

# How uncertainties in the atomic potential affect DIRAC results

Mikhail Zhabitsky

Joint Institute for Nuclear Research, Dubna, Russia

December 8, 2014

## Abstract

DIRAC experiment reconstructs lifetime of  $\pi^+\pi^-$  atoms ( $A_{2\pi}$ , ponium) through the measurement of their ionization (break-up) probability  $P_{\text{ion}}$  in a thin target. Method relies on the fact that dependence  $P_{\text{ion}}(\tau)$  can be calculated with sufficient precision. The value of  $P_{\text{ion}}$  is a result of competitive processes: ponium annihilation vs. ponium ionization in the Coulomb field of target atoms. This note estimates impact of uncertainties in the potential of a target atom on DIRAC results.

## 1 Interaction of the ponium with targets atoms

To calculate coherent scattering of a ponium on a target atom we use the first Born approximation [1]:

$$\sigma_i^f = \frac{1}{2\pi\beta^2} \int_0^\infty |U(\vec{q})|^2 |F_{if}(\vec{q}/2) - F_{if}(-\vec{q}/2)|^2 q dq. \quad (1)$$

Here  $i$  and  $f$  are initial and final ponium states,  $\beta$  — the ponium velocity,  $F_{if}$  is the ponium form factor as a function of the momentum transfer  $\vec{q}$ ,  $U(\vec{q})$  stands for the target atomic potential (see Sec. 2).

By using completeness of the atomic states basis [1]

$$\sum_f |F_{if}(\vec{q}/2) - F_{if}(-\vec{q}/2)|^2 = 2 - 2F_{ii}(\vec{q}), \quad (2)$$

one can derive the total cross section for the ponium to transit from the initial state  $i$  into any bound state or to get ionized [1]

$$\sigma_i^{\text{tot}} = \sum_f \sigma_i^f + \sigma_i^{\text{ion}} = \frac{1}{\pi\beta^2} \int_0^\infty |U(\vec{q})|^2 (1 - F_{ii}(\vec{q})) q dq. \quad (3)$$

## 2 Atomic potential

The atomic form factor as a function of the momentum transfer is the Fourier transform of its  $U(\vec{r})$  representation:

$$U(\vec{q}) = \int U(\vec{r}) e^{i\vec{q}\vec{r}} d^3r. \quad (4)$$

For a spherically symmetrical atom

$$U(q) = 4\pi \int_0^\infty U(r) \frac{\sin(qr)}{qr} r^2 dr. \quad (5)$$

The electrostatic atomic potential of a neutral atom with a nucleus as a point charge  $Z$

$$U(r) = \frac{Z}{r} + \int_0^\infty \frac{\rho(r')}{\max\{r, r'\}} d^3r' = \frac{Z}{r} + \frac{4\pi}{r} \int_0^r \rho(r') r'^2 dr' + 4\pi \int_r^\infty \rho(r') r' dr' = \frac{Z}{r} \phi(r), \quad (6)$$

where  $\rho(r)$  — the radial atomic electron density. Screening function  $\phi(r)$  is linked to the atomic density through Poisson's equation

$$\nabla^2 U(r) = -4\pi\rho(r), \quad (7)$$

$$\frac{d^2\phi(r)}{dr^2} = -\frac{4\pi r}{Z}\rho(r). \quad (8)$$

So as soon as the electron density  $\rho(r)$  is defined, the atomic potential  $U(q)$  is determined.

For completeness

$$F(q) = 4\pi \int_0^\infty \rho(r) \frac{\sin(qr)}{qr} r^2 dr \quad (9)$$

is an atomic form factor for a spherically symmetrical atom.

In this work we use cubic-spline interpolation to reconstruct the accurate electronic density  $\rho_{\text{DF}}$  from tabulated densities provided with ELSEPA program [2], where electron densities  $\rho_{\text{DF}}$  for free atoms were calculated by [3] through the self-consistent multiconfiguration relativistic Dirac-Fock (DF) method. This approach is compared to simple analytic approximations of the electronic density.

