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TRANSITION RATES DEPENDENCE ON THE TURNING POINT

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ABSTRACT. In the case of the short-range potential [1, 5, 10, 11], the estimation of the transition rate of ionization of atoms is defined taking into account Keldysh approximation, which states that this kind of potential does not affect the energy of the final states f of the ejected electron in the laser field, because electron is far enough from the nucleus. When the Coulomb potential is taken into account, it can be treated as a perturbation to the energy of the final state [1, 10]. So there are three different transition rates, one obtained for short range potential, the other for the ADK-theory and third for ADK result with turning point corrected with the Coulomb interaction. If plotted for the fields from $10^{12}\ \mathrm{W/cm^2}$ to $10^{17}\ \mathrm{W/cm^2}$ the three variants give behavior which were predicted many times theoretically, but still with rather poor experimental support, see [11]. Yet result for short range potential is not realistic at all for greater fields and it is given here only to be compared with more realistic results shown in Figs 2 and 3. Indeed in Fig 3 one has corrected result of ADK-theory, which includes the turning point calculated with the Coulomb correction, and gives the saturation effect after 10^{13} W/cm^2, differing from the ADK case which gives this effect after 10^{14} W/cm^2 . Which of two is correct only experiment can decide.

1. INTRODUCTION

In the late XX Century tunneling ionization (Keldysh's [6] parameter γ□1) of atoms and ions by strong low-frequency laser fields has become the subject of intensive research. In that period, one of the most utilized theories was Ammosov-Delone-Krainov (ADK) theory [1], which uses the concept of a quasi-stationary external field ejecting valence electrons via tunneling. Recently [8, 12, 13], this theory has been extended to the barrier-suppression ionization of complex atoms and atomic ions, i.e. to the case of super-strong fields. Before that, the ADK-theory has been used to describe ionization which occurs when the laser intensities, in experiments, were up to 10^{12} W/cm^2 (atomic field is approximately 10^{16} W/cm^2). Nowdays, when we are dealing with field strengths of the order of atomic and even higher, the ADK theory had to be adjusted to the situation.

Using Landau-Dykhne adiabatic approximation [10 - 13] the ADK-theory [1] starts with the transition amplitude between initial and final states ($E_f > E_i$ on real axes)

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

where ω_{if} is frequency of the transition from i - initial to f - final state in the presence of the external field, and τ is the complex turning point in the time plane.

The complex turning point is obtained from equation which is classically forbidden [11]:

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

Also, the transition rate $i \rightarrow f$ is given by expression [1, 11]

$$W_{if} = |A_{if}|^2 = \exp\{-2 \cdot \mathrm{Im}\,\delta S(\tau)\} . \qquad (3)$$

In the case of the short-range potential [11, 12], the estimation of the transition rate of ionization of atoms using (3) is performed taking into account the Keldysh approximation, which states that this kind of potential does not affect the energy of the final state f of the ejected electron in the electromagnetic field, because the electron is far enough from the nucleus. When the Coulomb potential is taken into account, it can be treated as a perturbation to the energy of the final state [1, 10]. Yet, originally [1, 10], the Coulomb potential in this kind of estimation was not included into calculating the turning point from (2). This was done in [7], but only for the fields below the atomic field (up to 10^{14} W/cm^2). Now we are extending our calculation that included the Coulomb correction into the estimating the turning point to the fields that are much stronger (up to 10^{17} W/cm^2), which is justified by the results of [12, 13]. That results in the shift of the position of the turning point τ. So the paper is comparing the results of the influence of that shift on the transition rate for atoms in super-strong low frequency laser fields, with the results obtained for the same rate in the "pure" ADK-theory.

