Dynamics of the pionium with the density matrix formalism

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Abstract
The evolution of pionium, the $\pi^+\pi^-$ hydrogen-like atom, passing through matter is described by the density matrix formalism in the first Born approximation. We compare the probability-based calculations with the more precise density matrix formalism which takes into account the interference effects, and consider their influence on the pionium break-up probability. We apply our general result to the specific conditions of the DIRAC experiment at CERN.

1. Introduction

Due to its importance for the DIRAC–PS 212 experiment at CERN [1], the interaction of the pionium atom, the hydrogen-like Coulomb bound state of $\pi^+\pi^-$ mesons, with target materials has been studied in great detail in recent years [2–8]. The DIRAC experiment is dedicated to measuring the pionium lifetime, which is closely linked to the strong interaction scattering lengths, as will be shown in section 2. These values are precisely predicted by the chiral perturbation theory, and thus the validity of the latter will be tested.

Earlier the propagation of pionium in matter was always treated using a classical probability-based formalism, which neglected the quantum mechanical interference between energy degenerated states. The interference effects are of particular importance for the case of hydrogen-like atoms since the accidental degeneracy of the Hamiltonian increases the number of states among which the interference can be significant.

The density matrix formalism has been used in [9] to advance a new set of equations describing the pionium evolution with account of the interference effects. In this paper, we get the numerical solution of these equations in the context of the DIRAC experiment.

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2. Propagation of pionium in matter

Due to the short pion lifetime, pionium cannot be produced at rest in the laboratory frame. It can, however, originate from the collisions of high-energy projectiles with atoms of a fixed target. The production cross section can be found in [10] and is given by

$$\frac{d\sigma^i}{dP} = (2\pi)^3 |\psi_i(0)|^2 \frac{E}{M} \frac{d\sigma^0}{d\tilde{p}d\tilde{q}} |_{\tilde{p} = \tilde{q} = P/2},$$

(1)

where the rightmost term describes the production of $\pi^+\pi^-$ pairs of equal momenta ($\tilde{p} = \tilde{q}$).

The pionium state is defined by the centre-of-mass momentum $P$ and its quantum numbers $n_i, l_i$, and $m_i$. For the sake of simplicity in this paper, we have considered monochromatic atoms of 4.6 GeV/c, corresponding to the average laboratory momentum of pionium in DIRAC. The influence of using the experimental pionium spectrum is small, as shown in [8]. The yield of a particular state is proportional to its wavefunction squared at the origin. It has been shown in [11] that the effect of the strong interaction between the two pions of the atom significantly modifies the magnitude of $|\psi_i(0)|$, as compared to the pure Coulomb wavefunction. However, the ratio of the production rates for different states was shown to be the same as for the Coulomb wavefunctions [12]. Thus, considering that the Coulomb functions follow

$$|\psi_i^{(C)}(0)|^2 = \begin{cases} 0 & \text{if } l_i \neq 0, \\ (\alpha M\pi / 2)^3 \pi n_i^3 & \text{if } l_i = 0, \end{cases}$$

(2)

one can observe that only the S states are being created, and the creation probability has $1/n_i^3$ dependence.

We assume that the atom propagates along the $z$ direction, through the target foil of certain thickness and of infinite transverse $(x, y)$ size. The target is assumed to be composed of a chemically pure material, such as nickel, platinum or titanium. Our goal is then to find the population probability of any bound state as a function of the $z$ position in the target, from which other results, such as the break-up probability, would follow. Ordinarily, a classical approach is utilized to solve this problem [3, 7]. One considers the total cross section $\sigma_i^{\text{tot}}$ and discrete-state transition cross sections for a pionium–target atom scattering $\sigma_{i,l}$. The probabilistic evolution equation is then applied:

$$\frac{dP_i(z)}{dz} = -\frac{1}{\beta \gamma} \Gamma_i P_i(z) - n_0 \sum_l c_{i,l} P_l(z),$$

(3)

where $P_i(z)$ is the classical probability for the atom to be found in the $i$ state, $\beta \gamma = 16.48$ is the Lorentz centre-of-mass to laboratory transition factor for momentum $P = 4.6$ GeV/c, $n_0$ is the number of target atoms per unit volume and $c_{i,l}$ are the transition coefficients. The value of $n_0$ can be expressed via the target density $\rho$, the Avogadro number $N_0$ and the atomic mass of the target atoms $A$:

$$n_0 = \frac{\rho N_0}{A}.$$

(4)

The transition coefficients depend on the pionium–target atom cross sections as

$$c_{i,l} = \delta_{i,l} \sigma_i^{\text{tot}} - \sigma_{l,l}.$$

(5)

