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Femtosecond Collisional and Radiative Phenomena in Atomic Systems Interacting with Ionic Beams and Intense Laser Pulses

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During the reporting period our group performed investigations in the following directions:

1. An asymptotic theory of one- and two-electron capture in slow ion-molecule collisions
2. A relativistic spherical model of the Stark effect in H-like ions
3. The relativistic Coulomb problem in two spatial dimensions
4. Measurement and R-matrix calculation of electron-impact de-excitation of the $(3s3p)^3P_{0,1,2}$ states in Mg

The following results were obtained.

Task T1

1. An Asymptotic Theory of One- and Two-Electron Capture in Slow Ion-molecule Collisions

The method of the asymptotic approach for the study of inelastic processes (one- and two-electron capture) in slow ion-molecule collisions has been elaborated. For the Green's function of the two-centre Coulomb problem, exact and asymptotically exact representations are obtained. An analytic expression for the matrix element for the two-electron exchange in the interaction of a highly charged ion with a molecule is obtained. The cross sections for one- and two-electron capture at slow ion-molecule collisions with different final states are calculated using the method of strong-coupling channels and the linear trajectories approximation for the colliding particles. Different ways of two-electron transfer (one-step: $A_2 + B^{Zb+} \to A_2^{2+} + B^{(Zb-2)+}$ and two-step: $A_2 + B^{Zb+} \to A_2^{+} + B^{(Zb-1)+} \to A_2^{2+} + B^{(Zb-2)+}$) and their relative contributions to the total cross-section of the process are investigated.

In the theory of atomic collisions and particularly in the theory of inelastic processes in ion - molecule collisions it is necessary to know a Green's function for the two-centre Coulomb problem:

$$\left[-\frac{1}{2}\Delta - \frac{Z_1}{r_1} - \frac{Z_2}{r_2} - E(R)\right] G_E(\vec{r},\vec{r}';R) = \delta(\vec{r}-\vec{r}'), \tag{1.1}$$

In our work, the expansions of the Green's function for the two-centre Coulomb potential over spheroidal functions are built. We represent the Green's function $G_E(\vec{r},\vec{r}';R)$ in the form of an expansion over a complete orthonormalised system of oblate angular spheroidal functions $\bar{S}_{m\ell}(p,\eta)$ [1]:

$$G_E(\vec{r},\vec{r}';R) \equiv G_E(\xi,\eta,\varphi;\xi',\eta',\varphi'|R) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} G_{m\ell}(\xi,\xi';E)\bar{S}^*_{m\ell}(p,\eta)\bar{S}_{m\ell}(p,\eta')\frac{e^{im(\varphi-\varphi')}}{2\pi}, \tag{1.2}$$

and the radial part of the Green's function $G_{m\ell}(\xi,\xi';E)$ satisfies the following differential equation:

$$\left\{\frac{d}{d\xi}\left[(\xi^2-1)\frac{d}{d\xi}\right] + \left[-\lambda^{(\eta)}_{m\ell}(p^2) - p^2(\xi^2-1) + 2p\alpha\xi - \frac{m^2}{\xi^2-1}\right]\right\} G_{m\ell}(\xi,\xi';E) = -\frac{4}{R}\delta(\xi-\xi'), \tag{1.3}$$

where $p = \frac{1}{2}R(-2E)^{1/2}$, $\alpha = (Z_1+Z_2)(-2E)^{-1/2}$ and $\lambda^{(\eta)}_{m\ell}$ denote the eigenvalues of the angular wavefunction, corresponding to the oblate spheroidal functions $\bar{S}_{m\ell}(p,\eta)$ [1]. The expression for the radial Green's function $G_{m\ell}(\xi,\xi';E)$ (see Refs. [4, 6]) can be given by

$$G_{m\ell}(\xi,\xi';E)=\frac{4Z}{\alpha}\left(\frac{x_+x'_+}{x_+x'_+}\right)^{m/2}\tilde{\Pi}^{(1,\pm)}_{m\ell}(x_{\pm<})\tilde{\Pi}^{(2,\pm)}_{m\ell}(x_{\pm>}),\ Z=Z_1+Z_2. \tag{1.4}$$

Here $\tilde{\Pi}^{(1,\pm)}_{m\ell}(x_\pm)$ and $\tilde{\Pi}^{(2,\pm)}_{m\ell}(x_\pm)$ are the two linearly independent solutions of the homogeneous part of Eq. (1.3), (after performing the variable substitution $x_\pm = p(\xi\pm 1)$) and can be given as the following infinite sums:

$$\tilde{\Pi}^{(1,\pm)}_{m\ell}(x_\pm)=\sum_{s=-\infty}^{\infty}h^{(\pm)}_s(p|\alpha,\lambda_{m\ell})R^{(1)}_{s+\nu}(x_\pm),\quad \tilde{\Pi}^{(2,\pm)}_{m\ell}(x_\pm)=\sum_{s=-\infty}^{\infty}\tilde{h}^{(\pm)}_s(p|\alpha,\lambda_{m\ell})R^{(2)}_{s+\nu}(x_\pm), \tag{1.5}$$

where the expansion coefficients $h^{(\pm)}_s$ and $\tilde{h}^{(\pm)}_s$ are to be determined.

In many physical problems whose examples are considered in [1], the asymptotic behaviour of the Green's function $G_E(\vec{r},\vec{r}';R)$ at small values of the internuclear distance needs to be known. Hence the necessity to construct the asymptotic expansions of $S_{m\ell}(p,\eta)$, $\tilde{\Pi}^{(1,\pm)}_{m\ell}(x_\pm)$ and $\tilde{\Pi}^{(2,\pm)}_{m\ell}(x_\pm)$ functions over a small parameter p at fixed quantum numbers ℓ and m arises. We use an asymptotic method, proposed by Abramov and Slavyanov [3], to search for such expansions.

Let us to consider the oblate angular spheroidal function $S_{m\ell}(p,\eta)$. The expansion for normalised angular spheroidal functions can be written in a form:

$$\bar{S}_{m\ell}(p,\eta)=N^{-1}_{m\ell}(p)\sum_{n=Ent[(m-\ell)/2]}^{\infty}d^{m\ell}_{2n+\delta}P^m_{\ell+2n+\delta}(\eta);\quad \delta=\begin{cases}0 & if \quad \ell-m=2k,\\ 1 & if \quad \ell-m=2k+1,\ k=0,1,2...\end{cases} \tag{1.6}$$

Here $P^m_\ell(\eta)$ are the associated Legendre polynomials, $N_{m\ell}(p)$is the normalisation factor and $\mathrm{Ent}[\rho]$ is the integer part of the real number ρ. We search for the separation constant $\lambda^{(\eta)}_\delta$ and the expansion coefficients $d^{m\ell}_{2n+\delta}$ in the form of asymptotic series over the powers of a small parameter p^2:

$$\lambda^{(\eta)}_\delta=\sum_{j=0}^{\infty}[\lambda_\delta]_{2j}p^{2j};\quad d^{m\ell}_{2n+\delta}=p^{|2n|}\sum_{j=0}^{\infty}\left[d^{m\ell}_{2n+\delta}\right]_{2j}p^{2j},\quad d_\delta=1. \tag{1.7}$$

On the basis of recurrence relations for the coefficients $d^{m\ell}_{2n+\delta}$, using the standard asymptotic technique (see refs. [3]), we can obtain analytic representations for the expansion coefficients $\left[d^{m\ell}_{2n+\delta}\right]_{2j}$ and $[\lambda_\delta]_{2j}$. Some coefficients are given below:

$$[\lambda_\delta]_0=(\ell+\delta)(\ell+\delta+1),\quad [\lambda_\delta]_2=1-(B_{-1+\delta}E_\delta+B_\delta E_{1+\delta}),$$

$$[\lambda_\delta]_4=\frac{E_\delta E_{-1+\delta}B_{-1+\delta}B_{-2+\delta}}{2(2\ell+2\delta-1)}-\frac{B_\delta B_{1+\delta}E_{1+\delta}E_{2+\delta}}{2(2\ell+2\delta+3)},$$

$$[d_{2+\delta}]_0=\frac{E_{1+\delta}E_{2+\delta}}{2(2\ell+2\delta+3)},\ [d_{2+\delta}]_2=\frac{E_{1+\delta}E_{2+\delta}}{4(2\ell+2\delta+3)^2}[B_{1+\delta}E_{2+\delta}+B_{2+\delta}E_{3+\delta}-B_{-1+\delta}E_\delta-B_\delta E_{1+\delta}].$$

$$B_k=\frac{\ell+k+m+1}{2\ell+2k+3},\quad E_k=\frac{\ell+k-m}{2\ell+2k-1},\quad d^{m\ell}_{m-\ell-2+\delta}=0.$$

Here, we represent only a few coefficients of the expansion (1.7), but in the numerical calculation for Z_1eZ_2 systems we keep up to ten coefficients in each expansion. The same approach was applied for

the calculation of the coefficients $h_s^{(\pm)}$ and $\tilde{h}_s^{(\pm)}$. We have checked the applicability of our approximate results with numerical solutions obtained for Z_1eZ_2 systems in [5, 8]. Some of the results are represented in tables 1-6. For a more convenient presentation of the results, the values of the separation constants are recalculated in the notation system chosen in Ref. [5]. The normalisation for the coefficients $d^{m\ell}_{2n+\delta}$, accepted in [5] is used here. In tables 1-4 we present the separation constant for the systems Z_1eZ_2 calculated using our asymptotic formulae (1.7) in comparison with the exact numerical data from Refs. [5, 8]. In tables 5 and 6 we present the expansion coefficients for the oblate angular spheroidal function, calculated using our asymptotic expansion for the $Z_1=Z_2=1$ system.

