

CERN Summer Student Report

First step in the process of calculating the cross section for muonic antihydrogen

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Introduction

The end goal of the project is to measure the charge radius of the antiproton with muons. However a necessary step first is to calculate cross section of Muonium and antiprotons in the production of antihydrogen to determine the feasibility of such an experiment.

$$\bar{p} + Mu \rightarrow \bar{H}_\mu + e^- \quad (1)$$

Muonium (Mu) is a bound neutral atom consisting of an antimuon (μ^+) and electron (e^-). This is of great interest due to recent results by ETH [1] in the measurement of the charge radius of the proton which was seven standard deviations away from the expected value. Muonic antihydrogen would also present the opportunity to verify or falsify the CPT conservation law where CPT refers to the product of three symmetry operations: charge transformations, parity-inversion and time reversal [2].

The reaction for positronium(Ps) and antiprotons is of the same form as (1):

$$\bar{p} + Ps \rightarrow \bar{H} + e^- \quad (2)$$

where positronium consists of an electron and a positron.

It is on this premise that the work on calculating cross sections began given that there are many published results for $\bar{H}$ cross sections with positronium including that for excited states[3]. The next step is to then adapt the method to take into account the muon's additional mass of $105.7 MeV/c^2 \sim 207m_e = \frac{1}{9}m_p$ and short lifetime of $2.2\mu s$ [4].

Antihydrogen Formation

To form antihydrogen, a very low velocity for the incoming beam of particles is required in order to approach the target which is close to rest. If the incoming particle has a high velocity the probability of Rutherford scattering increases and the cross section diminishes. Rutherford scattering is the single elastic scattering of charged particles due to the Coulomb interaction. The use of perturbation techniques to analyse the interaction in antihydrogen formation is inappropriate as the particle velocities are below 10au. Initially it was thought that the Born approximation could be used for $\bar{H}$ however due to the low energies being considered in the keV range this was abandoned. Nevertheless time was spent analysing [3] which uses the Born approximation to treat $\bar{H}$ formation with Ps in excited states. This yielded a greater understanding of the Bethe integral with [5] and its use in calculating the transition matrix.

The relation between reaction cross sections is:

$$\sigma(\bar{p} + Ps \rightarrow \bar{H} + e^-) = \sigma(p + Ps \rightarrow H + e^+) = \frac{k_e^2}{k_{Ps}^2} \sigma(e^+ + H \rightarrow Ps + p) \quad (3)$$

k_e and k_{Ps} are the wavenumbers of e^+ and Ps

The significance of the transition(T) matrix lies in its relationship to the cross section which can be solved numerically

$$\sigma_{ji}^{(1)} = \frac{2l+1}{2\pi^2} \frac{k_j}{k_i} \left| \int_{-1}^1 T_{ji} P_l(\mu) d\mu \right|^2 \quad (4)$$

$\mu = \mathbf{k}_i \cdot \mathbf{k}_j / k_i k_j$ and $\mathbf{k}_i$ and $\mathbf{k}_j$ are momentum vectors.

The T matrix element is calculated by the following formula where $\sigma(e^+ + H(nl) \rightarrow Ps(\nu\lambda) + p)$ is used as the cross section:

$$T_{ji} = \int d^3x d^3r \exp(-i\mathbf{k}_j \cdot \mathbf{R}) \psi_j^*(s) \left(\frac{1}{x} - \frac{1}{r} \right) \exp(i\mathbf{k}_i \cdot \mathbf{x}) \psi_i(r) \quad (5)$$

where $\psi_i = \psi_{nlm_i}(\mathbf{r})$ and $\psi_j = \psi_{\nu\lambda\mu_\lambda}(\mathbf{s})$ are H and Ps wavefunctions, the Coulomb potential V is $\left(\frac{1}{x} - \frac{1}{r} \right)$
 $\mathbf{r}$ and $\mathbf{x}$ are the e^- and e^+ vectors (relative to p) while $\mathbf{s} = \mathbf{r} - \mathbf{x}$ and $\mathbf{R} = (\mathbf{r} + \mathbf{x}) / 2$
The relation between the wave numbers is:

$$k_j^2 = 2k_i^2 - \frac{2}{n^2} + \frac{1}{\nu^2} \quad (6)$$

which can be derived using [6]

$$k^2 - 1 = \frac{1}{2}(\kappa^2 - 1) \quad \bar{H} \text{ and Ps are in the ground state}$$

$$k_i^2 - 1 = \frac{1}{2}(k_j^2 - 1)$$

$$k_i^2 - \frac{1}{n^2} = \frac{1}{2}(k_j^2 - \frac{1}{\nu^2}) \quad \text{for excited states}$$

