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PREFACE

This proceedings comprises the talks presented at the 19^{th} *SMALL TRIANGLE MEETING on theoretical physics* conference, which was held in Medzilaborce, Slovakia, on October 15–18, 2017.

This year, it was already the 19^{th} STM conference, which is organized annually since 1999.

The aim of the conference is to serve as a forum for meeting between theoretical and experimental physicists from Ukraine, Russia, Finland, Hungary, Czech Republic, Poland and Slovakia, where scientists from different research areas of physics met together. This provided an ideal opportunity to exchange knowledge, ideas and experiences. We believe that it helps us in our future work and that we find joint tasks in the following scientific collaboration.

The scientific programme presented at this year's meeting covered the research areas from solid state physics, through nonlinear dynamical systems, atomic, nuclear, high energy physics to biophysics. The final programme included 31 oral presentations. We would like to thank the authors for their cooperation and we are looking forward for the following STM meeting.

All articles published in this proceedings were peer reviewed.

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Contents

The Coulomb Green's Function in the Theory of One-Electron Charge Exchange

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Abstract

Our work is devoted to the theoretical study of the single-electron charge exchange process during collisions of multiply charged ions with atoms or molecules of the target. To describe the single-electron charge exchange process we use semi-classical eikonal approximation, which takes into account the screening of the core of the incident multi-charged ion. The summation of the spectrum of degenerate finite states is carried out using the technique of the Coulomb Green's function. We explored the influence of the shielding effects of the incident ion on the cross section of single-electron capture in fast ion-atomic collisions, which affect both the value of cross sections, and the nature of their dependence on the collision energy. Calculations of the charge exchange cross sections for hydrogen atoms on carbon, nitrogen and oxygen ions have been performed, and their comparison with experimental data has been carried out.

1 Introduction

Processes of electron capture by fast ions in collisions with atoms relate to the important region of physics of ion-atom interactions, that has evoked considerable interest for the development of the theory of collisions in general, and, at the same time, has many applications in related fields. The phenomenon of the single-electron capture is very diverse: it includes capture during symmetrical and asymmetrical collisions, corresponding to a different ratios between the charges of the target and the incident particle; capture at resonant and nonresonant transitions depending on the ratio of the bond energies of the electron in the initial and final states; the capture from single-electron and many-electron atoms and ions in a wide range of energies of the colliding particles.

Currently there is no unified theory of electron capture, describing all the variety of these processes. Therefore, development of approximate methods of theoretical consideration of electron capture, establishing dependence of cross sections on the basic parameters of collision and consistent with experimental data still remains relevant. Methods for describing electron capture in the field of intermediate and large velocities of colliding particles develop especially intensively. Among the most successful approaches to solve this problem it is necessary to note, on the one hand, the numerical solution of equations of the strong-coupling channels using the expansion of the wave function of an electron by an atomic basis, on the other hand – methods that take into account multiple rescattering of captured electron. The latter should include the different variants of the method of distorted waves, used to describe symmetric or almost symmetric collisions [1, 2, 3, 4], and the Born approximation of strong potential that takes into account a strong paired interaction potential in all orders of perturbation theory, and the weak potential - in the first order and, therefore, applied in the description of asymmetric processes. Note, however, that all these approximations require highly complex numerical calculations and realized only in the simplest cases. Note also that detailed developed methods, asymptotic in a large impact parameter, of the theory of atomic collisions are not applicable for the calculation of single-electron charge exchange at high energies, as in this case, on the contrary, small impact distances are essential. Therefore, an important task is to develop a simple theoretical approaches that would take into account the specifics of the processes involving multiply charged ions, approaches that would be illustrative and efficient to use, and enable to receive the single-electron capture cross sections in analytical form.

2 General relations

Our work is devoted to the theoretical study of the single-electron charge exchange process during collisions of multiply charged ions B^{Z_p+} with atoms A^{Z_t+} of the target:

$$B^{Z_p+} + A^{Z_t+} \to \left\{B^{(Z_p-1)+}\right\}^* + A^{(Z_t+1)+}. \tag{1}$$

To describe the electron capture process at the collision velocities $v \gg v_0$ we use a modified eikonal approximation, which takes into account additional interaction of the captured electron with the atomic core $A^{(Z_t+1)+}$ in the output reaction channel. As was shown in [5], accounting of this interaction leads to the appearance in the full cross section

$$\sigma_{capt}(v) = \widetilde{\alpha}(Z_p, v) \sum_{n'} \sigma^{\text{OBK}}_{1S\to n'}(Z_p, v) \tag{2}$$

of the correction factor $\widetilde{\alpha}$, which value is to be calculated.