2. CALCULATING THE COMPLEX TURNING POINT, BY TAKING INTO ACCOUNT THE COULOMB INTERACTION

The method for calculating the transition rate using the Landau-Dykhne adiabatic approximation is given in [10, 11]. 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. Because external field F is much smaller than the atomic field F_{at} (and that is so even in the case of superstrong fields - 10^{17}W/cm^2 is the highest value we are taking into account, see explanation in the paragraph after equation 19 - because as shown in [8], and in this paper, after intensities of laser fields of 10^{14}W/cm^2 the atoms are ionized so that Z~10, thus producing the atomic field much stronger then external), we will take in consideration influence of external field only on final state E_f, while assuming that initial state is non-perturbed (see [6]) . In the case of linear field polarization $E_i(\tau) = -E_i$, where E_i is the ionization potential of the ground state of valence electron, and energy of final state E_f is given as:

$$E_f(\tau) = \frac{1}{2}\left(p - \frac{F}{\omega}\sin\omega\tau\right)^2 - \frac{Z}{\eta(\tau)},$$

where the last term in the above expression is due to Coulomb interaction. From (4), it follows:

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

As Coulomb term in (5) is small compared to other terms, we will be using iteration. In approximation of zero order, only the external electric field is taken into account

$$\frac{d^2z}{dt^2}=-F\cdot\cos\omega\tau,$$

which, after integration and remembering that $z=\eta/2$ (we are using parabolic coordinates, as in [11]), gives

$$\eta(\tau)=-2i\sqrt{2E_i}\cdot\tau-\frac{2F}{\omega^2}\cdot(1-\cos\omega\tau). \qquad (6)$$

First term in (6) was chosen in such way as to make it possible that, at the initial time $t=0$, energy of the electron equals atomic energy $-E_i$. By neglecting a second term in (6), as was done earlier in ADK theory [1], one has $\eta(\tau_0)=-2i\sqrt{2E_i}\cdot\tau_0$, where τ_0 is the turning point in the zero-order approximation

$$\tau_0=\frac{p+i\sqrt{2E_i}}{F}. \qquad (7)$$

But, if we form a power series of cosine: $\cos\omega\tau\approx1-\omega^2\tau^2/2$, expression (6) becomes

$$\eta(\tau)=-2i\sqrt{2E_i}\cdot\tau+F\tau^2. \qquad (8)$$

By following an iteration procedure, we put τ_0 instead of τ and obtain

$$\eta(\tau_0)=\frac{p^2+2E_i}{F}. \qquad (9)$$

Now, let us go back to expression (5): because external field has a low-frequency ($\omega<<\omega_{at}$), we are allowed to expand sine in power series, $\sin\omega\tau\approx\omega\tau$. Thus we get following expression

$$p-F\tau=-i\sqrt{2E_i}\cdot\sqrt{1-\frac{1}{\eta(\tau)}\cdot\frac{Z}{E_i}}. \qquad (10)$$

If, in expression (10), we substitute $\eta(\tau_0)$, because of iteration, we will obtain

$$p-F\tau=-i\sqrt{2E_i}\cdot\sqrt{1-\frac{F}{p^2+2E_i}\cdot\frac{Z}{E_i}}. \qquad (11)$$

As Coulomb correction under the root of the above expression is small compared with ionization potential E_i there follows another expanding: $\sqrt{1-x}\approx1-x/2$, which gives

$$p-F\tau=-i\sqrt{2E_i}\cdot\left(1-\frac{1}{2}\cdot\frac{F}{p^2+2E_i}\cdot\frac{Z}{E_i}\right),$$

i.e.

$$\tau=\frac{p}{F}+\frac{i\sqrt{2E_i}}{F}\cdot\left(1-\frac{Z}{2E_i}\cdot\frac{F}{p^2+2E_i}\right),$$

and, finally, an expression for Coulomb-correction-included turning point, already obtained in [7]

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

3. RATES OF TUNNELING IONIZATION OF ATOMS IN VARIUOS APPROACHES

The transition rate in the adiabatic approximation of Landau-Dykhne in the case of an atom in an external electromagnetic field is given by expression (3), where $S(\tau)$is time dependent part of the classical action, defined as:

$$S(\tau) = \int_0^\tau \{E_f(t) - E_i(t)\} dt,$$

or, using Keldysh approximation:

$$S_{sr}(\tau) = \int_0^\tau \left\{\frac{1}{2}(p\text{-}Ft)^2 + E_i\right\} dt.$$

