Quasibound states of an antiproton and a hydrogen atom

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Abstract

Accurate three-body quantal calculations of the system composed of a proton, an antiproton, and an electron are performed in perimetric coordinates with the Lagrange-mesh method, an approximately variational calculation with the simplicity of a calculation on a grid. Quasibound states with respect to the $\bar{p} + H(n = 2)$ threshold are obtained for $L = 60 - 73$ for various vibrational excitations. Their energies have accuracies up to about $10^{-14}$ atomic units while less precise energies are determined for $L = 56 - 59$ broader resonances. Their structure is analyzed with the help of mean distances between the particles. These mean distances indicate that the proton-electron subsystem is in excited states, mostly $n = 2$, as predicted by Sakimoto (Phys. Rev. A 98, 042503, 2018) with the Born-Oppenheimer approximation. A comparison performed with this approximation provides the accuracies of its energies and of its proton-antiproton mean distances.

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I. INTRODUCTION

The existence of low-energy antiproton beams allows the start of the realization of a long-awaited goal, the study of antimatter. Of particular interest is the simplest system, antihydrogen, which is now available in experiments [1]. It will allow testing a number of basic properties of antimatter [2]. Other systems involving antiprotons are very informative such as the hydrogenlike protonium [3, 4] or antiprotonic atoms where an antiproton replaces an electron. Among these atoms, antiprotonic helium composed of a helium nucleus, an antiproton, and an electron has been studied in very accurate experiments [5–7] and theoretical calculations [8–12]. Together, they provided a very precise measurement of the antiproton mass. Within the present experimental and theoretical error bars, this mass is found equal to the proton mass.

Antiprotonic helium presents a variation of structures with increasing angular momenta: successively hydrogenlike atom, quasistable pseudomolecule, and quasistable Rydberg pseudoatom [12]. An interesting question is what happens in such a system where the helium nucleus is replaced by a proton, i.e., the antiprotonic H$^-$ ion. Because of the smaller charge of the proton, the existence of this antiproton-hydrogen system is far from obvious. In a study based on the Born-Oppenheimer approximation, Sakimoto has deduced that the binding of an antiproton by an hydrogen atom in its ground state is unlikely [13]. In a further work, however, he has shown that this binding could be possible at very high angular momenta when the hydrogen atom is in its first excited Stark-like state [14]. The reason is that the antiproton-hydrogen Born-Oppenheimer potential for this excited state has a much slower decrease at large distances than for hydrogen in its ground state. It may then be attractive enough to allow bound states. In a careful study of the decay processes, Sakimoto has shown that long-lived states could exist for total orbital momenta between 60 and 73.

The aim of the present paper is to establish the existence of these quasistable states of the proton-antiproton-electron system in a fully quantal three-body calculation. To this end, we employ the Lagrange-mesh method [15–20] in the perimetric coordinate system [21, 22], a numerical method with the simplicity of a mesh calculation and the accuracy of a variational calculation. This method does not require analytical evaluations of integrals and computer times remain reasonable. It is found accurate in a variety of spectroscopic or collision applications [20]. In particular, in the case of antiprotonic helium, the accuracy on
the energies matches the best available results in the literature and some other properties of the system can easily be computed [12].

The Lagrange-mesh method is briefly summarized in Sec. II and the conditions of the numerical calculations are determined. Energies and mean distances are presented in Sec. III. These results are compared with the Born-Oppenheimer approximation and discussed in Sec. IV. Section V contains a summary and a conclusion. Atomic units are used throughout.

II. THE LAGRANGE-MESH METHOD

A. Summary

We study the quantal three-body system formed by a proton of mass \( m_p = 1836.152 \, 667 \, 5 \), an antiproton of same mass \( m_{\bar{p}} = m_p \), and an electron of mass \( m_e = 1 \) in atomic units, interacting only through Coulomb forces. Fine structure and relativistic effects are not taken into account.