We assume that the incident particle B^{Z_p+} is moving along a straight trajectory $\mathbf{R}(t) = \mathbf{b} + \mathbf{v}t = \mathbf{b} + \mathbf{Z}_R(t)$ ($\mathbf{b}$ - impact parameter, $\mathbf{b} \cdot \mathbf{Z}_R(t) = 0$) in the reference frame associated with the nucleus of the target A^{Z_t+}. Suppose $\mathbf{r}$, $\mathbf{r}_t = \mathbf{r} + \alpha\mathbf{R}$ and $\mathbf{r}_p = \mathbf{r} - (1-\alpha)\mathbf{R}$ represent, respectively, the radius vector of the electron relative to the center of mass of the system $A^{Z_t+} + B^{Z_p+}$, target atom A^{Z_t+} and the incident particle B^{Z_p+}, and the value of $\alpha = M_p/(M_p + M_t)$. Then the amplitude of the single-electron charge exchange process can be written as follows:

$$\Re_{fi}(\mathbf{b}, v) = -i \int_{-\infty}^{+\infty} \langle \Psi_f | \hat{V}_p | \Psi_i \rangle \, dt. \tag{3}$$

Wave functions

$$\Psi_i = \varphi_i(\mathbf{r}_t)\, \exp\left\{-iE_t t - i\alpha \mathbf{v}\mathbf{r} - i\alpha^2 v^2 t/2\right\}, \tag{4}$$

$$\Psi_f = \varphi_f(\mathbf{r}_p)\, \exp\left\{-iE_p t + i(1-\alpha)\mathbf{v}\mathbf{r} - i(1-\alpha^2)v^2 t/2\right\} \exp\left\{i\chi(t)\right\} \tag{5}$$

are localized around the various centers and include translation factors, taking into account the momentum transfer effects by electron at the transition from one center to another. The wave function (7) contains eikonal factor $\exp\{i\chi(t)\}$, where

$$\chi(t) = \int_t^{+\infty} V_t(\mathbf{r}_t)\, dt, \tag{6}$$

which takes into account the interaction $V_t(\mathbf{r}_t)$ of the electron in a bound state of $\varphi_f(\mathbf{r}_p)$ with the atomic residue $A^{(Z_t+1)+}$ in the final channel of charge exchange reaction (1). The potential of the field, in which an exciting electron was located before the collision, will be chosen in the form of effective Coulomb potential

$$V_t(\mathbf{r}_t) = -Z_t^{'}/r_t. \tag{7}$$

In the calculation of the amplitude $\Re_{fi}(\mathbf{b}, v)$ we use the integral representation for the distorting eikonal factor ($\eta = 1/v$) [5]

$$\exp\left(i\int_t^{+\infty} \frac{Z_t^{'}}{r_t} dt\right) = \frac{1}{\Gamma(-i\eta Z_t^{'})} \int_0^{+\infty} \lambda^{-1-i\eta Z_t^{'}} \exp[-\lambda(r_t - z_t)]\, d\lambda. \tag{8}$$

Assuming that the incident ion B^{Z_p+} consists of N electrons moving in the field of a nucleus with a charge of Z, potential of the field affecting to the electron being captured by the nucleus and the residue of the incident multiply charged ion is selected as screened Coulomb potential:

$$V_p(\mathbf{r}_p) = -\frac{Z_p^{'}}{r_p} - \frac{N}{r_p} \exp\left(-a r_p\right); \quad Z_p^{'} = Z - N; \quad a \approx Z^{1/3}. \tag{9}$$

The first term on the right side of (9) has the form of the Coulomb potential with an effective charge $Z_p^{\prime}$. The second term takes into account the deviation of the electrostatic field of the atomic core of the Coulomb type. Potential (9) follows from the statistical theory of Thomas-Fermi, it has a simple form and ensures the correct behavior in $r_p \to 0$ and $r_p \to \infty$.

In the momentum representation, the amplitude of the charge exchange (5) then shall be rewritten as follows:

$$\Re_{fi} = 2\pi i\eta\, Z_p^{'} \int \delta(p_z - p_{0z})\, \exp(-i\, \mathbf{p}\, \mathbf{b})\, g_f^{*}(\mathbf{p} + \mathbf{v})\, M_i(\mathbf{p})\, d\mathbf{p}, \tag{10}$$

where we introduce the following notations

$$g_f(\mathbf{q}) = g_f^{'}(\mathbf{q}) + \frac{N}{Z_p^{'}} g_f^{''}(\mathbf{q}), \tag{11}$$

$$g'_f(\mathbf{q}) = (2\pi)^{-3/2} \int \exp(i\mathbf{qr}) \frac{\varphi_f(\mathbf{r})}{r} d\mathbf{r}, \tag{12}$$

$$g''_f(\mathbf{q}) = (2\pi)^{-3/2} \int \exp\left(i\mathbf{qr} - ar\right) \frac{\varphi_f(\mathbf{r})}{r} d\mathbf{r}, \tag{13}$$

$$M_i(\mathbf{p}) = \frac{(2\pi)^{-3/2}}{\Gamma(-i\eta Z'_t)} \int_0^{+\infty} d\lambda \int d\mathbf{r}\, \varphi_i(\mathbf{r})\, \lambda^{-1-i\eta Z'_t} \exp\left[i\mathbf{pr} - \lambda(r - \mathbf{rn})\right], \tag{14}$$

$$p_{0z} = \eta E - v/2, \quad E = E_p - E_t, \quad \mathbf{p} = p_z \frac{\mathbf{v}}{v} + p_b \frac{\mathbf{b}}{b}. \tag{15}$$

Here $\mathbf{n}$ is the unit vector along the axis z of reference system associated with the atomic nucleus A^{Z_t+}; $\mathbf{b}$ is the impact parameter. To describe the interaction of the electron with the atomic core $A^{(Z_t+1)+}$ we applied the concept of effective charge $Z'_t \neq Z_t$. Unperturbed wave function $\varphi_f(\mathbf{r}_p)$ in the case of the final state $Z'_p = Z$ is taken in the form of hydrogen-like function, while $Z'_p < Z$ is taken in the form of hydrogen-like functions with an effective charge Z'_p defined by the Slater's rules.