## 2.1 Analytic models to approximate the atomic potential

There is a simple analytic approximation [4], which describes the electrostatic atomic potential by a sum of three Yukawa potentials (this class of approximations is often called the Molière-like parametrization). In this approach the screening function  $\phi(r)$  has a simple form [4]:

$$\phi(r) = \sum_{i=1}^3 A_i e^{-\alpha_i r}. \quad (10)$$

Corresponding parametrization for the electron atomic density is

$$\rho(r) = -\frac{Z}{4\pi r} \sum_{i=1}^3 A_i \alpha_i^2 e^{-\alpha_i r}. \quad (11)$$

For the atomic form factor and the atomic potential:

$$F(q) = -Z \sum_{i=1}^3 \frac{A_i \alpha_i^2}{q^2 + \alpha_i^2}, \quad (12)$$

$$U(q) = 4\pi Z \sum_{i=1}^3 \frac{A_i}{q^2 + \alpha_i^2}. \quad (13)$$

Normalization

$$4\pi \int_0^\infty \rho(r) r^2 dr = Z \Rightarrow F(0) = Z \Rightarrow \sum_{i=1}^3 A_i = 1. \quad (14)$$

Thus a Molière-like potential is described by five parameters.

Coefficients  $\alpha_i$  and  $A_i$  for the Molière-like parametrization of the Dirac-Hartree-Fock-Slater (DHFS) potential are tabulated in [4] for atoms in the range  $Z = 1 \div 92$  (see Tab. 1 for elements used in DIRAC as target's materials).

The original Molière parametrization [5] of a screening function for the Thomas-Fermi potential reads

$$\phi_{\text{TFM}}(r) = \sum_{i=1}^3 B_i e^{-\beta_i r/b}, \quad (15)$$

Table 1: Parameters of the Molière-like parametrization of the Dirac-Hartree-Fock-Slater (DHFS) potential [4]

$Z$	$A_1$	$A_2$	$\alpha_1$	$\alpha_2$	$\alpha_3$
4	0.3278	0.6722	4.5430	0.9852	
28	0.0474	0.7294	34.758	3.8299	1.2209
78	0.2230	0.6176	22.994	3.7346	1.4428

where  $b = \frac{(3\pi)^{2/3}}{2^{7/3}}Z^{-1/3} = 0.885Z^{-1/3}$  in atomic units and

$$B_1 = 0.35, \quad B_2 = 0.55, \quad B_3 = 0.10, \quad (16)$$

$$\beta_1 = 0.3, \quad \beta_2 = 4\beta_1, \quad \beta_3 = 20\beta_1. \quad (17)$$

TFM screening function is described by two parameters and is universal for all elements heavier than helium. Corresponding electron density, atomic form factor and potential are

$$\rho_{\text{TFM}}(r) = -\frac{Z}{4\pi r b^2} \sum_{i=1}^3 B_i \beta_i^2 e^{-\beta_i r/b}, \quad (18)$$

$$F_{\text{TFM}}(q) = -Z \sum_{i=1}^3 \frac{B_i \beta_i^2}{b^2 q^2 + \beta_i^2}, \quad (19)$$

$$U_{\text{TFM}}(q) = 4\pi Z \sum_{i=1}^3 \frac{B_i}{q^2 + \beta_i^2/b^2}. \quad (20)$$

As shown on Fig. 1 electron radial densities and corresponding form factors for simple Molière-like approximations are significantly different from corresponding distributions calculated through more accurate Dirac-Fock method. Nevertheless for the atomic potential  $U(q)$  these differences are mostly cancelled during integration (5). The Molière-like parametrization of the DHFS potential is much closer to the accurate solution, while the Thomas-Fermi-Molière potential diverges away from it already at distance of the order of one atomic unit.

