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DIRECT CALCULATION OF THE PROBABILITY OF PIONIUM IONIZATION IN THE TARGET

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Прямое вычисление вероятности ионизации пиония в мишени

Целью эксперимента DIRAC, проводимого в CERN, является измерение времени жизни пиония ($\pi^+\pi^-$-атома). Время жизни пиония определяется аннигиляцией атома в результате зарядово-обменного процесса $\pi^+\pi^- \to \pi^0\pi^0$. Вычисления в рамках киральной теории возмущений предсказывают значение времени жизни пиония в основном состоянии с высокой точностью: $\tau_{1S} = (2{,}9 \pm 0{,}1) \cdot 10^{-15}$ с. Экспериментальный метод основан на выделении $\pi^+\pi^-$-пар, возникших в результате ионизации (развала) пиония в мишени, из спектра пионных пар с малым относительным импульсом в системе центра масс. Пионии, рожденные в протон-ядерных столкновениях, обладают релятивистскими скоростями ($\gamma > 10$). При заданных импульсе пиония и толщине мишени вероятность ионизации пиония в мишени является однозначной функцией его времени жизни, что позволяет определить время жизни пиония из экспериментального значения вероятности ионизации. Впервые произведено прямое (основанное на сечениях ионизации) вычисление вероятности ионизации пиония в веществе мишени.

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Direct Calculation of the Probability of Pionium Ionization in the Target

The goal of the DIRAC experiment at CERN is the lifetime measurement of pionium ($\pi^+\pi^-$ atom). Its lifetime is mainly defined by the charge-exchange process $\pi^+\pi^- \to \pi^0\pi^0$. Value of the lifetime in the ground state is predicted in the framework of Chiral Perturbation Theory (ChPT) with high precision: $\tau_{1S} = (2.9 \pm 0.1) \cdot 10^{-15}$ s. The method used by DIRAC is based on the analysis of $\pi^+\pi^-$-pairs spectra with small relative momenta in their center-of-mass system in order to find out signal from pionium ionization (break-up) in the target. Pioniums are produced in proton–nuclei collisions and have relativistic velocities ($\gamma > 10$). For fixed values of the pionium momentum and the target thickness the probability of pionium ionization in the target depends on its lifetime in a unique way, thus the pionium lifetime can be deduced from the experimentally defined probability of pionium ionization. Based on ionization cross sections of pionium with target atoms we performed the first direct calculation of the pionium ionization probability in the target.

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INTRODUCTION

Pionium is the hydrogen-like Coulomb bound system of two oppositely charged pions. Its lifetime is determined by strong $\pi^+\pi^- \to \pi^0\pi^0$ annihilation, but it interacts mainly electromagnetically with the target atoms, while propagating through the target material with the relativistic velocity. The DIRAC experiment at CERN [1] detects $\pi^+\pi^-$ pairs with low relative momenta in their center-of-mass system. From the low-momentum part of the spectrum, the probability of the pionium ionization (break-up) in the target, which is the probability for the pionium to be converted into an unbound $\pi^+\pi^-$ pair on the exit of the target, is determined. If the dependence of the pionium ionization probability in the target as a function of its lifetime is established, this measurement will test in a model-independent way the understanding of chiral symmetry breaking in QCD.

The main task of this work is the direct (based on ionization cross sections) calculation of the pionium ionization probability in the target. The formalism of pionium dynamics based on a set of the probabilistic kinetic equations is reminded in Sec. 1. Section 2 is devoted to the direct calculation of the ionization probability.

