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Interaction of Electrons with Atoms in Ground and Excited States; Potential of Interaction, Momentum Transfer Cross-Sections

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Abstract

In this paper the potential of the electron-atom interaction was presented which may be useful both in the case of the ground state of an atom with one optical electron and in the case of the excited state of any atom, and which is given by expressions suitable for operational use. The presented potential is used in calculating the transport cross sections for the elastic electron scattering on the atoms of H, Li and Na respectively, in the ground and excited states.

1 Introduction

The determination of kinetic coefficients, thermodynamic functions and of a number of other important characteristics of partially ionized plasma generally requires the knowledge of the potential of interaction of electron with the atoms in the ground, as well as in the excited states. In literature we find potentials describing the interaction of the electron with the ground state atom which are not suited for the description of the interaction of the electron with excited and, particularly, highly excited atoms. However, depending on the conditions within the plasma, the relative contribution of the ground state atoms as well as excited atoms to the kinetic coefficients can significantly change. This is particularly manifested in the transition from plasma in LTE state into a remarkably unstable, laser-generated plasma, where a considerable number of atoms is in highly excited states [1, 2]. In addition, more or less realistic potentials do not have a universal character and are rather developed for particular atoms. As such we often find different forms of the polarisation potential [3, 4].

This paper presents a model potential of the electron-atom interaction which represents one of the results of our investigations in the area of influence of the neutral component on the kinetic coefficients of a partially ionized plasma.

The form of the presented potential allows the application to the excited state of any atom, including the ground state of the atom with one optical electron. In present work, the potential has been tested in the case of hydrogen, lithium and sodium atoms, respectively. For these atoms transport cross sections are determined (as energy functions of the incoming electron), which are necessary to calculate the kinetic coefficients of a particular plasma.

All formulas in the paper are given in atomic units.

2 The Properties of the Interaction of the Electron with the Atom in a Given State

We propose to explore interaction of a free electron with an atom described by Hamiltonian $\hat{H}_{at}(\mathbf{x})$, where $\mathbf{x}$ denotes the coordinates (space as well as spin) of atomic electrons. It is assumed that the atom is in the given state $|a>$ with energy W_a. Note that the following considerations do not apply to excited states of hydrogen, treated in next section.

In order to determine the basic properties of the electron-atom interaction, let us initially consider the atom in the field of the trial negative electric charge, that is, point electric charge equal to that of an electron. It is assumed that the atomic centre coincides with the beginning of laboratory coordinate system and that the trial electric charge is fixed at the point with radius vector $\mathbf{r}$. This system will be described by means of Schrödinger's equation

$$[\hat{H}_{at} + \hat{V}(\mathbf{x}, \mathbf{r})]\Phi(\mathbf{x}, \mathbf{r}) = E(\mathbf{r})\Phi(\mathbf{x}, \mathbf{r}) \tag{1}$$

where $\hat{V}(\mathbf{x}, \mathbf{r})$ is the operator of the interaction of the atom with the trial electric charge, and $\Phi(\mathbf{x}, \mathbf{r})$ - the wave function of the perturbed atom state. Here, the function $\Phi(\mathbf{x}, \mathbf{r})$ is taken to be the superposition of the given state $|a>$ and some other state $|b>$ with energy W_b. The criterion by which the state $|b>$ is selected will be given later. In the approximation of the two states we obtain

$$\Phi(\mathbf{x}, \mathbf{r}) = c_a(\mathbf{r})\phi_a(\mathbf{x}) + c_b(\mathbf{r})\phi_b(\mathbf{x}), \qquad (|c_a|^2 + |c_b|^2 = 1), \tag{2}$$

where $\phi_a(\mathbf{x})$ and $\phi_b(\mathbf{x})$ are the wave functions of the states $|a>$ and $|b>$.

In the following discussion the spherical coordinate system will be used and it will be assumed that the polar axis is directed along the radius vector $\mathbf{r}$. Additionally, it is assumed that $W_a \neq W_b$ and by means of $E_a(\mathbf{r})$ we denote the energy of the state of our system asymptotically correlated with the state $|a>$, which assumes that $E_a(\mathbf{r}) \to W_a$ when $r \to \infty$.

From equations (1) and (2) the term $E_a(\mathbf{r})$ is obtained to be

$$\begin{aligned} E_a(\mathbf{r}) &= \frac{1}{2}\Big\{W_b + W_a + V_{bb} + V_{aa} - (W_b - W_a + V_{bb} - V_{aa}) \\ &\times \Big[1 + \frac{4|V_{ab}|^2}{(W_b - W_a + V_{bb} - V_{aa})^2}\Big]^{1/2}\Big\}, \end{aligned} \tag{3}$$

where $V_{aa} =< a|V(\mathbf{x}, \mathbf{r})|a >$, $V_{bb} =< b|V(\mathbf{x}, \mathbf{r})|b >$ and $V_{ab} =< a|V(\mathbf{x}, \mathbf{r})|b >$. The value $U_a(\mathbf{r}) = E_a(\mathbf{r}) - W_a$ should then be interpreted as the energy of the interaction of the trial electric charge with the atom in the given state $|a>$, namely

$$\begin{aligned} U_a(\mathbf{r}) &= \frac{1}{2}\Big\{W_b - W_a + V_{bb} + V_{aa} - (W_b - W_a + V_{bb} - V_{aa}) \\ &\times \Big[1 + \frac{4|V_{ab}|^2}{(W_b - W_a + V_{bb} - V_{aa})^2}\Big]^{1/2}\Big\}. \end{aligned} \tag{4}$$

In the further discussion dimensions and structure of the atomic core will be ignored and, consequently, the operator $V(\mathbf{x}, \mathbf{r})$ will be of the form

$$V(\mathbf{x}, \mathbf{r}) = -\frac{1}{r} + \frac{1}{|\mathbf{r} - \mathbf{x}|} = \begin{cases} -\dfrac{1}{r} + \dfrac{1}{r}\displaystyle\sum_{k=0}^{\infty} P_k(\cos\theta)\left(\frac{x}{r}\right)^k, & \text{for} \quad r > x, \\ -\dfrac{1}{r} + \dfrac{1}{x}\displaystyle\sum_{k=0}^{\infty} P_k(\cos\theta)\left(\frac{r}{x}\right)^k, & \text{for} \quad r < x, \end{cases} \tag{5}$$

where $\mathbf{x}$ now denotes the radius vector of the optical electron, θ is the angle between $\mathbf{x}$ and $\mathbf{r}$, and $P_k(\cos\theta)$ is the k-th polynom Legendre. Matrix elements V_{aa}, V_{bb} and V_{ab} have been calculated with wave functions by means of Coulomb approximation, keeping the first few addents in Eq. (5).