The pionium decay is strongly dominated by the $\pi^+\pi^- \rightarrow \pi^0\pi^0$ decay channel (BR $> 99\%$ [10]). Taking this into account, the width of the $i$ state is proportional to the isospin 0 and 2 pion–pion scattering length difference [14]:

$$\Gamma_i = \frac{16\pi}{9} \sqrt{M_\pi^2 - M_{\pi^0}^2 - \frac{1}{4} M_\pi^2 m_\pi^2} (a_0^0 - a_0^2) (1 + \delta_i) |\psi_i^{(C)}(0)|^2,$$

(6)
where $M_\pi$ and $M_\pi^0$ are the masses of the charged and the neutral pion and $\delta_\Gamma = 0.058$ is the next-to-leading-order correction that includes the effect of the strong interaction between the two pions. Considering the usual relationship between the decay width $\Gamma_i$ and the corresponding lifetime $\tau_i$ of a given state $\Gamma_i = \tau_i^{-1}$ and using equation (2), we find that pionium atoms decay only from the S states and that the lifetime of an S state is related to the ground state lifetime as

$$\tau_{00} = n^3 \tau.$$  \hfill (7)

The lifetime of pionium is hence the only parameter necessary as input for the evolution equation and which can be related to any of its outputs. In this paper, we will develop the relationship between the break-up probability and the lifetime.

DIRAC’s experimental results will be used to test the precise prediction of the scattering length difference by the chiral perturbation theory with $a_0^0 - a_2^0 = 0.265 \pm 0.004 \, (5\% \text{ accuracy})$, which corresponds to the lifetime of $\tau = (2.9 \pm 0.1) \times 10^{-15} \text{ s}$ \cite{15}.

3. The density matrix evolution equation

Equation (3) has an exact solution set containing the eigenvalues and the eigenvectors of the matrix $c_{i,l}$ \cite{3}. Alternatively, it can be solved by applying Monte Carlo methods \cite{8} for the bound states with $n < 8$, which is enough to precisely calculate the break-up probability, as explained in \cite{8}. However, the classic probabilistic methods neglect the quantum interference between the pionium states during their passage through the target, as demonstrated by Voskresenskaya \cite{9}, and are, thus, imprecise.

A more precise description of the dynamics of the system may be given in terms of the density matrix $\rho_{ik}$. Within this framework, the evolution equation can be written as \cite{9}

$$\frac{\partial \rho_{ik}}{\partial z} = \frac{1}{\beta \gamma} \left[ i(\epsilon_k - \epsilon_i) - \frac{1}{2}(\Gamma_i + \Gamma_k) \right] \rho_{ik}(z) - n_0 \sum_{l,m} \Omega_{ik,lm} \rho_{lm}(z),$$ \hfill (8)

where $\epsilon_k$ indicates the binding energy of the $k$th state and $\Omega_{ik,lm}$ is the matrix of transition coefficients. This equation reduces to (3), if one replaces $\rho_{ii}(z)$ with $P_i(z)$ and the $\Omega_{ik,lm}$ cross terms (obeying $i \neq k$ or $l \neq m$) are set to zero.

The goal of this work is to find the solution to this equation and determine what corrections to (3) are to be made to the break-up probability under the particular conditions of the DIRAC experiment.

4. The matrix elements

In order to calculate the matrix elements $c_{i,l}$ and $\Omega_{ik,lm}$, we apply the coherent, pure electrostatic first Born approximation. It has been found in \cite{8} that in order to achieve the precision of 1%, relativistic and multiphoton exchange neglected in the first Born approximation must be taken into account. However, for the purpose of establishing the relevance of the effects of quantum interference, the Born approximation is sufficiently accurate.

The expression for the pionium–target cross sections in the electrostatic first Born approximation was obtained by Mrówczyński using classical methods \cite{2}:

$$\sigma_i = \frac{2}{\beta^2} \int |U(q)|^2 \left[ 1 - F_i^i(q) \right] d^2q,$$ \hfill (9)

$$\sigma_{i,l} = \frac{1}{\beta^2} \int |U(q)|^2 \left| F_i^l \left( \frac{q}{2} \right) - F_i^l \left( - \frac{q}{2} \right) \right|^2 d^2q,$$ \hfill (10)
where $q$ is the momentum transfer between the target and the pionium atoms. Due to the symmetry of the collisions with respect to the scattering axis, the cross section depends only on the two transverse momentum coordinates. We have chosen the Fourier transform of the target atom potential $U(q)$ to have the Molière parametrization of the Thomas–Fermi equation [16]:

$$U(q) = 4\pi Z\alpha \left( \frac{0.35}{q^2 + q_0^2} + \frac{0.55}{q^2 + 16q_0^2} + \frac{0.10}{q^2 + 400q_0^2} \right) q_0 = \frac{0.32Z^{1/3}}{0.885a_0}.$$  

with $a_0 = 0.529 \times 10^{-10}$ cm being the Bohr radius of the hydrogen atom, $\alpha$ being the fine structure constant and $Z$ being the atomic number of the target atoms. The $F_l^i(q)$ are the pionium form factors:

$$F_l^i(q) = \int \psi^*_l(\vec{r}) e^{i\vec{q}\cdot\vec{r}} \psi^i(\vec{r}) d\vec{r},$$

calculated in [3] and [4]. In this work, we use the code developed by [17] based on results of [3].