The transition matrix can be rewritten with $\mathbf{x} = \mathbf{r} - \mathbf{s}$ and $\mathbf{R} = (\mathbf{r} + \mathbf{x}) / 2$ in the form:

$$T_{ji} = \int d^3s d^3r \psi_j^*(s) \left(\frac{1}{|\mathbf{r} - \mathbf{s}|} - \frac{1}{r} \right) \psi_i(r) \exp[i(\mathbf{k} \cdot \mathbf{r} - \mathbf{K} \cdot \mathbf{s})] \quad (5)$$

where $\mathbf{k} = \mathbf{k}_i - \mathbf{k}_j$ and $\mathbf{K} = \mathbf{k}_i - \frac{1}{2}\mathbf{k}_j$

These terms can then be separated into two terms, with the second being written in terms of Fourier transforms. For the second term:

$$T_{ji}^{(2)} = F[\psi_j^*(s); \mathbf{K}] F[\psi_i(r)/r; -\mathbf{k}] = \int d^3s \psi_j^*(s) \exp(-i\mathbf{K} \cdot \mathbf{s}) \int d^3r \frac{\psi_i(r)}{r} \exp(i\mathbf{k} \cdot \mathbf{r}) \quad (6)$$

The first term can then be written as:

$$T_{ji}^{(1)} = 4\pi \int d^3r e^{(-\frac{1}{2}\mathbf{k}_j \cdot \mathbf{r})} \psi_i(r) \bar{\psi}_j(\mathbf{r}; \mathbf{K}) \quad (7)$$

$$\bar{\psi}_j(\mathbf{r}; \mathbf{K}) = (2\pi)^{-3} \int d^3p \frac{F_j^*(\mathbf{p}) e^{i\mathbf{p} \cdot \mathbf{r}}}{|\mathbf{p} - \mathbf{K}|^2} \quad (8)$$

The reasoning behind equation (7) involves the Bethe integral:

$$\frac{1}{|\mathbf{r} - \mathbf{R}|} = \frac{1}{2\pi^2} \int \frac{d^3s}{s^2} e^{i\mathbf{s} \cdot \mathbf{r}} e^{-i\mathbf{s} \cdot \mathbf{R}} \quad (9a)$$

In this case:

$$\frac{1}{|\mathbf{r} - \mathbf{s}|} = \frac{1}{2\pi^2} \int \frac{d^3p}{p^2} e^{i\mathbf{p} \cdot \mathbf{r}} e^{-i\mathbf{p} \cdot \mathbf{R}} \quad (9b)$$

$$T_{ji} = \int d^3s d^3r \psi_j^*(s) \left(\frac{1}{|\mathbf{r} - \mathbf{s}|} \right) \psi_i(r) \exp[i(\mathbf{k} \cdot \mathbf{r} - \mathbf{K} \cdot \mathbf{s})]$$

$$T_{ji} = \int d^3s d^3r \psi_j^*(s) \left(\frac{1}{2\pi^2} \int \frac{d^3p}{p^2} e^{i\mathbf{p} \cdot \mathbf{r}} e^{-i\mathbf{p} \cdot \mathbf{R}} \right) \psi_i(r) \exp[i(\mathbf{k} \cdot \mathbf{r} - \mathbf{K} \cdot \mathbf{s})]$$

Letting $\mathbf{p} = \mathbf{p} - \mathbf{K}$

$$T_{ji} = \int d^3s \psi_j^*(s) e^{-i\mathbf{p} \cdot \mathbf{s}} d^3r \left(\frac{1}{2\pi^2} \int \frac{d^3p}{|\mathbf{p} - \mathbf{K}|^2} e^{i\mathbf{p} - \mathbf{K} \cdot \mathbf{r}} e^{-i\mathbf{K} \cdot \mathbf{s}} \right) \psi_i(r) \exp[i(\mathbf{k} \cdot \mathbf{r} - \mathbf{K} \cdot \mathbf{s})] \quad (10)$$