3 The Potential of the Electron-Atom Interaction

Considering the arguments in the previous section, as well as the numerical analysis of the expression (4) and a number of approximative expressions, we realised that the potential $U_a(r)$, when the state $|a>$ is spherically symmetrical, was fitted to the following form:

$$U_a(r) = \begin{cases} U_a^{(0)}(r) = -\dfrac{1}{r} + \dfrac{1}{r+x_a} + u & \text{for} \quad 0 < r < x_a, \\ U_a^{(as)}(r) = -\dfrac{\alpha_a}{2(r^2+f^2)^2} & \text{for} \quad x_a^{(as)} < r < \infty, \end{cases} \tag{10}$$

where $U_a^{(0)}(r = x_a) = U_a^{(as)}(r = x_a)$, $x_a =< x >_a$ is the mean radius of the atom. In other cases the fitting form is

$$U_a(r) = \begin{cases} U_a^{(0)}(r) = -\dfrac{1}{r} + \dfrac{1}{r+x_a} + u & \text{for} \quad 0 < r < x_a, \\ U_a^{(m)}(r) & \text{for} \quad x_a < r < x_a^{(as)}, \\ U_a^{(as)}(r) = \dfrac{\alpha_a}{2(r^2+f^2)^2} - \dfrac{Q_{zz}^{aa}}{2(r^2+f^2)^{3/2}} & \text{for} \quad x_a^{(as)} < r < \infty, \end{cases} \tag{11}$$

where $U_a^{(0)}(r = x_a) = U_a^{(m)}(r = x_a)$ and $U_a^{(m)}(r = x_a^{as}) = U_a^{(as)}(r = x_a^{as})$, $x_a^{(as)} > x_a$, and the connective function $U_a^{(m)}(r)$ is defined below.

The characteristic lenght f is close to or at least of the order of magnitude x_a in both (10) and (11). Notice that these expressions do not apply to the excited states of the atomic hydrogen.

Term $U_a^0(r)$ in (10) and (11) is here taken in the same form from purely physical reasons. It is noticed that in this form the interaction potential in accordance with (9) behaves similarly to the cut-off Coulomb potential in the vicinity of point $r = 0$. The purpose of the term $1/(r + x_a)$, conditioning the violation $U_a^{(0)}(r)$ from the cut-off Coulomb potential is to take into account the deformation of the orbit of the outer atomic electron when the electric charge - perturber is placed within the orbit.

Then, it is observed that the form of the term $U_a^{as}(r)$ in (10) and (11) provides the behaviour of the potential of the electron-atom interaction according to (8). It is to be noted here that the quadrupole momentum Q_{zz}^{aa} of the atom in the spherically symmetrical state equals zero, and in other cases it is expressed as

$$Q_{zz}^{aa} = 2\frac{3m^2 - l(l+1)}{(2l-1)(2l+3)}\langle nlm|x^2|nlm\rangle, \tag{12}$$

where n, l and m are spherical quantum numbers characterising the state $|a>$. It is the exact form of Q_{zz}^{aa} used in our calculations. In addition, let us note that in these expressions, in contrast to (8), α_a is assumed to be the real polarizability of the atom in state $|a>$ whenever such data exist in literature. In the opposite case, we may assume that $\alpha_a = \alpha_a^{(b)}$, where $\alpha_a^{(b)}$ is given through the expression (7), which is quite sufficient in a number of cases.

The purpose of the parameters u and f in the expressions (10) is to provide the continuity of the potential at point $r = x_a$, with the greatest possible similarity of its behaviour in the vicinity of this point to the behaviour obtained in (4). In the expressions (11) the purpose of these parameters is reduced to provide the continuity if the interaction potential at points $r = x_a$ and $r = x_a^{(as)}$, whereas the greatest possible similarity of the behaviour of

We will now consider the behaviour of the matrix elements V_{aa}, V_{bb} and V_{ab} when $r \to \infty$ and when $r \to 0$. From the preceding arguments, in the asymptotic region the following expressions are obtained:

$$V_{aa} \overset{r\to\infty}{=} -\frac{Q_{zz}^{aa}}{2r^3} + O(r^{-5}), \quad V_{bb} \overset{r\to\infty}{=} -\frac{Q_{zz}^{bb}}{2r^3} + O(r^{-5}),$$

$$V_{ab} \overset{r\to\infty}{=} \frac{z_{ab}}{r^2} + O(r^{-4}),$$

where $z_{ab} =< a|z|b >$, $z = x\cos\theta$, and coefficients Q_{aa}^{zz} and Q_{bb}^{zz} denote quadrupole momentum and are non-zero when the states $|a >$ and $|b >$ are not spherically symmetrical. In the region of small r we have

$$V_{aa} \overset{r\to 0}{=} -\frac{1}{r} + \langle\frac{1}{x}\rangle_a + O(r^2), \quad V_{bb} \overset{r\to 0}{=} -\frac{1}{r} + \langle\frac{1}{x}\rangle_b + O(r^2),$$

$$V_{ab} \overset{r\to 0}{=} A_{ab} z_{ab} r + O(r^2),$$

where $\langle 1/x\rangle_a = \langle a|1/x|a\rangle$ and $\langle 1/x\rangle_b = \langle b|1/x|b\rangle$, and the coefficient A_{ab} depends on the quantum numbers characterising the states $|a >$ and $|b >$. It follows from here that in (4) we have

$$\frac{|V_{ab}|}{W_b - W_a + V_{bb} - V_{aa}} \longrightarrow 0,$$

when $r \to \infty$ and when $r \to 0$, so according to (4) in both the asymptotic region and in the vicinity of point $r = 0$ we obtain

$$U_a(r) \approx V_{aa}(r) - \frac{|V_{ab}(r)|^2}{W_b - W_a + V_{bb}(r) - V_{aa}(r)}. \tag{6}$$

Considering that in the asymptotic region $|V_{ab}(r)|^2/(W_b - W_a) \approx \alpha_a^{(b)}/2r^4$, where

$$\alpha_a^{(b)} = \frac{|z_{ab}|^2}{W_b - W_a}, \tag{7}$$

we obtain for $U_a(r)$ the following asymptotic expression:

$$U_a(r) \approx -\frac{Q_{zz}^{aa}}{2r^3} - \frac{\alpha_a^{(b)}}{2r^4}, \tag{8}$$

where Q_{zz}^{aa} is a zz-component of the quadrupole momentum of the atom in state $|a >$. In this expression the coefficient $\alpha_a^{(b)}$ according to definition (7) represents the partial polarizability of the atom in state $|a >$, determined solely by means of state $|b >$. From here we derive the searched criterion for the selection of state $|b >$: namely, the selection of state $|b >$ must be such that $\alpha_a^{(b)}$ contributes most to the total polarizability of the atom in state $|a >$.

From the expressions given previously, as well as the expression (4), it can be demonstrated that in the vicinity of point $r = 0$

$$U_a(r) \approx -\frac{1}{r} + \langle\frac{1}{x}\rangle_a. \tag{9}$$

This indicates that in the region of very small r this potential behaves similarly to the cut-off Coulomb potential with the cut-off radius of $< 1/x >_a^{-1}$.

