DIRAC NOTE 2018–02
Draft February 5, 2019

A constructive way to calculate a yield of $\pi^+\pi^-$-atoms from the Be target

M. Zhabitsky
Joint Institute for Nuclear Research, Dubna, Russia

February 5, 2019

Abstract

This note describes details of a constructive approach to calculate with sufficient precision a yield of $\pi^+\pi^-$-atoms from the Be target.

Variables and main equations are as in the paper [6].

A work mainly focuses on the way to solve an infinite system of kinetic (transport) equations, which describes dynamic of $\pi^+\pi^-$ atoms crossing the Be foil.

1 Solution A

A straightforward way to solve the system of transport equations, which contains infinite number of equations, is to take into account all quantum levels with principal quantum number $n \in [1, \ldots, n_{\max}]$ and analyze the behavior of numerical solutions as a cut on $n_{\max}$ is increased. We will call this "Solution A".

We define following distinct sums of final states.

An estimation of total probability to leave a target in a bound state with the principal quantum number $n \leqslant n_{\max}$:

$$P_{\text{dsc}}(n_{\max}) = \sum_{n=1}^{n_{\max}} P_{\text{dsc}}(n) = \sum_{n=1}^{n_{\max}} \sum_{l,m} |nlm\rangle^2. \tag{1}$$

An estimation of total probability to annihilate from bound states with the principal quantum number $n \leqslant n_{\max}$:

$$P_{\text{anh}}(n_{\max}) = \sum_{n=1}^{n_{\max}} P_{\text{anh}}(n) = \sum_{n=1}^{n_{\max}} P_{\text{anh}}(|n00\rangle). \tag{2}$$

An estimation of total probability for an atom to got ionized from bound states with the principal quantum number $n \leqslant n_{\max}$:

$$P_{\text{ion}}(n_{\max}) = \sum_{n=1}^{n_{\max}} P_{\text{ion}}(n) = \sum_{n=1}^{n_{\max}} \sum_{l,m} P_{\text{ion}}(|nlm\rangle). \tag{3}$$

$P_{\text{unrec}}(n_{\max})$ is an estimation of the probability for an atom to reach a highly-excited states with $n > n_{\max}$. This artificial level is an effective trap: atoms can reach it, but never leave it. This level doesn't change Solution A, it is introduced to verify unitarity of a numerical solution of the limited system of transport equations (with it system becomes complete). Probability $P_{\text{unrec}}(n_{\max})$ is expected to converge to zero as we increase $n_{\max} \to \infty$.

Limited systems of transport equations were numerically solved for all $n_{\max} \in [1, \ldots, 10]$. Sums of distinct final states as a function of $n_{\max}$ are shown in Figs. 1–2. Distributions were fitted by a function $(p_0 \exp(-p_1 n_{\max}) + p_2)$ to analyze convergence of solutions as $n_{\max} \to \infty$. The most precise solution at $n_{\max} = 10$ is shown in Tab. 1.

As expected only low lying levels 1S, 2S and 3S contribute to annihilation. If one uses $n_{\max} \geqslant 4$ then the probability of annihilation is known with absolute precision better than 10^{-4}.

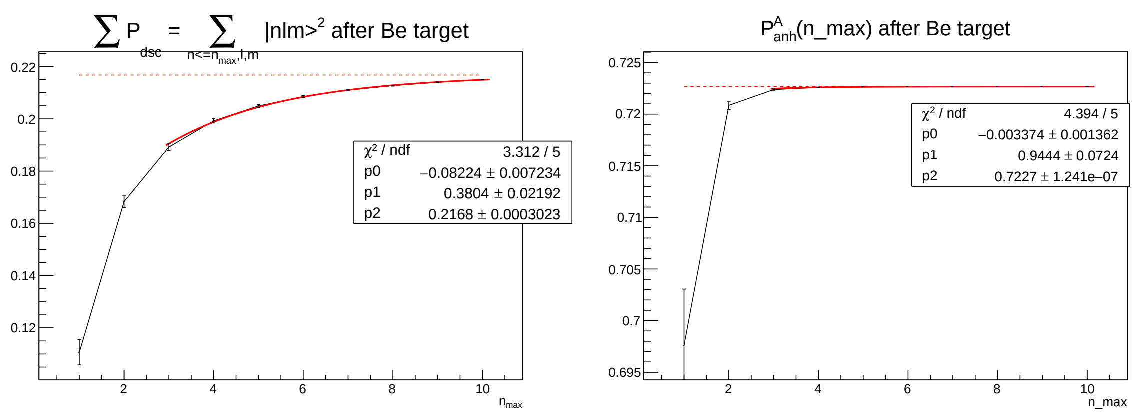

Figure 1: Estimated probability of pionium to leave the Be target in a bound state P_{dsc} (left) or annihilate P_{anh} (right) as a function of $n_{\max}$.