For the case of a short-range potential, the transition rate (3) is:

$$W_{sr} = \exp\left(-\frac{2\cdot(2E_i)^{3/2}}{3F}\right). \qquad (13)$$

Including the Coulomb interaction [1] into the time-dependant part of the action, will lead to the following expression for energy of the final state:

$$E_f(t) = \frac{1}{2}(p - Ft)^2 - \frac{2n_2 - 1}{n^* \eta(t)}, \qquad (14)$$

where $\eta(t) = -2i\sqrt{2E_i} + Ft^2$, n_2 being one of parabolic quantum numbers that define a given state, and $n^* = Z/\sqrt{2E_i}$ is an effective principal quantum number – all these follow from our expressing the Coulomb interaction in parabolic coordinates.

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

$$\delta S_C = -\int_0^\tau \frac{(2n_2 + 1)\cdot\sqrt{2E_i}}{2\cdot\eta(t)\cdot Z}\cdot dt. \qquad (15)$$

which we shall divide into two parts [7]

$$\delta S_C = \delta S_0 + \delta S_a = \int_0^{t_a} + \int_{t_a}^{\tau}. \qquad (16)$$

where t_a represents time related to arbitrary turning point $\eta_a = 2r_a$, that we are allowed to use because, at this distance from atom, the influence of atomic residue on ejecting electron is already small, and the external field can still be neglected. Now, in a region $\eta < \eta_a$, which corresponds to time $t < t_a$, quantum effects are very strong, so it should be treated in a completely different manner than region $\eta > \eta_a$, which corresponds to time $t > t_a$.

Corresponding gain to the action by δS_0 can be obtained using semiclassical approximation, and by taking into account that, for $t < t_a$, the wave function can be treated as unperturbed atomic function

$$\mathrm{Im}\,\delta S_0 = -\frac{2n^*-1}{2}\cdot \ln\left(\frac{2Ze}{n^{*2}}\cdot\sqrt{2E_i}\cdot t_a\right).$$

Analogous gain to the action by δS_a can be obtained by integrating:

$$\delta S_a = \int_{t_a}^{\tau} \frac{(2n_2+1)\sqrt{2E_i}}{\eta(t)}\cdot dt\,.$$

After substituting a turning point $\eta(\tau)$, and a few elementary transformations, we have

$$\delta S_a = i\cdot\frac{2n_2+1}{2}\cdot\ln\left(\frac{\tau-\frac{2i\sqrt{2E_i}}{F_0}}{\tau}\cdot\frac{t_a}{t_a-\frac{2i\sqrt{2E_i}}{F_0}}\right).$$

As $\tau \approx i\sqrt{2E_i}/F_0 >> t_a$, we can neglect t_a in the denominator of above fraction, and shall include expression (7) for the turning point in the zero-order approximation. Taking into account that $\ln i = i\pi/2$, using a fact $n_{2\max} = n^*-1$, it follows from (16):

$$-2\,\mathrm{Im}\,\delta S_c = (2n^*-1)\ln\left(\frac{4Ze}{Fn^{*2}}\cdot 2E_i\right).$$

Remembering that $\sqrt{2E_i} = Z/n^*$ and including part of action due to already mentioned short-range potential, the transition rate is now given as:

$$W_{ADK} = \left(\frac{4Z^3e}{Fn^{*4}}\right)^{2n^*-1}\exp\left(-\frac{2Z^3}{3Fn^{*3}}\right). \qquad (17)$$

At the end, we have to examine the influence of turning point on a pre-exponent obtained in ADK theory. For that purpose, we shall include an expression for Coulomb-corrected turning point (12) in formulae for δS_a; after rather cumbersome but pretty much straightforward procedure, we obtain expression for imaginary part of action:

$$\mathrm{Im}\,\delta S_a = \frac{2n^*-1}{2}\cdot\ln\left\{\left[1+\frac{2ZF}{(p^2+2E_i)^2}+\frac{Z^2F^2}{2E_i\cdot(p^2+2E_i)^3}\right]\cdot\left(\frac{Fn^{*2}}{4\cdot Ze\cdot 2E_i}\right)\right\}, \qquad (18)$$