In the region of mean r, i.e. those r of the order of magnitude of the characteristic radius of the observed atom, the behaviour of the potential $U_a(r)$, as opposed to the two aforementioned cases, requires the numerical analysis of the initial expression (4). This is allowed by the fact that the parameters of the atomic states are $|a >$ and $|b >$ for each r.

the potential in region $x_a < r < x_a^{(as)}$ to the one we could obtain through expression (4) is provided by the parameters included in the connective function $U_a^{(m)}$. Here the function $U_a^{(m)}$ was used in the following form

$$U_a^{(m)} = \frac{c_2 r^2 + c_1 r + c_0}{r^2 + d}. \tag{13}$$

All the parameters that we used to describe the potential $U_a(r)$ for $ns-$ and $np-$ states of the atoms Li and Na, concluding with the principal quantum number $n = 9$, are given in the Tables 1-4. For the ground state of the hydrogen atom we found out that in the expressions (10) one should take $u = -0.0625$, $f = (2/3)x_a' = 1$ and $\alpha = 4.5$.

Table 1: Parameters which are necessary for the calculation of the potential $U_a(r)$ for $ns-$states of Li

	$2s$	$3s$	$4s$	$5s$
x_a	.374E+1	.101E+2	.194E+2	.317E+2
α	.163E+3	.424E+4	.372E+5	.193E+6
u	.454E−1	.160E−1	.827E−2	.507E−2
f	.405E+1	.122E+2	.256E+2	.447E+2
	$6s$	$7s$	$8s$	$9s$
x_a	.470E+2	.653E+2	.866E+2	.111E+3
α	.728E+6	.221E+7	.579E+7	.133E+8
u	.343E−2	.248E−2	.188E−2	.148E−2
f	.700E+2	.102E+3	.141E+3	.186E+3

Table 2: Parameters which are necessary for the calculation of the potential $U_a(r)$ for $ns-$states of Na

	$3s$	$4s$	$5s$	$6s$
x_a	.391E+1	.104E+2	.199E+2	.324E+2
α	.154E+3	.335E+4	.267E+5	.130E+6
u	.498E−1	.193E−1	.104E−1	.660E−2
f	.401E+1	.115E+2	.236E+2	.407E+2
	$7s$	$8s$	$9s$	
x_a	.479E+2	.663E+2	.878E+2	
α	.471E+6	.139E+7	.354E+7	
u	.450E−2	.330E−2	.250E−2	
f	.633E+2	.916E+2	.125E+3	

The excited states of the atomic hydrogen As is known, in the presence of the outer electric field (realised in plasma conditions) the splitting of energetic levels of the hydrogen atoms with the same principal quantum numbers n occurs. Therefore, in describing the excited atomic hydrogen in plasma, it is fitting to use, instead if the spherical basis consisting of states $|nlm>$, the parabolic basis, that is, the states $|n_1 n_2 m>$ where n_1 and n_2 are parabolic quantum numbers. Namely, nearly all such states have a non-zero dipole moment, which in the presence of an electric field (always existing in plasma) causes splitting of energy levels of atomic hydrogen. Considering this aspect, a procedure similar to that given in the previous section can be applied to the excited states of the atomic hydrogen as well,

Table 3: Parameters which are necessary for the calculation of the potential $U_a(r)$ for np–states of Li

	2p		3p		4p	
	$m=0$	$m=\pm1$	$m=0$	$m=\pm1$	$m=0$	$m=\pm1$
x_a	.475E+1	.475E+1	.121E+2	.121E+2	.224E+2	.224E+2
Q	−.284E+2	.109E+2	−.136E+3	.676E+2	−.458E+3	.229E+3
α	.139E+3	.104E+3	.337E+5	.253E+5	.332E+6	.249E+6
u	.546E−1	.325E−1	.136E−1	.332E−2	.514E−2	−.273E−4
c_2	−.134E−1	.000E+0	.000E+0	.000E+0	.000E+0	.000E+0
c_1	.421E+0	.884E−1	.497E−1	.951E−1	.485E−1	.102E+0
c_0	−.218E+1	−.213E+1	−.520E+1	−.822E+1	−.111E+2	−.171E+2
d	.000E+0	.946E+0	.194E+2	.396E+2	.825E+2	.162E+3
f	.605E+1	.000E+0	.311E+2	.352E+2	.700E+2	.617E+2
	5p		6p		7p	
	$m=0$	$m=\pm1$	$m=0$	$m=\pm1$	$m=0$	$m=\pm1$
x_a	.358E+2	.358E+2	.522E+2	.522E+2	.716E+2	.716E+2
Q	−.116E+4	.577E+3	−.244E+4	.122E+4	−.458E+4	.229E+4
α	.175E+7	.132E+7	.656E+7	.492E+7	.200E+8	.150E+8
u	.275E−2	−.371E−3	.176E−2	−.325E−3	.125E−2	−.239E−3
c_2	.000E+0	.000E+0	.000E+0	.000E+0	.000E+0	.000E+0
c_1	.466E−1	.105E+0	.457E−1	.108E+0	.447E−1	.111E+0
c_0	−.187E+2	−.288E+2	−.282E+2	−.437E+2	−.396E+2	−.616E+2
d	.241E+3	.468E+3	.583E+3	.111E+4	.121E+4	.230E+4
f	.126E+3	.111E+3	.199E+3	.176E+3	.293E+3	.260E+3
	8p		9p			
	$m=0$	$m=\pm1$	$m=0$	$m=\pm1$		
x_a	.938E+2	.938E+2	.119E+3	.119E+3		
Q	−.787E+4	.393E+4	−.127E+5	.635E+4		
α	.515E+8	.386E+8	.126E+9	.946E+8		
u	.940E−3	−.170E−3	.738E−3	−.122E−3		
c_2	.000E+0	.000E+0	.000E+0	.000E+0		
c_1	.445E−1	.111E+0	.428E−1	.114E+0		
c_0	−.528E+2	−.828E+2	−.676E+2	−.107E+3		
d	.228E+4	.432E+4	.388E+4	.733E+4		
f	.406E+3	.362E+3	.571E+3	.495E+3		

Table 4: Parameters which are necessary for the calculation of the potential $U_a(r)$ for np–states of Na

