Low-energy Antiproton Interaction with Helium

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Abstract

An ab initio potential for the interaction of the neutral helium atom with antiprotons and protons is calculated using the Born-Oppenheimer approximation. Using this potential, the annihilation cross section for antiprotons in the energy range 0.01 µeV to 1 eV is calculated.

1 Introduction

Recent work on the trapping of low-energy antiprotons [1] presented the measurement of the annihilation rate on helium atoms which remained in the partial vacuum. It was found that the rate increased sharply as the cooling took place and then suddenly dropped to the background level. There has been some speculation concerning the cause of this sudden decrease in the rate. One possibility could be that there is a barrier of a few millivolts which would only be important when the energy of the antiprotons reaches this level.

While these observations formed the initial motivation for the work presented here there are additional reasons why the knowledge of this potential is interesting.

First, the experiment mentioned above points out the possibility of carrying out experiments in which this annihilation cross section could be measured and, in a more advanced version, the x-ray transitions might be measured as well.

Second, there are more general reasons for knowing this potential. For example in the particle remnants of the big bang there could well be some antiprotons left in space. To the extent that these antiprotons remained free they would have thermalized with the ambient background of photons and so would have an average energy corresponding to a temperature of around 2.7 K. Their interactions would be with naturally occurring hydrogen and helium.

As a third reason, it is conceivable that there could exist pockets of potential or perhaps changes in slope in the antiproton-atom potential which could allow metastable states to be formed. These might be associated with configurations of the electrons which are strongly deformed from a spherical distribution. Such pockets of potential
are perhaps more probable in larger aggregates of matter but this simple case of helium provides an entry into the subject.

There exist some calculations \cite{2, 3} of a nature related to this reaction but the author knows of no calculation of this precise process.

The calculation of the annihilation cross section as a function of energy requires the knowledge of the electrostatic potential between the $\bar{p}$ and the neutral helium atom, the annihilation potential of the nucleus and the solution of the Schrödinger equation with these two potentials.

It is natural to approach the problem of antiproton-helium electrostatic interaction, considering at the same time the proton-helium potential. In this way a check on the calculation is provided. The calculation of the proton-helium ab initio (variational) potential by Kolos and Peek\cite{6} is considered to be the standard reference.

While one might at first think that the calculations are almost the same (just the charge of the external particle is changed), because of the art of choosing the variational wave function they can be very different. For instance, Kolos and Peek (following earlier work by Kolos\cite{5} and Wolniewicz\cite{7}) chose a trial electron wave function which was elliptical in form, thus naturally tending to surround the two positive charges. This function is quite appropriate for the two nuclei separated by small or intermediate distances. For large distances, where the electrons are nearly spherically distributed around the helium nucleus, this wave function can be expected to less efficient. For the case of the antiproton this form is perhaps less appropriate.

Since it is desirable to do both calculations on the same footing, a single trial function has been use for both cases. It is based on an expansion in spherical coordinates about the helium nucleus. This function is very efficient for small or large distances between the two nuclei. It has more difficulty representing the wave function well at intermediate distances where it may require a large number of terms.

In the following section the expressions for the calculation of the variational ratio are derived. In section 2 the results of the potentials are given and in section 3 the annihilation cross section is computed.

\section{Calculation of the potentials}

The trial wave function chosen for this work is based on a spherical expansion about the helium nucleus in terms of spherical harmonics and orthogonal polynomials in the (scaled) radial distance of the electrons from the center. It is taken of the same form for the proton and antiproton problem so that a direct comparison can be made. This partial wave expansion goes over into the polarizability expansion naturally.

\subsection{Variational Integrals}

A completely general form of the wave function for two electrons can be expressed as

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \sum \psi_{\ell_1, m_1, \ell_2, m_2, n_1, n_2} Y_{\ell_1}^{m_1}(\hat{r}_1) Y_{\ell_2}^{m_2*}(\hat{r}_2) L_{n_1}(y_1) L_{n_2}(y_2) e^{-\frac{1}{2}(y_1+y_2)}$$  \hspace{1cm} (1)
where $L_n(r)$ is the Laguerre polynomial of order 2 (usual notation $L_n^{(2)}(r)$) and $y_1 = r_1/a$, $y_2 = r_2/a$, “a” being a variational parameter which sets the scale of the system. The quantities $\psi_{\ell_1,m_1,\ell_2,m_2,n_1,n_2}$ are the components of the wave function in this basis and embody (reduced by one index, see below) the other variational parameters of the calculation. It has been assumed, as usual \cite{4}, that the singlet spin state dominates the lowest energy configuration leaving the spatial wave function symmetric.