The Schrödinger equation is solved in perimetric coordinates to avoid numerical problems with the singularities of the kinetic-energy operator and of the Coulomb interactions. The system of perimetric coordinates [21, 22] is defined by the three Euler angles \( \psi, \theta, \phi \) and the three coordinates

\[
\begin{align*}
    x &= r_{p\bar{p}} + r_{pe} - r_{\bar{p}e}, \\
    y &= r_{p\bar{p}} - r_{pe} + r_{\bar{p}e}, \\
    z &= -r_{p\bar{p}} + r_{pe} + r_{\bar{p}e},
\end{align*}
\]

involving the distances \( r_{p\bar{p}}, r_{pe}, \) and \( r_{\bar{p}e} \) between the particles. The coordinates \( x, y \) and \( z \) vary over the \((0, \infty)\) interval. In perimetric coordinates, the Coulomb potential reads

\[
V(x, y, z) = -\frac{2}{x+y} - \frac{2}{x+z} + \frac{2}{y+z}.
\]

The kinetic energy operator for \( S \) states is given, e.g., in Ref. [23]. The general expression for arbitrary states can be found in Ref. [19].

The wave function with total orbital momentum \( L \), natural parity \((-1)^L\), and projection \( M \) on the fixed \( z \) axis is expanded as [19]

\[
\Psi_M^L = \sum_{K=0}^L D_{MK}^L(\psi, \theta, \phi)\Phi_K^L(x, y, z),
\]
where $K$ is the projection on the intrinsic axis 3 of the system and $D_{MK}^L(\psi, \theta, \phi)$ with $K \geq 0$ is a parity-projected and normalized Wigner angular function. In some cases, for $L > 0$, the sum can be truncated with excellent accuracy at some value $K_{\text{max}}$. For $K_{\text{max}} = 0$, the wave function presents a cylindrical symmetry along the $p\bar{p}$ axis. The value of $K_{\text{max}}$ gives information about the departure from this symmetry.

Let $u_i, v_j, w_k$ be the zeros of Laguerre polynomials of respective degrees $N_x, N_y, N_z$, and $h_x, h_y, h_z$ be three scale parameters with the dimension of a length in atomic units. The Lagrange-mesh method combines the three-dimensional mesh of $N_x N_y N_z$ points $(h_x u_i, h_y v_j, h_z w_k)$, a set of Lagrange functions $F_{ijk}^K(x, y, z)$ associated with each mesh point, and a Gauss quadrature consistent with this mesh [12, 15, 20]. The Lagrange functions are constructed from Laguerre polynomials and their exponential weight function [24]. They verify the Lagrange conditions

$$F_{ijk}^K(h_x u_i', h_y v_j', h_z w_k') \propto \delta_{ii'}\delta_{jj'}\delta_{kk'},$$

(4)

i.e. each $F_{ijk}^K(x, y, z)$ vanishes at all mesh points except at the $ijk$ point. These functions are normed at the Gauss-Laguerre quadrature approximation which is used everywhere. The $\Phi_L^K(x, y, z)$ functions in Eq. (3) are expanded in the Lagrange basis as

$$\Phi_L^K(x, y, z) = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} C_{L}^{Kijk} F_{ijk}^K(x, y, z).$$

(5)

For each $L$ value, the coefficients are given by the mesh equations

$$\sum_{K_{ij}k} \{ \langle F_{ijk'}^{K'} | T_{K'K}^L | F_{ijk}^K \rangle + [V(h_x u_i, h_y v_j, h_z w_k) - E_{L\nu}] \delta_{KK'} \delta_{ii'} \delta_{jj'} \delta_{kk'} \} C_{L}^{Kijk} = 0,$$

(6)

where $T_{K'K}^L$ is the matrix element of the kinetic-energy operator between functions $D_{MK'}^L$ and $D_{MK}^L$. The matrix elements of operator $T_{K'K}^L$ between Lagrange functions are computed with the Gauss quadrature associated with the mesh [19]. The potential part in Eq. (6) is diagonal at this approximation because of the Lagrange property (4) while the kinetic-energy part has a tridiagonal block structure with many zeros in the blocks. The matrix of this system is thus rather sparse. Its size is $N_x N_y N_z (K_{\text{max}} + 1)$. A limited number of eigenvalues of such big matrices can be obtained in rather short computing times with the code of Ref. [25]. The longest present computations with $K_{\text{max}} = 3$ take about half an hour on a fast workstation. By increasing order, the physical eigenvalues $E_{L\nu}$ are labeled with the quantum number $\nu$ starting from zero. Other eigenvalues are discarded as explained in
Sec. II B. The eigenvectors corresponding to physical eigenvalues provide, from Eqs. (5) and (3), square-integrable approximations of the wave functions.