	3p		4p		5p	
	$m=0$	$m=\pm1$	$m=0$	$m=\pm1$	$m=0$	$m=\pm1$
x_a	.569E+1	.569E+1	.137E+2	.137E+2	.247E+2	.247E+2
Q	−.312E+2	.156E+2	−.173E+3	.865E+2	−.552E+3	.276E+3
α	.325E+3	.244E+3	−.644E+4	−.483E+4	−.759E+5	−.569E+5
u	.410E−1	.204E−1	.416E−1	.385E−1	.235E−1	.213E−1
c_2	−.100E−1	−.137E−1	−.162E−1	−.115E−1	−.120E−1	−.854E−2
c_1	.405E+0	.558E+0	.884E+0	.538E+0	.119E+1	.769E+0
c_0	−.371E+1	−.655E+1	−.857E+1	−.514E+1	−.208E+2	−.136E+2
d	.445E+1	.242E+2	−.870E+2	−.156E+3	−.239E+3	−.459E+3
f	.939E+1	.000E+0	.178E+2	.100E+2	.365E+2	.307E+2
	6p		7p		8p	
	$m=0$	$m=\pm1$	$m=0$	$m=\pm1$	$m=0$	$m=\pm1$
x_a	.386E+2	.386E+2	.556E+2	.556E+2	.755E+2	.755E+2
Q	−.134E+4	.672E+3	−.277E+4	.138E+4	−.510E+4	.255E+4
α	−.420E+6	−.315E+6	−.162E+7	−.121E+7	−.497E+7	−.373E+7
u	.151E−1	.135E−1	.105E−1	.930E−2	.770E−2	.680E−2
c_2	−.811E−2	−.635E−2	−.545E−2	−.436E−2	−.379E−2	−.321E−2
c_1	.127E+1	.916E+0	.125E+1	.939E+0	.120E+1	.946E+0
c_0	−.349E+2	−.256E+2	−.496E+2	−.379E+2	−.650E+2	−.527E+2
d	−.534E+3	−.959E+3	−.112E+4	−.190E+4	−.218E+4	−.325E+4
f	.644E+2	.581E+2	.103E+3	.946E+2	.152E+3	.143E+3

	9p	
	$m=0$	$m=\pm1$
x_a	.985E+2	.985E+2
Q	−.866E+4	.433E+4
α	−.131E+8	−.982E+7
u	.590E−2	.520E−2
c_2	−.262E−2	−.220E−2
c_1	.111E+1	.876E+0
c_0	−.790E+2	−.644E+2
d	−.434E+4	−.580E+4
f	.214E+3	.201E+3

if as $|a>$ and $|b>$ the corresponding parabolic states are taken. In this case, however, for the dipole moment and the polarizability of the parabolic states there exist analytical expressions derived from a stricter approach. Namely, in the case when the point charge - perturber is far away from the observed atom the potential energy of their interaction can be presented as a potential energy of the atom in the homogeneous electrical field (whose intensity is the same as the intensity of the field of the charge - perturber in the centre of the atom) with the correction which describes the influence of inhomogenity of the real field of the charge - perturber. The potential energy of the excited hydrogen atom in the mentioned homogeneous electrical field is described in the familiar way, i.e. with the help of the dipole moment d^{aa} and the polarizability α_a in state $|a>=|n_1n_2m>$ which are given by expressions [5]

$$d^{aa} = d_z^{aa} = -\frac{3}{2}n(n_1 - n_2), \tag{14}$$

$$\alpha_a = \frac{n^4}{8}[17n^2 - 3(n_1 - n_2)^2 - 9m^2 + 19] \tag{15}$$

where $n = n_1+n_2+|m|+1$. We will take the influence of the inhomogenity of the real field of the charge - perturber on the potential energy of its interaction with the excited hydrogen atom in the quadrupole approximation, i.e. with the help of the quadrupole momentum Q_{zz}^{aa}, where

$$\begin{aligned} Q_{zz}^{aa} = \langle n_1n_2m|Q_{zz}|n_1n_2m\rangle = -\frac{n}{4}\frac{(n_1+|m|)!(n_2+|m|)!}{(|m|!)^4n_1!n_2!} \times \\ [I_m(|m|+3,n_1)I_m(|m|,n_2) - 3I_m(|m|+2,n_1)I_m(|m|+1,n_2) - \\ 3I_m(|m|+1,n_1)I_m(|m|+2,n_2) + I_m(|m|,n_1)I_m(|m|+3,n_2)], \end{aligned} \tag{16}$$

where

$$I_m(p,q) = \int_0^\infty t^p e^{-t}[F(-q,|m|+1,t)]^2 dt, \tag{17}$$

and $F(-q,|m|+1,t)$ is the corresponding degenerate hypergeometric function [6]. On the basis on this and from the numerical analysis, the function $U_a^{(as)}(r)$ representing the interaction potential of the excited atomic hydrogen with point electric charge in the region of large r will be taken in following form

$$U_a^{(as)}(r) = -\frac{d_z^{aa}}{(r^2+x_a^2)} - \frac{\alpha_a}{2(r^2+x_a^2)^2} - \frac{Q_{zz}^{aa}}{2(r^2+x_a^2)^{3/2}}, \tag{18}$$

where d_z^{aa}, α_a and Q_{zz}^{aa} are given by expressions (14)-(17), and x_a is, as before, the mean radius of the observed atom

$$x_a = \frac{5n^2+1}{4}. \tag{19}$$

We shall now take into account that when the point electric charge is located within the orbit of the excited electron the difference between hydrogen and non-hydrogen states actually ceases to affect the form in which the interaction potential $U_a(r)$ in the region of small r is sought. Consequently, in the region $0 < r < x_a$ this potential is described in terms of the function $U_a^{(0)}(r)$ taken in the same form as in expressions (10) and (11). Proceeding from this, we established that the function $U_a(r)$, describing the interaction potential of the excited atomic hydrogen with point electric charge in the entire region $r > 0$, can be taken in the form (10), where $U_a^{(as)}(r)$ is given by the expression (18). The parameter u in the

function $U_a^{(0)}(r)$ is, as before, determined from the conditions of sewing together at point $r = x_a$. From (10) and (18) the parameter u is now given by the expression

$$u = \frac{1}{2x_a}\left[1 - \frac{d_z^{aa}}{x_a} - \frac{Q_{zz}^a}{2\sqrt{2}x_a^2} - \frac{\alpha_a}{4x_a^3}\right], \tag{20}$$

where α_a, Q_{zz}^a and x_a are given by the expressions (15) - (17) and (19).

In the connection with the fact that for the determination of the potential $U_a(r)$ the two states approximation was used, we want to emphasize that here this approximation has a secondary role. Its purpose is in the determination (on the qualitative level) of the relevant properties of the potential $U_a(r)$ and its connections with the basic characteristics of the observed atomic state. The two states approximation is quite sufficient for this purpose from two reasons. The first reason is that the inclusion of the third state in the consideration does not bring the qualitative change (which was confirmed by the direct calculations). The second reason is the treatment of the parameters which influence the behaviour of the potential $U_a(r)$ as the function of r. Namely, all these parameters are treated as a quantities which must be determined on the basis of the whole available information on the observed atom. The exceptions are the cases when the approximation of the two states itself provides good results on the quantitative level (as in the case of s-states of alkali metals, where this approximation provides about 90 percent of the atomic polarizability). The behaviour of