1. DYNAMICS OF A PIONIUM IN THE TARGET

The pionic atoms can be created in inelastic proton-nuclei collisions with the probability given by [2]

$$\frac{d\sigma_A}{d\vec{P}_A} = (2\pi)^3 \left|\Psi(0)\right|^2 \frac{E}{M} \left.\frac{d\sigma_s^0}{d\vec{p}_+ d\vec{p}_-}\right|_{\vec{p}_+ \approx \vec{p}_-},$$

where $\dfrac{d\sigma_s^0}{d\vec{p}_+ d\vec{p}_-}$ is the double inclusive cross section of $\pi^+\pi^-$ pairs without interaction in the final state with both pions produced either directly in hadronic processes or through short-lived resonances. Production of the pionium atoms with the angular momentum $l > 0$ is suppressed. The square of the S-wave function modulus at zero separation can be approximated as follows [3]:

$$\left|\Psi_{n0}(0)\right|^2 = (1+\delta_n)\left|\Psi_{n0}^C(0)\right|^2,$$

where $\Psi^C_{n0}(0)$ is the pure Coulomb wave function of the $\pi^+\pi^-$ atom at zero distance and the correction factor $(1+\delta_n)$ takes into account the effect of finite-size of the pion production region and the two-pion strong interaction in the final state. It was found that this correction shifts the probability of ionization on per mille level, therefore we will use pure Coulomb wave functions hereafter. For them only nS states are nonzero in the origin

$$\left|\Psi^C_{nlm}(0)\right|^2 = \begin{cases} \dfrac{(\alpha m_\pi/2)^3}{\pi n^3} & \text{if } l=0, \\ 0 & \text{otherwise.} \end{cases}$$

If we normalize probability of atom production to unity then the probability of atom production in the $|nlm\rangle$ state reads

$$p_{nlm}(0) = \frac{\left|\Psi^C_{nlm}(0)\right|^2}{\sum_{k=1}^{\infty}\left|\Psi^C_{kS}(0)\right|^2} = \frac{\delta_{l0}}{n^3\sum_{k=1}^{\infty}1/k^3} = \frac{\delta_{l0}}{n^3\zeta(3)}, \qquad (1)$$
$$p_{100}(0) = 0.832, \quad p_{200}(0) = 0.104, \quad p_{300}(0) = 0.031.$$

After production atom can either annihilate (mainly through $\pi^+\pi^- \to \pi^0\pi^0$ process*) or electromagnetically interact with target atoms.

The partial decay width of the pionium in $1S$ state is [6]:

$$\Gamma_{2\pi^0} = \frac{2}{9}\alpha^3\sqrt{m^2_{\pi^+} - m^2_{\pi^0} - \frac{1}{4}m^2_{\pi^+}\alpha^2}(a^0_0 - a^2_0)^2 m^2_{\pi^+}(1+\delta_\Gamma),$$
$$\delta_\Gamma = (5.8 \pm 1.2)\cdot 10^{-2}.$$

The $(a^0_0 - a^2_0)$ difference of the pion–pion S-wave scattering lengths with isospin 0 and 2 have been calculated [7] within the framework of the standard chiral perturbation theory (ChPT) [8]

$$a^0_0 - a^2_0 = (0.265 \pm 0.004)m^{-1}_{\pi^+}.$$

This difference leads to the predicted value of the pionium lifetime in the ground state

$$\tau_{1S} = (2.9 \pm 0.1)\cdot 10^{-15}\ \text{s}. \qquad (2)$$

Lifetime in nS states reads $\tau_{nS} = \tau_{1S}\dfrac{|\Psi_{1S}(0)|^2}{|\Psi_{nS}(0)|^2} = \tau_{1S}n^3$. Therefore the probability for a pionium with the laboratory momentum p_A to annihilate per unit

*Another annihilation channel $\pi^+\pi^- \to 2\gamma$ amounts only about 0.3% [4,5].

length is

$$W^{\text{anh}}_{nlm} = \frac{1}{\lambda^{\text{anh}}_{nlm}} = \begin{cases} \dfrac{1}{\gamma\beta\tau_n} = \dfrac{2m_\pi}{p_A\tau_{1S}n^3} & \text{in } nS \text{ states,} \\ 0 & \text{in other states.} \end{cases}$$

While crossing the target a pionium electromagnetically interacts with target atoms. As a result, $\pi^+\pi^-$ atom can be either ionized or transit from the initial bound state $|n_i l_i m_i\rangle$ to another bound state $|n_f l_f m_f\rangle$ (excitation/deexcitation). Hereafter we will denote initial and final bound states as $|i\rangle$ and $|f\rangle$, respectively.