The cross section of single-electron capture from an arbitrary $|i\rangle \equiv |nlm\rangle$ state of the hydrogenlike atom in a state with given quantum numbers $|f\rangle \equiv |n'l'm'\rangle$ of the incident ion is determined by the transition amplitude $\Re_{fi}$ by integrating along the plane of impact parameters:

$$\sigma_{(nlm \to n'l'm')} = \int |\Re_{fi}(\mathbf{b}, v)|^2 \, d^2\mathbf{b}. \tag{16}$$

The special interest for applications are the cross sections, summed over all final electronic states of the ion $B^{(Z_p-1)+}$ formed by one-electron capture:

$$\sigma_{(nlm)} = \sum_{n'l'm'} \sigma_{(nlm \to n'l'm')}. \tag{17}$$

In mathematical physics, apparatus of Green's functions, which are determined by the decomposition

$$G(\mathbf{r}_1, \mathbf{r}_2; \omega) = \sum_f \frac{\varphi^*_f(\mathbf{r}_1)\varphi_f(\mathbf{r}_2)}{\omega - \omega_f + i0}, \tag{18}$$

is commonly used to calculate the sums of spectral type (18). It is assumed that $\sum_f(...)$ includes the sum over the states of the discrete spectrum and the integral – over the states of the continuum. Given the ratio of

$$\frac{1}{\omega - \omega_f + i0} = P\frac{1}{\omega - \omega_f} - i\pi\, \delta(\omega - \omega_f), \tag{19}$$

where P is the symbol of the principal value, the total probability and cross section charge exchange (18) can be written then as follows:

$$W_{nlm}(\mathbf{b};v) = -4\pi\eta Z_p^{'2}\iint d\mathbf{p}_1\, d\mathbf{p}_2\, \delta(p_{1z}-p_{2z})M_{nlm}(\mathbf{p}_1)M^*_{nlm}(\mathbf{p}_2)\times$$
$$\times \exp\left[i\mathbf{b}(\mathbf{p}_2-\mathbf{p}_1)\right] \mathrm{Im}\Big\{G^{11}\left(\mathbf{p}_2+\mathbf{v},\mathbf{p}_1+\mathbf{v};\mathbf{p}_1\mathbf{v}+v^2/2+E_t\right)+$$
$$+(2N/Z_p^{'})\, G^{12}\left(\mathbf{p}_2+\mathbf{v},\mathbf{p}_1+\mathbf{v};\mathbf{p}_1\mathbf{v}+v^2/2+E_t\right)+$$
$$+(N^2/Z_p^{'2})\, G^{22}\left(\mathbf{p}_2+\mathbf{v},\mathbf{p}_1+\mathbf{v};\mathbf{p}_1\mathbf{v}+v^2/2+E_t\right)\Big\}, \qquad (20)$$

$$\sigma_{nlm} = -2^4\pi^3\eta Z_p^{'2}\int d\mathbf{p}\left|M_{nlm}(\mathbf{p})\right|^2 \mathrm{Im}\Big\{G^{11}(\mathbf{p}+\mathbf{v},\mathbf{p}+\mathbf{v};\mathbf{p}\mathbf{v}+v^2/2+E_t)+$$
$$+(2N/Z_p^{'})\, G^{12}\left(\mathbf{p}+\mathbf{v},\mathbf{p}+\mathbf{v};\mathbf{p}\mathbf{v}+v^2/2+E_t\right)+$$
$$+(N^2/Z_p^{'2})\, G^{22}\left(\mathbf{p}+\mathbf{v},\mathbf{p}+\mathbf{v};\mathbf{p}\mathbf{v}+v^2/2+E_t\right)\Big\}. \qquad (21)$$

The following notations are used here:

$$G^{ij}(\mathbf{p}_2+\mathbf{v},\mathbf{p}_1+\mathbf{v};\mathbf{p}_1\mathbf{v}+v^2/2+E_t) = (2\pi)^{-3}\iint d\mathbf{r}_1\, d\mathbf{r}_2\, \exp\left[-i\mathbf{r}_2(\mathbf{p}_2+\mathbf{v})\right]\times$$
$$\times f_i(\mathbf{r}_2)\, G(\mathbf{r}_2,\mathbf{r}_1;\mathbf{p}\mathbf{v}+v^2/2+E_t)\, f_j(\mathbf{r}_1)\, \exp\left[i\mathbf{r}_1(\mathbf{p}_1+\mathbf{v})\right], \quad \{i,j\}=1,2, \quad (22)$$

$$f_k(\mathbf{r}) = \exp\left(-\mu_k r\right)/r, \quad \mu_1 = 0, \quad \mu_2 = a, \quad k=1,2. \qquad (23)$$