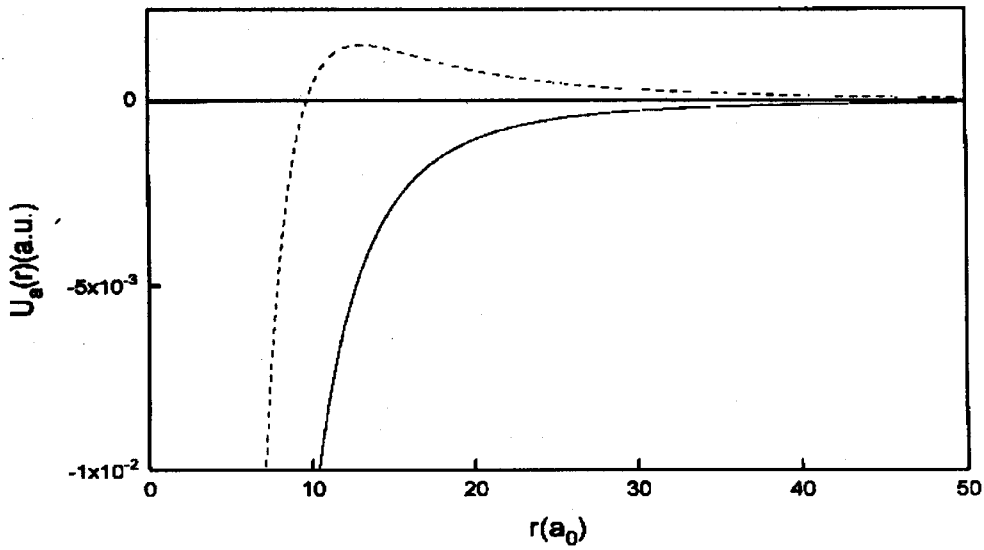

Figure 1: Typical shapes of potentials of electron-atom interaction $U_a(r)$: —— case of the purely attractive potential; - - - case of potential with repulsive terms.

the potential $U_a(r)$ is illustrated in Fig. 1, which shows that $U_a(r)$ can have either a purely attractive character (lower curve), or a barrier (upper curve) in the region of relatively large r. Notice that the repulsive character of $U_a(r)$ in the general case can be related both to the quadrupole and polarization terms, and in the case of hydrogen to the dipole terms, in the expressions (11) and (18) for $U_a^{as}(r)$.

4 The Transport Cross Section for the Electron Scattering on the Potential $U_a(r)$

The above described potential $U_a(r)$ can be used for the consideration of the different physical problems, which are connected with the electron-atom interaction. Having in mind the needs of our current investigation, which requires the knowledge of the plasma kinetic coefficients, this potential has been tested here on the problem of determining the transport cross section for the elastic electron scattering from the observed atom, which is defined by the expression

$$\sigma_a^{tr}(E) = 2\pi \int_0^{\pi} |A_a(\theta; E)|^2 (1 - \cos\theta) \sin\theta d\theta, \tag{21}$$

where E is the free electron energy, and $A_a(\theta; E)$ is an adequately defined amplitude of the elastic electron scattering for angle θ. Namely, we had in mind that the plasma electrical conductivity, as well as some of the other plasma kinetic coefficients, is determined with the help of the $\sigma^{tr}(E)$.

In the general case the description of the elastic electron - atom scattering means that the inelastic channels (which could be opened or closed depending on the energy of the electron) are to be taken into account. According to that, the electron - atom transport cross section in the general case is determined on the basis of the close-coupling theory which is, for example, given in the [7] (see also [8, 9]). However, on the basis of the consideration from the previous part of this work, the electron - atom scattering has been treated here as the scattering of the electron on the above described potential $U_a(r)$, which means that there exist only the channel for the elastic scattering. According to that, the amplitude $A_a(\theta; E)$ in the expression (21) will be determined here in a standard way by employing the partial wave method for the potential scattering [10]. On the basis of this, in the case when the optical electron of the observed atom is in s - state (excluding the excited hydrogen states), the transport cross section is obtained in the form

$$\sigma_a^{tr}(E) = \frac{2\pi}{k^2} \sum_{j=0}^{\infty} (j+1) \sin^2(\delta_j - \delta_{j+1}), \tag{22}$$

where δ_j is the phase shift for the j-th partial wave.

In the case of other non-hydrogen states in the expression (21) it is assumed that: $A_a(\theta) = (2l+1)^{-1} \sum_{m=-l}^{l} A_{a;lm}(\theta)$ where l and m are orbital and magnetic quantum numbers of the observed state, and $A_{a;lm}(\theta)$ is the corresponding scattering amplitude which is also determined by the partial wave method. Then, we have

$$\sigma_a^{tr}(E) = \frac{1}{2l+1} \sum_{m=-l}^{l} \sigma_{a;lm}^{tr}(E), \tag{23}$$

where $\sigma_{a;lm}^{tr}(E)$ is the transport cross section for the electron scattering from the atom in the observed state with the given l and m, which is determined by an expression similar to (22). This kind of approach (resulting in a transport cross section averaged over the magnetic quantum numbers) takes into account that the application of the potential $U_a(r)$ in describing the electron-atom scattering is equivalent to the application of the approximation of the rotating polar axis which connects the center of the target atom and that of the projected electron. The purpose of this approximation is that in the case of $l > 0$ the collision for each m is described as if taking place in a centrally symmetrical field. We expect the errors resulting from such approximation to be substantially corrected in determining $\sigma_a^{tr}(E)$ given by the expression (23).

In the case of the excited hydrogen states the procedure is assumed to be similar to the one described in the previous case. Particularly, in this case the final result represents $\sigma_a^{tr}(E)$, where now

$$\sigma_a^{tr}(E) = \frac{1}{n^2} \sum_{m=-n+1}^{n-1} \sum_{n_1=0}^{n-|m|-1} \sigma_{a;n_1|m|}^{tr}(E). \tag{24}$$

In this expression $\sigma_{a;n_1|m|}^{tr}(E)$ are transport cross sections for the electron scattering from the atom in states with given quantum numbers $n_1, n - n_1 - |m| - 1$ and $|m|$. The cross sections themselves $\sigma_{a;n_1|m|}^{tr}(E)$ are also determined by means of an expression similar to (22)

5 Results and Discussion

From the expressions (22),(23) and (24) the transport cross sections for the ground and a number of the excited states of the atomic Li, Na and H have been calculated. The results of the calculation in the case of the ground states of these atoms, in the energy range of the incoming electron from 0.001 to 10 eV, are represented in Figs. 2, 3 and 4. These Figures indicate the presence of a particular interference structure of the transport cross section in the region $0.1 \leqslant E \leqslant 1$ eV in the case of Li and Na, and the absence of such a structure in the case of hydrogen. This is in accordance with the results of the papers concerned with the elastic scattering on the atomic H and Cs, as shown in paper [11] with all the necessary references. From these results it follows that in the case of the atomic Cs the transport cross section in the region $0.1 \leqslant E \leqslant 1$ eV has a similar, but a considerably more remarkable structure, whereas in the case of the atomic H such a structure does not exist. The values of the transport cross section in this paper in the case of the ground state of the atomic H are given in Fig. 4 together with the results of our own estimates, which enables them to be compared and thus seen to be in good agreement. In the case of hydrogen apart from these there are estimates of the total cross section for the elastic scattering [12] which have been verified experimentally (see [13]). Out of these in Fig. 4 the limit of this total cross section is given for $E = 0$, equalling the value of the transport cross section at zeroth energy.