The obtained result is used for the asymptotic form of the one-electron three-centre wave function. Using this function, exchange matrix elements are calculated which correspond to the following processes of one- and two-electron capture at slow ion-molecule collisions:

$$\begin{array}{ccc} H_2 + C^{n+} & \rightarrow & 2p + C^{(n-2)+} \\ \downarrow & & \uparrow \\ \rightarrow & H_2^+ + C^{(n-1)+} & \rightarrow \end{array} \qquad n = 3,4,5. \tag{1.8}$$

In Fig.1, we present the matrix elements of the two-electron exchange interaction between a C^{4+} ion and a H_2 molecule, reaction (1.8, n=4).

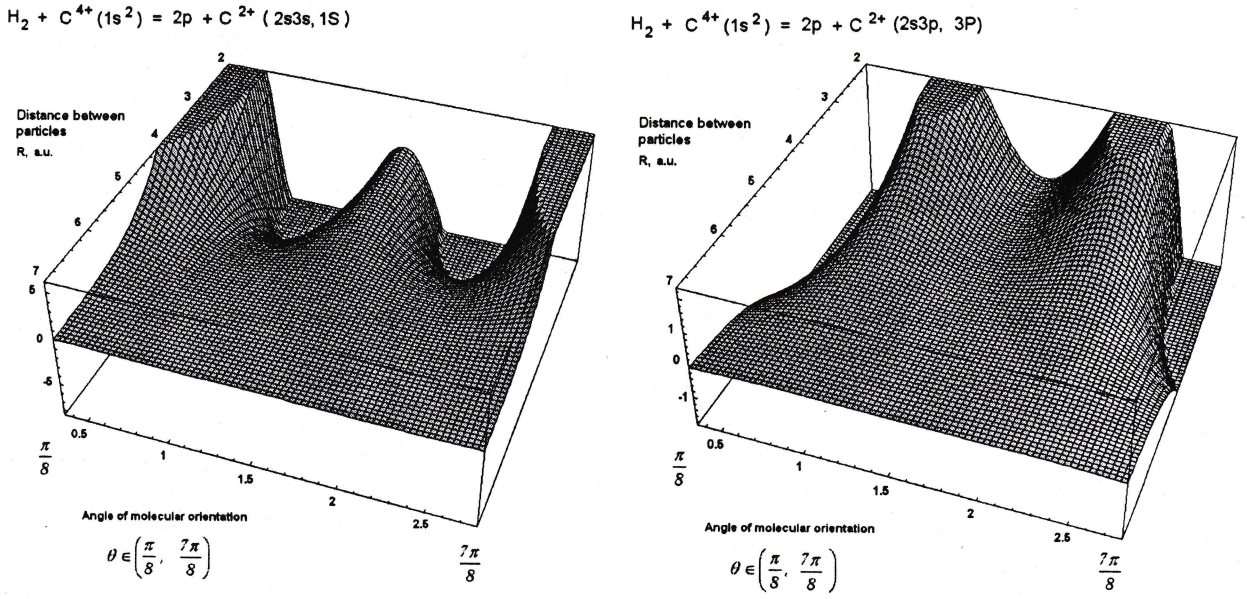

Figure1: The matrix elements of the two-electron exchange interaction for the reaction (1.8 b) as a function of the distance between the colliding particles and the angle of orientation of a molecular axis with respect to the projectile velocity vector.

The cross sections are found to be in good agreement with the experimental data. As in the case of ion-atom collisions, the following types of two-electron capture processes are possible: one-step mode $H_2 + C^{4+} \rightarrow 2p + C^{2+}$, and two-step mode $H_2 + C^{4+} \rightarrow H_2^+ + C^{3+} \rightarrow 2p + C^{2+}$. The calculations show that the two-step mode plays an important role and significantly influences the total cross section of the reaction, as in the case of ion-atom collisions. Experimental investigations of the above-mentioned reactions were performed by the group of prof. B. Kikiani (P6)

Table 1. Separation constants $\lambda_{m\ell}^{(\eta)} - p^2$ of the angular equation for the oblate spheroidal function, $\lambda_{m\ell}^{(\eta)} = \Lambda_{m\ell} \times 10^n$, for the $\ell = m = 0$ and $\ell = 1, m = 0$ states. $Z_1=Z_2=1$.

	Our calculation		Ref. [5]		Our Calculation		Ref. [5]	
p	Λ_{00}	n	Λ_{00}	n	Λ_{01}	n	Λ_{01}	n
0.1	-3.33482	-3	-3.34	-3	1.99400	0	1.99400	0
0.5	-8.42666	-2	8.427	-2	1.84957	0	1.84957	0
1	-3.48605	-1	-3.4860	-1	1.39321	0	1.39321	0
1.5	-8.29869	-1	-8.2987	-1	6.16041	-1	6.1604	-1
2	-1.59451	0	-1.59449	0	-5.05240	-1	-5.0524	-1
2.5	-2.73297	0	-2.73476	0	-1.99986	0	-1.99990	0
3	-4.31034	0	-4.34329	0	-3.89916	0	-3.89940	0
3.5	-6.19528	0	-6.47733	0	-6.23271	0	-6.23325	0

Table 2. Separation constants $\lambda_{m\ell}^{(\eta)} - p^2$ of the angular equation for the oblate spheroidal function, $\lambda_{m\ell}^{(\eta)} = \Lambda_{m\ell} \times 10^n$, for the $\ell = m = 1$ and $\ell = 2, m = 1$ states. $Z_1=Z_2=1$.

	Our calculation		Ref. [5]		Our calculation		Ref. [5]	
p	Λ_{11}	n	Λ_{11}	n	Λ_{12}	n	Λ_{12}	n
0.1	1.99800	0	1.99800	0	5.99571	0	5.99571	0
0.5	1.94971	0	1.94971	0	5.89261	0	5.89261	0
1	1.79530	0	1.79531	0	5.56753	0	5.56753	0
1.5	1.52542	0	1.52542	0	5.01589	0	5.01589	0
2	1.11854	0	1.11855	0	4.22275	0	4.22275	0
2.5	5.38653	-1	5.3890	-1	3.16700	0	3.16699	0
3	-2.7174	-1	-2.6942	-1	1.82165	0	1.82154	0
3.5	-1.40178	0	-1.38633	0	1.55051	-1	1.5432	-1

Table 3. Separation constants for the ground state $1s\sigma$, $Z_1=1$, $Z_2=2$.

		Our calc.	Ref. [8]
R	p	$\lambda_{00}^{(\eta)}$	$\lambda_{00}^{(\eta)}$
0.2	0.290953	0.049553	0.049553
0.4	0.554405	0.175242	0.175244
0.6	0.794506	0.347491	0.347538
0.8	1.01837	0.546972	0.547375
1	1.23153	0.760295	0.762415
1.2	1.43806	0.976566	0.984442

Table 4. Separation constants for the state $2p\sigma$, $Z_1=1$, $Z_2=2$.

		Our calc.	Ref. [8]
R	p	$\lambda_{00}^{(\eta)}$	$\lambda_{00}^{(\eta)}$
0.2	0.150799	2.01311	2.01311
0.4	0.306268	2.05382	2.05382
0.6	0.469837	2.12594	2.12594
0.8	0.64160	2.23417	2.23415
1	0.818029	2.38169	2.38156
1.2	0.994205	2.56837	2.56895

Table 5. Expansion coefficients for the oblate angular spheroidal function calculated for the ground state ($\ell = m = 0$), $d_r^{m\ell} = D_r \times 10^n$. $Z_1=Z_2=1$.