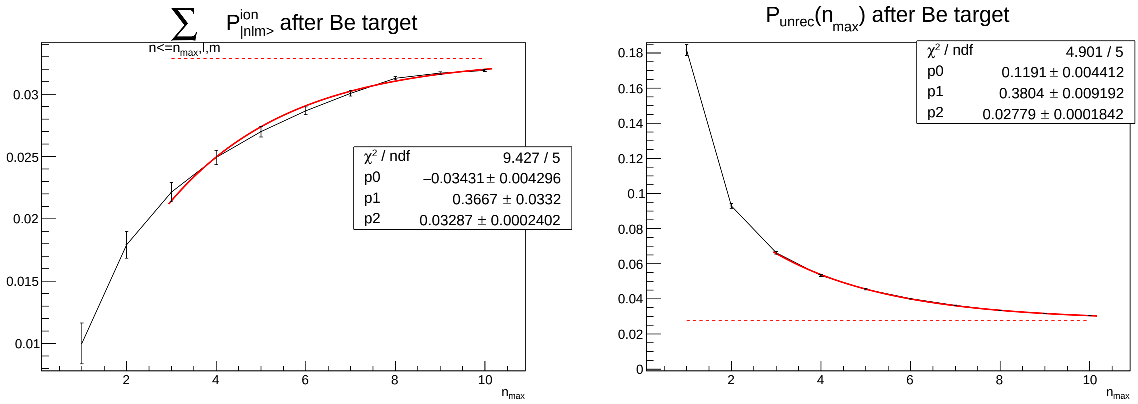

Figure 2: Estimated probability of pionium to got ionized P_{ion} (left) or reach highly excited bound states with $n > n_{\max}$ P_{unrec} (right) as a function of $n_{\max}$.

Table 1: Sums of distinct final states at $n_{\max} = 10$ for solution A.

P^A_{dsc}	P^A_{anh}	P^A_{ion}	P^A_{unrec}	$\left\|1 - \left(P^A_{\text{dsc}} + P^A_{\text{anh}} + P^A_{\text{ion}} + P^A_{\text{unrec}}\right)\right\|$
0.2150	0.7227	0.0319	0.0305	$< 7 \cdot 10^{-14}$

If we further increase $n_{\max}$, we refine precision of contributions to leave a target in any bound state or got ionized, namely we try to find out how the value $(1 - P_{\text{anh}})$ is shared between P^A_{dsc} and P^A_{ion}. The striking feature of the solution A is that the expected convergence of $P^A_{\text{unrec}}(n_{\max})$ to zero is not obvious. As the numerical solution is sufficiently accurate (unitarity is conserved with precision better than 10^{-13} — see Tab. 1), round-off errors do not affect the result. This means that

$$\lim_{n_{\max}\to\infty} P^A_{\text{unrec}} = P^A_{\text{unrec},\infty} = 0.028$$

is an estimation of the unitarity violation by the Solution A due to the truncation of the infinite system of kinetic equations. Term $P^A_{\text{unrec},\infty}$ will provide an additional not yet accounted impact on aggregate sums of P_{ion} and P_{dsc}.

By its construction, solution A provides only lower estimates on aggregate probabilities P_{ion} and P_{dsc}.

The profile of bound state populations on the principal quantum number n, estimated by solution A at $n_{\max} = 10$, is in Tab. 2. With respect to the "true" profile (Fig. 3) there is a decrease in populations $P_{\text{dsc}}(n)$, which becomes larger as $n \to n_{\max}$. This decrease affects the profile slope on n as well.