This calculation is not variational for two reasons of different natures: (i) all eigenstates of \( p\bar{p}\) are unbound and (ii) the Gauss quadrature approximation is not exact. Nevertheless, some eigenvalues and eigenvectors of this system may provide approximate but accurate energies and eigenfunctions of quasibound states or narrow resonances. The difficulty is to isolate these eigenvalues from those corresponding to square-integrable approximations of continuum states which are named unphysical eigenvalues below. The separation of eigenvalues with a physical meaning is easily performed by computing the mean distances between the particles. For example, the mean distance between the proton and antiproton is simply given with the Gauss-Laguerre quadrature \[24\] by

\[
\langle r_{\bar{p}p} \rangle = \frac{1}{2} \sum_{Kij} (C_{Kij}^L)^2 (h_x u_i + h_y v_j).
\]

(7)

Unphysical eigenvalues are indicated by very large electron-proton and electron-antiproton distances. Another consistent criterion is obtained from the probabilities of the different \( K \) components of the wave functions

\[
P_L(K) = \sum_{ijk} (C_{Kij}^L)^2.
\]

(8)

One observes below that physical states always have \( P_L(0) \) close to unity in contrast with square integrable approximations of continuum states. This indicates that these physical states have an almost cylindrical symmetry along the intrinsic axis 3 of the two heavy particles. Because many channels are open below the energies we are looking for, it is important to have an idea of the energy domain where to search. This is provided by the Born-Oppenheimer results of Ref. \[14\]. They suggest the existence of quasibound states or narrow resonances in the domain \( 59 \leq L \leq 73 \).

B. Conditions of the numerical calculations

The painful part of the calculation is to determine near-optimal values of seven parameters: \( h_x, h_y, h_z, N_x, N_y, N_z, \) and \( K \). Once these choices have been made, it becomes easy to reproduce our calculations. Since the method is not variational, eigenvalues exist below the physical ones for given \( L \). We found them unstable with respect to variations of the number
of mesh points and of the scale parameters. The physical eigenvalues are thus searched for in limited energies intervals and discriminated by their stability with respect to variations of the parameters and by the criteria discussed above. The choice of these intervals is usefully guided by the Born-Oppenheimer study of Ref. [14]. Searches in other energy domains have also been performed but did not provide usable results.

We have adopted the following strategy. First, since the system has a symmetry close to cylindrical, the Euler angles are chosen in such a way that the intrinsic axis 3 is chosen along the $p\bar{p}$ direction. With this convention, values of $K$ can be limited to a small $K_{\text{max}}$ for the high accuracies obtained here. Here, results are obtained with $K_{\text{max}} = 3$ but there is no difference with $K_{\text{max}} = 2$ for $L \geq 68$. Second, the scale parameters $h_x, h_y, h_z$ are selected. To this end, for each $L$, a number of calculations are performed with relatively small matrices where these parameters are varied to find plateaus of stability, i.e., regions such that small variations of these parameters do not affect a number of stable digits of the lowest quasibound eigenvalue ($\nu = 0$) found in the present study.

These fast preliminary calculations were performed with $N_x = N_y = N_z = 20$ and $K_{\text{max}} = 2$. The parameters $h_x, h_y, h_z$ need not be known with a high accuracy, typically one or two decimal digits are enough as displayed in Table I. They depend on the total orbital momentum $L$. Third, the best possible accuracy is searched for by increasing $N_x, N_y, N_z$. These numbers of mesh points are then optimized on the second excited quasibound state ($\nu = 2$). Accurate results for the next excited states ($\nu = 3 - 5$) are obtained by increasing $N_y$ only, up to 38, and for a few levels close to the $\bar{p} + H(n = 2)$ threshold by simultaneously increasing $h_y$.