	Our calc.		Ref.[5]		Our calc.		Ref.[5]		Our calc.		Ref.[5]	
p	D_0	n	D_0	n	D_2	n	D_2	n	D_4	n	D_4	n
0.1	1.0006	0	1.0006	0	1.1121	-3	1.1121	-3	1.90667	-7	1.9066	-7
0.2	1.0022	0	1.0021	0	4.4599	-3	4.4595	-3	3.0593	-6	3.0590	-6

0.3	1.0050	0	-	-	1.0079	-2	-	-	1.5562	-5	-	-
0.4	1.0090	0	1.0090	0	1.8029	-2	1.8028	-2	4.9519	-5	4.9517	-5
0.5	1.0142	0	1.0142	0	2.8394	-2	2.8393	-2	1.2196	-4	1.2194	-4
0.6	1.0205	0	1.0205	0	4.1281	-2	4.1283	-2	2.5558	-4	2.5555	-4
0.7	1.0282	0	-	-	5.6837	-2	-	-	4.7954	-4	-	-
0.8	1.0373	0	1.0373	0	7.5231	-2	7.5232	-2	8.3022	-4	8.2977	-4
0.9	1.0478	0	-	-	9.6662	-2	-	-	1.3523	-3	-	-
1	1.0599	0	1.0599	0	1.2138	-1	1.2138	-1	2.1004	-3	2.0975	-3
1.1	1.0736	0	-	-	1.4965	-1	-	-	3.1404	-3	-	-
1.2	1.0892	0	1.0892	0	1.8182	-1	1.8182	-1	4.5523	-3	4.5385	-3
1.3	1.1067	0	-	-	2.1825	-1	-	-	6.4318	-3	-	-
1.4	1.1264	0	1.1264	0	2.5940	-1	2.5940	-1	8.8950	-3	8.8418	-3
1.5	1.1483	0	1.1484	0	3.0571	-1	3.0573	-1	1.2080	-2	1.1983	-2

Table 6. Expansion coefficients for the oblate angular spheroidal function, calculated for the first excited state ($\ell = 1$, $m = 0$), $d_r^{m\ell} = D_r \times 10^n$. $Z_1=Z_2=1$.

	Our calc.		Ref.[5]		Our calc.		Ref.[5]		Our calc.		Ref.[5]	
p	D_1	n	D_1	n	D_3	n	D_3	n	D_5	n	D_5	n
0.1	1.0006	0	1.0006	0	4.0020	-4	4.0020	-4	4.5373	-8	4.5373	-8
0.2	1.0024	0	1.0024	0	1.6033	-3	1.6033	-3	7.2701	-7	7.2700	-6
0.3	1.0054	0	-	-	3.6165	-3	-	-	3.6892	-6	-	-
0.4	1.0097	0	1.0097	0	6.4528	-3	6.4526	-3	1.1700	-5	1.1699	-5
0.5	1.0151	0	1.0151	0	1.0128	-2	1.0129	-2	2.8684	-5	2.8684	-5
0.6	1.0219	0	1.0219	0	1.4668	-2	1.4667	-2	5.9797	-5	5.9792	-5
0.7	1.0299	0	-	-	2.0096	-2	-	-	1.1147	-4	-	-
0.8	1.0393	0	1.0393	0	2.6451	-2	2.6451	-2	1.9154	-4	1.9150	-4
0.9	1.0501	0	-	-	3.3770	-2	-	-	3.0934	-4	-	-
1	1.0623	0	1.0623	0	4.2099	-2	4.2097	-2	4.7584	-4	4.7557	-4
1.1	1.0759	0	-	-	5.1486	-2	-	-	7.0375	-4	-	-
1.2	1.0911	0	1.0911	0	6.1996	-2	6.1998	-2	1.0079	-3	1.0068	-3
1.3	1.1079	0	-	-	7.3693	-2	-	-	1.4052	-3	-	-
1.4	1.1264	0	1.1264	0	8.6652	-2	8.6655	-2	1.9151	-3	1.9114	-3
1.5	1.1466	0	1.1467	0	1.0095	-1	1.0096	-1	2.5596	-3	2.5533	-3

Task T4

2. A Relativistic Spherical Model of the Stark Effect in H-like Ions

The properties of the energy spectrum of hydrogen and other atoms in external electromagnetic fields have been thoroughly studied since the late 1920s. However, relativistic aspects of the problem were not considered. In our papers, we attempt to partially fill that gap for the example of Stark ionisation of atomic systems with a high degree of ionisation (highly charged ions). As in such systems relativistic effects cause non-negligible corrections and essentially define orders of the spectral

characteristics, a consistent theory of the Stark effect should be based on relativistic equations.

We solve the Dirac equation with a spherically symmetric potential $V=-eA_0(r)$ in the WKB approximation framework. The solution of the Dirac equation can be represented in the form [9]

$$\Psi(\vec{r})=\frac{1}{r}\begin{pmatrix} F(r)\Omega_{jlm}(\vec{n}) \\ (-1)^{\frac{1+l-l'}{2}} G(r)\Omega_{jl'm}(\vec{n}) \end{pmatrix}, \quad l=j\pm 1/2, \quad l'=2j-l, \quad \vec{n}=\vec{r}/r.$$

where j and l are the total electron and orbital angular moments, respectively, m is the projection of j onto the internuclear axis Oz and the functions $F(r)$ and $G(r)$ satisfy the equations ($m_e=\hbar=c=1$):

$$\frac{dF}{dr}=-\frac{\aleph}{r}F+(1+\varepsilon-V)G, \quad \frac{dG}{dr}=(1-\varepsilon+V)F+\frac{\aleph}{r}G,$$

$\aleph=\mp(j+1/2)$ for states with $j=l\pm 1/2$.

In order to obtain the quasiclassical solutions of the system, it is convenient to write equations (2.2) in the matrix form:

$$\psi'=\frac{1}{\hbar}D\psi, \quad \psi=\begin{pmatrix} F \\ G \end{pmatrix}; \quad D=\begin{pmatrix} -\hbar\aleph/r & \varepsilon+1-V(r) \\ 1-\varepsilon+V(r) & \hbar\aleph/r \end{pmatrix}.$$

Here we use again $\hbar$ in order to obtain the WKB approximation and the prime denotes the derivative with respect to r. For the solution of the matrix equation (2.4) we look at the formal expansion in powers of $\hbar$:

$$\psi=\varphi\exp\left(\int^{r} y\,dr\right), \quad y(r)=\frac{1}{\hbar}y_{-1}(r)+y_0(r)+\hbar y_1(r)+\dots, \quad \varphi(r)=\sum_{n=0}^{\infty}\hbar^n\varphi^{(n)}(r), \tag{2.4}$$

where the upper (lower) component $\varphi_F^{(n)}$ ($\varphi_G^{(n)}$) of the vector $\varphi^{(n)}$ corresponds to the radial wave function F (G). By substituting (2.5) into (2.4) and equating the coefficient of each power of $\hbar$ to zero, we obtain a recursive set of equations

$$\begin{aligned} &(D-y_{-1})\varphi^{(0)}=0, \\ &(D-y_{-1})\varphi^{(n+1)}=\varphi^{(n)'}+\sum_{k=0}^{n}y_{n-k}\varphi^{(k)}, \quad n=0,1,\dots \end{aligned} \tag{2.5}$$

Taking the first two equations of system (2.5) using the left- and right-vectors technique, we find the terms y_{-1}, y_0 and $\varphi^{(0)}$. Solving the next equations of the system (2.5) by a similar procedure, one can sequentially find the terms y_2, y_3,..., $\varphi^{(2)}$, $\varphi^{(3)}$,... in the expansions (2.4). However, the expressions for them are rather cumbersome and therefore, in applications one usually restricts oneself to the first terms only. Actually, the reason for this is the fact that the expansions in powers of $\hbar$ (2.4) generally do not converge but are asymptotic series with a finite

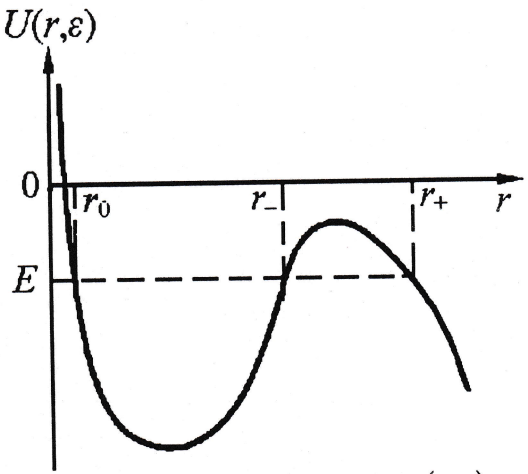

Fig. 2. The effective potential $U(r,\varepsilon)$

number of terms, which gives a good approximation for the wave function, if the parameter of an expansion (the Dirac constant $\hbar$) is rather small. So we obtained (apart from a normalisation constant)

$$\psi = \frac{1}{\sqrt{qQ_+}} \exp\left[\int^r \left(\pm q + \frac{V'(r)}{2qQ_+}\right) dr\right] \begin{pmatrix} 1+\varepsilon - V(r) \\ \mp Q_+ \end{pmatrix}, \qquad q = \left[1 + \varkappa^2/r^2 - (\varepsilon - V(r))^2\right]^{1/2}. \tag{2.6}$$

If we represent the quantity q as $q = \sqrt{2(U-E)}$, then $E = (\varepsilon^2 - 1)/2$ is the electron binding energy and

$$U(r,\varepsilon) = \varepsilon V - V^2/2 + \varkappa^2/2r^2$$

is the effective potential. For the potential

$$V(r) = -\frac{Z\alpha}{r} - Fr, \tag{2.7}$$

$U(r,\varepsilon)$ is a potential with a barrier (see Fig. 2).

The wavefunction of quasistationary states differs in the different regions.