In terms of $\Omega_{ik,lm}$ elements of the density matrix, equation (5) can be written as

$$\Omega_{ik,lm}^{(1)} = \Omega_{ik,lm} - \Omega_{ik,lm}^{(2)},$$

where

$$\Omega_{ik,lm}^{(1)} = \frac{\delta_{ik}}{2\beta^2} \int |U(q)|^2 \left[ 2\delta_{ij} - F_l^i(q) - F_l^i(-q) \right] d^2q$$

and

$$\Omega_{ik,lm}^{(2)} = \frac{1}{2\beta^2} \int |U(q)|^2 \left[ 2\delta_{ik,m} - F_m^i(q) - F_m^i(-q) \right] d^2q,$$

plays the role of the total cross section, while

$$\Omega_{ik,lm}^{(2)} = \frac{1}{2\beta^2} \int |U(q)|^2 \left[ F_m^l(q) - F_m^l(-q) \right] \left[ F_m^l(q) - F_m^l(-q) \right]^* d^2q,$$

is the analogue of the transition cross section. In fact, $\Omega_{ik,lm}^{(1)}$ yields the total cross section if $i = k$ and $l = m$ in $\Omega_{ik,lm}^{(2)}$ gives the transition cross section when $i = k$ and $l = m$.

Equations (14) and (15) are our main tools for the numerical calculations and their derivation from the original formulae of [9] can be found in the appendix A.

### 4.1. Selection rules and transition elements examples

As pointed out in [9], and due to the properties of the form factors under the parity transformation, the $\Omega_{ik,lm}$ coefficients are different from zero only if

$$m_i - m_k - m_l + m_m = 0, \quad l_i - l_k - l_l + l_m = 2s,$$

where it should be recalled that $m_{i(k,l,m)}$ and $l_{i(k,l,m)}$ are the magnetic and orbital quantum numbers of the states $|i(k,l,m)\rangle$. The index $s$ is an arbitrary integral number.

The choice of the $z$ direction as the quantization axis means that the transitions between states of different $z$-parity are strongly suppressed [3]. It then follows that only the states with even $l - m$ are populated since pionium atoms are produced in S states exclusively. Considering (16), this means that

$$\rho_{ik}(z) \neq 0 \quad \text{if} \quad m_i = m_k, \quad l_i = l_k + 2s.$$  

This rule could be violated by the complex coefficient in (8):
which produces an oscillatory term in the solutions. However, for the ground and the lowest excited states the condition

\[ n_0 |\Omega_{ik,ik}| \ll |\epsilon_k - \epsilon_i| \beta \gamma \]

can be applied and in a small interval the \( \rho_{ik}(z) \) solution oscillates rapidly compared to the electromagnetic transition range (defined by \( n_0 |\Omega_{ik,ik}| \)) and can be considered to average to zero:

\[ \rho_{ik}(z) \approx 0. \]

Since the energy of the hydrogen-like system depends only on the principal quantum number, in the exceptional case of the \( i \) and \( k \) states belonging to the same shell \( \epsilon_k - \epsilon_i \) is equal to 0. Hence, for the low energy states, one can complete relation (17) as

\[ \rho_{ik}(z) \neq 0 \quad \text{if} \quad \epsilon_i = \epsilon_i \left( n_i = n_k \right), \quad m_i = m_k, \quad l_i = l_k + 2s. \quad (18) \]

On the other hand, if the principal quantum numbers of the \( i \) and \( k \) states obey the \( n_{i,k} \geq 6 \) relationship, then

\[ n_0 |\Omega_{ik,ik}| \sim |\epsilon_k - \epsilon_i| \beta \gamma \]

and the solution for \( \rho_{ik}(z) \) is non-zero even though \( i \) and \( k \) do not belong to the same shell.

In figure 1, we can see that while \( \rho_{100(200)}(z) \) oscillates more than six times in 0.1 \( \mu \text{m} \), \( \rho_{600(700)} \) does not oscillate at all in a fairly large interval.

To illustrate the individual matrix elements, we consider the subspace formed by the \( \langle 211 \rangle, \langle 300 \rangle \) and \( \langle 320 \rangle \) states. The \( \Omega \) matrix restricted to this subspace is shown in table 1. One observes that for this restricted sample, the \( \langle 320 \rangle \langle 300 \rangle \) mixed state matrix elements are of the same order of magnitude as for the same pure shell states.