Numerical integration (Eqs. 6 and 1) was performed by the Gauss-Kronrod adaptive method while the Fourier transform (5) — through the indefinite integration of oscillatory functions using the Chebyshev series expansion. Computer codes incorporated in GNU Scientific Library have been used to calculate above integrals.

Integration towards cross sections (1) and (3) is effectively the triple integral. To control numeric precision, the Molière-like atomic density (11) was tabulated on the same grid as  $\rho_{\text{DF}}$  and the result of the triple integral was compared to the result obtained by using the analytic atomic potential (13). Relative precision of the triple integral is better than  $10^{-4}$ .

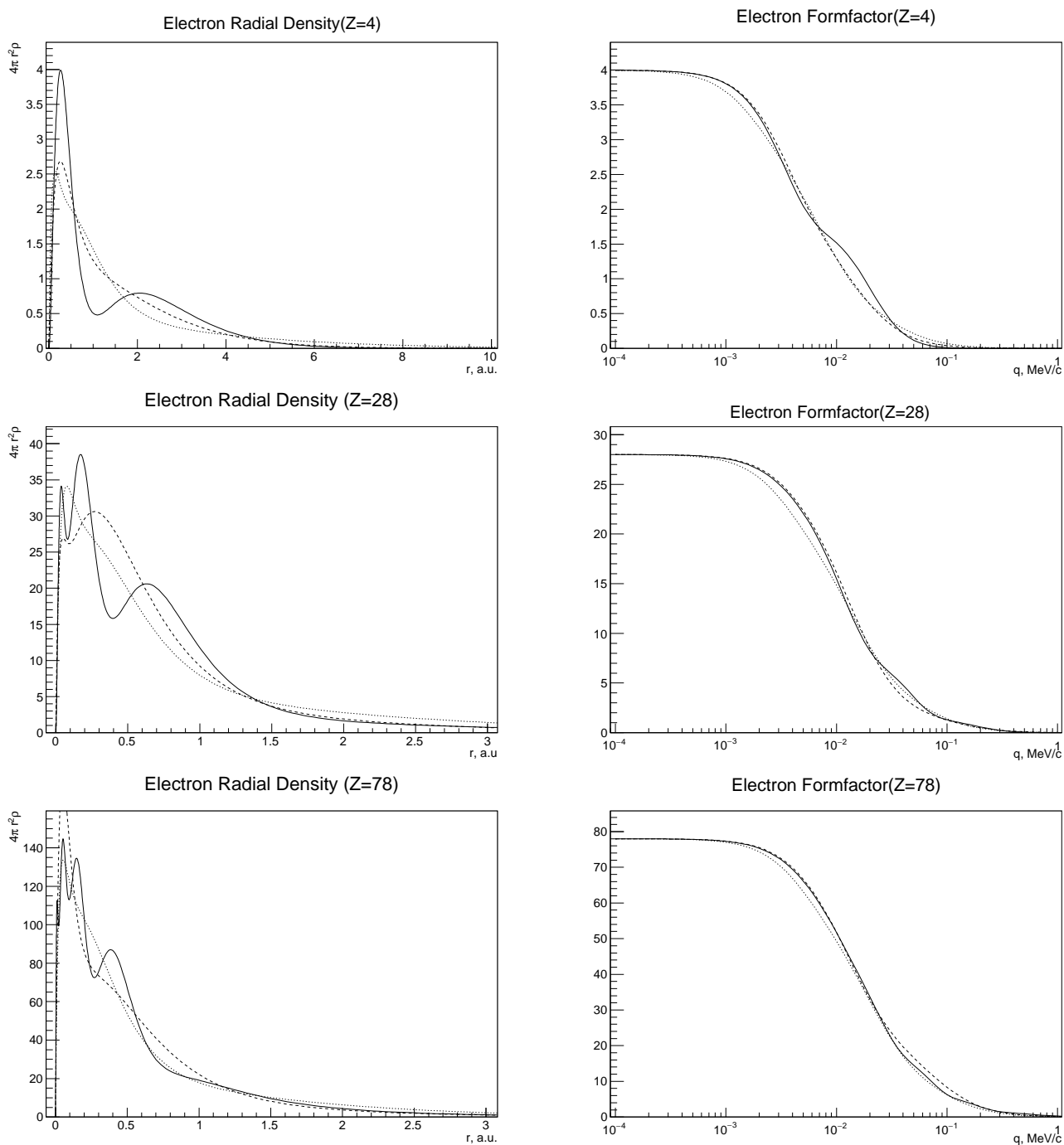


Figure 1: Electron radial densities (left) and corresponding atomic form-factors (right). Dirac-Fock (solid line), the Molière parametrization of DHFS (dash line), the Molière parametrization of TF (dotted line).