I. The region $r_0 < r < r_-$ is classically allowed; there the wave function (2.6) oscillates.

II. The below-barrier region $r_- < r < r_+$ is classically forbidden. Here, $p=iq$ and the quantities q, y_{-1} i y_0 are real. As it is known [10], the wavefunction should exponentially decrease in this region.

III. In the region $r > r_+$, a divergent wave corresponds to the quasistationary state (emission of a positron). In order to obtain the solutions we use the usual method [10]. Close to r_- i r_+, the system (2.2) reduces to the Schrödinger equation with an effective potential which depends linearly on $r - r_\pm$, the solution of which is expressed through the Airy function, as can be seen when using the more elegant Zwaan method. As we consider the electric field F not to be strong, the normalisation of the wavefunctions can be performed by connecting the quasiclassical solutions in the below-barrier region $r_- < r < r_+$ with the asymptotic expansions of the unperturbed one-centre Coulomb wavefunction

$$\left.\begin{matrix} F_{as}(r) \\ G_{as}(r) \end{matrix}\right\} = \pm A_{as}\sqrt{1 \pm \varepsilon_0}\left[1 + B_\pm r^{-1} + \ldots\right] r^{\varepsilon_0 Z\alpha/\lambda_0} e^{-\lambda_0 r},$$

$$\varepsilon_0 = \left[1 + \frac{(Z\alpha)^2}{\left(n_r + \sqrt{\varkappa^2 - (Z\alpha)^2}\right)^2}\right]^{-1/2}, \qquad \lambda_0 = \sqrt{1-\varepsilon_0^2}.$$

Although the formulae for the wavefunctions essentially differ from the formulae in the non-relativistic quasiclassical case and are more complicated, their application for concrete problems does not create difficulties, because all quantities in the functions $F(r)$ and $G(r)$ appear quadratically.

Let us now consider the problem of quasistationary states. For the determination of the quasistationary states, the solution of the Dirac equation is usually demanded to be

a divergent wave that corresponds to a particle that is emitted from a decaying system. The required absence of a convergent solution selects complex energy eigenvalues:

$$\varepsilon_{njlm} = \varepsilon - i\frac{\tilde{A}}{2}, \tag{2.8}$$

where ε defines the position of the quasistationary level and Γ defines its width. The quantity Γ is positive and characterises the decay (ionisation) probability of quasistationary state per unit time interval: $W = \tilde{A}/\hbar$.

Neglecting the penetrability of a barrier in the region $r_- < r < r_+$ we obtain the quantization condition:

$$\int_{r_-}^{r_+}\left(p + \frac{\varkappa\omega}{pr}\right)dr = \pi\left(n + \frac{1}{2}\right), \qquad n=0, 1, 2,... \tag{2.9}$$

Equation (2.9) determines the real part ε of the level energy. It is easy to show that condition (2.13) reproduces the exact expression of the energy spectrum in the case of a Coulomb potential $V = -Z\alpha/r$ ($\alpha = e^2 \approx 1/137$ is the fine structure constant).

Let us now consider the level width $\tilde{A} = -2Im\varepsilon_{njlm}$. From equations (2.2) and the obtained formulae for F and G in the region $r > r_+$, we obtain an expression for Γ

$$\tilde{A} = \frac{1}{T}exp\left[-2\int_{r_-}^{r_+}\left(q - \frac{\varkappa\omega}{qr}\right)dr\right].$$

Let now us apply expressions (2.13), (2.14) to the Stark ionisation of an atom in a weak external constant electric field $F << 1$.
Calculating the integral in (2.13) for the potential (2.7) we obtain an equation for ε:

$$\varepsilon = \varepsilon_0 + \frac{F}{2Z\alpha}\left[\varkappa - \varepsilon_0\left(\frac{3Z^2\alpha^2}{\lambda_0^2} - \varkappa^2\right) + A\right],$$

$$A = \frac{Z\alpha\, sgn\varkappa}{\lambda_0}\left(1 - \varepsilon_0 + 2\varepsilon_0^2 - \frac{Z^2\alpha^2(1-\varepsilon_0)^2}{\varkappa^2(1+\varepsilon_0)}\right)\Bigg], \tag{2.11}$$

Note that the perturbation calculations lead to expression (2.11), where $A = 0$. (2.12)
Calculating the integral in (2.10) we obtain

$$\tilde{A} = 2\lambda_0|A_{as}|^2\left(\frac{2\lambda_0^2}{F}\right)^{\frac{2\varepsilon Z\alpha}{\lambda_0}} exp\left[-\frac{\Phi(\varepsilon)}{F} + 2Z\alpha\, arccos\varepsilon\right],$$

$$\Phi(\varepsilon) = arccos\varepsilon - \varepsilon\sqrt{1-\varepsilon^2}. \tag{2.13}$$

(2.14)

3. The Relativistic Coulomb Problem in Two Spatial Dimensions

3.1. Introduction

It is known [9, 11] that in three spatial dimensions the expression for the electronic ground-state energy in the Coulomb field of a point-charge $Z|e|$ becomes purely imaginary for $Z>137$ and that its interpretation as electron energy no longer has a physical meaning. In order to determine the electron-energy spectrum in the Coulomb field with such a charge we need to eliminate the singularity of the Coulomb potential of a point-charge at $r = 0$ by cutting off the Coulomb potential at small distances. This is equivalent to taking into account the size of the nucleus. In three space dimensions the electron-energy spectrum in the Coulomb field regulated at small distances was first considered in [12]. With increasing Z in the region $Z>137$, the electron energy levels in such a field were found to decrease, become negative, and may cross the boundary of the lower energy continuum, $E = -mc^2$. The value of $Z|e|=Z_{cr}|e|$ at which the lowest electron-energy level crosses the boundary of the lower energy continuum is called the critical charge for the electron ground state [11, 13, 14]. If Z continues to grow and enters the transcritical region with $Z>Z_{cr}$, the lowest electron energy level "sinks" into the lower energy continuum, which results in a rearrangement of the vacuum of the QED. This rearrangement is constrained by Pauli's exclusion principle. If the electron ground state at $Z<Z_{cr}$ is vacant, two electron-positron pairs are created; if it is half-occupied, one pair is created and if it is occupied, no pairs are created. The Coulomb potential is repulsive for the created positrons, so they escape the system. Hence, at $Z>Z_{cr}$ a quasistationary state appears in the lower energy continuum and the new vacuum of QED, which corresponds to the filling of all the electronic states with $E<-mc^2$, has the total electric charge $2e$ [11, 13, 14]. Indeed, all the electronic states with $E<-mc^2$ (the Dirac sea) were filled at $Z<Z_{cr}$, so electrons created by the strong Coulomb field with $Z>Z_{cr}$ cannot be described by means of a convenient wavefunction, and the notion of a charged vacuum was introduced to describe these states [13-17]. In terms of the new vacuum, the density of electric charges $\rho(r)$ is classical. It is a function which characterises the spatial distribution of the real electric charge appearing in the new (charged) vacuum, while in terms of the old (uncharged) vacuum, this function should be interpreted as the probability of two electrons (with charge $2e$) being present at a given point in space.

We would like to see how the same system behaves in two dimensions. With this aim we shall apply the WKB method to the Dirac equation in a strong Coulomb field. Such an approach works rather well for states with energy both $0< \varepsilon < 1$ and $\varepsilon < -1$ (in mc^2 units). The obtained quasiclassical formulae for the energy of quasistationary levels of solutions of the Dirac equation in the lower continuum in (2+1) dimensions allow the treatment of a wide range of problems in the theory of supercritical atoms.

3.2. The Dirac Equation in an External Coulomb Field in 2+1 Dimensions

Since [18] the Dirac algebra in (2+1) dimensions may be represented in terms of the Pauli matrices as $\gamma^0=\sigma^3$, $\gamma^k=i\sigma^k$. The Dirac equation for an electron minimally coupled to an external electromagnetic field has the form ($\hbar=c=m=1$)

$$(i\partial/\partial t - H_D)\Psi = 0, \tag{3.1}$$

$$H_D = \vec{\alpha}\vec{p} + \beta - eA^0 I = \sigma^1 p_2 - \sigma^2 p_1 + \sigma^3 - eA^0 I \tag{3.2}$$

is the Dirac Hamiltonian, $p_\mu = i\partial_\mu + eA_\mu$ is the operator of the generalised momentum of the electron, $-e$ is the electric charge of the electron ($e>0$), A_μ the vector potential of the external electromagnetic field and the conserved total angular momentum has only a single component, namely, $J_z=L_z+S_z$, where $L_z = -i\partial/\partial\varphi$ and $S_z = \sigma^3/2$.

Let us apply the Dirac equation (1), (2) to study two-dimensional hydrogen-like ions with nuclear charge $eZ >> 1$. We neglect the size of the nucleus and assume the vector potential to be a Coulomb potential

$$A^0(r) = -Ze/r, \quad A^x = A^y = 0 \tag{3.3}$$

for $0 \le r < \infty$.