5. Solving the equations

Using the Runge–Kutta method [18], we were able to numerically solve the systems of differential equations (3) and (8). Finding the eigenvalues, as was done in [3], was considered to be too lengthy due to the size of the density matrix system. The Monte Carlo method of
Table 1. $\Omega$ matrix elements in the $|211\rangle$, $|300\rangle$, $|320\rangle$ subspace in units of $10^{-20}$ barn.

| $\Omega_{ijkl}^m$ | $|211\rangle\langle 211|$ | $|300\rangle\langle 300|$ | $|320\rangle\langle 320|$ |
|------------------|-----------------|-----------------|-----------------|
| $|211\rangle\langle 211|$ | -4.66 | 0.044 | -0.083 | 0.234 |
| $|300\rangle\langle 300|$ | 0.044 | -18.2 | 2.41 | 0 |
| $|320\rangle\langle 320|$ | -0.083 | 2.41 | -13.7 | 2.41 |
| $|320\rangle\langle 320|$ | 0.234 | 0 | 2.41 | -9.10 |

[7] cannot be applied to the density matrix formalism since the system (8) does not obey the relationship

$$\Omega_{ik,ik} \geq \sum_{lm \neq ik} |\Omega_{ik,lm}|.$$ (19)

We have considered a 95 $\mu$m nickel target and a monochromatic 4.6 GeV/c atom sample. In accordance with the theoretical prediction [15], the lifetime of the ground state of pionium was taken to be $\Gamma^{-1} = 2.9 \times 10^{-15}$ s. The initial conditions are given by

$$P_i(0) = \rho_{ii}(0) = n_i^{-3}/\zeta(3) \quad \text{if } l_i = 0,$$
$$P_i(0) = \rho_{ij}(0) = 0 \quad \text{otherwise},$$ (20)

with $\zeta(3) = \sum n^{-3} \approx 1.202$. The system has been restricted to the bound states with $n \leq 7$. This means considering 84 mixed states and 353 088 $\Omega$ matrix elements different from zero. Cutting the number of states under consideration was found [7] to have only a minor effect on the solution for the last two shells, i.e. the states with $n = 6$ and $n = 7$.

To achieve a very good accuracy of the final results, we have considered the following sequence of step lengths in the numerical integration of the equations:

$$h = 2 \times 10^{-3}, 1 \times 10^{-3}, 0.5 \times 10^{-3}, 0.25 \times 10^{-3}, 0.1 \times 10^{-3} (\mu m)$$

and made a polynomial extrapolation to the limit $h = 0$ [18]. The precision in calculation is obtained as the difference between the extrapolation and the $h = 0.1 \times 10^{-3}$ (\mu m) results. This is, of course, a pure mathematical precision. The physics result accuracy is dominated by the input used for $\Omega$ and $\sigma$. This has been thoroughly discussed in [7]. As we are focusing our interest on the discrepancy between the probabilistic and density matrix approaches, we only quote the numerical precision of the equation solutions.

As we will explain below, we are mainly interested in the averaged integrals of $\rho_{ii}(z)$ and $P_i(z)$ over the target thickness $W$:

$$p_i^{\text{disc}} = \frac{1}{W} \int_0^W \rho_{ii}(z) \, dz.\quad (21)$$

We can switch to the $P$ representation in this equation by changing $\rho_{ii}(z) \rightarrow P_i(z)$. In table 2, the $P_{\text{disc}}$ results are shown as a function of the principal and angular quantum numbers summed over the magnetic quantum number $m$ for a 95 $\mu$m nickel target. The differences are not very large, especially for the ground and lowest excited states. However, for some particular states the difference can rise up to 20%. In figure 2, we see the discrepancy between $\rho$ and $P$ in an example of the $|320\rangle$ state.

5.1. Obtaining the break-up probability

Our goal is to obtain the break-up probability $P_{\text{br}}$ of the pionium atom in the target. As we have seen in the previous sections, the atoms in the target can undergo transitions between
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Figure 2. The solution of (3) and (8) for the |320⟩ state.

bound states and annihilate. However, in collisions with target atoms they can also make transitions to a continuum state. The coefficients $c_{i,j}$ and $\Omega_{k,lm}$, taking into account transitions between discrete and continuum states, are more difficult to compute than the discrete–discrete ones since the atomic form factors are more involved [4]. However, as shown in [7] using the probabilistic approach, the direct calculation of the break-up probability from the system solutions is not satisfactory since it decreases very slowly as a function of the principal quantum number of the broken discrete state and only a finite number of shells ($n \leq 7$) are considered when solving either (3) or (8). One would have to guess the break-up probability for any shell with $n > 7$ and would likely make a sizable error in the determination of the total break-up probability.