Since the two-electron wave function can depend only on the relative value of the $\phi$ angles, because of the symmetry around the $^4\text{He}-\bar{p}$ axis, the most general form reduces to

$$\psi(r_1, r_2) = \sum \psi_{m,\ell_1,\ell_2,n_1,n_2} Y_{\ell_1}^m(r_1) Y_{\ell_2}^{m*}(r_2) L_{n_1}(y_1)L_{n_2}(y_2)e^{-\frac{1}{2}(y_1+y_2)}. \quad (2)$$

It is this expression which will be used in the following work. The sums on $\ell$ and $n$ are taken to $\ell_{\text{max}}$ and $n_{\text{max}}$. The condition that the spatial electron wave function is symmetric requires that the $\psi$’s are symmetric under the interchange $(\ell_1, n_1) \leftrightarrow (\ell_2, n_2)$.

The normalization of the wave function is given by

$$\sum (n_1 + 1)(n_1 + 2)(n_2 + 1)(n_2 + 2)\psi_{m,\ell_1,\ell_2,n_1,n_2}^2. \quad (3)$$

The hamiltonian for the problem is

$$H = -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{|r_1 - r_2|} \pm \frac{e^2}{|r_1 - \mathbf{R}|} \pm \frac{e^2}{|r_2 - \mathbf{R}|}, \quad (4)$$

where $\mathbf{R}$ is the vector separating the antiproton (proton) from the helium nucleus.

In order to carry out the variational calculation the computation of the expectation value of the trial wave function of each of these terms is needed.

The radial derivative part of the kinetic energy can be expressed as

$$\frac{-\hbar^2}{2ma^2} K(n_1, n_1', n_2, n_2')\delta_{\ell_1,\ell_1'} \delta_{\ell_2,\ell_2'} \delta_{m,m'} \quad (5)$$

where $K$ is an integer. Twice the contribution to the kinetic energy for one of the electrons is given by

$$KK(n', n) = \delta_{n,n'} \frac{(n_1 + 1)(n_1 + 2)}{2} - 2na_{n',n} + 2(n + 2)a_{n',n-1} - 2(n + 1)b_{n',n} \quad (6)$$

so that the contribution to both will be

$$K(n_1, n_1', n_2, n_2') = \frac{1}{2} \left[ KK(n_1', n_1)(n_2 + 1)(n_2 + 2)\delta_{n_2',n_2} 
+ KK(n_2', n_2)(n_1 + 1)(n_1 + 2)\delta_{n_1',n_1} \right], \quad (7)$$

with

$$a_{n_1,n_2} \equiv \int_0^\infty e^{-y} L_{n_1}(y)L_{n_2}(y)dy \quad (8)$$

$$a_{n,n} = \frac{(n + 1)(n + 2)(2n + 3)}{6}; \quad a_{n,n+m} = a_{n,n} + \frac{m(n + 1)(n + 2)}{2} \quad (9)$$

3
can be found by using the explicit expression of the Laguerre polynomials

\[ b_{n_1, n_2} = \int_0^\infty ye^{-y}L_{n_1}(y)L_{n_2}(y)dy = \frac{(n+1)(n+2)}{2}; \quad n = \min \text{ of } (n_1, n_2) \quad (10) \]

The angular momentum part contributes

\[ K_L(m, m', \ell_1, \ell_1', \ell_2, \ell_2', n_1, n_1', n_2, n_2') = \delta_{m, m'}\delta_{\ell_1, \ell_1'}\delta_{\ell_2, \ell_2'} \]

\[ \times \left[ \ell_1(\ell_1+1)(n_2+1)(n_2+2)a_{n_1, n_1', n_2, n_2'} + \ell_2(\ell_2+1)(n_1+1)(n_1+2)a_{n_2, n_2', n_1, n_1'} \right]. \quad (11) \]

The contribution to the potential energy of the electron-He interaction is given by

\[ \frac{2e^2\delta_{m, m'}\delta_{\ell_1, \ell_1'}\delta_{\ell_2, \ell_2'}}{a} \left[ (n_1+1)(n_1+2)b_{n_2, n_2'}\delta_{n_1, n_1'} + (n_2+1)(n_2+2)b_{n_1, n_1'}\delta_{n_2, n_2'} \right]. \quad (12) \]