The numbers of mesh points and scale parameters are displayed in Table I. One observes that $h_x$ and $h_y$ monotonically increase with $L$. Parameter $h_z$ is significantly larger for $L < 70$ and presents a minimum near $L = 65$. While $N_x$ remains remarkably constant and rather small, $N_y$ and $N_z$ have contrasted evolutions. Above $L = 60$, $N_y$ increases and $N_z$ decreases. These tendencies are not valid below $L = 60$ because the smaller number of stable digits makes results poorly sensitive to the numbers of mesh points. Since the perimetric coordinates have no intuitive interpretation, the evolution of all these parameters is mainly phenomenological.
| Table I. Parameters of the Lagrange meshes. |
|---|---|---|---|---|---|---|
| $L$ | $N_x$ | $N_y$ | $N_z$ | $h_x$ | $h_y$ | $h_z$ |
| 56 | 20 | 24 | 20 | 0.24 | 0.12 | 1.5 |
| 57 | 20 | 24 | 20 | 0.25 | 0.15 | 1.5 |
| 58 | 20 | 24 | 20 | 0.27 | 0.17 | 1.5 |
| 59 | 20 | 28 | 24 | 0.27 | 0.17 | 1.4 |
| 60 | 20 | 28 | 32 | 0.28 | 0.17 | 1.4 |
| 61 | 20 | 28 | 32 | 0.28 | 0.18 | 1.3 |
| 62 | 20 | 28 | 32 | 0.28 | 0.21 | 1.3 |
| 63 | 20 | 28 | 32 | 0.29 | 0.24 | 1.2 |
| 64 | 20 | 30 | 30 | 0.30 | 0.26 | 1.2 |
| 65 | 20 | 30 | 30 | 0.30 | 0.28 | 1.1 |
| 66 | 20 | 32 | 28 | 0.31 | 0.30 | 1.1 |
| 67 | 20 | 32 | 24 | 0.35 | 0.36 | 1.1 |
| 68 | 20 | 32 | 24 | 0.38 | 0.45 | 1.2 |
| 69 | 20 | 32 | 24 | 0.45 | 0.57 | 1.2 |
| 70 | 20 | 32 | 20 | 0.58 | 0.90 | 1.3 |
| 71 | 20 | 32 | 20 | 0.70 | 1.30 | 1.3 |
| 72 | 20 | 38 | 20 | 0.70 | 2.10 | 1.6 |
| 73 | 18 | 42 | 18 | 0.70 | 3.00 | 1.6 |

III. ENERGIES AND MEAN DISTANCES

Energies are obtained from the three-body Schrödinger equation for $L = 56 - 73$. Their accuracies are based on the stability of digits when comparing calculations with $(N_x, N_y, N_z)$, $(N_x + 2, N_y, N_z)$, $(N_x, N_y + 2, N_z)$, and $(N_x, N_y, N_z + 2)$ mesh points. Variations of $h_x$, $h_y$, and $h_z$ appear to be a less good indicator of the accuracy.

The convergence of the energies with respect to the number of mesh points is illustrated in Table II for the $\nu = 0$ and $\nu = 5$ levels at $L = 65$. The parameters $h_x = 0.30$, $h_y = 0.28$, and $h_z = 1.1$ are located in a plateau of stability and small variations such as 0.01 for $h_x$ and $h_y$ and 0.1 for $h_z$ do not modify the significant digits. The $K = 3$ contribution is smaller than $10^{-10}$. Thirteen stable digits are obtained for $\nu = 0$ with $N_x = 20$, $N_y = 30$, and $N_z = 30$ while an error of a few times $10^{-9}$ for $\nu = 5$ requires $N_y = 40$.

Unexpectedly, the easiest calculation concerns $L = 70$ where the matrix size $N_x N_y N_z (K_{\text{max}} + 1)$ is smaller and the physical energies are easy to find because they are not mixed with other eigenvalues. For $L$ smaller than about $60 - 62$, on the contrary, the physical eigenvalues are mixed with many non-physical ones and their localization requires more efforts.
Table II. Example of convergence for two levels at $L = 65$. The parameters are $h_x = 0.30$, $h_y = 0.28$, and $h_z = 1.1$.

| $K$ | $N_x$ | $N_y$ | $N_z$ | $\nu = 0$         | $\nu = 5$         |
|-----|-------|-------|-------|-------------------|-------------------|
| 2   | 20    | 20    | 20    | -0.12900486696001 | -0.12652861745    |
| 20  | 30    | 20    | 20    | -0.12900487223390 | -0.12652861644    |
| 20  | 40    | 30    | 20    | -0.12900487206534 | -0.12658040389    |
| 3   | 20    | 20    | 20    | -0.129004867004739| -0.126528617590   |
| 20  | 30    | 30    | 20    | -0.129004872109936| -0.126580396162   |
| 20  | 38    | 30    | 20    | -0.129004872109875| -0.126580395179   |
| 22  | 38    | 30    | 20    | -0.129004872109937| -0.126580403986   |
| 20  | 40    | 30    | 20    | -0.129004872109928| -0.126580396162   |

cases of $L = 73$ and the highest $\nu$ values for $L = 72$, the convergence may not have been reached.