The standard strategy for obtaining the break-up probability is to, first, calculate the probability of the atom to leave the target in a discrete state ($P_{\text{dsc}}$) and the probability of

Table 2. Summed $P_{\text{dsc}} = \sum_{m} P_{\text{dsc}}^{lm}$ results in the probabilistic ($P$) and density matrix ($\rho$) representations. The average is over $W = 95 \mu$m and the target material is nickel. The accuracy of the result does not account for the physical uncertainty of $\Omega$ and $\sigma$, as discussed in section 5.

| $n$ | $P_{\text{dsc}}$ | $P$ | $\rho$ |
|-----|-----------------|-----|-------|
| 1   | 0.072854        | 0.072860 |
| 2   | 0.0050676       | 0.008500 |
| 3   | 0.00087163      | 0.0016366 |
| 4   | 0.00024899      | 0.0006270 |
| 5   | 0.0000489072    | 0.00006445 |
| 6   | 0.0000038357    | 0.000003979 |
| 7   | 0.0000034640    | 0.0000043716 |

$\rho_{320,320} \rangle < 320 \rangle < \rho_{320}$
annihilation \( (P_{\text{anh}}) \) and then make use of the relation:
\[
1 = P_{\text{br}} + P_{\text{dsc}} + P_{\text{anh}}.
\] (22)
As both \( P_{\text{dsc}} \) and \( P_{\text{anh}} \) decrease rapidly with \( n \), we can obtain an accurate result taking into account only those events with \( n \leq 7 \). A small correction will be introduced for \( P_{n>7}^{\text{dsc}} \).

Under the experimental conditions, the atoms are not created close to the front face of the target but uniformly distributed along the target thickness. The probability of the atom leaving the target in a discrete state can be, however, linked to the solutions of the initial conditions (20) by
\[
P_{\text{dsc}} = \sum_i \frac{f_0^W \rho_{ii}(W - z) \, dz}{W} = \sum_i \frac{f_0^W \rho_{ii}(z) \, dz}{W},
\] (23)
where \( W \) is the target thickness (of 95 \( \mu \text{m} \) in our case).

The annihilation probability calculation is slightly more involved. If the atom is created at \( z_0 \), the probability that it reaches point \( z \) and annihilates is given by \( \Gamma_i \rho_{ii} \). But \( z \) can take on any value between \( z_0 \) and the target thickness \( W \). Meanwhile, if the atom production points are distributed uniformly between 0 and \( W \), the annihilation probability is then given by
\[
P_{\text{anh}} = \sum_i \frac{\Gamma_i}{W} \int_0^W \int_{z_0}^W \rho_{ii}(z - z_0) \, dz \, dz_0 = \sum_i \frac{\Gamma_i}{W} \int_0^W (W - z) \rho_{ii}(z) \, dz.
\] (24)
Evidently, the probabilistic representation can be recovered by substituting \( P_i(z) \) for \( \rho_{ii}(z) \) in (23) and (24).

As was done for the case of \( P_{\text{dsc}} \) (21), we can define the annihilation probability from a certain state as
\[
P_{\text{anh}}^i = \frac{\Gamma_i}{W} \int_0^W (W - z) \rho_{ii}(z) \, dz,
\] (25)
where again replacing \( \rho_{ii}(z) \rightarrow P_i(z) \) restores the \( P \) representation. Of course, \( P_{\text{anh}}^i \) is 0 for any state with \( l_i \neq 0 \).

The results for the annihilation probability from the S states up to \( n = 7 \) are shown in table 3 and complete those of the \( P_{\text{dsc}} \) in table 2.

In figure 4, we show the dependence of \( P_{\text{dsc}}^n \) and \( P_{\text{anh}}^n \) on the principal quantum number. The results have been summed over every bound state. We can check that while \( P_{\text{anh}}^n \) rapidly...
Table 3. $P_{\text{anh}}$ results in the $P$ and $\rho$ representations. The average is over $W = 95 \, \mu\text{m}$ and the target material is nickel. The lifetime of pionium was assumed to be $2.9 \times 10^{-15} \, \text{s}$. The precision of the results has the same meaning as in table 2.

| $n$ | $P_{\text{anh}}$ | $P / \rho$ |
|-----|------------------|------------|
| 1   | 0.072 854        | 0.072 860  |
| 2   | 0.005 067 6      | 0.005 087 8|
| 3   | 0.000 871 63     | 0.000 869 09|
| 4   | 0.000 248 99     | 0.000 246 20|
| 5   | 0.000 092 377    | 0.000 089 072|
| 6   | 0.000 038 357    | 0.000 034 640|
| 7   | 0.000 015 300    | 0.000 013 706|

Table 4. Probability results in the $P$ and $\rho$ representations. The average is over $W = 95 \, \mu\text{m}$ and the target material is nickel. The lifetime of pionium was assumed to be $2.9 \times 10^{-15} \, \text{s}$.