The function G^{ij} can be expressed through the convolution of the Green's function recorded in the momentum representation:

$$G^{ij}(\mathbf{p}_2+\mathbf{v},\mathbf{p}_1+\mathbf{v};\mathbf{p}_1\mathbf{v}+v^2/2+E_t) = (2\pi)^{-6}\iint d\mathbf{q}_1\, d\mathbf{q}_2\, \tilde{f}_i(\mathbf{q}_2-\mathbf{p}_2-\mathbf{v})\times$$
$$\times G(\mathbf{q}_2,\mathbf{q}_1;\mathbf{p}_1\mathbf{v}+v^2/2+E_t)\, \tilde{f}_j(\mathbf{q}_1-\mathbf{p}_1-\mathbf{v}); \qquad (24)$$

$$\tilde{f}_k(\mathbf{q}) = 4\pi/(q^2+\mu_k^2). \qquad (25)$$

Results of (20)–(26) in the framework of the model used are accurate. Further approximations under specific calculations related to the use for the evaluation of the functions G^{ij} instead of the eigenfunctions of Hamiltonian with the potential (9) of hydrogen-like wave functions with selected variational parameters. The advantage of this simplification is the use of the Coulomb Green's functions of inbound (22) and (24), of closed integral representations. One such integral representations found by Hostler [8], has the following form

$$G(\mathbf{r}_2,\mathbf{r}_1;\omega) = \frac{ip\,\exp(-\pi\lambda/p)}{8\pi\, sh(\pi\lambda/p)}\int_{+\infty}^{(1+)} d\xi\left(\frac{\xi+1}{\xi-1}\right)^{i\lambda/p} D(\mathbf{r}_2,\mathbf{r}_1;\omega), \qquad (26)$$

$$\arg(\xi\pm 1) = 0,$$

where

$$D(\mathbf{r}_2, \mathbf{r}_1; \omega) = I_0 \left\{ \sqrt{-ip(x^2 - y^2)(\xi^2 - 1)} \right\} \exp(ipx\xi),$$
$$x = r_1 + r_2, \quad y = |\mathbf{r}_2 - \mathbf{r}_1|, \quad (\mathbf{p})^2 = -2m(\omega + i0), \quad \operatorname{Re} p > 0. \tag{27}$$

Through integration with respect to $\mathbf{r}_1$ and $\mathbf{r}_2$ in the expression of (22) for G^{ij}, after the substitution of integral representation (26) for the Green function $G(\mathbf{r}_2, \mathbf{r}_1; \omega)$, we find:

$$G^{ij}(\mathbf{k}_2, \mathbf{k}_1; \omega) = \frac{2\tilde{p}}{\pi^2} \left\{ \frac{i \exp(i\pi\lambda/\tilde{p})}{2 \sin(\pi\lambda/\tilde{p})} \right\} \times$$
$$\times \int_1^{(0+)} dz \frac{z^{-\lambda/\tilde{p}}}{A_1 z^2 - 2Bz + A_2} \Bigg|_{\mu_1=\lambda_i, \mu_2=\lambda_j}, \tag{28}$$

where

$$A_{1,2} = \left[(\tilde{p} \mp \mu_1)^2 + k_1^2 \right] \left[(\tilde{p} \mp \mu_2)^2 + k_2^2 \right], \tag{29}$$

$$B = 4\tilde{p}^2(\mathbf{k}_1 \, \mathbf{k}_2) + (\mu_1^2 + k_1^2 - \tilde{p}^2)(\mu_2^2 + k_2^2 - \tilde{p}^2), \tag{30}$$

$$\lambda_1 = 0, \quad \lambda_2 = a, \quad \tilde{p}^2 = -2(\omega + i0), \quad \operatorname{Re} \tilde{p} > 0; \quad \omega = \mathbf{p}_1 \mathbf{v} + v^2/2 + E_t. \tag{31}$$

Integration contour in (28) runs along the unit circle from $z = 1 + i0$ to $z = 1 - i0$.

According to the formula (28), the imaginary component of the $G^{ij}(\mathbf{k}_2, \mathbf{k}_1; \omega)$ function has a different appearance depending on the type of its pole characteristics corresponding to the energy spectrum of the incident particle. Since these features have different origins in the occupation of electronic states of discrete and continuous spectra, it is advisable to consider them separately.