The expectation value of the electron-electron interaction involves calculating

\[ \frac{e^2}{a} \int dy_1 dy_2 \frac{Y_{\ell_1}'(\hat{y}_1)Y_{\ell_2}'(\hat{y}_2)L_{n_1}'(y_1)L_{n_2}'(y_2)e^{-(y_1+y_2)}}{|y_1-y_2|} Y_{\ell_1}^m(\hat{y}_1)Y_{\ell_2}^m(\hat{y}_2)L_{n_1'}(y_1)L_{n_2'}(y_1). \quad (13) \]

\[ \frac{e^2}{a} \sum \sqrt{\frac{(2\ell_1+1)(2\ell_2+1)}{(2\ell_1'+1)(2\ell_2'+1)}} C_{\ell_1, L, \ell_1'} C_{\ell_2, L, \ell_2'} C_{\ell_1, L, \ell_1'} C_{\ell_2, L, \ell_2'} I(n_1, n_1', n_2, n_2', L), \quad (14) \]

where

\[ I(n_1, n_1', n_2, n_2', L) \equiv \int y_1^2 dy_1 y_2^2 dy_2 e^{-(y_1+y_2)} L_{n_1}(y_1)L_{n_2}(y_2) L_{n_1'}(y_1) L_{n_2'}(y_2) \quad (15) \]

The coefficient for the expansion of a product of Laguerre polynomials

\[ L_{n_1}(y)L_{n_2}(y) = \sum A_{n_1, n_2, n_3} L_{n_3}(y) \quad (16) \]

can be found by using the explicit expression of the Laguerre polynomials

\[ L_n(y) = \sum_{m=0}^n (-1)^m \begin{pmatrix} n+2 \\ n-m \end{pmatrix} \frac{y^m}{m!} = \sum_{m=0}^n d_{n,m} y^m \quad (17) \]

\[ (n_3+1)(n_3+2)A_{n_1, n_2, n_3} = (n_1+2)(n_2+2)(n_3+2)! \]

\[ \times \sum_{m_1, m_2, m_3=0}^{n_1, n_2, n_3} \frac{(-1)^{m_1+m_2+m_3}(m_1+m_2+m_3+2)!}{(n_1-m_1)!(m_1+2)!m_1!(n_2-m_2)!(m_2+2)!m_2!(n_3-m_3)!(m_3+2)!m_3!} \quad (18) \]
With the definition

\[ I_{k,n} = \int_0^\infty y^k e^{-y} dy \int_0^y x^n e^{-x} dx \]  

(19)

\[
I_{k,n} = \begin{cases} 
  n! \sum_{m=n+1}^{\infty} \frac{(k+m)!}{m! 2^{m+k+1}} & k \leq 0 \\
  n! \left[ k! - \sum_{m=0}^{n} \frac{(k+m)!}{m! 2^{m+k+1}} \right] & k \geq 0 
\end{cases}
\]  

(20)

we have

\[
I(n_1, n_1', n_2, n_2', L) = \sum A_{n_1', n_1, j_1} A_{n_2', n_2, j_2} d_{j_1,k_1} d_{j_2,k_2} \left[ I_{k_1+L-1,k_2-L+1} + I_{k_2-L-1,k_1+L-1} \right].
\]  

(21)

To evaluate the interaction energy with the antiproton (proton) we need

\[
\int_0^\infty \frac{y^n e^{-y}}{|Y - Y'|} dy = \sum P_L(\cos \theta) \left[ \int_0^Y \frac{y^{n+L}}{Y^{L+1}} e^{-y} dy + \int_Y^\infty y^{n-L-1} e^{-y} dy \right]
\]  

(22)

\[
= Y^n \sum P_L(\cos \theta) \left[ \int_0^1 t^{n+L} e^{-Yt} dt + \int_1^\infty t^{n-L-1} Y^L e^{-Yt} dt \right]
\]  

(23)

where \( Y \) is the distance from the He nucleus to the antiproton in units of \( a \) along the z-axis.

If we define

\[
\alpha_m(Y) \equiv \int_1^\infty t^m e^{-Yt} dt; \quad m \geq 0,
\]  

(24)

then

\[
\alpha_0(Y) = \frac{e^{-Y}}{Y}; \quad Y \alpha_m(Y) = e^{-Y} + m \alpha_{m-1}(Y).
\]  

(25)

Note

\[
\int_0^1 t^m e^{-Yt} dt = \frac{m!}{Y^{m+1}} - \alpha_m(Y) \equiv \gamma_m(Y)
\]  

(26)

If \( m < 0 \) then the exponential integral is needed

\[
E_m(Y) = \int_1^\infty t^{-m} e^{-Yt} dt; \quad E_{m+1} = \frac{e^{-Y} - YE_m(Y)}{m}
\]  

(27)

\( E_1(Y) \) must be calculated to high accuracy.