| Picture | $P_{\text{br}}$ | $P_{\text{anh}}$ | $P_{\text{ani}}^{<7}$ | $P_{\text{ani}}^{\geq7}$ |
|---------|-----------------|-------------------|------------------------|------------------------|
| $P$     | 0.459 254       | 0.444 536         | 0.094 7916             | 0.001 418             |
| $\rho$  | 0.459 268       | 0.444 575         | 0.094 9106             | 0.001 245             |

converges to zero, and can be neglected for $n_i > 4$, $P_{\text{ani}}^{i}$ decreases more slowly. This leads us to introduce an extrapolation for $P_{\text{ani}}^{\geq7}$ [3]:

$$P_{\text{ani}}^{\geq7} = \frac{a}{n^2} + \frac{b}{n^3},$$

(26)

where $a$ and $b$ are obtained by fitting $P_{\text{ani}}^{n}$ at $n = 5$ and $n = 6$. This extrapolation is also used for $n = 7$ because neglecting the following shells in the systems of equations changes the solutions for this particular shell.

The results of the extrapolation are summed over $n$ and, together with $P_{\text{ani}}^{<7}$ and $P_{\text{anh}}$, subtracted from 1 to yield the break-up probability:

$$P_{\text{br}} = 1 - P_{\text{anh}} - P_{\text{ani}}^{<7} - P_{\text{ani}}^{\geq7}.$$  

(27)

For our particular example of atoms propagating in a 95 $\mu\text{m}$ Ni target with the lifetime of $2.9 \times 10^{-15} \, \text{s}$, we obtain $P_{\text{br}} = 0.459 254$ in the probabilistic picture and $P_{\text{br}} = 0.459 268$ in the density matrix formalism. The other probabilities are shown in table 4.

6. Discussion and conclusions

We have found that for DIRAC’s experimental conditions, the effect of the quantum interference between states does not change the result of the break-up probability of pionium.
in the target. Hence, the results obtained with the classical methods are accurate enough to safely perform the experimental measurement.

The break-up probability is unchanged despite the fact that for some discrete states, as $|320\rangle$, the effect of interference can significantly increase the population of the state by a value of up to 20%. However, the affected states are sparsely populated and, hence, are not relevant for the final results.

These results might change if most of the atoms were not created in the ground state, as the latter is non-degenerate and interference effects appear only after the first transition. We have considered the scenario when all the atoms are created in the $|300\rangle$ state and have not observed any significant changes using the probabilistic approach. One possible explanation is that, while the interference is most likely to occur between the states with the same magnetic quantum number $m$, and comparable to the transition cross sections, the dominant transitions are those that increase $l$ and $m$ by one unit, free of interference with the parent state. Moreover, the interference only affects states with $n \geq 3$. For these states, the annihilation probability per unit length is much smaller than the electromagnetic (ionization or discrete) scattering probability per unit length. As the highly excited atoms will finish being ionized, the transition between two discrete states does not affect the final break-up probability result.

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Appendix. The $\Omega$ matrix elements in the first Born approximation

Here we will show the method of obtaining the discrete matrix elements of the $\Omega$ matrix in the first Born approximation from the original equations of [9]. The $\Omega$ operator is originally defined as a function of the transverse position of the atom wavefunctions $\vec{s}_1, \vec{s}_2$. If one splits the operator into two parts:

$$\Omega(\vec{s}_1, \vec{s}_2) = \Omega^{(1)}(\vec{s}_1, \vec{s}_2) + \Omega^{(2)}(\vec{s}_1, \vec{s}_2),$$  \hspace{1cm} (A.1)

its definition can then be given as

$$\Omega^{(1)}(\vec{s}_1, \vec{s}_2) = \int \left[ \Gamma(\vec{b}, \vec{s}_1) + \Gamma^*(\vec{b}, \vec{s}_2) \right] d^2b,$$  \hspace{1cm} (A.2)

$$\Omega^{(2)}(\vec{s}_1, \vec{s}_2) = -\int \Gamma(\vec{b}, \vec{s}_1)\Gamma^*(\vec{b}, \vec{s}_2) d^2b.$$  \hspace{1cm} (A.3)