If one takes into account all levels up to sufficiently large $n_{\max}$ (e.g. $n_{\max} > 4$), solution A provides a strict range on an unknown true sum of all bound states populations

$$P^A_{\text{dsc}}(n_{\max}) < P^{\text{true}}_{\text{dsc}} < P^A_{\text{dsc}}(n_{\max}) + P^A_{\text{unrec}}(n_{\max}), \tag{4}$$

$$0.2150 < P^{\text{true}}_{\text{dsc}} < 0.2454 \quad \text{at } n_{\max} = 10.$$

Table 2: $P_{\text{dsc}}(n) = \sum_{l,m} |nlm\rangle^2$ at $n_{\max} = 10$ for solution A.

n	1	2	3	4	5	6	7	8	9	10
$P^A_{\text{dsc}}(n)$	0.1108	0.0596	0.0217	0.0099	0.0053	0.0032	0.0020	0.0013	0.0008	0.0004

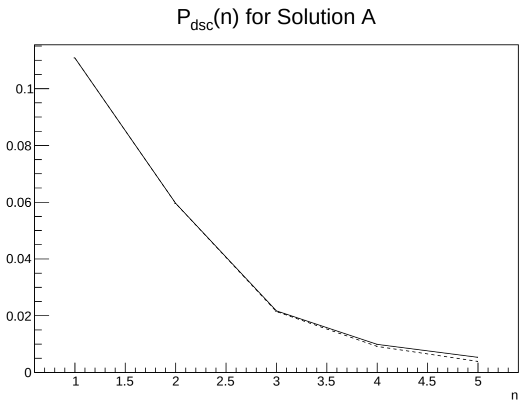

Figure 3: Estimated probabilities for pionium to leave the Be target in a bound state with the particular principal number n, if $n_{\max} = 5$ is used in calculations A (dotted line). Solid line — an estimation of a "true" solution for the system of kinetic equations without cut ($n_{\max} \to \infty$).

2 Solution B

Rather than try to solve the infinite system of transport equations directly, there is an another approach [6], called "solution B", which provides strict upper and lower bounds on aggregate probabilities $P_{\rm dsc}$ and $P_{\rm ion}$. Solution B takes into account dynamics of highly-excited states with $n > n_{\rm max}$. It replaces infinite number of bound states with $n > n_{\rm max}$ by one effective level (see [6] for details). The cross-section of ionization from this effective level is set to be less than from any bound state $n > n_{\rm max}$. The probability for an atom to be de-excited from states with $n > n_{\rm max}$ into states with $n \leqslant n_{\rm max}$ is taken into account as well.

In solution B the system of kinetic equations is constructed in the way that ionization is *underestimated* and all competitive processes including de-excitation 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.

As the probability of annihilation is very well known for solutions with $n_{\rm max} \geqslant 4$, the sum $P_{\rm dsc} + P_{\rm ion} = 1 - P_{\rm anh}$ is almost constant. This way the *lower bound* on the probability of ionization leads to the *upper bound* on the aggregate probability to leave a target in any bound state.

Limited systems of transport equations were numerically solved for all $n_{\rm max} \in [1, \ldots, 8]$, as the set of ionisation cross-sections is known up to $n = 8$ [4]. Sums of distinct final states as a function of $n_{\rm max}$ are shown in Figs. 4–5. Distributions were fitted by a function $(p_0 \exp(-p_1 n_{\rm max}) + p_2)$ to analyze convergence of solutions as $n_{\rm max} \to \infty$. The most precise solution at $n_{\rm max} = 8$ is shown in Tab. 3.

Solution B provides the correct zero asymptotic value for the aggregate sum of high-n states as $n_{\rm max} \to \infty$. Convergence of the ionisation sum $P^B_{\rm ion}(n_{\rm max})$ is slow, nevertheless the asymptotic value $P^B_{\rm ion}$ can be estimated. The asymptotic value for $P^B_{\rm dsc}$ is more difficult to estimate (see Fig. 7).

The profile of bound state populations on the principal quantum number n, estimated by solution B at $n_{\rm max} = 8$, is in Tab. 4. With respect to the "true" profile (Fig. 6) there is a positive perturbation in populations $P_{\rm dsc}(n)$, which becomes larger as $n \to n_{\rm max}$.