3 Bound-bound transitions

At the real value of the parameter $\tilde{p}$, which corresponds to an electron capture by the incident ion in the states of the discrete spectrum, the imaginary component of $G^{ij}(\mathbf{k}_2, \mathbf{k}_1; \omega)$ is determined by the singularity of the factor in parentheses in front of a contour integral in the (28). In this case, in the calculation of Im G^{ij} we should take into account the ratio

$$\operatorname{Im} G^{ij} \left(\mathbf{p}_1 + \mathbf{v}, \mathbf{p}_2 + \mathbf{v}; \mathbf{p}_1 \mathbf{v} + v^2/2 + E_t \right) \sim$$
$$\sim \operatorname{Im} \frac{1}{\sin(\pi\lambda/\tilde{p} - i0)} = \sum_{n'} (-1)^{n'} \, \delta(\lambda/\tilde{p} - n'), \tag{32}$$

where

$$\tilde{p} = \left[-2(\mathbf{p}_1 \mathbf{v} + E_t + v^2/2) \right]^{1/2}. \tag{33}$$

Substituting in the right side of (20) the following expression for ImG^{ij}, we obtain the following for the total (in all states) charge exchange probability

$$W_{nlm}(\mathbf{b}, v) = \sum_{n'} W_{nlm \to n'}(\mathbf{b}, v). \tag{34}$$

The probability of electron capture in the states with a given value of the principal quantum number n' is defined by the formula

$$W_{nlm\to n'}(\mathbf{b},v) = -\frac{i}{v^2}\frac{4Z_p^3 Z_p'^2}{\pi n'^4}\iint d^2\mathbf{p}_{1b}\, d^2\mathbf{p}_{2b}\,\exp\left[i\mathbf{b}(\mathbf{p}_2-\mathbf{p}_1)\right]\times$$
$$\times\left[M_{nlm}(\mathbf{p}_1)\,M^*_{nlm}(\mathbf{p}_2)\right]\Big|_{p_{1z}=p_{2z}=p_{0z}}\times$$
$$\times\int_1^{(0+)} dz\cdot z^{-n'}\left\{T(\lambda_1,\lambda_1)+\frac{2N}{Z_p'}T(\lambda_1,\lambda_2)+\frac{N^2}{Z_p'^2}T(\lambda_2,\lambda_2)\right\}. \quad (35)$$

Here we have introduced the notations

$$T(\lambda_i,\lambda_j) = \frac{1}{A_1z^2-2Bz+A_2}\Big|_{\lambda_i=\mu_1,\,\lambda_j=\mu_2}, \quad \lambda_1=0, \quad \lambda_2=a, \quad (36)$$

$$A_{1,2} = \left[\left(\frac{Z_p}{n'}\mp\mu_1\right)^2+p_{1b}^2+(p_{0z}+v)^2\right]\times$$
$$\times\left[\left(\frac{Z_p}{n'}\mp\mu_2\right)^2+p_{2b}^2+(p_{0z}+v)^2\right], \quad (37)$$

$$B = \frac{4Z_p^2}{n'^2}\left[\mathbf{p}_{1b}\,\mathbf{p}_{2b}+(p_{0z}+v)^2\right]+\left[\mu_1^2+p_{1b}^2+(p_{0z}+v)^2-\frac{Z_p^2}{n'^2}\right]\times$$
$$\times\left[\mu_2^2+p_{2b}^2+(p_{0z}+v)^2-\frac{Z_p^2}{n'^2}\right]. \quad (38)$$

To calculate the contour integral of the first term on the right side (35) we use the following ratio:

$$\left(z^2-2xz+1\right)^{-1} = \frac{1}{z}\sum_{\mu=0}^{\infty} z^\mu\, C^1_\mu(x). \quad (39)$$

$C^\nu_\mu(x)$ – Gegenbauer polynomials. Roots of square trinomials in the denominators of the other two members of the integrand (35) are complex and in modulus greater than one. Therefore, for electron capture into the states of the discrete spectrum of standing under the contour integral in $W_{nlm\to n'}$ the function has no singularities other than pole of n'-th order at the point $z=0$. The circuit at the point $z=1$ can be closed and then the theorem of residues can be applied for calculation of the integral. As a result, for the probability of electron capture in a states with a definite value of the principal quantum number n' we obtain

$$W_{nlm\to n'}(\mathbf{b},v) = \frac{8Z_p^3 Z_p'^2}{v^2 n'^4}\iint d^2\mathbf{p}_{1b}\, d^2\mathbf{p}_{2b}\,\exp\left[i\mathbf{b}(\mathbf{p}_2-\mathbf{p}_1)\right]\Big\{F(\lambda_1,\lambda_1)+$$
$$+\frac{2NF(\lambda_1,\lambda_2)}{Z_p'}+\frac{N^2F(\lambda_2,\lambda_2)}{Z_p'^2}\Big\}\left\{M_{nlm}(\mathbf{p}_1)\,M^*_{nlm}(\mathbf{p}_2)\right\}\Big|_{p_{1z}=p_{2z}=p_0z}. \quad (40)$$

Here

$$F(\lambda_i, \lambda_j) = \frac{\sin(n'\Phi)}{\sin\Phi} A_1^{\frac{n'-1}{2}} A_2^{-\frac{n'+1}{2}} \Bigg|_{\substack{\mu_1=\lambda_i,\\ \mu_2=\lambda_j}}, \quad \Phi = \mathrm{arctg}\left(\frac{A_1 A_2}{B^2} - 1\right)^{1/2}. \tag{41}$$

For further specification of the obtained expressions we represent the wave functions $\varphi_{nlm}(\mathbf{r}_t)$, describing the initial bound state of the electron, in the form of

$$\varphi_{nlm}(\mathbf{r}_t) = \hat{D}_{nlm}(\beta, \mu) \exp(-\beta r_t + i\mu\mathbf{r}_t)\Big|_{\beta=Z_t/n,\, \mu=0}. \tag{42}$$