Applied to the case of the $\pi^+\pi^-$-atom, the interaction operator of the Glauber theory is given by

$$\Gamma(\vec{b}, \vec{s}) = 1 - \exp[i\chi(\vec{b} - \vec{s}/2) - i\chi(\vec{b} + \vec{s}/2)],$$  \hspace{1cm} (A.4)

where

$$\chi(\vec{B}) = \frac{1}{\beta} \int_{-\infty}^{\infty} U(\sqrt{B^2 + z^2}) dz,$$  \hspace{1cm} (A.5)

with $U(r)$ being the potential of the target atoms given by the inverse Fourier transform of (11).
First, let us re-write $\Omega^{(1)}(\vec{s}_1, \vec{s}_2)$. It is convenient to split $\Gamma(\vec{b}, \vec{s})$ into real and imaginary parts:

$$\Gamma(\vec{b}, \vec{s}_1(2)) = \text{Re} \Gamma(\vec{b}, \vec{s}_1(2)) + i \text{Im} \Gamma(\vec{b}, \vec{s}_1(2)), \quad (A.6)$$

$$\text{Re} \Gamma(\vec{b}, \vec{s}_1(2)) = 1 - \cos[\chi(\vec{b} - \vec{s}/2) - \chi(\vec{b} + \vec{s}/2)]$$

$$= \frac{1}{2} \Gamma(\vec{b}, \vec{s}_1(2)) \Gamma^* (\vec{b}, \vec{s}_1(2)), \quad (A.7)$$

$$\text{Im} \Gamma(\vec{b}, \vec{s}_1(2)) = -\sin[\chi(\vec{b} - \vec{s}/2) - \chi(\vec{b} + \vec{s}/2)], \quad (A.8)$$

where the integral over the imaginary part tends to zero

$$\int \text{Im} \Gamma(\vec{b}, \vec{s}_1(2)) \, d^2 b = 0, \quad (A.9)$$

due to the odd nature of the sin function and the even nature of $\chi(\vec{b} \pm \vec{s}/2)$. Taking this into account, we have

$$\Omega^{(1)}(\vec{s}_1, \vec{s}_2) = \frac{1}{2} \int [\Gamma(\vec{b}, \vec{s}_1) \Gamma^* (\vec{b}, \vec{s}_1) + \Gamma(\vec{b}, \vec{s}_2) \Gamma^* (\vec{b}, \vec{s}_2)] \, d^2 b. \quad (A.10)$$

Our final goal is to obtain the matrix elements $\Omega^{(1,2)}_{ik,lm}$, defined as

$$\Omega^{(1,2)}_{ik,lm} = \int \psi_i^*(\vec{r}_1) \psi_l(\vec{r}_1) \psi_k(\vec{r}_2) \psi_m^*(\vec{r}_2) \Omega^{(1,2)}(\vec{s}_1, \vec{s}_2) \, d\vec{r}_1 \, d\vec{r}_2. \quad (A.11)$$

In particular, we can define the profile-function $\Gamma_{il}(\vec{b})$:

$$\Gamma_{il}(\vec{b}) = \int \psi_i^*(\vec{r}) \psi_l(\vec{r}) \Gamma_{il}(\vec{b}, \vec{s}) \, d\vec{r}, \quad (A.12)$$

and its Fourier transform, the amplitude:

$$A_{il}(\vec{q}) = \frac{1}{2\pi} \int e^{i\vec{q} \cdot \vec{b}} \Gamma_{il}(\vec{b}) \, d^2 b, \quad (A.13)$$

$$\Gamma_{il}(\vec{b}) = \frac{1}{2\pi} \int e^{-i\vec{q} \cdot \vec{b}} A_{il}(\vec{q}) \, d^2 q. \quad (A.14)$$

It is easy to check that

$$\Omega^{(2)}_{ik,lm} = - \int \Gamma_{il}(\vec{b}) \Gamma^*_{km}(\vec{b}) \, d^2 b = - \int A_{il}(\vec{q}) A^*_{km}(\vec{q}) \, d^2 q. \quad (A.15)$$

More involved calculation is required in order to obtain an analogue of (A.15) for $\Omega^{(1)}_{ik,lm}$. By definition,

$$\Omega^{(1)}_{ik,lm} = \frac{\delta_{km}}{2} \int \left[ \int \psi_i^*(\vec{r}) \psi_l(\vec{r}) \Gamma(\vec{b}, \vec{s}) \Gamma^* (\vec{b}, \vec{s}) \, d\vec{r} \right] \, d^2 b$$

$$+ \frac{\delta_{il}}{2} \int \left[ \int \psi_k^*(\vec{r}) \psi_m(\vec{r}) \Gamma(\vec{b}, \vec{s}) \Gamma^* (\vec{b}, \vec{s}) \, d\vec{r} \right] \, d^2 b. \quad (A.16)$$