With the definition

\[
\beta_m(Y) \equiv \begin{cases} 
  \alpha_m(Y) & m \geq 0 \\
  E_{-m}(Y) & m < 0 
\end{cases}
\]  

(28)

we can write
\[
\int_0^\infty \frac{y^n e^{-y}}{|y - y'|} = \sum P_L(\cos \theta) Y_n^m [\gamma_{n+L}(Y) + \beta_{n-L-1}(Y)]
\] (29)

and

\[
\int dy \frac{Y_n^{m'}(y) Y_l^m(y) L_{n'}(y) L_n(y)}{|y - y'|} = \delta_{mm'} \sum A_{n,n',\ell} d_{n,m} C_{\ell,L,L'} C_{l_{\ell'},\ell} \sqrt{\frac{2l + 1}{2l'} + 1} [\gamma_{m+2+l}(Y) + \beta_{m-L+l}(Y)]
\] (30)

Figure 1: Proton helium potential. The solid line is from Ref. [8]. The solid boxes are from the (4,4) calculation, the open circles from the Padé extension and the crosses and x symbols are from [5, 6].

\[2.2 \text{ Results for the proton potential}\]

The results for the proton potential are shown in Fig. [4]. Calculations were made at various radii for the pair \((\ell_{max}, n_{max}) = (2, 2), (3, 3)\) and \(4, 4\). The \((4,4)\) results (solid squares) are shown in the figure. Also shown are the results of ref. [5, 6] and the parameterization of their potential by Bosanac and Knesarek [7]. The \((4,4)\) results give an adequate representation of the previous results except in the minimum where
there is a significant cancellation between the electronic potential energy and the direct proton-nucleus interaction.

A [1,1] Padé approximate was used with the three determinations mentioned above to estimate the result of the limit of the sequence. This result is shown as the open circles in Fig. 1. While this last extrapolation is significant the result gives a satisfactory agreement with the previous work.

A specific comparison was made with ref. [5, 6] at R=3.704 Å. They found –8.32 meV while the present work gives –8.10 meV for the (4,4) search.

2.3 Results for the antiproton potential

The potential energy for the electrons alone is shown in Fig. 2. It is seen to vary between the limits $E_0$ at $R = 0$ (approximately equal to the binding energy of $H^-$) to $E_1$ (the binding energy of isolated helium) at large distances.

Writing the electron potential as a ratio of two fourth-order polynomials, including the direct He-$\bar{p}$ electrostatic potential, assuming that the potential varies as $1/R^4$ at large values of $R$ and subtracting the asymptotic value, $E_1$, the full antiproton-helium atom electrostatic potential can be expressed as

$$V(R) = -\frac{\beta z(z^3 + \frac{d}{E_0-E_1}z^4)}{1 + gz + \frac{\beta}{E_0-E_1}z^4} \quad (31)$$
where $z \equiv 1/R$.

In the fit $E_0 = -14.3477$ eV and $E_1 = -78.9847$ eV were used. The constant “d” ($= e^2$) has the value 28.798 eV Å$^{-1}$. By searching on parameters in this form against the (4,4) results, a best fit was found for $g = 0.6474$ Å and $\beta = 1595$ meV-Å$^4$. The last value can be compared with 1557 meV-Å$^4$ from Ref [9] and 1678 meV-Å$^4$ from Ref [10].

The antiproton potential is shown in Figs. 3 and 4. It is seen that there is no apparent change in slope which might aid in the formation of a metastable state. Since any such effect would be expected to be small (perhaps in the few meV range) it would have to be active at moderately large distances to be visible, say beyond 3 Å. We can perhaps understand why it is likely that there is no such effect by looking at the structure of the electron wave function.

The variation in the scale parameter “a” with R is shown if Fig. 5. It is seen that the system undergoes a rapid growth for a baryonic separation inside of 1 Å. Figure 6 shows the first dipole component of the wave function which provides a measure of the deformation of the electron cloud from spherical symmetry. It also shows little effect outside of 1 Å. Thus any possible inflection in the potential curve would occur inside of 1 Å when the potential is completely dominated by the simple coulomb attraction of the He-$\bar{p}$ system.