We seek the solutions of the Dirac equation (1) in the field (3) in polar coordinates in the form

$$\Psi(t,\vec{x}) = \frac{1}{\sqrt{2\pi}} \exp(-i\varepsilon t + il\varphi)\psi(r,\varphi), \qquad \psi(r,\varphi) = \frac{1}{\sqrt{r}} \begin{pmatrix} F(r) \\ G(r)e^{i\varphi} \end{pmatrix} \tag{3.4}$$

where ε is the energy and l is an integer number. Note that the function (3.4) is an eigenfunction of the the Dirac Hamiltonian H_D and J_z is the total angular momentum with eigenvalues ε and $l+1/2$, respectively.

The functions $F(r)$ and $G(r)$ satisfy the equations

$$\frac{dF}{dr} - \frac{l+1/2}{r}F + (\varepsilon + 1 - V(r))G = 0, \quad \frac{dG}{dr} + \frac{l+1/2}{r}G - (\varepsilon - 1 - V(r))F = 0, \tag{3.5}$$

where $V(r) = -Z\alpha/r$ and $\alpha = e^2 \approx 1/137$ is the fine structure constant.

The exact solutions and the energy eigenvalues with $\varepsilon<1$ corresponding to stationary states of the Dirac equation may be found in full analogy to the case of three spatial dimensions [9]. Let us consider the functions F and G in the form

$$F = \sqrt{1+\varepsilon}\ e^{-\rho/2}\rho^\gamma (Q_1 + Q_2), \quad G = \sqrt{1-\varepsilon}\ e^{-\rho/2}\rho^\gamma (Q_1 - Q_2), \tag{3.6}$$

$$\rho = 2\lambda r, \qquad \lambda = \sqrt{1-\varepsilon^2}, \quad \gamma = \sqrt{(l+1/2)^2 - (Z\alpha)^2}. \tag{3.7}$$

The value of γ is to be found by studying the behaviour of the wavefunction at small values of r. The functions Q_1 and Q_2 which render the solutions of (3.6) to a finite value at $\rho=0$ are given in terms of the confluent hypergeometric function $F(a; b; z)$ as:

$$Q_1 = AF(\gamma - \varepsilon Z\alpha/\lambda, 2\gamma + 1; \rho), \qquad Q_2 = BF(\gamma - \varepsilon Z\alpha/\lambda + 1, 2\gamma + 1; \rho),$$

$$B = \frac{\gamma - \varepsilon Z\alpha/\lambda}{l + 1/2 + Z\alpha/\lambda} A.$$

It is easy to show that the following values of the quantum number n_r are allowed: $n_r=0,1,2,\ldots$, if $l \ge 0$, and $n_r=1,2,3,\ldots$ if $l < 0$. The electron-energy spectrum in the Coulomb field (3.3) is

$$\varepsilon_0 = \left[1 + \frac{(Z\alpha)^2}{\left(n_r + \sqrt{(l+1/2)^2 - (Z\alpha)^2}\right)^2}\right]^{-1/2}.$$

It can be seen that for $l=n_r=0$ ε_0 becomes zero at $Z\alpha = 1/2$, whereas in three spatial dimensions ε_0 equals zero at $Z\alpha = 1$. Thus, in two space dimensions the expression for the electron ground-state energy in the Coulomb field of a point-charge $Z|e|$ no longer has a physical meaning at a much lower value than $Z\alpha = 1/2$ and the corresponding solution of the Dirac equation oscillates near the point $r \to 0$.

In order to determine the electron-energy spectrum in the Coulomb field with the charge $2Z>137$, we need to eliminate the singularity of the Coulomb potential of a point charge at $r=0$ by cutting off the Coulomb potential at small distances of r_N. This is equivalent to taking into account the size of the nucleus. We consider the Coulomb potential in the form:

$$V(r) = \begin{cases} -\dfrac{Z\alpha}{r}, & r > r_N, \\ -\dfrac{Z\alpha}{r} f\left(\dfrac{r}{r_N}\right), & r \le r_N. \end{cases}$$

(3.8)

Here $f(x)$ is the cut-off function and $0 \le x = r/r_N \le 1$. Very often the following models are used: $f(x)=1$ and $f(x)=(3-x^2)/2$. In the given paper the first model $f(x)=1$ is considered.

In the region $r < r_N$, the finite solution at $r = 0$ of this equation is

$$F(r) = \sqrt{r} J_{|l|}(kr), \qquad G(r) = sgn\left(l + \frac{1}{2}\right) \frac{k\sqrt{r}}{\varepsilon + Z\alpha/r_N + 1} J_{|l+1|}(kr).$$

(3.9)

In the external region $r > r_N$, the potential $V(r)$ is a Coulomb potential but we take into account both signs of the quantity γ. Thus, the finite solutions at $r \to \infty$ of the Dirac system (3.6) are determined by (3.7) and the functions Q_1 and Q_2 are

$$Q_j = C_j \Psi(1/2 - \chi_j + \gamma, 2\gamma + 1; \rho), \quad j = 1,2,$$

$$\chi_1 = Z\alpha\varepsilon/\lambda + 1/2, \quad \chi_2 = Z\alpha\varepsilon/\lambda - 1/2, \quad \rho = 2\lambda r, \quad C_2/C_1 = Z\alpha/\lambda - l - 1/2,$$

(3.10)

where $\Psi(a; b; z)$ is the irregular solution of the confluent hypergeometric equation.

Matching the internal and external solutions at the point $r=r_N$ gives the equation

$$\frac{\sqrt{1-\varepsilon}}{\sqrt{1+\varepsilon}} \frac{Q_1 - Q_2}{Q_1 + Q_2}\bigg|_{r = r_N} = sgn(l + 1/2) \frac{k}{\varepsilon + Z\alpha/r_N + 1} \frac{J_{|l+1|}(kr)}{J_{|l|}(kr)},$$

(3.11)

which determines the Dirac equation spectrum. At $\varepsilon \to -1$ equation (3.11) is transcendental for Z_{cr} [19].

In order to find a solution of the Dirac equation in the energy range $\varepsilon < -1$ and for quasistationary states we apply the WKB method. It can be seen that the system (3.8) can be obtained from (2.2) by substituting $G \to -G$ and $\varkappa \to -(l+1/2)$. So it is worthwhile to use the results obtained in section 2. In this case the effective potential has the form of a potential with a barrier, too (see figure 3)

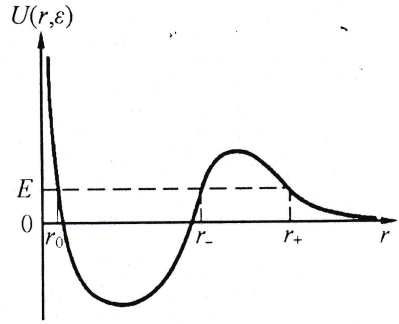

Fig. 3. The effective potential $U(r,\varepsilon)$ at $\varepsilon \le -1$.

Calculating the integral in (2.9) for the potential (3.8) and taking into account that $|\varepsilon| << Z\alpha/r_N$, we obtain the transcendental equation for ε:

$$\frac{\varepsilon Z\alpha}{2k} ln\frac{|\varepsilon| Z\alpha + kg}{|\varepsilon| Z\alpha - kg} - g ln\frac{r_N e\mu}{2g^2} + \sigma \arccos\frac{g^2 - \varepsilon\varkappa^2}{Z\alpha\mu} + I = \pi\left(n + \frac{1}{2}\right), \tag{3.12}$$

$$I = Z\alpha \int_{x_0}^{1} \left[\sqrt{f^2(x) - \frac{\rho^2}{x^2}} + \frac{\varkappa}{2(Z\alpha)^2}\left(\frac{f'(x)}{f(x)} + \frac{1}{x}\right)\frac{1}{\sqrt{x^2 f^2(x) - \rho^2}}\right] dx, \quad e = 2.718.. \tag{3.13}$$

The numerical solutions of equations (3.11)-(3.13) (for model I) for the three lowest states are shown in figure 4. Let us now pass to consider the level width $\tilde{A} = -2Im\varepsilon_{nl}$ that coincides with the probability of the spontaneous creation of positrons. Substituting the obtained quasiclassical formulae for G and F into (2.10) we have obtained

$$\tilde{A} = \tilde{A}_0 \exp\left\{-2\pi Z\alpha\left|\sqrt{1+1/k^2} - \sqrt{1-\rho^2}\right|\right\}, \tag{3.14}$$

$$T = \frac{1}{\tilde{A}_0} = -\frac{2}{k^2}\left[\varepsilon g + \frac{Z\alpha}{2k} ln\left(\frac{|\varepsilon| Z\alpha + kg}{|\varepsilon| Z\alpha - kg}\right)\right]. \tag{3.15}$$

3.3. Conclusions

In this paper, by an exact solution of the Dirac equation with a strong Coulomb field in (2+1) dimensions, we constructed the discrete energy spectrum in the range $-1 \le \varepsilon \le 1$. The WKB-solutions of the two-dimensional Dirac equation were