The differential operator $\hat{D}_{nlm}(\beta, \mu)$ is a linear combination of the operators $\partial/\partial\beta$, $\partial/\partial\mu_x$, $\partial/\partial\mu_y$, $\partial/\partial\mu_z$ and their higher derivatives. Then from (14) it follows:

$$M_{nlm}(\mathbf{p}) = \hat{D}_{nlm}(\beta, \mu)\, \Lambda(\mathbf{p}, \beta, \mu)\Big|_{\beta=Z_t/n,\, \mu=0}, \tag{43}$$

where

$$\begin{aligned}\Lambda(\mathbf{p}, \beta, \mu) =& \frac{2\sqrt{2\pi}}{\Gamma(-i\eta Z_t')\,\mathrm{sh}(\pi\eta Z_t')} \left[\beta^2 + (\mathbf{p}+\mu)^2\right]^{-2-i\eta Z_t'} \times \\ & \times \left[2\beta - 2i(p_z+\mu_z)\right]^{i\eta Z_t'} \left\{ i\beta(1+i\eta Z_t') + \frac{\eta Z_t'}{2} \frac{\beta^2 + (\mathbf{p}+\mu)^2}{\beta - i(p_z+\mu_z)} \right\}.\end{aligned} \tag{44}$$

Using formulas (40)–(44), we can derive a number of simpler relations for some important special cases. One of them concerns the probability of capturing of an electron by a bare nucleus ($N = 0$, $Z_p = Z_p'$):

$$\begin{aligned}W_{1s\to n'}(\mathbf{b}, v) =& \frac{2^8 \pi Z_p^5 Z_t^5}{v^2 n'^3} \frac{\eta Z_t'}{\mathrm{sh}(\pi\eta Z_t')} \exp\left[-2\eta Z_t' \,\mathrm{arctg}(-p_{0z}/Z_t)\right] \times \\ \times & \left| \frac{\eta Z_t'/Z_t}{2Z_t - 2ip_0} \left(\frac{b}{2\sqrt{p_{0z}^2 + Z_t^2}}\right)^{1+i\eta Z_t'} \frac{\mathcal{K}_{1+i\eta Z_t'}(b\sqrt{p_{0z}^2+Z_t^2})}{\Gamma(2+i\eta Z_t')} + \right. \\ & \left. + i(1+i\eta Z_t') \left(\frac{b}{2\sqrt{p_{0z}^2 + Z_t^2}}\right)^{2+i\eta Z_t'} \frac{\mathcal{K}_{2+i\eta Z_t'}(b\sqrt{p_{0z}^2+Z_t^2})}{\Gamma(3+i\eta Z_t')} \right|^2.\end{aligned} \tag{45}$$

$\mathcal{K}_\nu(z)$ – modified Bessel function. Hence the approximate equality for all finite $\mu_{1,2}$:

$$\sin(n'\,\Phi) \simeq n' \sin\Phi. \tag{46}$$

Note that, at $\mathbf{p}_1 = \mathbf{p}_2$ equality of (46) is realized accurately.

In the case when $Z_t' \to 0$ (OBK – approximation without eikonal corrections) from the (45) we obtain the following expression for the partial probabilities:

$$W_{1s\to n'}^{\mathrm{OBK}}(\mathbf{b}, v) = \frac{4Z_t^5\, Z_p^5}{v^2 n'^3} \left(\frac{b}{\sqrt{p_{0z}^2 + Z_t^2}}\right)^4 \mathcal{K}_2^2\left(b\sqrt{p_{0z}^2 + Z_t^2}\right). \tag{47}$$

Here is also an expression for the cross section of capture from the $|nlm\rangle$-shell of the target into an arbitrary n'-shell of the incident particle:

$$\sigma_{nlm\to n'} = \frac{2^5\pi^2 Z_p^3\, Z_p'^2}{v^2 n'^3} \int d^2\mathbf{p}_b\, |M_{nlm}(\mathbf{p})|^2 \left\{ \left[p_b^2 + (p_z+v)^2 + \left(\frac{Z_p}{n'}\right)^2 \right]^{-1} + \right.$$

$$\left. + \frac{N}{Z_p'} \frac{\left[p_b^2 + (p_z+v)^2 + (\frac{Z_p}{n'} - Z^{1/3})^2\right]^{(n'-1)/2}}{\left[p_b^2 + (p_z+v)^2 + (\frac{Z_p}{n'} + Z^{1/3})^2\right]^{(n'+1)/2}} \right\}^2 \Bigg|_{p_z=p_{0z}}. \tag{48}$$