For each $L$ value, the ground quasibound state and a number of its vibrational excited states are shown in Table III. The last presented digit may be uncertain within a few units. When stability of an excited eigenvalue could not be reached, the location is left empty in the table. The large number of stable digits indicates that all couplings with continuum states are weak in this range of $L$ values in agreement with the findings of Ref. [14]. This is also confirmed by the absence or small number of non-physical eigenvalues among the physical energies for $L \geq 60$. The number of stable digits gives a rough indication of the width of the level. In the antiprotonic helium case, it was observed that $N$ stable decimal digits roughly correspond to a width $10^{-(N-1)}$ [12]. We expect that the same property holds here. Notice that, for eigenvalues with 14 stable digits, the width can even be smaller since this number of digits is limited by the computer accuracy.

The widths assumed here correspond to the decay of the $\bar{p}pe$ system into $\bar{p}\bar{\nu} + e$ (Auger electron emission or autodetachment) and $\bar{p} + H$ (dissociation). According to Ref. [14], $\bar{p} + H$ dissociation is the main separation process. This is confirmed by the mean values of the distances between particles shown below. Notice however that the main decay channel according to Ref. [14] is due to spontaneous radiation, i.e., photon emission from the $pe$ subsystem to the hydrogen ground state leading to a dissociation into $\bar{p} + H(1s)$. Let us recall that the structure of the $pe$ subsystem is modeled as the lowest $n = 2$ Stark state in
the Born-Oppenheimer study of Ref. [14]. The widths are found to be a little smaller than
the radiative width of the 2p state of a free hydrogen atom. This radiative channel is absent
in the present study and thus not included in the assumed width. Since the wave functions
are available in a rather simple form, this channel could be studied in the present approach
but is delayed to an ulterior work including other electromagnetic transitions.

From \( L = 56 \) to 59, the number of stable digits is small. The widths are expected to be
large. No or few excited states could be obtained. They should be resonances too broad for
the present static calculations. From $L = 60$ to 72, we display five vibrational excited states
(see Sec. IV for a justification of this interpretation). The states become narrower when $L$
increases and broader when $\nu$ increases. For $L = 72$, the $\nu = 5$ energy is very close to the $\bar{p} + H(n = 2)$
dissociation threshold and its binding energy with respect to that threshold is
not accurate. For $L = 73$, we only obtain the $\nu = 0$ state as clearly quasibound.

The binding energies $-E_{L\nu} + E_{Hn=2}^H$ with respect to the $\bar{p} + H(n = 2)$
dissociation threshold, where $E_{Hn=2}^H = -0.12493196$, are displayed in logarithmic scale in Fig. 1. One observes that
they decrease monotonically, faster than exponentially, as a function of $L$. For each $L$
value, the points in the figure present an almost constant spacing. This corresponds to
exponentially decreasing binding energies as a function of $\nu$ in the considered range $\nu \leq 5$. A similar behavior has been observed in Ref. [26] for several muonic and pionic three-body
systems (see the discussion in section IV).

![Figure 1. Binding energies $-E_{L\nu} + E_{Hn=2}^H$ with respect to the $\bar{p} + H(n = 2)$ threshold as a function of $L$. The curves are labeled by the vibrational quantum number $\nu$.](image)

In Table IV are presented mean values of the distances $\langle r_{pp} \rangle$ between proton and antiproton,
$\langle r_{pe} \rangle$ between proton and electron, and $\langle r_{\bar{p}e} \rangle$ between antiproton and electron. Here
also, only stable digits are kept except the last one which may be uncertain within a few
units. The number of presented decimal digits is limited to a maximum of seven. In all
cases, the accuracy does not exceed 9 decimal places in the range $65 – 70$. Indeed, since the
method is approximately variational, an error $\epsilon$ on wave functions and mean values corre-
sponds to an error of about $\epsilon^2$ on energies. A $10^{-9}$ accuracy on the distances means that
the accuracy of the energies in this range could be better than $10^{-14}$ if quadruple precision
arithmetic was used.

Let us first consider $\langle r_{pe} \rangle$. This mean distance decreases monotonically from the large value 12.5 at $L = 56$ to 5.55 at $L = 73$ (see also Fig. 2). It decreases when $\nu$ increases. Around $L = 69$, $\langle r_{pe} \rangle$ is very close to 6, i.e., the mean distance between the proton and electron of an infinite-proton-mass hydrogen atom in an $n = 2$ state. With increasing $L$, it tends to the mean distance 5.5 of the $n = 2$ Stark state. This nicely corresponds to the assumption in the model of Ref. [14]. For lower $L$ values, higher excitations of hydrogen also play a role. Beyond $L = 69$ and for some higher vibrational states, a significant component of hydrogen in its ground state must also be present.