Finally, for the improved transition rate one has (S_{sr} being the part of the action due to the short-range potential, and S_c the part of the action due to Coulomb potential):

$$W_{CADK} = \exp\left(-2\cdot\mathrm{Im}\,\delta S_{sr}\right)\cdot\exp\left(-2\cdot\mathrm{Im}\,\delta S_C\right) =$$
$$= \left[\frac{4Z^3e}{Fn^{*4}}\cdot\frac{1}{1+\frac{2ZF}{(p^2+2E_i)^2}+\frac{Z^2F^2}{2E_i\cdot(p^2+2E_i)^3}}\right]^{2n^*-1}\cdot\exp\left(-\frac{2}{3}\cdot\frac{Z^3}{Fn^{*3}}\right). \qquad (19)$$

Here we denoted by W_{CADK} the transition rate obtained in ADK-theory which was corrected by introducing Coulomb interaction into estimation of the turning point τ. In expression (19) for transition rate W_{CADK}, the second rational term in the parentheses is a correction due to the Coulomb interaction which was obtained in [7]. 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 [5], it is 0.10876478, [7]), but for greater fields (in [7] the fields were used up to 10^{14} W/cm^2 $< I_{at} \sim 10^{16}$ W/cm^2, because at that time the ADK-theory was not extended to the fields that are greater than the atomic [12, 13]) this correction gains in amount (for instance, 10^{14} W/cm^2 gives 1.340258, and 10^{17} W/cm^2 gives 314.185).

If plotted for the fields from 10^{10} W/cm^2 to 10^{17} W/cm^2 (because for 10^{18} W/cm^2 and higher fields relativistic effects become predominant [9], and, also, it is extremely difficult to obtain so strong laser pulses as continuous, and for higher intensities that is even impossible, for the moment), transition rate (17) gives behavior which were predicted many times theoretically, but with rather poor experimental support yet, see [13]. One has, after strong increase of the transition rate of ionization of atoms, until the field intensities of 10^{14} W/cm^2, rapid decreasing at intensities of order 10^{14} W/cm^2 (which can be explained by the ionization via tunneling effect of all available electrons in the last orbits that, in the cases of alkali metals or noble gases, give nuclear charge of the residuum $Z \approx 10$, so ADK- theory is still valid [8, 12]), then a saturation at very low level of transition rate for fields from 10^{15} W/cm^2 to 10^{17} W/cm^2 - see Fig 2. Because $Z \approx 10$ the Keldysh approximation is still valid [12], and ADK-theory can be used to describe ionization of electrons from deeper orbits. Yet result for short range potential is not realistic at all for greater fields and it is given here only to be compared with more realistic results shown in Figs. 2 and 3. Indeed in Fig. 3 one has corrected result of ADK-theory, which includes the turning point calculated with the Coulomb correction (therefore transition rate has an index *CADK*: W_{CADK}), and gives the saturation after 10^{13} W/cm^2, and Fig.2 gives this saturation only after intensities of 10^{14} W/cm^2. Which of two is correct only experiment can decide.

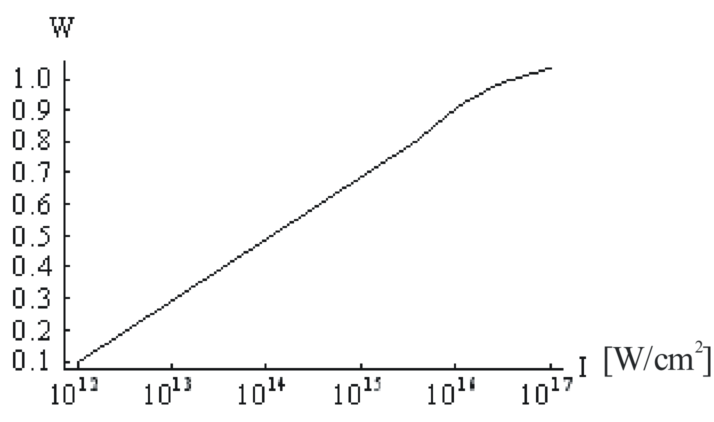

Figure 1.W_{sr} plotted vs. intensity of the field [W/cm^2]