The behaviour of the transport cross section in the case of the excited states we have illustrated here on the example of ns- states of Na atom for $n = 5, 7, 9$. The corresponding curves are shown in Fig. 5. Besides that, here we have compared the behaviour of the transport cross section determined by the above mentioned partial wave method and the behaviour of the same cross section which was determined within the Born approximation. The behaviour of these cross sections is illustrated in the Fig. 6 where we have given the curves for the scattering of the electron by the atom $Na(5s)$. This picture shows that the Born approximation is not useful in the range of relatively low electron energies $E < 5$ eV in the case of the potential $U_a(r)$.

In order to present the behaviour of the $\sigma_a^{tr}(E)$ we have determined the corresponding expressions which, in the range $0.1 \leqslant E \leqslant 10$ eV, approximate the results of our calculations (with the accuracy within a few percent) in the case of atom $Li(n \geqslant 2)$, $Na(n \geqslant 3)$ and $H(n \geqslant 1)$.These expressions are suitable for use both in theoretical studies and in the interpretation of the experimental results. For all considered cases, these expressions are given in the form

$$\sigma_a^{tr}(E) = \frac{A}{E^2} \ln(1 + BE^2)[1 + C\exp(-D\sqrt{E})], \tag{25}$$

where parameters A, B, C and D depend on the kind of atom and the observed state. The form of this approximative expression guarantees the correct behaviour of the $\sigma^{tr}(E)$ in the region of large E, i.e. proportionably with $E^{-2}\log(E)$ (see e.g. [5]), as well as the finiteness

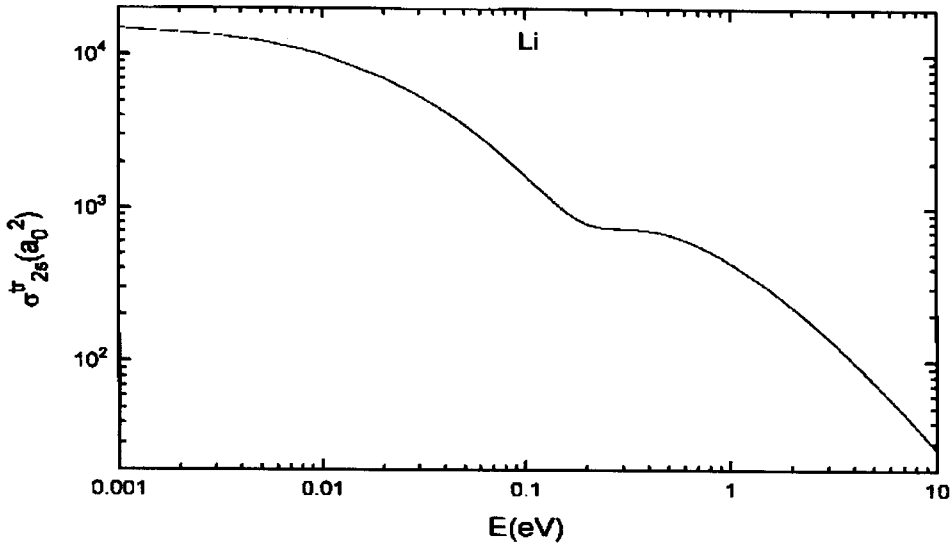

Figure 2: Momentum transfer cross-section for elastic scattering of electrons by atom Li in the ground state.

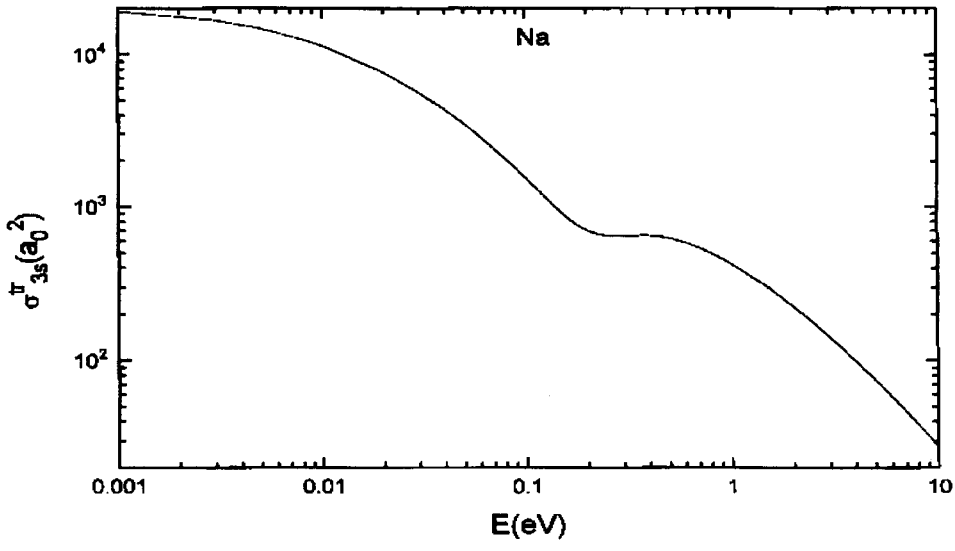

Figure 3: Momentum transfer cross-section for elastic scattering of electrons by atom Na in the ground state.

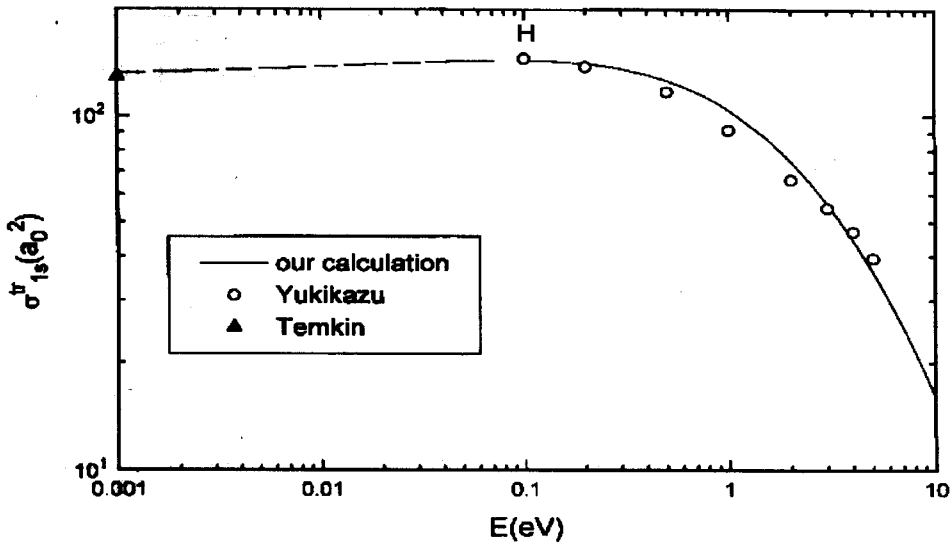

Figure 4: Momentum transfer cross-section for elastic scattering of electrons by atom H in the ground state.