Figure 2. Mean distances $\langle r_{pp} \rangle$, $\langle r_{pe} \rangle$, and $\langle r_{\bar{p}e} \rangle$ between the particles for $\nu = 0$.

Let us now turn to the proton-antiproton mean distance $\langle r_{pp} \rangle$. It monotonically increases with both $L$ and $\nu$. The increase with $L$ follows from the centrifugal effect. The increase with $\nu$ corresponds to a broadening due to vibrational excitation. This is discussed in another way in Sec. IV.

The antiproton-electron mean distance $\langle r_{\bar{p}e} \rangle$ is always larger than the proton-electron one $\langle r_{pe} \rangle$ as expected from the electrostatic repulsion between these particles. It also increases with the vibrational quantum number $\nu$.

As mentioned before, the probabilities of $K$ components give indications about the cylindrical symmetry of the system. The $K > 0$ probabilities are displayed with a maximum of ten decimal digits in Table V and illustrated by Fig. 3. They are quite inaccurate for $L < 60$. For $L > 65$, an excellent accuracy on the energies is already obtained with $K_{\text{max}} = 2$, or even $K_{\text{max}} = 1$ for $L \geq 70$. On the contrary, for $L < 60$, values larger then 3 could be necessary in more elaborate calculations of resonance properties.
Table IV. Mean distances between the particles as a function of $L$ and $\nu$.

| $L$ | $\nu$ | $\langle r_{pb}\rangle$ | $\langle r_{pe}\rangle$ | $\langle r_{pe}\rangle$ |
|-----|-------|--------------------------|--------------------------|--------------------------|
| 56  | 0     | 3.96                     | 12.5                     | 15.4                     |
| 57  | 0     | 4.23                     | 10.6                     | 13.8                     |
|     | 1     | 4.5                      |                          |                          |
| 58  | 0     | 4.504                    | 9.6                      | 13.0                     |
|     | 1     | 4.7                      |                          |                          |
| 59  | 0     | 4.80035                  | 8.985                    | 12.677                   |
|     | 1     | 5.208                    | 8.82                     | 12.88                    |
|     | 2     | 5.6                      |                          |                          |
| 60  | 0     | 5.12423                  | 8.5280                   | 12.5026                  |
|     | 1     | 5.5792                   | 8.266                    | 12.650                   |
|     | 2     | 6.06                     | 8.1                      | 13.0                     |
| 61  | 0     | 5.4865215                | 8.127147                 | 12.421703                |
|     | 1     | 5.993173                 | 7.87762                  | 12.62937                 |
|     | 2     | 6.5430                   | 7.6553                   | 12.9061                  |
| 62  | 0     | 5.897680                 | 7.77372                  | 12.43425                 |
|     | 1     | 6.465661                 | 7.54210                  | 12.71805                 |
|     | 2     | 7.085388                 | 7.32942                  | 13.07158                 |
| 63  | 0     | 6.3720818                | 7.4546917                | 12.5407382               |
|     | 1     | 7.0153989                | 7.2428201                | 12.9163477               |
|     | 2     | 7.7208651                | 7.049496                 | 13.3718622               |
| 64  | 0     | 6.9301622                | 7.1637094                | 12.7541037               |
|     | 1     | 7.6689101                | 6.9717212                | 13.2414497               |
|     | 2     | 8.4837312                | 6.7978713                | 13.8224752               |
| 65  | 0     | 7.6027009                | 6.8961919                | 13.0991423               |
|     | 1     | 8.4665215                | 6.7237866                | 13.7271771               |
|     | 2     | 9.425775                 | 6.5691080                | 14.468225                |
| 66  | 0     | 8.4389209                | 6.6486442                | 13.6196868               |
|     | 1     | 9.4736262                | 6.4955777                | 14.4335341               |
|     | 2     | 10.63183                 | 6.359864                 | 15.388694                |
| 67  | 0     | 9.5236837                | 6.4183166                | 14.3951181               |
|     | 1     | 10.804703                | 6.2846998                | 15.4698911               |
|     | 2     | 12.251974                | 6.1681192                | 16.729417                |
| 68  | 0     | 11.018548                | 6.2031032                | 15.5807073               |
|     | 1     | 12.680887                | 6.0897259                | 17.0520249               |
|     | 2     | 14.578629                | 5.9930624                | 18.778600                |
| 69  | 0     | 13.275801                | 6.0018471                | 17.5208472               |
|     | 1     | 15.588816                | 5.9106846                | 19.6608992               |
|     | 2     | 18.25717                 | 5.8355943                | 22.17830                 |
| 70  | 0     | 17.221213                | 5.8160442                | 21.1321144               |
|     | 1     | 20.798740                | 5.7508863                | 24.5630015               |
|     | 2     | 24.959507                | 5.6997582                | 28.601044                |
| 71  | 0     | 25.8842807               | 5.6568797                | 29.4453979               |
|     | 1     | 32.3448483               | 5.6214789                | 35.8029457               |
|     | 2     | 39.938984                | 5.5948039                | 43.314436                |
| 72  | 0     | 50.4129254               | 5.5542954                | 53.6702664               |
|     | 1     | 65.4809                  | 5.5416528                | 68.6858                  |
|     | 2     | 83.8                     | 5.53223                  | 87.0                     |
| 73  | 0     | 150                      | 5.513                    | 153                      |
Table V. Probabilities $P_{L\nu}(K)$ of the $K > 0$ components as a function of $L$ and $\nu$. The $K = 0$ probability is always close to 1.