To derive the final result we will need the completeness equation of the form:

$$\delta(\vec{r} - \vec{r}') = \sum_j \psi_j(\vec{r}) \psi_j^*(\vec{r}'). \quad (A.17)$$
which allows one to express the inside integrals in (A.16) in terms of the profile-function $\Gamma_{ij}(\vec{b})$:
\[
\int \psi_i^*(\vec{r}) \psi_j(\vec{r}) \Gamma(\vec{b}, \vec{z}) \Gamma^*(\vec{b}, \vec{z}) \, d\vec{r}
\]
\[
= \int \psi_i^*(\vec{r}) \psi_j(\vec{r'}) \delta(\vec{r} - \vec{r'}) \Gamma(\vec{b}, \vec{z}) \Gamma^*(\vec{b}, \vec{z'}) \, d\vec{r} \, d\vec{r'}
\]
\[
= \sum_j \left[ \int \psi_i^*(\vec{r}) \Gamma(\vec{b}, \vec{z}) \psi_j(\vec{r}) \, d\vec{r} \right] \left[ \int \psi_j^*(\vec{r'}) \Gamma^*(\vec{b}, \vec{z'}) \psi_j(\vec{r'}) \, d\vec{r'} \right]
\]
\[
= \sum_j \Gamma_{ij}(\vec{b}) \Gamma_{jj}^*(\vec{b}),
\]
where one can make the substitution
\[
\int \sum_j \Gamma_{ij}(\vec{b}) \Gamma_{jj}^*(\vec{b}) \, d^2 b = \int \sum_j A_{ij}(\vec{q}) A_{ij}^*(\vec{q}) \, d^2 q,
\]
(A.18)
to obtain
\[
\Omega_{ik,lm}^{(1)} = \frac{\delta_{km}}{2} \int \sum_j A_{ij}(\vec{q}) A_{ij}^*(\vec{q}) \, d^2 q + \frac{\delta_{il}}{2} \int \sum_j A_{mj}(\vec{q}) A_{mj}^*(\vec{q}) \, d^2 q.
\]
(A.20)
In the Born approximation
\[
A_{ij}(\vec{q}) = \frac{1}{\beta} U(\vec{q}) \left[ F_i^j \left( \frac{\vec{q}}{2} \right) - F_i^j \left( -\frac{\vec{q}}{2} \right) \right],
\]
(A.21)
with the form factors defined in (12).
We now perform the summation:
\[
\sum_j A_{ij}(\vec{q}) A_{ij}^*(\vec{q}) = \sum_j \left[ F_i^j \left( \frac{\vec{q}}{2} \right) - F_i^j \left( -\frac{\vec{q}}{2} \right) \right] \left[ F_i^j \left( \frac{\vec{q}}{2} \right) - F_i^j \left( -\frac{\vec{q}}{2} \right) \right]^*
\]
\[
= \sum_j \left[ \int \psi_i^*(\vec{r}) (e^{i\vec{q} \cdot \vec{r}}/2 - e^{-i\vec{q} \cdot \vec{r}}/2) \psi_j(\vec{r}) \, d\vec{r} \right]
\]
\[
\times \left[ \int \psi_j^*(\vec{r'}) (e^{-i\vec{q} \cdot \vec{r'}}/2 - e^{i\vec{q} \cdot \vec{r'}}/2) \psi_j(\vec{r'}) \, d\vec{r'} \right]
\]
\[
= \int \psi_i^*(\vec{r}) (e^{i\vec{q} \cdot \vec{r}}/2 - e^{-i\vec{q} \cdot \vec{r}}/2) \psi_j(\vec{r}) \, d\vec{r}
\]
\[
= \int \psi_i^*(\vec{r}) (2 - e^{-i\vec{q} \cdot \vec{r}} - e^{i\vec{q} \cdot \vec{r}}) \psi_j(\vec{r}) \, d\vec{r} = 2\delta_{ij} - F_i^j(\vec{q}) - F_i^j(-\vec{q}).
\]
(A.22)

From equations (A.15), (A.16), (A.18), (A.19), (A.21) and (A.22), one can derive the final expressions in the Born approximation:
\[
\Omega_{ik,lm} = \Omega_{ik,lm}^{(1)} + \Omega_{ik,lm}^{(2)},
\]
\[
\Omega_{ik,lm}^{(1)} = \frac{\delta_{km}}{2\beta^2} \int |U(q)|^2 \left[ 2\delta_{il} - F_i^j(\vec{q}) - F_i^j(-\vec{q}) \right] \, d^2 q
\]
\[
+ \frac{\delta_{il}}{2\beta^2} \int |U(q)|^2 \left[ 2\delta_{km} - F_k^m(\vec{q}) - F_k^m(-\vec{q}) \right] \, d^2 q,
\]
(A.14)
\[
\Omega_{ik,lm}^{(2)} = \frac{1}{\beta^2} \int |U(q)|^2 \left[ F_i^j \left( \frac{\vec{q}}{2} \right) - F_i^j \left( -\frac{\vec{q}}{2} \right) \right] \left[ F_k^m \left( \frac{\vec{q}}{2} \right) - F_k^m \left( -\frac{\vec{q}}{2} \right) \right] \, d^2 q.
\]
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