Figure 3: Antiproton He potential. The triangles are the result of the (3,3) calculation and the solid circles are from the (4,4) case. The solid line is calculated from Eq. 31.
3 Annihilation cross section

The energy of the antiproton at the nuclear surface will be given by the incident energy plus the gain due to the acceleration in the coulomb potential. Since (at 1 fm) the coulomb energy is 2.88 MeV, in the range of incident energies considered here the annihilation takes place at constant energy to a good approximation. The nuclear potential was taken to be the product of a purely absorbed single nucleon strength with a Woods-Saxon density with radius 2 fm and diffuseness 0.5 fm for 4 nucleons.

The system was treated from the point of view of a nuclear optical model, i.e. no consideration was given to the possibility of the knock-out of electrons or the electromagnetic transition into atomic bound states. In general such corrections might be expected to increase slightly the annihilation cross section.

The problem could be treated in a perturbation approach. In that case one would solve the problem of scattering from the purely electrostatic potential generated in the previous section and calculate the annihilation rate from the expectation value of the potential just introduced. Since the nuclear potential is very short ranged, the amplitude will be proportional to the square of the wave function at the origin. It was found in calculating this quantity that it had very nearly the same value as the pure coulomb case

\[
C_0^2(\eta) = 2\pi\eta(e^{2\pi\eta} - 1)^{-1} \approx -2\pi\eta; \quad \eta = -\alpha c/v
\]  

(32)
for energies above 10 \( \mu V \). From these considerations it is seen that the cross section should vary as \( 1/v^2 \). Since the potential is strongly absorbing the wave function will be modified significantly in the region of the nuclear potential so that it is better to solve the full equation as now described.

Since there exists no known analytic form for the solution of the Schrödinger equation in these potentials at short range or in the region of the “surface” of the atom, the wave function was calculated over the entire region from 0 to 80 Å. The step size was changed by an order of magnitude 4 times with 20,000 points calculated in each of the first four (overlapping) regions and 160,000 points in the region of largest distance from the helium nucleus.

The results for the annihilation cross section are presented in Fig. 7. It is seen that there is a change in energy dependence around 10\( \mu V \). Above that energy the cross section is proportional to \( 1/v^2 \) as can be expected for a coulomb system. Below that energy the cross section varies as \( 1/v \) as expected for a low-energy neutral system.

One can estimate this transition point using the asymptotic form of the potential. We can define a radius representing the “surface” of a potential as that value where the incident wave number is significantly affected by the potential, say where the potential becomes a fraction, \( f \), of the incident kinetic energy. In the present case the radius \( R_0 \) will be defined by

\[
E = \frac{k^2}{2m} = f \beta / R_0^4.
\]  
(33)
The long wave length limit is reached at $kR_0 < 1$. Combining these conditions, it is seen that the transition should take place around $2/f \mu V$ or about $20 \mu V$ for $f=0.1$.

The s-wave cross section above $10^{-5}$ eV can be represented by the expression

$$\sigma_{abs} = \frac{0.536\pi}{k^2}$$

(34)

Since this is greater than half of the unitarity limit the full cross section cannot be much larger than this. While the overall accuracy of the present calculation does not justify the three significant figures quoted in Eq. (34), the result is stable to this precision in this energy range. Thus if the absolute cross section can be established at any one value of the energy it will be known over a wide range. The measurement of the annihilation rate on a small, known, amount of helium introduced into a trap could thus provide a direct measurement of the temperature over a certain region of energy.

4 Conclusion

The authors in Ref. [1] estimate that the pressure in the container was of the order of $10^{-11}$ Torr. If we assume that the helium and antiprotons are cooled to 4.2 °K then the annihilation rate calculated using the cross section from Fig. 6 is $\sim 1.2 \times 10^{-3}$ 1/sec. Since a maximum rate of $\sim 8 \times 10^{-3}$ 1/sec was observed, there is a slight discrepancy.
Figure 7: Absorption cross section for antiprotons incident on neutral helium atoms. The solid curves gives the result due to the sum of all partial waves while the separated dashed curve gives the p-wave contribution. The dashed curve almost coincident with the solid curve represents the s-wave contribution alone. The short dashed curve gives the product of the velocity and the cross section normalized to the cross section at 1 meV.

Possible explanations of this discrepancy include the existence of a higher pressure than estimated or the presence of heavier material.

It was seen that no barrier or inflection of the potential occurred. However, the possible corrections beyond the Born-Oppenheimer approximation have not yet been considered and could influence this conclusion.

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