$$T_{ji} = \int d^3r \psi_j^*(p) \left(\frac{1}{2\pi^2} \int \frac{d^3p}{|\mathbf{p} - \mathbf{K}|^2} e^{i\mathbf{p} - \mathbf{K} \cdot \mathbf{r}} \right) \psi_i(r) \exp[i(\mathbf{k} \cdot \mathbf{r})]$$

$$T_{ji} = \int d^3r \psi_j^*(p) \frac{1}{2\pi^2} \int \frac{d^3p}{|\mathbf{p} - \mathbf{K}|^2} e^{i\mathbf{p} \cdot \mathbf{r}} \psi_i(r) \exp[i(-\mathbf{k}_i \cdot \mathbf{r} + \frac{1}{2}\mathbf{k}_j \cdot \mathbf{r} + \mathbf{k}_i \cdot \mathbf{r} - \mathbf{k}_j \cdot \mathbf{r})]$$

$$T_{ji} = \int d^3r \psi_j^*(p) \frac{1}{2\pi^2} \int \frac{d^3p \exp(i\mathbf{p} \cdot \mathbf{r})}{|\mathbf{p} - \mathbf{K}|^2} \psi_i(r) \exp[i(-\frac{1}{2}\mathbf{k}_j \cdot \mathbf{r})]$$

$$T_{ji} = \int d^3r \psi_i(r) \exp(-\frac{1}{2}i\mathbf{k}_j \cdot \mathbf{r}) \frac{1}{2\pi^2} \int d^3p \frac{\psi_j^*(p) \exp(i\mathbf{p} \cdot \mathbf{r})}{|\mathbf{p} - \mathbf{K}|^2}$$

This is the same as equation (7).

Numerical solution

Instead of the Born approximation, the close coupling approximation was implemented using code from [7],[8] which has evolved over the years. The code is written in Fortran 77 and is to be executed on a linux/unix system. The commands required can be found in the appendix. The Runge Kutta method is used to solve Ordinary Differential Equations (ODEs) generated from the expansion of states and solving the Schrodinger function. The program was created to model the interaction between a proton and hydrogen. Slater orbitals are used which are of the form :

$$R(r) = N r^{n-1} e^{-\zeta r} \quad (11)$$

The output from the Fortran code gives the velocity values (v), impact parameter values(b) and the probability of b(P(b))in each state in columns. The final column is the sum all the probabilities in each row for each b value so should give 1.

The cross section can then computed using the following formula:

$$\sigma = \int_0^{b_{max}} P(b) b db \quad (12)$$

The input file provides values for the impact parameter which can be selected depending on the required result, velocity, number of target states and further parameters for the solving the ODEs. The form required in the program to supply additional states is shown below taking the 2p+ state as an example:

2	1	1	-0.125	0.0,0.0 :	(i)
1					(ii)
0.204124					(iii)
-0.5					(iv)
1					(v)

The Radial wavefunction for Hydrogen of the above state is:

$$R_{21} = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_0} \right)^{\frac{3}{2}} \left(\frac{Zr}{a_0} \right) e^{-\frac{Zr}{2a_0}} \quad (13)$$

(i) n=2 l=1 m=1, due to symmetry m=1 is equivalent to m=-1

The energy of the projectile -0.125au,calculated for each state from :

$$E(eV) = \frac{-E_0}{n^2} \text{ where } 1 \text{ au of energy} = 1 \text{ Hartree} = 0.0367493\text{eV}$$

(ii) number of entries in radial part of wavefunction - there is only one term in this example

(iii) coefficients : $0.204124 = \frac{1}{\sqrt{3}} \left(\frac{1}{2} \right)^{\frac{3}{2}}$ with Z=1

(iv) exponential coefficients

(v) the degrees of r present

The appendix contains a link to the other radial wavefunctions.

10ph is the name of input file which now contains all n=1,2,3 states which were added according to this rubric and the probabilities of being in ten different states for different b values are

calculated.