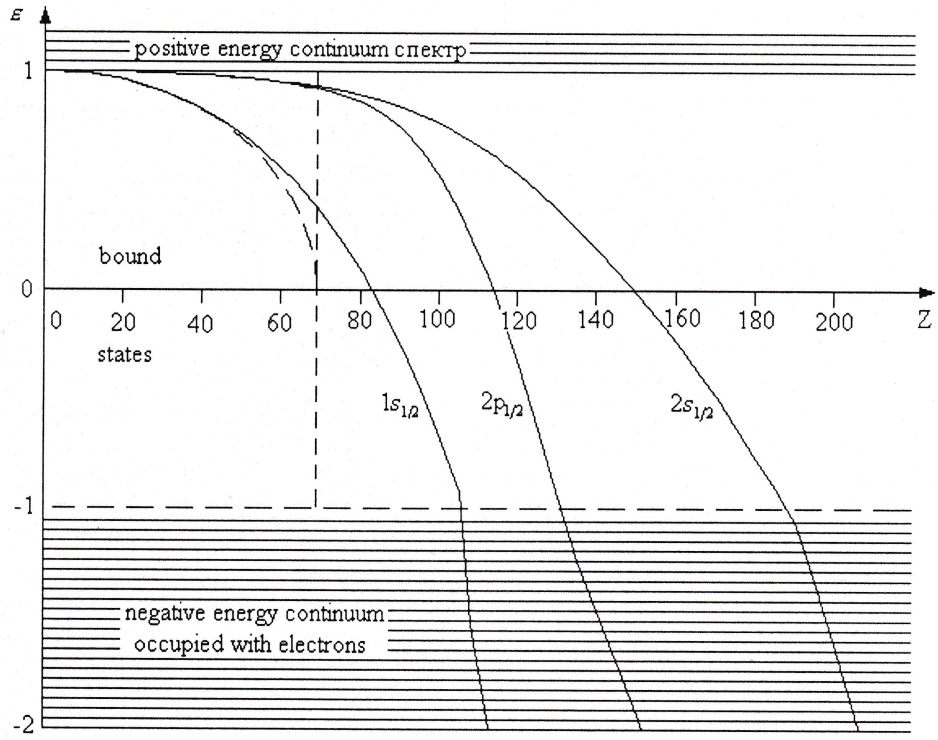

Figure 4: The energy eigenvalues of the Dirac system (3.6) manifest the three thresholds for the nuclear charge number Z: (I) at $Z \approx 1372$ solutions with l=0 dissappear for point nuclei (dashed curves), (II) at $Z \approx 83$ the 1s binding energy balances the electron rest mass if one takes into account the finite size of the nuclei (full curves), and (III) at the critical charge number $Z_{cr} \approx 107$ the 1s state enters the negative energy continuum.

obtained. Using the obtained quasiclassical formulae we find the spectrum of quasistationary levels (its position and width) in the lower energy continuum $\varepsilon < -1$ for a spherical superheavy nucleus with a charge $Z > Z_{cr}$ (see figure 4). The comparison of the values for a critical charge Z_{cr} which are obtained from exact solutions of the Dirac equation with Z_{cr} obtained from the quasiclassical formulae (3.12), (3.13), shows a good agreement (see figure 2). Note that in the ground state for the model I at r_N=0.03 $Z_{cr} \approx 107$ and 170 in (2+1)- and (3+1)-dimensional QED, respectively. Thus, the Dirac vacuum in two spatial dimensions in the presence of a strong Coulomb field is unstable against electron-positron production at significantly smaller values of the critical charge than in the case of three spatial dimensions. Another difference between these two cases results from the fact that electrons confined to a plane behave like a spinless fermion. So if the electronic ground state at $Z < Z_{cr}$ is vacant, one pair is created; if it is occupied, no pairs are created.

Task T2

4. Measurement and R-matrix Calculation of Electron-Impact De-Exitation of the $(3s3p)^3P_{0,1,2}$ States in Mg

In the performed investigation the energetic dependence of the cross section of the superelastic electron in collisions with metastable Mg atoms was determined for the first time [20]. In our experiments the superelastically scattered electrons were detected and the energy dependence of their formation cross section (Q^s) was determined by measuring the ratio of the current (i^s) of the scattered electron to the electron beam current (i_e), i.e. $Q^s = i^s/i_e$. In [21] the dependence of the superelastic electron scattering cross section on the electron energy is presented. The relative uncertainty in determining Q^s was ~ 8%, the energy scale calibration error 0.1 eV.

Magnesium atoms have two triplet metastable states 3s3p $^3P_0$, 3s3p $^3P_2$ with excitation energies of 2.71 eV and 2.72 eV. Both of these metastable states were present in the atomic beam with a the ratio of their concentration $N^m(3s3p\ ^3P_0) / N^m$ (, 3s3p $^3P_2$) = 1/5.

As a result of superelastic electron scattering, atoms may decay from the metastable state into the ground state $3s^2\ ^1S_0$. The corresponding reactions can be written in the form:

$$e + \mathrm{Mg}(3s3p\ ^3P_0) \rightarrow \mathrm{Mg}(3s^2\ ^1S_0) + e', \tag{4.1}$$

$$e + \mathrm{Mg}(3s3p\ ^3P_2) \rightarrow \mathrm{Mg}(3s^2\ ^1S_0) + e'', \tag{4.2}$$

where e is the incident electron with the energy E; e' and e'' are superelastically scattered electrons with energies of (E+2.71) eV and (E+2.72) eV. Taking into account that the difference between the energies of the scattered electrons is 0.01 eV, it must be said that the resulting cross section reflects an average cross section of reactions (4.1) and (4.2).
In order to explain the phenomenon of superelastic electron scattering in collisions with metastable atoms, the following model has been developed. According to it, the superelastic process proceeds by the following scheme:

$$e^-(E) + A_j^* \rightarrow A^{-*} \rightarrow \tilde{e}^-(E + \Delta E) + A_i^*, \tag{4.3}$$

where A^{-*} is the negative ion in the excited state.

For Mg atoms the reaction can be written in the following way:

$$\begin{aligned} e(E) + \mathrm{Mg}(3^3P_2) \rightarrow \mathrm{Mg}^- &\rightarrow \mathrm{Mg}(3\ ^3P_2) + e(E); \\ &\rightarrow \mathrm{Mg}(3\ ^1S_0) + e(E+\Delta E_1); \\ &\rightarrow \mathrm{Mg}(3\ ^3P_0) + e(E+\Delta E_2); \\ &\rightarrow \mathrm{Mg}(3\ ^1P_1) + e(E+\Delta E_3); \end{aligned} \tag{4.4}$$

$$\downarrow\!\rightarrow \mathrm{Mg}(3\,{}^1S_0) + h\nu.$$

We are limited only by the consideration of the metastable $3\,{}^3P_2$-state.

In our experiments negative ions were detected and the energy dependence of their formation cross section (Q_i^-) was determined by measuring the ratio of the negative-ion current (i^-) to the electron beam current (i_e), i.e. $Q_i^- = i^-/i_e$.

We used a R-matrix method with pseudo-states [22] in a 35-state intermediate-coupling approximation for the calculation of the electron-impact excitation cross sections in neutral Mg. A configuration-interaction representation with frozen core was used for the outer electrons of the target. The close-coupling expansion includes the 21 physical target states and 14 pseudo-states in the *LSJ* -coupling scheme.

The pseudo-states are introduced in the close-coupling expansion to represent, in some artifcal way, the remaining infinite number of bound states and continuum states of the target, which could not be included directly. In cases when the convergence of the close-coupling expansion is slow, these states can lead to considerable corrections. There is no unique way to determine the pseudo-states and different authors use different methods. In one of the more often used methods the states are obtained by diagonalisation of the model Hamiltonian in the final basis of some functions, e.g., the Laguerre functions, Slater functions and so on. In a more general way the higher-lying eigenvalues obtained from diagonalisation of the target Hamiltonian are used as pseudo-states. In CI calculations we obtain many eigenstates, where the first of them reproduce the low-lying physical states rather well. The rest of eigenvalues has energies which do not agree with any specific state and can be considered as pseudo-states, which represent, in some average manner, the residual states (both bound and continuum) of the target. This procedure was applied for Mg, where we use orbitals of Mg^+ for the construction of a basis set. The unsolved question is the accuracy of this representation because the number of pseudo states and their position strongly depends on the basis functions.

The present calculations are a direct extension of our previous *LS* calculations [23] of electron-impact excitation of the Mg atom to the case of intermediate coupling and have been undertaken in support of recent measurements of super-elastic scattering on the metastable 3s3p $^3P_{0,2}$ levels of Mg, as described above.