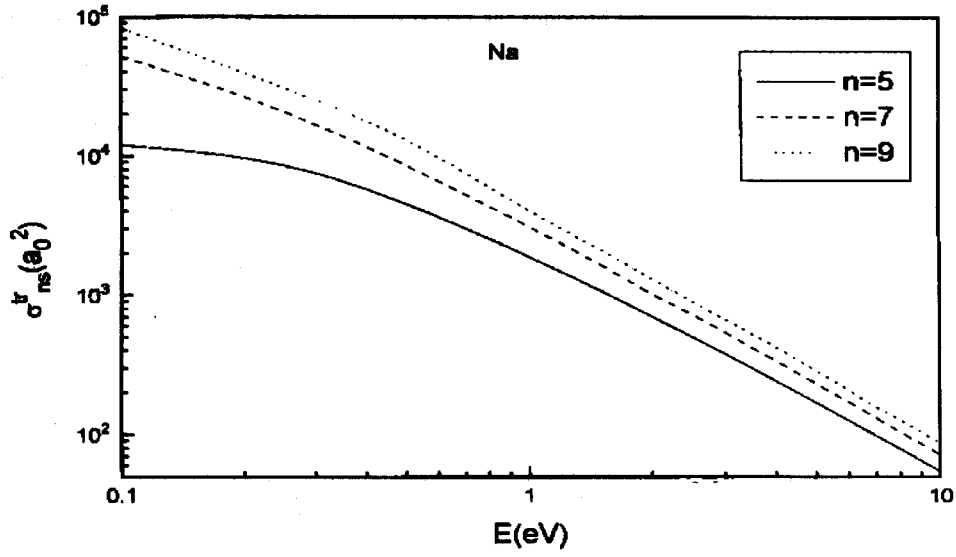

Figure 5: Typical behaviour of $\sigma_a^{tr}(E)$ in the case of elastic scattering of electrons by the highly-excited atoms.

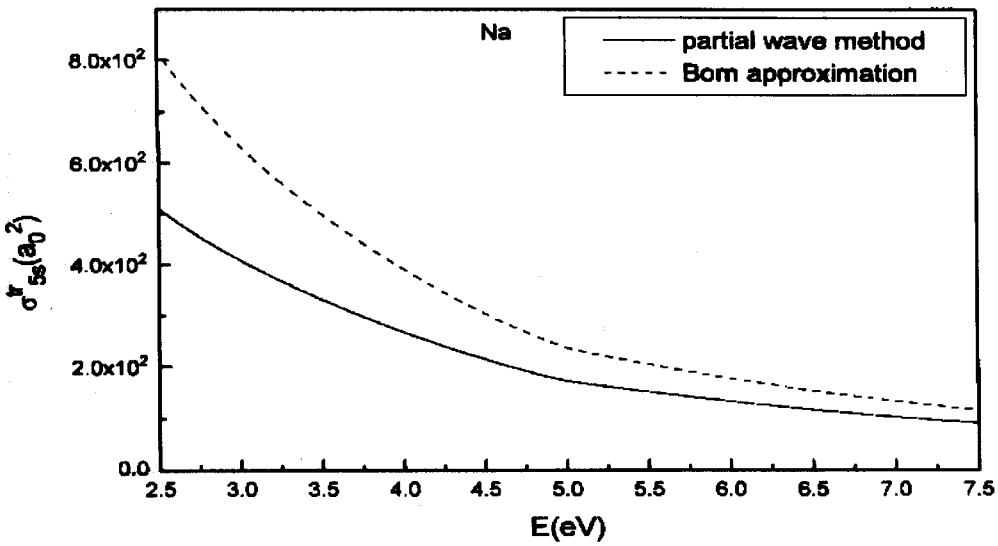

Figure 6: The comparison of the results of calculations $\sigma_a^{tr}(E)$ by the partial wave method and within the Born approximation for the atom Na in the $5s-$state.

of the $\sigma^{tr}(E)$ when we approach the point $E = 0$. Besides that, the factor in the square brackets in the expression (25) provides the necessary correction in the region of the energies of the order of $1eV$. The concrete values of the parameters A, B, C and D are determined by fitting the results which are obtained from the starting expressions (22), (23) and (24).

In the case of $s-$states of the atoms Li and Na the expression (25) is corresponding to the expression (22) with the $n \leqslant 9$ when the mentioned parameters are taken from the Tables 5,6. In the case of $p-$states of the same atoms the expression (25) corresponds to the expression (23), where $n \leqslant 9$ too, when the values of A, B, C and D are taken from the Tables 7,8. Finally, in the case of atom H the expression (25) corresponds to the expression (24) for $n \leqslant 10$ when the values of the parameters A, B, C and D are taken from the Table 9. Besides that, in the hydrogen case the values of these parameters for $n = 10$ enable us to apply the expression (25) up to $n = 15$ with the accuracy which is less or equal 10 percent.

Since data on the transport cross sections are scarce, equally scarce data on the total cross sections for the elastic scattering on the atomic H, Li and Na are of certain interest.

Table 5: Parameters A, B, C and D for the calculation of $\sigma_a^{tr}(E)$ for $Li(ns)$

	n							
	2	3	4	5	6	7	8	9
A	566.0	702.4	785.7	869.2	925.9	964.7	990.6	1018.5
B	0.062	0.051	0.039	0.028	0.020	0.019	0.017	0.016
C	7.00	2.38	2.62	7.24	10.16	12.05	12.96	13.36
D	3.98	3.29	3.36	4.48	5.53	6.50	7.41	8.46

Table 6: Parameters A, B, C and D for the calculation of $\sigma_a^{tr}(E)$ for $Na(ns)$

	n						
	3	4	5	6	7	8	9
A	582.3	712.1	787.7	907.7	930.1	953.7	1108.5
B	0.011	0.015	0.012	0.009	0.010	0.009	0.005
C	6.83	8.66	2.21	7.41	9.34	11.74	8.37
D	4.08	5.31	3.31	4.52	5.44	6.84	4.91

Table 7: Parameters A, B, C and D for the calculation of $\sigma_a^{tr}(E)$ for $Li(np)$

	n							
	2	3	4	5	6	7	8	9
A	615.6	724.2	827.4	926.5	1033.1	1138.0	1370.5	1186.1
B	0.078	0.087	0.067	0.041	0.021	0.011	0.004	0.004
C	0.36	3.45	9.10	14.75	20.04	23.79	45.76	29.70
D	1.68	3.49	5.31	6.03	6.21	6.35	6.56	6.71

Table 8: Parameters A, B, C and D for the calculation of $\sigma_a^{tr}(E)$ for $Na(np)$

	n						
	3	4	5	6	7	8	9
A	696.1	769.7	791.2	869.4	877.5	865.8	850.6
B	0.019	0.011	0.014	0.011	0.009	0.008	0.011
C	28.62	29.78	16.84	16.84	18.82	20.65	21.16
D	17.27	15.94	19.71	19.71	17.73	15.90	15.18