The probability of ionization per unit length from the state $|i\rangle$ is given by

$$W^{\text{ion}}_i = \frac{1}{\lambda^{\text{ion}}_i} = \frac{\rho N_A}{A}\sigma^{\text{ion}}_i,$$

where ρ is the target density, A is its atomic weight, N_A is the Avogadro constant and σ^{ion}_i is the ionization cross section.

The probability of a pionium excitation per unit length from the state $|i\rangle$ to the final state $|f\rangle$ is given by

$$W^f_i = \frac{1}{\lambda^f_i} = \frac{\rho N_A}{A}\sigma^f_i = W^i_f,$$

where σ^f_i is the discrete (bound–bound) transition cross section.

The total inelastic cross section gives the probability of an atom to undergo an inelastic electromagnetic interaction

$$\sigma^{\text{tot}}_i = \sum_f \sigma^f_i + \sigma^{\text{ion}}_i. \tag{3}$$

Total cross sections can be calculated owing to the completeness of the eigenstates of the Coulomb Hamiltonian.

Total and transition cross sections for any bound states were initially calculated in the Born approximation with the static potential of target atoms [9]. Later a more accurate set of cross sections was derived which takes into account relativistic effects and target excitations [10]. Moreover, in the latter work authors calculated ionization cross sections for any initial bound state with $n \leqslant 8$ which provides the possibility to perform direct calculation of the pionium ionization probability in the target, which is the subject of the present work. Comparison between different sets of cross sections was performed [11], where authors found that uncertainties in most precise sets of cross sections for Ni target will cause only 1% uncertainty in the pionium lifetime. Uncertainty due to the accuracy of cross sections is expected to dominate precision of the ionization probability dependence on the pionium lifetime.

The dynamics of the pionium interaction with target atoms is supposed to be described by a set of kinetic equations [9] using the probabilities $p_i(s)$ to find the $\pi^+\pi^-$ atom in the definite quantum state $|i\rangle$ at a distance s from the production point. This approach ignores any interference between different pionium bound states. For low n most of interference effects are suppressed at typical pionium momenta in DIRAC ($3 \div 8$ GeV$/c$) as the mean free path between pionium inelastic interactions is usually longer than the formation time of atomic system multiplied by its velocity. Nevertheless, even for low n some interference effects can take place due to the accidental degeneracy of energy levels of hydrogen-like atoms. This problem was considered in the framework of the density matrix formalism [12]. It was found that the interference between quantum states with small n does not change the result based on a set of probabilistic kinetic equations (their difference is less than per mille).

Eigenstates of the Coulomb Hamiltonian form a countable set of discrete levels. For numerical calculations we will take into account only levels with principal quantum number $n \leqslant n_{\text{max}}$. For a given principal quantum number n there are n^2 states $|nlm\rangle$ with different orbital and magnetic quantum numbers. We will denote the total number of discrete bound states taken for the calculation as N. To make the system complete we introduce a cross section σ_i^u which stands for the sum of transitions from state $|i\rangle$ to any discrete state with the principal quantum number $n_f > n_{\text{max}}$:

$$\sigma_i^u = \sum_{f:n_f>n_{\text{max}}} \sigma_i^f = \sigma_i^{tot} - \sigma_i^{\text{ion}} - \sum_{f:n_f\leqslant n_{\text{max}}} \sigma_i^f.$$

It is straightforward to write the probability of pionium production in all bound states above n_{max}:

