{2E_i}}\frac{1 - \dfrac{iZF}{\sqrt{2E_i}(p^2+2E_i)}}{1 - \dfrac{iZF}{\sqrt{2E_i}(p^2+2E_i)}}\frac{t_a}{(-2i\sqrt{2E_i})/F}\right). \tag{34}$$

As the transition rate is proportional to the square of the absolute value of the exponential function whose exponential factor is composed of expression (34) [see equation (3)], we can see that the term

$$\left|\frac{p - i\sqrt{2E_i}}{p + i\sqrt{2E_i}}\right|^{(2n_2+1)} = 1$$

does not have any influence at all on our expression for the transition rate.

Therefore, remembering that $\ln i = i\pi/2$ and that $2n_{2\,\max} = 2n^* - 2$, we obtain

$$\operatorname{Im}\delta S_a = \frac{2n^*-1}{2}\ln\left\{\left[1 + \frac{2ZF}{(p^2+2E_i)^2} + \frac{Z^2F^2}{2E_i(p^2+2E_i)^3}\right]\left(\frac{Ft_a}{2\sqrt{2E_i}}\right)\right\}, \tag{35}$$

where we expanded in power series the denominator of the ratio under the logarithm sign in expression (34), as Coulomb interaction could be considered small.

Thus, according to (23), we have

$$\operatorname{Im}\delta S_{\text{coul}} = \frac{2n^*-1}{2}\ln\left\{\left[1 + \frac{2ZF}{(p^2+2E_i)^2} + \frac{Z^2F^2}{2E_i(p^2+2E_i)^3}\right]\left(\frac{Fn^{*2}}{4Ze2E_i}\right)\right\}. \tag{36}$$

Finally, for the ionization probability one has (S_{sr} being the part of the action due to the short-range potential)

$$W = e^{-2\operatorname{Im}S_{\text{sr}}}e^{-2\operatorname{Im}S_{\text{Coul}}} = \left[\frac{4Z^3e}{Fn^{*4}}\frac{1}{1 + \dfrac{2ZF}{(p^2+2E_i)^2} + \dfrac{Z^2F^2}{2E_i(p^2+2E_i)^3}}\right]^{2n^*-1} \times e^{-\frac{2}{3}\frac{Z^3}{Fn^{*3}}}. \tag{37}$$

In expression (37), for ionization probability W the second rational term in the parentheses is a correction for the Coulomb interaction which we obtained. For the fields up to 10^{12} W/cm^2, the correction is small and could be neglected (for instance, in the case of potassium ionization in the laser field of 10^{12} W/cm^2 [4], it is 0.10876478), but for greater fields (up to 10^{14} W/cm$^2 \ll I_{\text{at}} \sim 10^{16}$ W/cm^2, so that the Keldysh approximation and, accordingly, the ADK theory can be considered yet valid) this correction gains in amount (1.340258).

If probability W from expression (37) were plotted as a function of field intensity I, it is obtained that for fields of $\sim 3.5 \times 10^{13}$ W/cm^2, one has some kind of saturation and even decreasing of the probability with growing of the field intensity (the behavior of probability for fields greater than 10^{14} W/cm^2 was not included, because the validity of the ADK theory is doubtful for those intensities). This is the behavior that is observed in the superstrong field case, but not for strong fields for

which the ADK theory is valid. The anomalous behavior is mostly due to the "short-range" term $\sim e^{-\frac{1}{F}}$, which earlier was not extended to greater distances; nevertheless, the effect is stronger with the correction we obtained in expression (37).

4. CONCLUSION

Dividing the proof in two parts, making the difference between the part of the classical action which was obtained out of the short-range potential and the part produced by Coulomb interaction, we have shown that approximations, connected with Coulomb interaction in the ADK theory, are well founded for fields up to 10^{12} W/cm^2, but that for higher field intensities ($\sim 10^{14}$ W/cm^2) the correction obtained by including more accurate determination of the turning point τ gains in its importance. The new expression (37) for ionization probability, obtained in this paper, shows controversial behavior when the intensity of the field is growing, indicating, thus, saturation in the ionization probability of the electron which is obtained in the case of superstrong fields.

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