In particular, for the electron capture from the K-shell of a hydrogen-like atom

$$\sigma_{1s\to n'} = \frac{2^8\pi^2\, Z_p'^2\, Z_p^3\, Z_t^5}{v^2 n'^3} \frac{\eta Z_t'}{\operatorname{sh}(\pi\eta Z_t')} \exp\left[-2\eta Z_t' \operatorname{arctg}\left(-\frac{p_{0z}}{Z_t}\right)\right] \times$$

$$\times \int_0^\infty d(p_b^2) \Bigg| \left(\frac{i - \eta Z_t'}{[p_b^2 + (p_{0z}+v)^2 + (Z_p/n')^2]^2} + \right.$$

$$\left. + \frac{\eta\, Z_t'/Z_t}{2(Z_t - ip_{0z})[p_b^2 + (p_{0z}+v)^2 + (Z_p/n')^2]} \right) \times$$

$$\times \Bigg([\, p_b^2 + (p_{0z}+v)^2 + (Z_p/n')^2]^{-1} + \frac{N}{Z_p'} \times$$

$$\times \frac{\left[p_b^2 + (p_{0z}+v)^2 + (\frac{Z_p}{n'} - Z^{1/3})^2\right]^{(n'-1)/2}}{\left[p_b^2 + (p_{0z}+v)^2 + (\frac{Z_p}{n'} + Z^{1/3})^2\right]^{(n'+1)/2}} \Bigg) \Bigg|^2 . \tag{49}$$

In the case of charge exchange on the bare nuclei ($N = 0$, $Z_p = Z_p'$) level-occupation cross section with any fixed value of n' is represented in closed form:

$$\sigma_{1s\to n'}^{\text{Coul}} = \alpha_{n'}(Z_t', Z_p, v)\ \sigma_{1s\to n'}^{\text{OBK}}(Z_t, Z_p, v), \tag{50}$$

where $\sigma_{1s\to n'}^{\text{OBK}}(Z_p, Z_t, v)$ is charge exchange cross section in OBK-approximation:

$$\sigma_{1s\to n'}^{\text{OBK}}(Z_p, Z_t, v) = \frac{2^8\pi Z_p^5 Z_t^5}{5n'^3 v^2 [Z_t^2 + (v/2 - E\eta)^2]^5}, \tag{51}$$

and the scale factor is determined by the following expression

$$\alpha_{n'} = \frac{\pi\eta Z_t'}{\operatorname{sh}(\pi\eta Z_t')} \exp\left[-2\eta Z_t' \quad \operatorname{arctg}\left(\frac{v/2 - E\eta}{Z_t}\right)\right] \left\{ 1 - \frac{5}{8}\frac{Z_t'}{Z_t} + \frac{5}{48}\left(\frac{Z_t'}{Z_t}\right)^2 + \right.$$

$$\left. + \left[\frac{Z_t'^2}{6} + \frac{5}{4}\frac{Z_t'}{Z_t}E - \frac{5}{12}\left(\frac{Z_t'}{Z_t}\right)^2 E \right] \eta^2 + \frac{5}{12}\left(\frac{Z_t'}{Z_t}\right)^2 E^2\, \eta^2 \right\}. \tag{52}$$

This result coincides with that from [5], obtained using electron density matrix in the momentum representation. An advantage of the expression (50) is that the perturbation of the electron wave function that occurs as a result of its interaction with the atomic residue $A^{(Z_t+1)+}$ of the target in the output channel, that is described by the factor $\alpha_{n'}(Z_t', Z_p, v)$, which is calculated analytically and is represented in closed form (52). This greatly simplifies the analysis of the perturbation effect on the electron capture cross section and allows to make a simple generalization to the case of electron capture from a variety of shells, making the formula (48) convenient for systematic calculations of cross sections of different processes.

The total cross sections, calculated as the sum of the partial ones, are represented in the following form

$$\sigma_t = \sum_{n'=1}^{n_{\max}} \sigma_{1s\to n'} + \sum_{n'>n_{\max}} \sigma^{\text{coul}}_{1s\to n'}, \tag{53}$$

since for large quantum numbers n' spectrum of any atom and ion can be considered as hydrogen-like. The value of $n_{\max}$ is chosen such that the error caused by the replacement of the $\sigma_{1s\to n'}$ for $\sigma^{\text{coul}}_{1s\to n'}$ when $n' > n_{\max}$ is not more than a few percent. The characteristic values of $n_{\max}$ lie between 10 and 20.

OBK theory usually gives higher values of absolute cross sections for $\sigma^{\text{OBK}}_{1S\to n'}$, but describes well the relative cross sections. Formula (50) is in much better agreement with the experimental data than (51). Expression (52) allows us to estimate the multiplier $\alpha_{n'}$ from (50) at different values of the parameters v, Z_p, Z_t', n' and leads to the following inequality $0.15 \le \alpha_{n'} \le 0.4$.

4 The results of charge exchange cross section calculations

The results of charge exchange cross section calculations in the reactions

$$H + \begin{cases} C^{q+} \\ N^{q+} \\ O^{q+} \end{cases} \to H^+ + \begin{cases} C^{(q-1)+} \\ N^{(q-1)+} \\ O^{(q-1)+} \end{cases}, \qquad q = 1, 2, 3, \tag{54}$$

performed in a modified eikonal approximation taking into account screening (the calculation according to the formula (49)) and on the basis of the usual eikonal approximation without allowance for screening (the calculation according to the formula (50)), are shown in Fig. 1 together with experimental data [6, 7]. For all three charge states ($q = 1, 2, 3$) cross section changes caused by screening, are correctly described by the theory. The effect of screening is significant at $q = 1$, noticeable at $q = 2$, small at $q = 3$ and usually unimportant at $q \ge 4$. These conclusions are easy to understand qualitatively: at high collision energies and small Z_p electron capture is performed mainly on the lower unfilled shells of the incident ion, which are highly susceptible to screening. With increasing charge Z_p and decreasing collision energy electron is captured in the states with large values of the principal quantum number n', for which influence of the screening effects is minor.