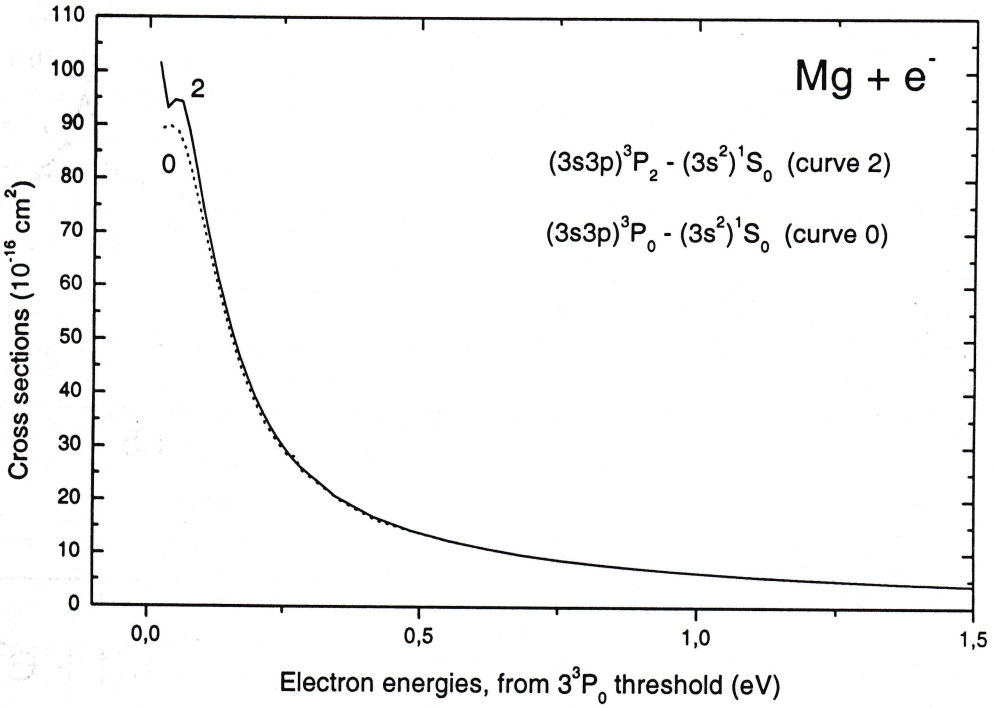

Figure 5: The de-excitation $(3s3p)^3P_{0,2}$ - $(3s^2)^1S_0$ cross sections: —— - $^3P_2$ - $^1S_0$ transition; ------ $^3P_0$ - $^1S_0$ transition.

In the experiment the part of the integral cross section for super-elastic scattering in the range of scattering angles from 0 to ~0.5 rad was measured. The energy dependence of these cross sections for super-elastic scattering from metastable $3^3P_{0,2}$ states of the Mg atom was obtained in the near-threshold region.

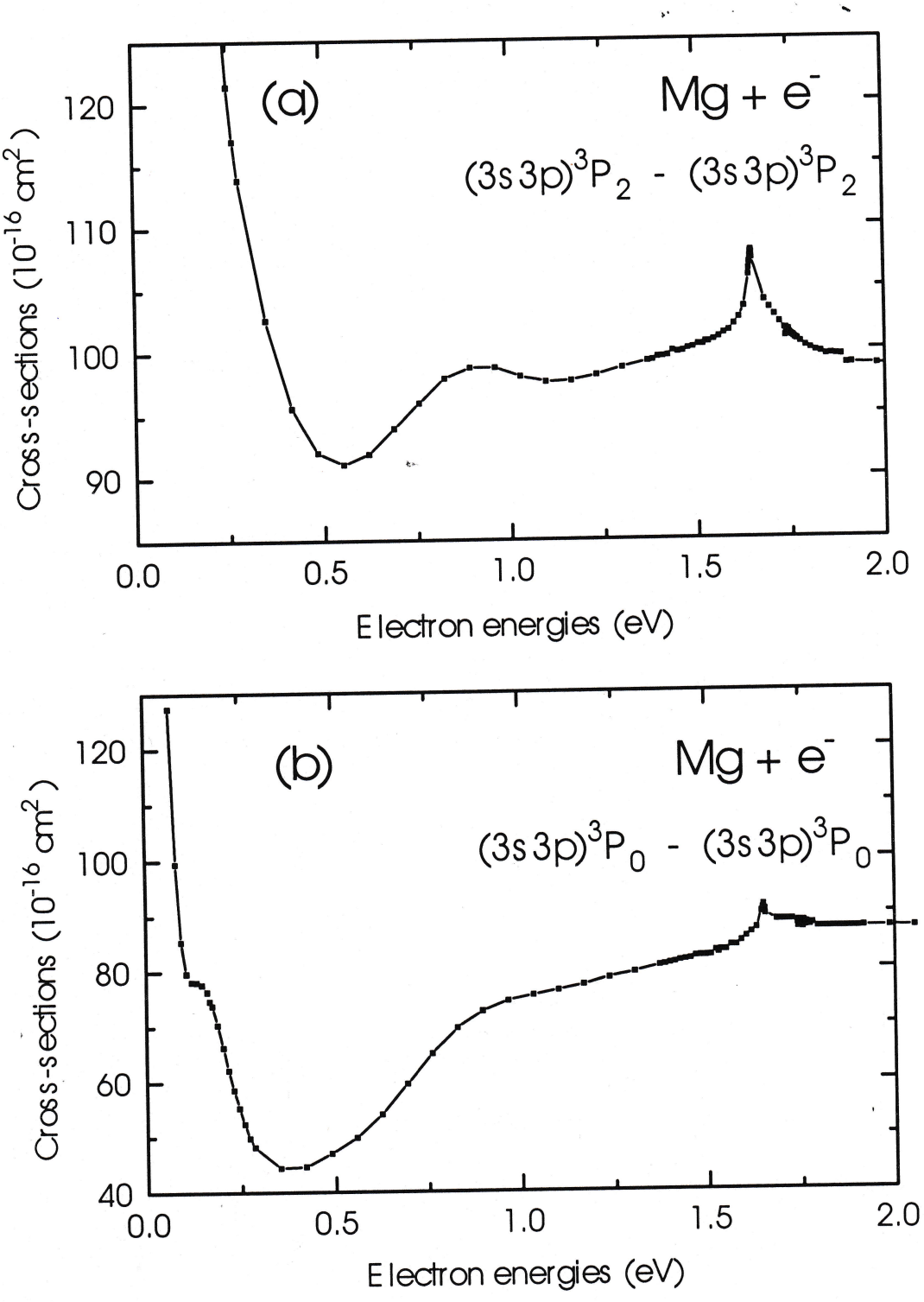

Figure 6: Excitation cross sections for the $(3s3p)^3P_2$ - $(3s3p)^3P_2$ elastic collision processes with the 3^3P_2 metastable state.

The results of our calculations for the $(3s^2)^1S_0$ - $(3s3p)^3P_0$, $(3s^2)^1S_0$ - $(3s3p)^3P_1$, $(3s^2)^1S_0$ - $(3s3p)^3P_2$ transitions and comparing the theoretical cross sections for the transition $(3s3p)^3P_2$ - $(3s^2)^1S_0$ with the relative measurements were represented in previous INTAS report. The $(3s3p)^3P_{0,1,2}$ - $(3s^2)^1S_0$ de-excitation integral cross sections is presented on Fig.5. As it is visible from a Fig.5, the de-excitation cross sections for transitions $(3s3p)^3P_0$ - $(3s^2)^1S_0$ and $(3s3p)^3P_2$ - $(3s^2)^1S_0$ iterate one another almost exactly. The small differences are watched during cross sections are watched only in area near a threshold. Let's mark, that the cross section of transition $(3s3p)^3P_1$ - $(3s^2)^1S_0$ essentially also coincides cross section of transition $(3s3p)^3P_0$ - $(3s^2)^1S_0$. As the course of a curves smoothly varying, without availability of any structure is visible from a figure, in the field of 0.5 eV see. It is qualitatively a course of integral cross section iterates a course of toted differential cross section for the transition $(3s3p)^3P_2$ - $(3s^2)^1S_0$. Apparently, for explanation of qualitative difference of the theory with experiment in the field of energies smaller ~0.5 eV it is necessary to conduct padding examinations.

In a Fig. 6 the cross sections of an elastic scattering for states $(3s3p)^3P_2$ (Fig. 6(a)) and $(3s3p)^3P_0$ (Fig. 6(b)) represented. The availability on a curves of transitions $(3s3p)^3P_0$ -$(3s3p)^3P_0$ and $(3s3p)^3P_2$ - $(3s3p)^3P_2$ of a broad sag with a minimum in the field of 0.4 - 0.5 eV can obliquely testify to formation of an negative ion of magnesium. The subsequent decay of this ion in underlying states can result in to diminution of sections of elastic collisions.

So, it is possible to make some deductions:

1) The experimental measurements of cross sections of formation of negatively ionized Mg-atoms, functions of excitation of spectral transition $(3s^2)^1S_0$ -$(3s3p)^3P_1$ and differential cross sections of an elastic scattering testify to availability of particular structure in the field of energies ~0.5 above a threshold of excitation. The origin of this structure can be bound to formation of a negative ion of magnesium, though, basically, the opportunity of the contribution and other effects is not eliminated.