$$p_u(0) = 1 - \sum_{i:n_i\leqslant n_{\text{max}}} p_i(0). \tag{4}$$

Finally, we will write the system of kinetic equations in the matrix form

$$\frac{d}{ds}\begin{pmatrix} p_1 \\ p_2 \\ \dots \\ p_N \\ p_u \\ p_{\text{ion}} \\ p_{\text{anh}} \end{pmatrix} = \begin{pmatrix} W_1^1 & W_2^1 & \dots & W_N^1 & 0 & 0 & 0 \\ W_1^2 & W_2^2 & \dots & W_N^2 & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & 0 & 0 & 0 \\ W_1^N & W_2^N & \dots & W_N^N & 0 & 0 & 0 \\ W_1^u & W_2^u & \dots & W_N^u & 0 & 0 & 0 \\ W_1^{\text{ion}} & W_2^{\text{ion}} & \dots & W_N^{\text{ion}} & 0 & 0 & 0 \\ W_1^{\text{anh}} & W_2^{\text{anh}} & \dots & W_N^{\text{anh}} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ \dots \\ p_N \\ p_u \\ p_{\text{ion}} \\ p_{\text{anh}} \end{pmatrix}. \tag{5}$$

Diagonal terms describe the total decrease of the level population

$$W_i^i = -\frac{\rho N_A}{A}\sigma_i^{\text{tot}} - W_i^{\text{anh}}.$$

System (5) is a system of linear ordinary differential equations with constant coefficients. The rank of the matrix is N, with three low lines being a linear combination of the first N lines. It is exactly solvable

$$p_i(s) = \sum_k c_k \alpha_i^{(k)} \mathrm{e}^{\lambda_k s}, \tag{6}$$

where $\lambda_1, \ldots, \lambda_N$ are eigenvalues and $\alpha^{(k)}$ their corresponding eigenvectors. Symmetry of the upper left N-by-N corner guaranties that all its eigenvalues are real [13]. Coefficients c_k are fixed from initial conditions (1), (4). The probability of pionium ionization at the distance s after the production point is expressed through the solution (6)

$$p_{\text{ion}}(s) = \sum_k \frac{c_k}{\lambda_k} \left(\mathrm{e}^{\lambda_k s} - 1\right) \sum_i W_i^{\text{ion}} \alpha_i^{(k)}.$$

DIRAC uses very thin targets (their nuclear efficiency is less than 10^{-3}), therefore atoms are produced nearly uniformly over the target thickness s_0. Hence the probability for a pionium to leave the target in the state $|i\rangle$ reads

$$P_i(s_0) = \sum_k c_k \alpha_i^{(k)} \frac{1}{\lambda_k s_0} \left(\mathrm{e}^{\lambda_k s_0} - 1\right),$$

while the probability of ionization on the exit of the target is

$$P_{\text{ion}}(s_0) = \sum_k \frac{c_k}{\lambda_k} \left(\frac{1}{\lambda_k s_0} \left(\mathrm{e}^{\lambda_k s_0} - 1\right) - 1 \right) \sum_i W_i^{\text{ion}} \alpha_i^{(k)}. \tag{7}$$

Expressions for the probability of annihilation P_{anh} and for the probability P_u to reach any excited state with $n > n_{\text{max}}$ on the exit of the target have the same form as (7) if one substitutes W_i^{ion} with W_i^{anh} and W_i^u, respectively.

In Table 1 we illustrate this solution as a function of n_{max} for a pionium atom produced in 95 μm thick Ni target with the momentum $p_A = 4.6\,\text{GeV}/c$, corresponding to the average laboratory momentum of produced pioniums in the kinematic range of the DIRAC experiment. Eigenvalues were numerically found by the appropriate function from LAPACK [14]. Here P_{dsc}^A is the probability for pionium to leave the target in a bound state with $n \leqslant n_{\text{max}}$. System of equations (5) is constructed in a way that as soon as an atom reaches the state with $n > n_{\text{max}}$ it effectively quits from calculations and is kept intact, though in reality it is expected to undergo further electromagnetic interactions, e.g., it can be ionized or deexcited to the low-lying states. Therefore, P_{u}^A is the probability for atoms to reach states with $n > n_{\text{max}}$, which amounts to about 20%. This

Table 1. Numerical solution with $n > n_{\max}$ states intact as a function of $n_{\max}$

$n_{\max}$	P^A_{dsc}	P^A_{anh}	P^A_{ion}	P^A_{u}
5	0.0928	0.4407	0.2438	0.2227
6	0.0937	0.4407	0.2586	0.2070
7	0.0943	0.4407	0.2715	0.1935
8	0.0947	0.4407	0.2828	0.1817

numerical value is in agreement with the earlier calculations [11] (Fig. 3, *d*). Numerical precision of the above solution can be estimated from the inequality

$$\left|1 - P^A_{\text{dsc}} - P^A_{\text{anh}} - P^A_{\text{ion}} - P^A_{\text{u}}\right| < 1 \cdot 10^{-12},$$

thus round-off errors do not affect the result.