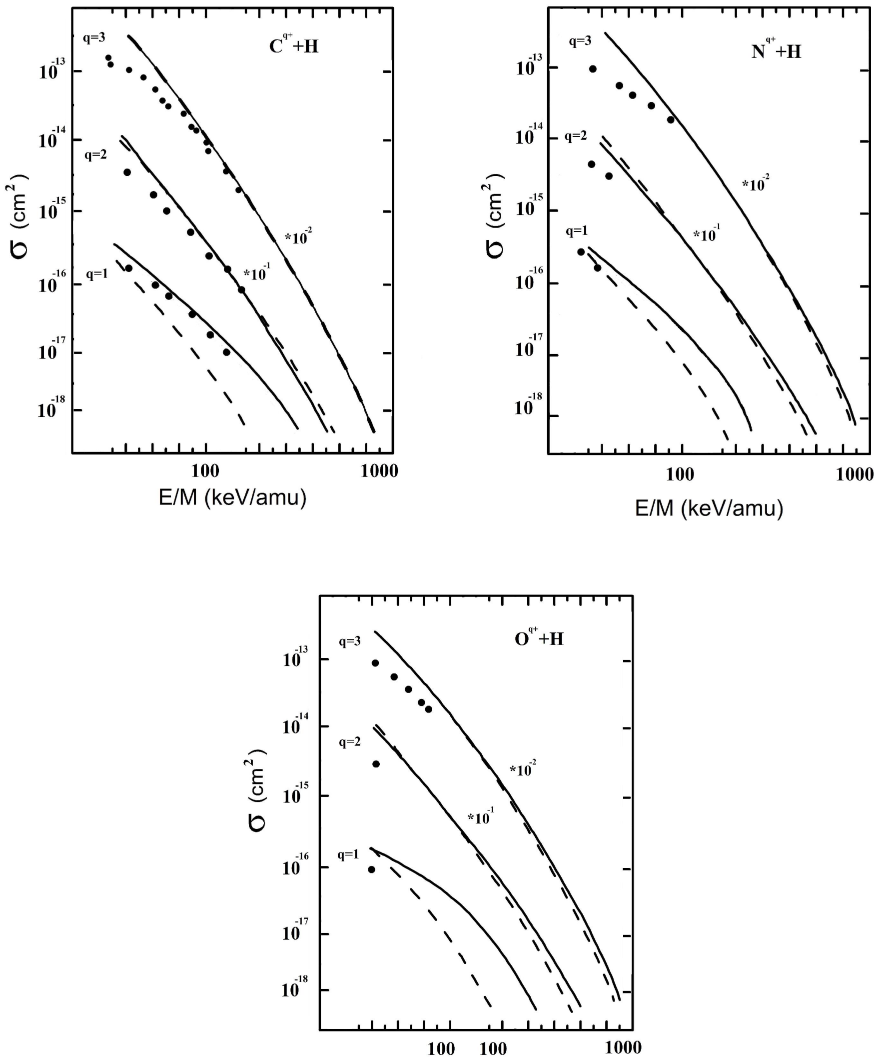

Figure 1: Charge exchange cross section of the hydrogen atoms on the ions C^{q+}, N^{q+}, O^{q+} ($q = 1, 2, 3$) as a function of energy divided by the atomic mass. Theory: the solid lines – calculation results in a modified eikonal approximation with allowance for screening; dashed lines – the results of calculations in the eikonal approximation without allowance for screening. Experiment (filled circles): C^{q+} – [6], (N^{q+}, O^{q+}) – [7].

Conclusion

The process of Coulomb charge exchange of bare or screened ion in collisions with light atoms was researched in the framework of the semi-classical eikonal theory. Potential of the field affecting the transiting electron by the nucleus and the core of the incident multiply charged ion is selected as screened Coulomb potential. For calculating probabilities and cross section for charge exchange summed over all final electronic states, we developed the method of Green's functions. The analytical expressions for the probability and electron capture cross sections from K-shell of a hydrogen atom in an arbitrary n'-shell of the bare and screened incident ion were obtained. For the probabilities of electron capture into continuous spectrum of the incident ion we found more simple analytical expression than previously known. Based on these results, we performed systematic calculations of electron capture cross sections of fast ions C^{q+}, N^{q+} and O^{q+} $(q = 1, 2, 3)$ during their collision with hydrogen atoms. The effects of shielding of the incident ion affect both the value of cross sections, and the nature of their dependence on the collision energy. This is especially strongly manifested in systems with small values of the incident ion charge states and large values of the energy of the incident particles.

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