Table 9: Parameters A, B, C and D for the calculation of $\sigma_a^{tr}(E)$ for $H(n)$

	n				
	1	2	3	4	5
A	528.6	755.6	757.2	772.7	798.6
B	0.019	0.038	0.047	0.037	0.030
C	18.68	34.04	32.04	23.73	11.08
D	0.73	4.54	7.81	8.60	7.58

	n				
	6	7	8	9	10
A	821.3	846.6	861.5	862.3	862.3
B	0.026	0.022	0.021	0.020	0.019
C	5.43	4.00	3.56	3.28	3.28
D	6.39	4.93	6.41	5.43	5.43

Therefore, in addition to the transport cross sections we have calculated a number of total cross sections for the elastic electron-atom scattering. For the ground state of the atomic H we found out that our calculations agree well with the results of the above mentioned paper in the considered energy range. In the case of the ground $(2s)$ and resonant $(2p)$ state of the atomic Li the results of our calculations have been compared with the results in paper [14], where the values of the corresponding total cross sections were obtained via close coupling theory, although they refer only to the region $E > 2$ eV. In the energy range $2 < E < 5$eV, which is relevant for partially ionized plasmas, our total cross section for the ground state changes in the interval $116.4 - 68.0\ [\pi a_0^2]$, whereas the corresponding total cross section in the stated paper changes in the interval $133.8 - 53.5\ [\pi a_0^2]$. For the resonant state our total cross section in the same energy range changes in the interval $146.6 - 86.6\ [\pi a_0^2]$ and the total cross section in the stated paper changes in the interval $232.0 - 85.0\ [\pi a_0^2]$. A more detailed comparison for the time being is not instructive since there are no available experimental data which would verify the results in paper [14].

To find out more about the mechanism of the elastic electron scattering on the excited atoms we have performed, besides the calculations with the potential $U_a(r)$, a number of calculations of the transport cross section with a modified potential

$$\tilde{U}_a(r) = \begin{cases} U_a(r) & \text{for } r < r_c, \\ 0 & \text{for } r \geqslant r_c, \end{cases}$$

for different values of r_c in the range $r_c \geqslant x_a$. We found out that with the increase in the main quantum number n the increase of r_c gradually diminishes its influence on the change in value of the transport cross section with respect to its value calculated with $r_c = x_a$, and that it is more so with the increase in energy of the incoming electron. This phenomenon suggests that with the increase in the main quantum number the inner part of the excited atom (i.e. the region $r < x_a$) starts to play a dominant role in the process of the elastic electron scattering on the excited atom. Therefore, with an increase in n there is necessarily a remarkable similarity of the function $U_a^{(0)}(r)$ with the cut-off Coulomb potential whose properties were examined in detail in papers [15, 16]. This is manifested through a similar interference structure of the differential cross section (depending on the scattering angle). This also explains the qualitative agreement between the differential cross section determined by the potential $U_a(r)$ and the differential cross section for the elastic electron scattering on the atomic Na in the resonant state [17]. In addition, the similarity of $U_a^{(0)}(r)$ with the cut-off Coulomb potential is manifested in yet another way. Namely, due to this similarity the influence of the excited atoms on the elastic electron scattering in plasma conditions becomes similar to the influence of ions taking into account the effects of screening within the plasma. This supports the view of those authors who take into account the effects of the excited atoms on the kinetic properties of a partially ionized plasma by treating highly excited atoms (from the aspect of the elastic electron scattering) in a similar way as the atomic ions [18].

In connection with the presented form of the potential $U_a(r)$ it is convenient to take note of those properties which as we think must be retained in the case of its possible modifications. Here we have in mind that in principle the very form of the potential $U_a(r)$ can be changed to a certain extent (primarily in the terms of the change of the connective function $U_a^{(m)}(r)$) so that new relevant information on the elastic electron-atom scattering can appear. However, we think that such possible changes cannot refer to the basic features of the functions $U_a^{(0)}(r)$ and $U_a^{(as)}(r)$. In particular, in the case of function $U_a^{(as)}(r)$ this assumes that the parameter f, which reflects a very important role of the dimensions of the atom itself, must be retained. In connection with this let us notice that a parameter similar to parameter f appears in some model potentials of other authors as well (see [3, 4]), where the polarization term is used in the whole region $r > 0$, that is, even there where it has no physical sense. In such cases the purpose of the parameter f is the elimination of singularity

at point $r = 0$.

In this paper, according to the obtained transport cross sections, the estimation has been made of the effects of the excited atoms on the static electrical conductivity of partially ionized hydrogen, lithium and sodium plasmas, respectively. In calculating the electrical conductivity the well-known approximative formula from paper [19] was used. In calculating the conductivity of plasma of alkali metals all states with $n \geqslant 10$ were treated as hydrogen. In addition, all lower lying states with the orbital quantum number $l \geqslant 2$ were treated in a similar way. The contribution of such states for the shell with $n < 10$ was estimated on the basis of their total statistical weight. The conclusion is that in case of an equilibrium plasma the effects of the block of the excited states on the electrical conductivity is very small. Thus, for the hydrogen plasma in the temperature range of $10000 - 30000$[K] and pressure $1 - 10$[atm] this effect does not exceed 0.7%. For lithium and sodium plasmas in the temperature range of $5000 - 20000$[K] and the same range of pressure the maximum effect of the block of the excited states is larger than 1% only by fraction. By establishing the contents of the observed plasmas it can be shown that this result is due to the fact that the total concentration of the excited atoms in the observed plasmas is small in relation to the total concentration of ions and atoms in the ground state. In connection with this one should have in mind the plasmas of different type, namely, laser-generated nonequilibrium plasmas of alkali metals [1, 2, 20, 21]), in which very large concentrations of the excited atoms are created. The effects of the excited atoms on the kinetic properties of such plasmas could be significant and therefore such plasmas are interesting from this aspect.

Finally, we wish to point out that the proposed potential of the electron-atom interaction $U_a(r)$ can be of interest with respect to some other properties of plasma as well. Thus, for example, it can be employed in studies of the spectrum of the continuous electromagnetic radiation which takes place during electron-atomic scattering (without change in the electronic state of the atom). Besides that, this potential can be used in determining the Stark parameters of a certain atomic lines.

6 Conclusions

In this paper the properties of the interaction of the atom with the negative point charge, for the different distances of this charge from the center of the atom, were analised. On the basis of this analysis the model potential of the electron-atom interaction was determined. This model potential is valid when the atom is in the ground, as well as in the excited states, and it can be applied for studying of the different problems from the field of the partially ionized plasmas. The parameters which define this potential are determined and tabulated here for the several groups of the states of the atoms H, Li and Na. On the basis of these parameters, by the partial wave method, the corresponding transport cross-sections were determined in the region of the impact electron energy relevant for the partially ionized plasmas (i.e. energies up to 10 eV). The compact analytical expressions were found for these cross-sections, the expressions which are suitable for the calculation of the transport coefficients. The parameters which appear in these expressions are determined by the fitting and they are also tabulated here.

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