If one takes into account all levels up to sufficiently large $n_{\rm max}$ (e.g. $n_{\rm max} > 4$), a strict upper bound on an unknown true sum of all bound states populations can be calculated

$$P^{\rm true}_{\rm dsc} < P^B_{\rm dsc}(n_{\rm max}) + P^B_{\rm unrec}(n_{\rm max}), \qquad (5)$$
$$P^{\rm true}_{\rm dsc} < 0.2349 \quad \text{at } n_{\rm max} = 8.$$

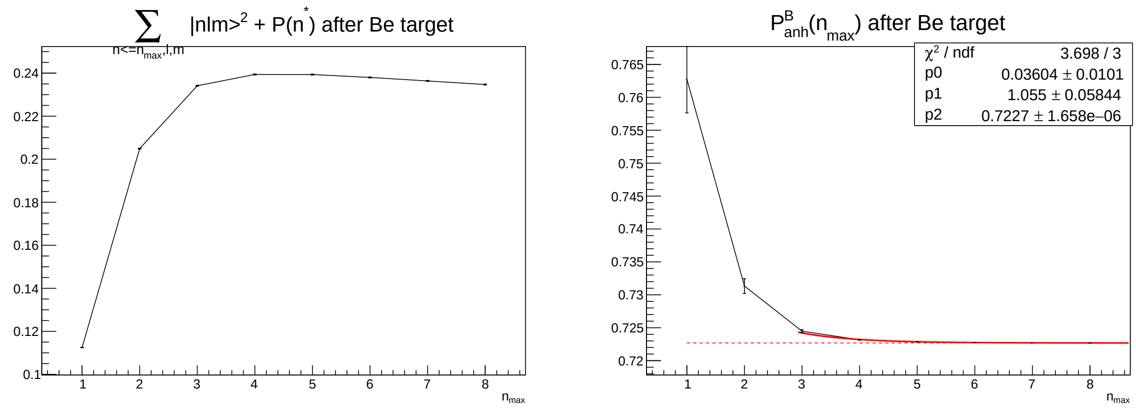

Figure 4: Estimated probability of pionium to leave the Be target in a bound state $P_{\rm dsc}$ (left) or annihilate $P_{\rm anh}$ (right) as a function of $n_{\rm max}$.

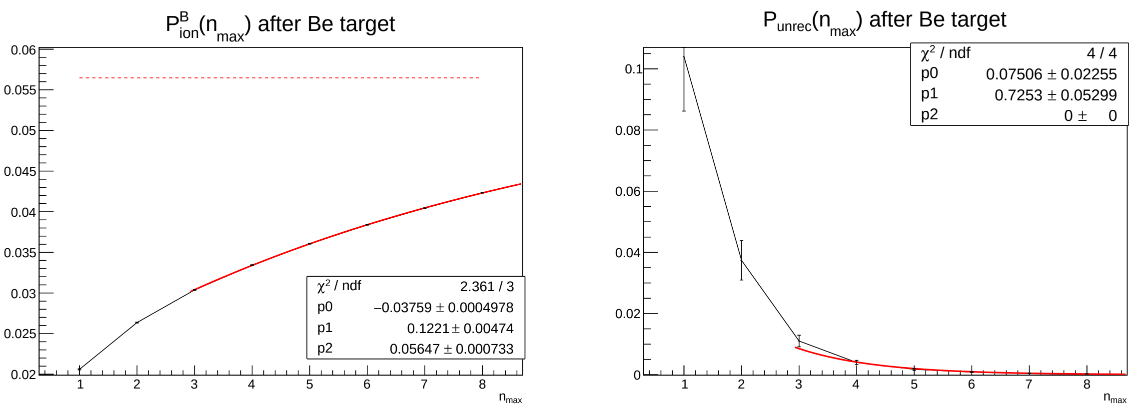

Figure 5: Estimated probability of pionium to got ionized P^B_{ion} (left) and probability P^B_{unrec} (right) as a function of $n_{\max}$.

Table 3: Sums of distinct final states at $n_{\max} = 8$ for solution B.