As an atom transits to the state $n_f > n_i$ its effective radius of electromagnetic interactions grows and its characteristic ionization length is getting shorter

$$\lambda^{\text{ion}}_{|n>n_{\max},lm\rangle} < \lambda^{\text{ion}}_{|n_{\max}=8,lm\rangle} \approx 2\ \mu\text{m}.$$

The target used in DIRAC is 95μm thick, therefore highly-excited atoms have a chance to leave the target in a bound state only if they were created close to the exit of the target. Otherwise these highly-excited atoms will be ionized. This allows us to set the range for the ionization probability in the target:

$$0.2828 = P^A_{\text{ion}} < P_{\text{ion}} < P^A_{\text{ion}} + P^A_u = 0.4645. \tag{8}$$

Here the upper bound corresponds to the case when all highly-excited atoms are ionized, while the lower bound P^A_{ion} is at least probability of ionization from states with $n \leqslant n_{\max}$.

From Table 1 one can conclude that above upper and lower bounds converge slowly with increase of $n_{\max}$ and in this way it would be difficult to increase $n_{\max}$ in order to achieve precision required by DIRAC (per cent level).

2. EVOLUTION OF HIGHLY-EXCITED STATES

Rather than trying to solve the system (5) directly we will modify it in order to get the *lower* bound of the ionization probability by taking into account

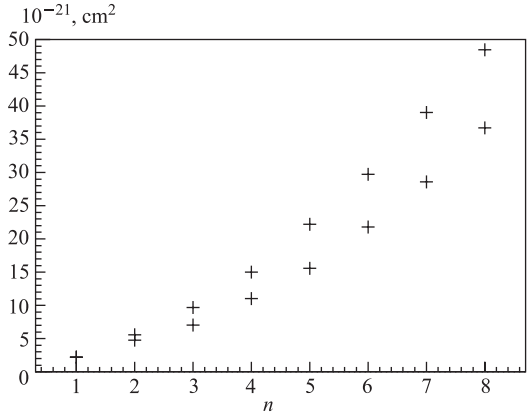

Fig. 1. $\min\limits_{l'm'}\left\{\sigma^{\text{ion}}_{|nl'm'\rangle}\right\}$ and $\max\limits_{l'm'}\left\{\sigma^{\text{ion}}_{|nl'm'\rangle}\right\}$ for different principal quantum numbers n

dynamics of highly-excited states with $n > n_{\text{max}}$:

$$\frac{d}{ds}\begin{pmatrix} p_1 \\ p_2 \\ \dots \\ p_N \\ p_u \\ p_{\text{ion}} \\ p_{\text{anh}} \end{pmatrix} = \begin{pmatrix} W_1^1 & W_2^1 & \dots & W_N^1 & W_u^1 & 0 & 0 \\ W_1^2 & W_2^2 & \dots & W_N^2 & W_u^2 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & 0 & 0 \\ W_1^N & W_2^N & \dots & W_N^N & W_u^N & 0 & 0 \\ W_1^u & W_2^u & \dots & W_N^u & W_u^u & 0 & 0 \\ W_1^{\text{ion}} & W_2^{\text{ion}} & \dots & W_N^{\text{ion}} & W_u^{\text{ion}} & 0 & 0 \\ W_1^{\text{anh}} & W_2^{\text{anh}} & \dots & W_N^{\text{anh}} & W_u^{\text{anh}} & 0 & 0 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ \dots \\ p_N \\ p_u \\ p_{\text{ion}} \\ p_{\text{anh}} \end{pmatrix}. \quad (9)$$