2) The theoretical calculations of differential sections conducted in *LSJ* coupling approach, and integrated on angles, practically have coincided with experiment (to within 10 %) in the field of energies from 2 up to 0.5 eV. However, to detect structures apparent on experiment, it was not possible to us. Probably, it is bound to features and (/or) deficiencies of theoretical approach, used by us. The area of conducted examinations is very close to a threshold, where manifestation of different threshold effects, as is known, is possible. At the same time, the availability of sags on curves of excitation cross sections of a elastic transitions $(3s3p)^3P_0$ -$(3s3p)^3P_0$ and $(3s3p)^3P_2$ - $(3s3p)^3P_2$ in the area of 0.5 eV can obliquely testify to formation of negatively ionized atoms of magnesium and, thus, confirm experiment.

In any case, as mentioned above, it is desirable to conduct padding examinations, both experimental, and theoretical, with the purpose of clearing up of the mechanism of process of excitation from metastable states by electron impact in threshold region.

References

1. I. V. Komarov, L. I. Ponomarev, and S. Yu. Slavyanov, Spheroid and Coulomb Spheroid Functions [in Russian], (Moscow: Nauka 1976).
2. L. Hostler, R. K. Pratt, *Phys. Rev. Lett.* **10,** 469 (1963); L. J. Hostler, *J.Math.Phys.* **5,** 591 (1964)
3. D.I. Abramov, S. Yu. Slavyanov, *J.Phys B* **11**, 2229 (1978).
4. B. J. Laurenzi, *J. Chem. Phys.* **55,** 2681 (1971).
5. C. Flammer, *Spheroidal Wave Functions* (Stanford, California 1957.)
6. P.M. Morse, H. Feshbach, *Methods of Theoretical Physics Vol.1* (New York: McGrew-Hill 1953).
7. H. Bateman, A. Erdelyi, *Higher Transcendental Functions Vol.1* (New York: McGraw-Hill 1953).
8. L.I. Ponomarev, T.P. Puzynina. *Quantum mechanical, two Coulomb centre problem III. Tables of terms.* (Preprint P4-3175. Dubna, 1967).
9. V.B. Berestetskii, E.M. Lifshitz, L.P. Pitaevskii, *Quantum Electrodynamics* (Oxford: Pergamon Press, 1982).
10. L.D. Landau, E.M. Lifshitz, Course of Theoretical Physics, v. 3, Quantum Mechanics. Non-Relativistic Theory, (London-Paris: Pergamon Press, 1958).
11. A.A. Grib, S.G. Mamaev, V.M. Mostapenko, Vacuum quantum effects in strong fields, (Moscow: Energoatomizdat, 1988).
12. I. Pomeranchuk, Ya. Smorodinsky, *J. Phys. USSR*, **9**, 97, (1945).
13. Ya.B. Zel'dovich and V.S. Popov, *Sov. Phys. Uspekhi*, **14**, 673, (1972).
14. A.B. Migdal, Fermions and bosons in strong fields, (Moscow: Nauka, 1978).
15. J. Reinhardt, W. Greiner, *Rep. Prog. Phys*, **40**, 219, (1977).
16. J. Rafelski, L.P. Fulcher, A. Klein., *Phys. Rep. C*, **38**, 227. (1978).
17. M. Soffel, B. Mueller, W. Greiner, *Phys. Rep.C*, **85**, p. 51, (1982).
18. A. Neagu and A.M.J. Schakel, *Phys.Rev. D*, **48**, 1785, (1993).
19. V.R. Khalilov and C.L. Ho, *Mod. Phys. Lett. A*, **13**, 615, (1998).
20. K. Bartschat, P. Burke, and M.P. Scott. *J. Phys. B*, **30**, 5915, (1997).
21. V. Gedeon, V. Lengyel, O. Zatsarinny, and C.A. Kocher, *Phys. Rev. A*, **59**, 2016, (1999).
22. I.I. Shafranyosh, V.I. Marushka, *Uzhhorod Univ. Scien. Herald, Series Physics*, Issue 8, Part 1, 125 (2000), (in Ukraine).
23. I.I. Shafranyosh, V.I. Marushka, *Journal of Physical Studies,* **4**, 415 (2000), (in Ukraine).

List of scientific publications

1. The Quantum-Mechanical Two-Coulomb-Centre Problem in the Dirac Equation Framework, O.K. Reity, V.Yu. Lazur, and A.V. Katernoha, J. Phys. B, 35 (2002), P. 1–17.
2. Asymptotic Methods in Relativistic Problems with Unseparable Variables, V.Yu. Lazur, O.K. Reity, A.V. Katernoha, Uzhhorod University Scientific Herald, Series Physics, Issue 7, P. 70-76, (2000), (*in Ukrainian*).
3. The Relativistic Hydrogen-Like Atom in 2+1 Dimensions, O.K. Reity, V.Yu. Lazur, is accepted for publication in Uzhhorod University Scientific Herald, Series Physics, Issue 9, (2001), (*in Ukrainian*).
4. Measurement and R-Matrix Calculation of Electron-Impact Deexcitation of the $(3s3p)^3p_{0,2}$ States in Mg, V.I. Marushka, I.I. Shafranyosh, V.F. Gedeon, V.Yu. Lazur, T.A. Zatsarinna, O.I. Zatsarinny and T.M. Zajac, Uzhhorod University Scientific Herald, Series Physics, Issue 9, (2001), (*accepted for publication*).
5. The Relativistic Two-Coulomb-Centre Problem at Small and Large Inter-Centre Separations, O.K. Reity, V.Yu. Lazur, Ukrainian Journal of Physics, Issue 3, (2002), (*accepted for publication*).

6. WKB Method for the Dirac Equation with Central-Symmetrical Potential and Its Application to the Theory of Two-Dimensional Supercritical Atoms, O.K. Reity, V.Yu. Lazur, Proceedings of Institute of Mathematics of NAS of Ukraine, (2002), (*accepted for publication*).
7. Asymptotic Expansions of the Potential Curves in the Relativistic Quantum-Mechanical Two-Coulomb-Centre Problem, O.K. Reity, Proceedings of Institute of Mathematics of NAS of Ukraine, (2002), (*accepted for publication*).
8. Green Function of the Problem of Two Coulomb Centers with Identical Charges, V.Yu. Lazur, M.V. Khoma, M.I. Karbovanets, Ukrainian Journal of Physics, 2001, 46. No 11, P.1201-1211. (*In Ukrainian*)
9. On the Asymptotic Solutions of the Two Coulomb Centers Problem at Small Intercenter Separation, V. Lazur, M. Khoma, M. Karbovanets, Ukrainian Journal of Physics, 2002, 47. No 3. (*accepted for publication*)
10. Green Function of the Model Two Center Quantum-Mechanical Problem, M.V. Khoma, V.Yu. Lazur, Journal of Physics Studies, 2002, 4. (*Accepted For Publication*)
11. Green Function of the Three Coulomb Centers in the Study of Inelastic Processes at Slow Ion-Molecule Collisions, M.V. Khoma, Lviv National University Scientific Herald, Series Physics, No 34, P.185-191.
12. Green Function for a Model Two-Centre Potentials in Molecular Physics, M.V. Khoma, Uzhhorod National University Scientific Herald, Series Physics, 2001, No 10, P.96-101.

Participation in conferences

1. O. K. Reity, V. Yu. Lazur. WKB method for the Dirac equation with central-symmetrical potential and its application to the theory of two dimensional supercritical atoms// Fourth International Conference "Symmetry in Nonlinear Mathematical Physics", July 9-15, 2001, Kiev, Ukraine.
2. O. K. Reity. Asymptotic Expansions of the Potential Curves in the Relativistic Quantum-mechanical Two-Coulomb-Centre Problem// Fourth International Conference "Symmetry in Nonlinear Mathematical Physics", July 9-15, 2001, Kiev, Ukraine.
3. A. V. Katernoha, V. Yu. Lazur, O. K. Reity. Asymptotic Methods in the Relativistic Two-Coulomb-Centre Problem// XXII International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC 2001), July 18-24, 2001, Santa Fe, New Mexico, USA.
4. O. K. Reity, V. Yu. Lazur. The relativistic Coulomb problem in two spatial dimensions// The Ukrainian Mathematical Congress, 21-23 серпня, 2001 р., Київ, Україна.
5. O.K. Reity, V.Yu. Lazur. WKB Method for the Dirac Equation with a Strong Coulomb Field and Its Application to the Theory of Two-Dimensional Supercritical Atoms// Small Triangle Meeting, September 25-26, 2001, Košice, Slovakia.
6. M.V. Khoma *Green Function of the Three Coulomb Centers in the Study of Inelastic Processes at Slow Ion-Molecule Collisions* // International Students and Young Scientist Conference in Theoretical and Experimental Physics EURECA-2001, 16-18 May, Lviv, Ukraine.
7. M V Khoma *Green Function for a Model Two-Centre Potentials in Molecular Physics* // International Young Scientist Conference IEP-2001, 11-13 October, Uzhhorod, Ukraine.
8. V Yu Lazur, M.V. Khoma, M.I. Karbovanets Two-Coulomb Centre Green Function in the Application for Inelastic Slow Ion-Molecule Collisions // XXII International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC 2001), July 18-24, 2001, Santa Fe, New Mexico, USA.