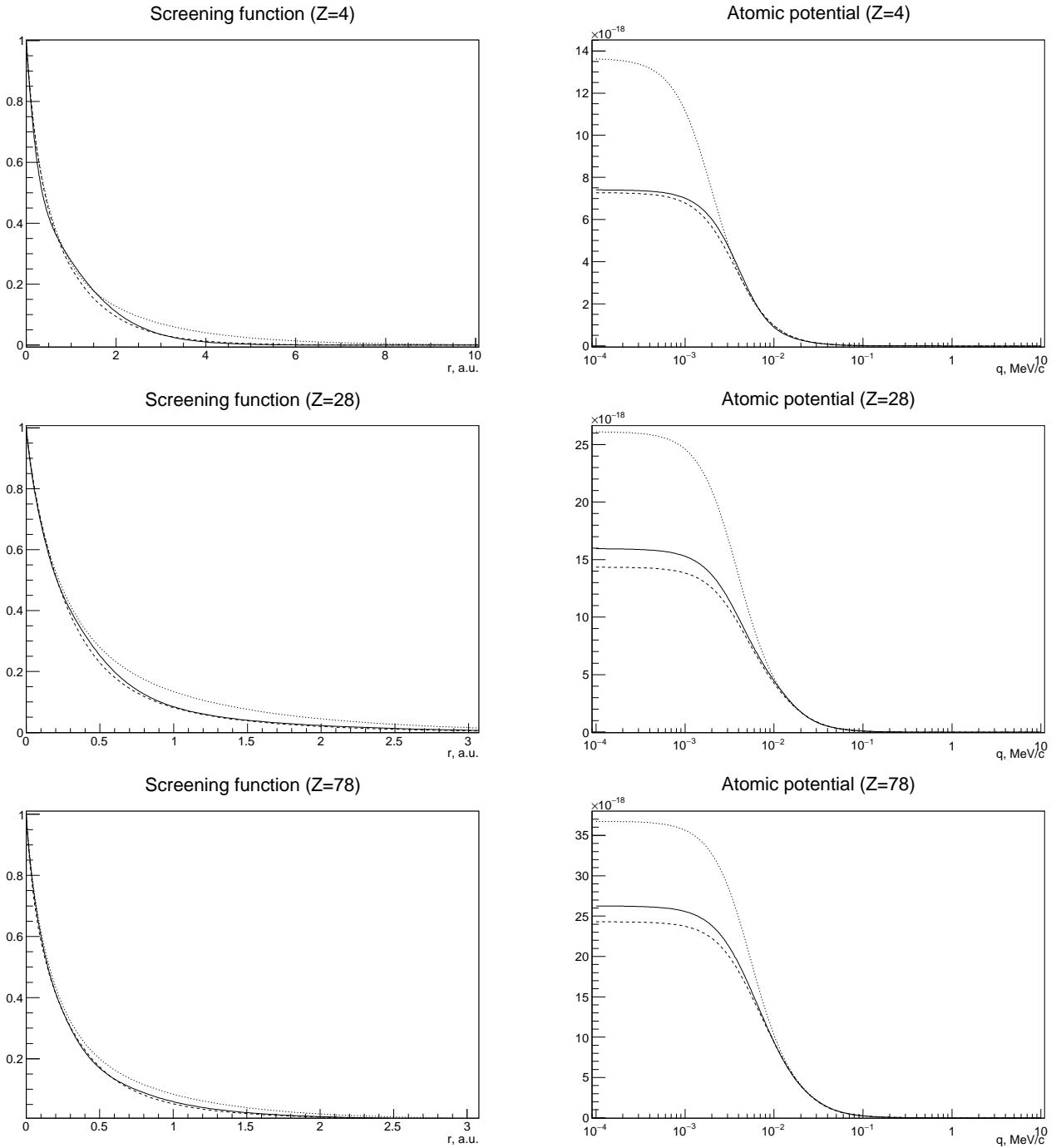


Figure 2: Atomic potentials (left) and corresponding  $U(q)$  (right). Dirac-Fock (solid line), the Molière parametrization of DHFS (dash line), the Molière parametrization of TF (dotted line).

### 3 Impact on DIRAC results

Use of different potentials modifies the integrand in (3) as shown in Fig. 3. Results for the total coherent cross-section of pionium in 1S state for different potential models and different target materials are in Tab. 2. Relative error in 1S total cross sections is less than 0.02.

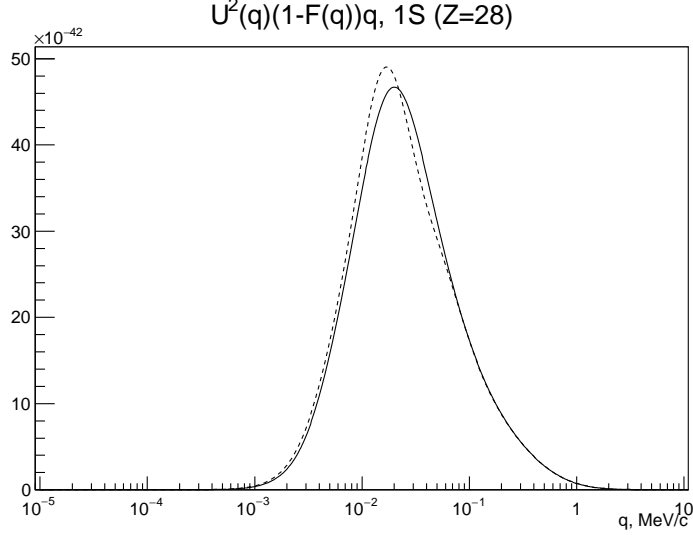


Figure 3: Integrand for the total coherent cross-section from 1S state: Dirac-Fock (solid line), the Molière-like parametrization of the DHFS potential (dash line).

Table 2: Total coherent cross-sections from 1S state for different potential models

$Z$	TFM	Molière-DHFS	Dirac-Fock
4	1.350e-22	1.359e-22	1.335e-22
28	5.599e-21	5.577e-21	5.528e-21
78	3.932e-20	3.769e-20	3.841e-20

We calculated all total and transition coherent cross-sections for pionium interacting with different targets in the parabolic basis upto the principal quantum  $n_{\max} = 8$ . It leads to an estimation of uncertainty in the probability of pionium ionization due to simplifications in potential models (Tab. 3). Cited probabilities are for the so-called maximal probability of ionization [6]. As expected uncertainty due to use of approximate potential models is worse for light- $Z$  Be than for heavier targets, like Ni or Pt.

Calculations of the ionization probability  $P_{\text{ion}}$ , shown in Tab. 3, don't include incoherent scattering on target atoms. Incoherent scattering (target atoms excitation) contributes about 4% for Ni [9], almost negligible for Pt, but amasses more than 1/3 of the cross-section value for Be.