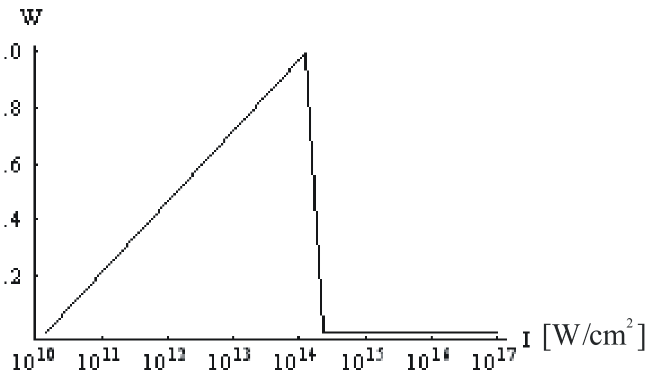

Figure 2.W_{ADK} plotted vs. intensity of field

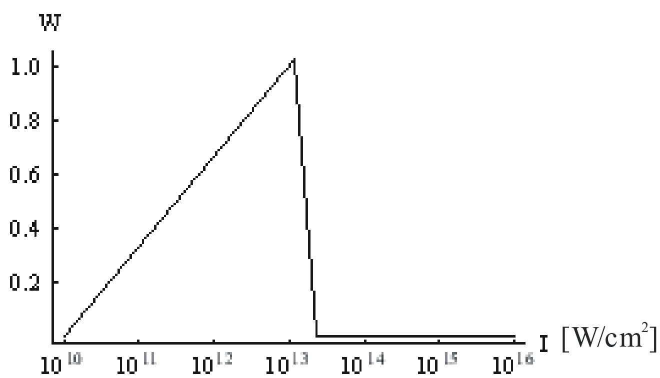

Figure 3.W_{CADK} plotted vs. intensity of field

4. CONCLUSION

For short-range potential, estimation of transition rate of ionization of atoms was made, based on assumptions of Keldysh approximation [6], that short-range potential does not affect energy of the final state of ejected electron, when it leaves the atom. Coulomb potential is then treated as perturbation of final state energy thus obtaining the ADK-theory. But not when calculating the turning point. This was done in [7], though only for fields with intensities below those of the atomic field. But as the ADK-theory was recently extended to the case of superstrong fields [12,13], our calculations now include extension of potential range up to $10^{17}\ \mathrm{W/cm^2}$, this leads to the shift of position of the turning point τ, which then influences transition rates for atoms in the low-frequency electromagnetic field of superstrong lasers.

Finally, we can conclude that, for the fields whose intensity vary from 10^{10} W/cm^2 to 10^{17} $\mathrm{W/cm^2}$, transition rates given by (17 and 19) show behavior which was predicted many times theoretically (but with rather poor experimental support so far, see [11]), i.e. in Figs. 2 and 3 (not in Fig. 1 which is not showing the realistic case, and is given here only for comparation with the other two, which are more realistic) the sudden decrease is shown at laser-field intensities of order $10^{14}\ \mathrm{W/cm^2}$ (but even after intensities of order 10^{13} W/cm^2, in the case of the ADK-theory with the turning point corrected to the Coulomb interaction, see formula 19 and Fig. 3), and then a saturation at a very low level of transition rate for fields from $10^{15}\ \mathrm{W/cm^2}$ to $10^{17}\ \mathrm{W/cm^2}$, which is, as mentioned above, all applicable only to multi-charged ions with the ion charge larger or equal to ten and with at least one electron left in a bound state (Z being 10 on both Figs. 2 and 3).

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