P^B_{dsc}	P^B_{anh}	P^B_{ion}	P^B_{unrec}	$\left\|1 - (P^B_{\text{dsc}} + P^B_{\text{anh}} + P^B_{\text{ion}} + P^B_{\text{unrec}})\right\|$
0.2347	0.7227	0.0423	0.0003	$< 3 \cdot 10^{-14}$

3 Range on real population of discrete states (Solutions A and B)

Combining lower (4) and upper (5) bounds we obtain a range of possible values of $P^{\text{true}}_{\text{dsc}}$

$$P^A_{\text{dsc}}(n_{\max}) < P^{\text{true}}_{\text{dsc}} < P^B_{\text{dsc}}(n_{\max}) + P^B_{\text{unrec}}(n_{\max}), \tag{6}$$

$$0.2150 < P^{\text{true}}_{\text{dsc}} < 0.2349.$$

Table 4: $P_{\text{dsc}}(n) = \sum_{l,m} |nlm\rangle^2$ at $n_{\max} = 8$ for solution B.

n	1	2	3	4	5	6	7	8
$P_{\text{dsc}}(n)$	0.1108	0.0597	0.0221	0.0109	0.0074	0.0068	0.0076	0.0094

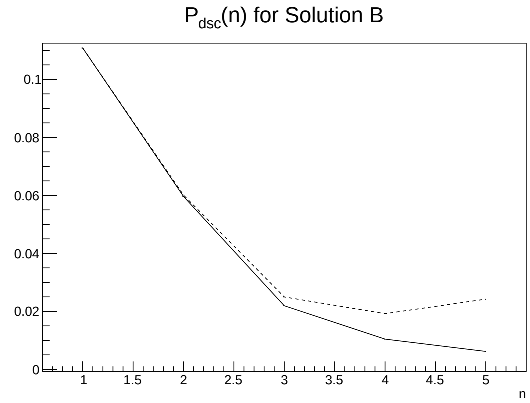

Figure 6: Estimated probabilities for pionium to leave the Be target in a bound state with the particular principal number n, if $n_{\max} = 5$ is used in calculations B (dotted line). Solid line — an estimation of a "true" solution for the system of kinetic equations without cut ($n_{\max} \to \infty$).

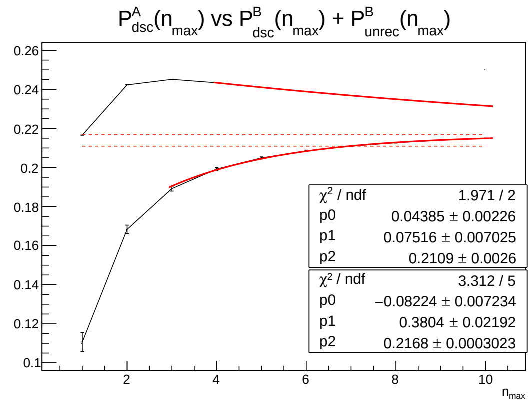

Figure 7: Range on real P_{dsc} after the Be target.

References

[1] J. Schweizer. Decay widths and energy shifts of $\pi\pi$ and πK atoms. Phys. Lett. **B 587** (2004) 33.

[2] St. Mrowczynski. Interaction of elementary atoms with matter. Phys. Rev. **A 33** (1986) 1549.

[3] L.G. Afanasyev and A.V. Tarasov. Passage of Atoms Formed by π^+ and π^- Mesons Through a Matter. Phys. Atom. Nucl. **59** (1996) 2130.

[4] Z. Halabuka, T. 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. Heim, K. Hencken, D. Trautmann and G. Baur. Coherent and incoherent atomic scattering: formalism and application to pionium interacting with matter. J. Phys. B: At. Mol. Opt. Phys. **33** (2000) 3583;
T. Heim, K. Hencken, D. Trautmann and G. Baur. Pionium interacting with matter: magnetic terms and relativistic corrections. J. Phys. B: At. Mol. Opt. Phys. **34** (2001) 3763.

[5] 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: At. Mol. Opt. Phys. **36**, 4273 (2003).

[6] M. Zhabitsky. Direct calculation of the probability of pionium ionization in the target. Phys. At. Nucl. **71** (2008) 1040; arXiv:0710.4416 [hep-ph].

[7] M. Zhabitsky. How uncertainties in the atomic potential affect DIRAC results. DIRAC-Note-2014-06 (2014) 7 p.; `http://cds.cern.ch/record/1987122`.

[8] G. H. Golub and C. Van Loan. Matrix computations. 3rd ed., — The Johns Hopkins University Press, 1996.

[9] E. Anderson *et al.*. LAPACK Users' Guide. 3rd ed., Society for Industrial and Applied Mathematics, Philadelphia, PA, 1999, ISBN 0-89871-447-8.