Cross section calculation

To compute the cross section a separate python program was written. The inputs is the output file generated from the Fortran code in the out folder. As expected the probability and cross section is greatest for the lowest excited states. First $P(b)$ vs b was plotted and a polynomial was fitted to the curve for using the `curve_fit` from the SciPy package. χ^2 tests were considered as a measurement for the good-fit of the curve but numbers greater than 5 were needed to give an accurate result so this idea was discarded. The polynomial was then used in (12) for the cross section and integrated using Gaussian quadrature. The program also produces subplots for each of the states as seen below:

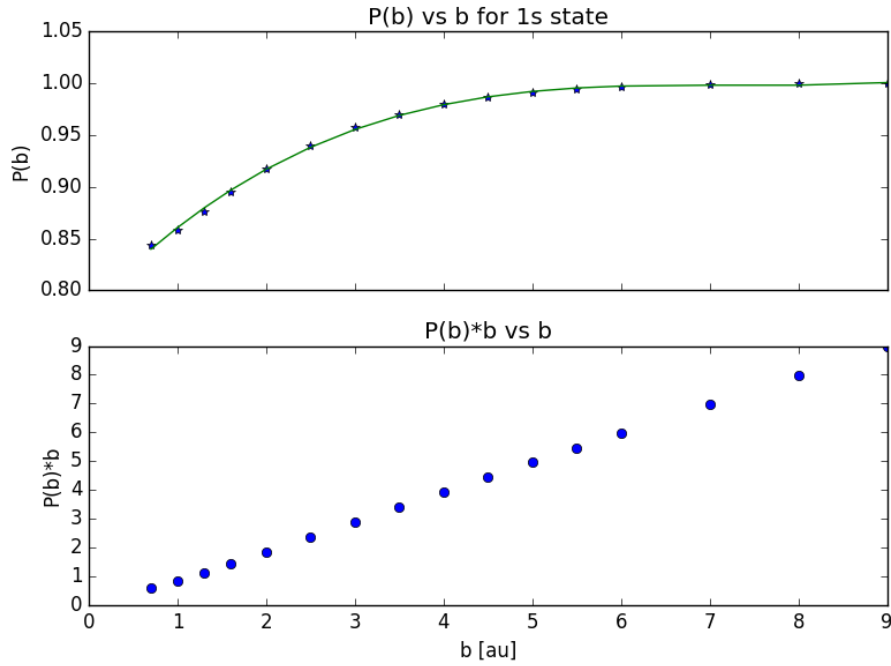


Fig.1 Above: $P(b)$ vs b with polynomial of degree 3 used to fit the curve,
Below: $P(b)*b$ vs b see what the complete function to be integrated looks like.

Each of the graphs are saved to files with the names of the states and an output file is also produced in the form of the table below:

State	Cross section[au]	Degree of polynomial
1s	249.22185	3
2s	1.534371	5
$2p_0$	1.497451	7
$2p_1$	0.5903671	7

Conclusion

From this project, I came to a much a greater understanding of scattering processes, the Born approximation and charge exchange reactions. The cross section of excited states from a proton- hydrogen interaction were calculated. The probability and the cross section was highest for states with the lowest energy. Plots were produced showing the probability amplitude vs the impact parameter for each state. A step by step use of the Bethe integral was shown. A clear process to add more states to the input file 10ph was provided. Future steps include looking at the 8ph file which contains excited states for before and after a collision in more detail and adapting the code and input parameters for positronium and antiproton collisions to compare to published data. Finally changing the equations and Fortran code required for μ and $\bar{p}$ interactions.

References

- [1] Aldo Antognini, François Nez et al. (2013) Proton structure from the measurement of $2S - 2P$ transition frequencies of muonic hydrogen
- [2] K.Nagamine(2005) Muonic Anti-Hydrogen-Formation and Test of CPT Theorem
- [3] G. Baur, G. Boero et al. Production of antihydrogen
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- [6] L. Kocbach, J. M. Hansteen and R. Gundersen(1980) Review of the SCA method for inner shell ionisation - results, limitations and possibilities
- [7] J W Humberston, M Charlton (1987) On antihydrogen formation in collisions of antiprotons with positronium
- [8] Jan. P Hansen, Alain Dubois (1991) Procedure for analytical and numerical calculations of Coulombic one and two -center integrals
- [9] J.P. Hansen(1989) General Subroutines for the calculation of atomic and molecular two-centre integrals

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Appendix

A.1

Commands for ubuntu 16.04 to run the fortran and python code:

```
f77 -std=legacy NEWgac.f  
cat 10ph — ./a.out testing.txt  
python lines.py
```

A Fortran 77 compiler is required.

Some packages may need to be installed in the linux terminal such as matplotlib depending what python interpreter is being used.

A.2

http://quantummechanics.ucsc.edu/ph130a/130_notes/node233.html for radial wavefunctions
H.A.Bethe, E.E Salpeter Quantum Mechanics of one and two electron systems