Here

$$W_u^{\text{ion}} = \frac{\rho N_A}{A}\sigma^{\text{ion}}_{n_{\text{max}}+1,\min}, \quad \sigma^{\text{ion}}_{n_{\text{max}}+1,\min} = \min_{l'm'}\left\{\sigma^{\text{ion}}_{|n_{\text{max}}+1,l'm'\rangle}\right\}$$

is the lower bound of the probability of ionization per unit length from any state with $n > n_{\text{max}}$, because the ionization cross section tends to grow with increasing of the principal quantum number n due to the corresponding expansion of the atomic radius. The minimal and maximal values of the ionization cross section for different principal quantum numbers are drawn in Fig. 1. To find the lower bound of the ionization probability, further we require all probabilities of ionization per unit length from any state $|nlm\rangle$ to be smaller than W_u^{ion}:

$$W^{\text{ion}}_{|nlm\rangle,\min} = \frac{\rho N_A}{A}\sigma^{\text{ion}}_{|nlm\rangle,\min}, \quad \sigma^{\text{ion}}_{|nlm\rangle,\min} = \min\left\{\sigma^{\text{ion}}_{|nlm\rangle},\ \sigma^{\text{ion}}_{n_{\text{max}}+1,\min}\right\}.$$

The diagonal term W_i^i, which describes the level depopulation, is changed accordingly to fulfill (3).

Upper bound of the probability of deexcitation per unit length from all states with $n > n_{\max}$ to a state f with $n_f \leqslant n_{\max}$ is obtained from the following inequality:

$$\sum_{i:n_i>n_{\max}} W_i^f p_i < \sum_{i:n_i>n_{\max}} W_i^f \cdot \sum_{i:n_i>n_{\max}} p_i = W_u^f p_u = W_f^u p_u.$$

Finally the diagonal term for the sum of discrete states with $n > n_{\max}$ is

$$W_u^u = -\frac{\rho N_A}{A}\sigma^{\text{ion}}_{n_{\max}+1,\min} - W_u^{\text{anh}} - \sum_{f:n_f\leqslant n_{\max}} W_u^f,$$

where $W_u^{\text{anh}} = \dfrac{2m_\pi}{p_A\tau_{1S}(n_{\max}+1)^3}$ is the upper bound of the probability for a pionium to annihilate from all states with $n > n_{\max}$ per unit length. The rank of the new system is $N+1$. The system (9) is constructed in the way that ionization is *underestimated* and all competitive processes including deexcitation from high n states (thus transitions to bound states with even lower ionization) are *overestimated*, therefore the solution is the *mathematical lower bound* of the probability of ionization. Numerical results for different $n_{\max}$ are presented in Table 2.

Table 2. Numerical solution for the lower bound of P_{ion} as a function of $n_{\max}$

$n_{\max}$	P^B_{dsc}	P^B_{anh}	P^B_{ion}	P^B_{u}
5	0.1109	0.4416	0.4468	0.00067
6	0.1068	0.4411	0.4517	0.00030
7	0.1041	0.4409	0.4548	0.00015
8	0.1023	0.4408	0.4567	0.00008

Upper (8) and lower bounds effectively squeeze the solution (Fig. 2), for $n_{\max} = 8$ they are

$$0.4567 = P^B_{\text{ion}} < P_{\text{ion}} < P^A_{\text{ion}} + P^A_u = 0.4645, \quad \frac{P^{\max}_{\text{ion}} - P^{\min}_{\text{ion}}}{2P_{\text{ion}}} \approx 0.8\cdot 10^{-2}. \quad (10)$$

Precision of the above calculated value of the pionium ionization probability in the target is comparable to the $\sim 1\%$ uncertainties in the P_{ion} value due to precision of the corresponding electromagnetic cross sections [11].