Table 3: Uncertainty in  $P_{\text{ion}}^*$  due to simplifications in  $U(q)$  ( $\tau = 2.9$  fs,  $n_{\max} = 8$ ,  $P_A = 4.5$  GeV/c)

Rel. uncertainty: $\delta = P_{\text{ion}}/P_{\text{ion}}(\text{Dirac-Fock}) - 1$						
$Z$	$s, \mu\text{m}$	Dirac-Fock	TFM	$\delta\text{TFM}, 10^{-2}$	M-DHFS	$\delta\text{M-DHFS}, 10^{-2}$
4	103.3	0.050652	0.051555	1.78	0.051778	2.22
28	108	0.46038	0.46319	0.61	0.46226	0.41
78	25.7	0.70976	0.71484	0.72	0.70564	-0.58

\* — only coherent scattering is taken into account

## 4 Discussion and Conclusions

So far there was a lot of work to increase precision in calculations of cross-sections and the probability of pionium ionization in the target, which include multiphoton exchange, density-matrix formalism and so on (see the review article [7] for references). Authors used either the Thomas-Fermi-Molière potential [8] or a more advanced Molière parametrization of the Dirac-Hartree-Fock-Slater potential [9]. Ultimate goal for DIRAC is to know  $P_{\text{ion}}(\tau)$  relation with precision better than 1%, otherwise this uncertainty will constitute a major systematic error in the experiment [10]. While for Ni, use of approximate parametrizations for the atomic potentials is tolerable, for Be target one should use a more accurate description of the potential.

## References

- [1] St. Mrówczyński. *Interaction of elementary atoms with matter*. Phys. Rev. **A** 33 (1986) 1549.
- [2] F. Salvat, A. Jablonski, C.J. Powell. *ELSEPA — Dirac partial-wave calculation of elastic scattering of electrons and positrons by atoms, positive ions and molecules*. Comput. Phys. Commun. 165 (2005) 157.
- [3] J.P. Desclaux. *A multiconfiguration relativistic DIRAC-FOCK program*. Comput. Phys. Commun. 9 (1975) 31; Erratum, Comput. Phys. Commun. 13 (1977) 71.
- [4] F. Salvat et al. *Analytical Dirac-Hartree-Fock-Slater screening function for atoms ( $Z=1-92$ )*. Phys. Rev. **A** 36 (1987) 467.
- [5] G. Molière. *Theorie der Streuung schneller geladener Teilchen I*. Z. Naturforschg. 2a. (1947) 133.
- [6] M. Zhabitsky. *Direct Calculation of the Probability of Pionium Ionization in the Target*. Phys. At. Nucl. 71 (2008) 1040.
- [7] C. Santamarina, M. Schumann, L.G. Afanasyev and T. Heim. *A Monte Carlo calculation of the pionium break-up probability with different sets of pionium target cross sections*. J. Phys. **B** 36 (2003) 4273.
- [8] L.G. Afanasyev, A.V. Tarasov. *Passage of Atoms Formed by  $\pi^+$  and  $\pi^-$  Mesons Through a Matter*. Phys. At. Nucl. 59 (1996) 2130.
- [9] Z. Halabuka, T.A. Heim, K. Hencken, D. Trautmann and R.D. Viollier. *Coulomb excitation and breakup of  $\pi^+\pi^-$ -atoms at high energies*. Nucl. Phys. **B** 554 (1999) 86;  
T.A. Heim, K. Hencken, D. Trautmann and G. Baur. *Coherent and incoherent atomic scattering: formalism and application to pionium interacting with matter*. J. Phys. **B** 33 (2000) 3583;  
T.A. Heim, K. Hencken, D. Trautmann and G. Baur. *Pionium interacting with matter: magnetic terms and relativistic corrections*. J. Phys. **B** 34 (2001) 3763;  
M. Schumann, T.A. Heim, K. Hencken, D. Trautmann and G. Baur. *Excitation cross sections for pionium in the Glauber approximation*. J. Phys. **B** 35 (2002) 2683.
- [10] B. Adeva et al. (DIRAC Collaboration). *Determination of  $\pi\pi$  scattering lengths from measurement of  $\pi^+\pi^-$  atom lifetime*. Phys. Lett. **B** 704 (2011) 24.