Upper and lower bounds of the probability of pionium ionization in the target as a function of its lifetime in the ground state is shown in Fig. 3. The

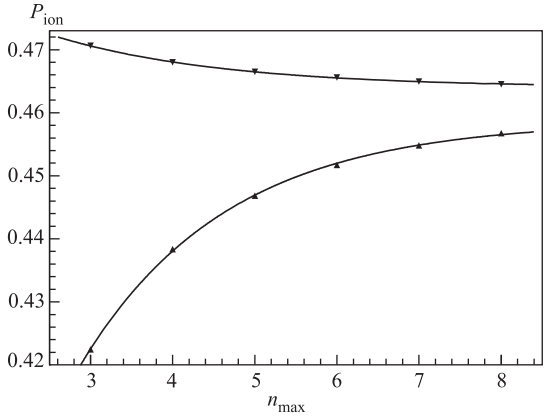

Fig. 2. Upper and lower bounds of P_{ion} as a function of $n_{\max}$, fitted by $a\mathrm{e}^{\alpha n_{\max}} + c$ functions to guide the eye

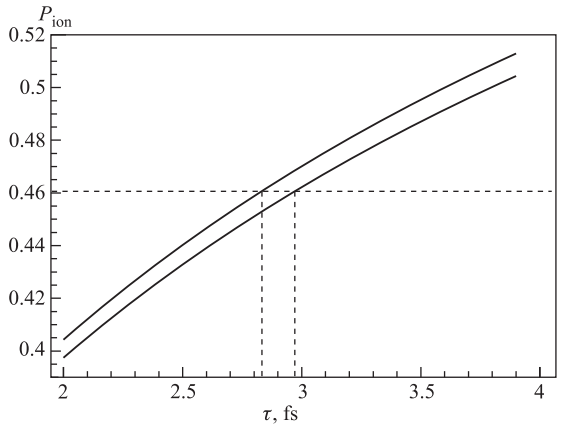

Fig. 3. Upper and lower bounds of P_{ion} as a function of the pionium lifetime in the ground state

corresponding uncertainties are shown by dotted lines around the value of the pionium lifetime (2) predicted by theory. The DIRAC collaboration reported the measured value of $P_{\text{ion}} = 0.452^{+0.025}_{-0.039}$ [15], based on part of the collected data. While further analysis will reduce uncertainties of the experimental result, uncertainties of the solution (10) are expected to be within precision, required by DIRAC. Range can be further shrunk by extrapolation as shown in Fig. 2.

We have to emphasize that upper and lower bounds of the ionization probability squeeze the solution with required precision due to the fact, that for atoms with the principal quantum number $n > 8$ the characteristic ionization length is

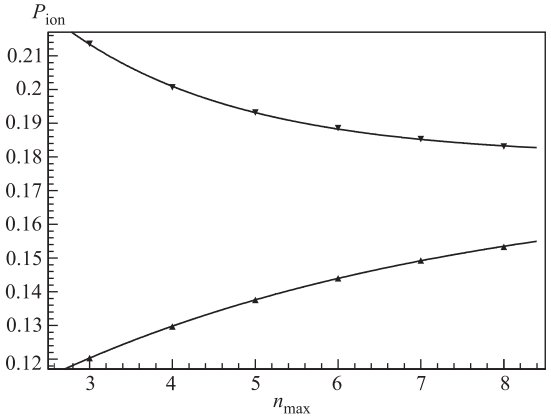

Fig. 4. Upper and lower bounds of P_{ion} as a function of n_{max} for 10 μm thick Ni target

less than 2 μm, which is much shorter than the target thickness of 95 μm. If one selects very thin target (e.g., 10 μm thick Ni) then the upper and lower bounds will show worse convergence (Fig. 4).

CONCLUSIONS

We derived a mathematical approach to solve a system of kinetic equations, which describes evolution of relativistic $\pi^+\pi^-$ atoms propagating through the target. In this approach we reduce the system of kinetic equations, which formally contains infinite number of equations, to the finite set of equations, which is solved exactly. The solution represents lower and upper bounds for the probability of pionium ionization in the target. These lower and upper bounds effectively squeeze the solution to the value of the probability of ionization with 1% precision, which is within requirements of the DIRAC experiment. Thus the first direct (based on ionization cross sections) calculation of the probability of ionization has been performed. We confirm that the contribution of highly-excited states (with the principal quantum number $n > 8$) to the probability of ionization is significant ($> 1/3$).

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