| $L$ | $\nu$ | $P_{L\nu}(K = 1)$ | $P_{L\nu}(K = 2)$ | $P_{L\nu}(K = 3)$ |
|-----|-------|-------------------|-------------------|-------------------|
| 56  | 0     | 0.082             |                   |                   |
| 57  | 0     | 0.047             | 0.003             |                   |
| 58  | 0     | 0.031             |                   | 0.0006            |
| 59  | 0     | 0.02162           | 0.000179          | 0.000003          |
|     | 1     | 0.024             |                   |                   |
| 60  | 0     | 0.015677          | 0.0000841         | 0.0000031         |
|     | 1     | 0.01551           | 0.000136          | 0.000003          |
|     | 2     | 0.0169            |                   | 0.0009            |
| 61  | 0     | 0.011536186       | 0.000033516       | 0.000000104       |
|     | 1     | 0.0110244         | 0.0000512         | 0.00000034        |
|     | 2     | 0.01050           | 0.00010           | 0.000010          |
| 62  | 0     | 0.0085988         | 0.0000161         | 0.00000003        |
|     | 1     | 0.0080172         | 0.00002199        | 0.00000007        |
|     | 2     | 0.0074112         | 0.00002714        | 0.00000013        |
| 63  | 0     | 0.0064633290      | 0.0000078829      | 0.0000000085      |
|     | 1     | 0.0059116281      | 0.0000098772      | 0.000000174       |
|     | 2     | 0.00536622        | 0.000011321       | 0.000000274       |
| 64  | 0     | 0.0048875929      | 0.0000038902      | 0.000000026       |
|     | 1     | 0.004401258       | 0.0000045151      | 0.000000047       |
|     | 2     | 0.003939311       | 0.0000048635      | 0.000000067       |
| 65  | 0     | 0.0037101822      | 0.0000019199      | 0.000000008       |
|     | 1     | 0.0032987199      | 0.0000020724      | 0.00000013        |
|     | 2     | 0.002920324       | 0.0000021061      | 0.00000017        |
| 66  | 0     | 0.0028202995      | 0.0000093994      | 0.000000002       |
|     | 1     | 0.002482245       | 0.0000094447      | 0.000000003       |
|     | 2     | 0.002179932       | 0.000009064       | 0.000000004       |
| 67  | 0     | 0.0021402927      | 0.000004505       | 0.000000001       |
|     | 1     | 0.0018698693      | 0.000004224       | 0.000000001       |
|     | 2     | 0.0016343534      | 0.000003824       | 0.000000001       |
| 68  | 0     | 0.0016148758      | 0.000002080       | 0.000000000       |
|     | 1     | 0.0014052474      | 0.000001819       | 0.000000000       |
|     | 2     | 0.0012276417      | 0.000001553       | 0.000000000       |
| 69  | 0     | 0.0012044099      | 0.000000895       | 0.000000000       |
|     | 1     | 0.0010494638      | 0.000000732       | 0.000000000       |
|     | 2     | 0.000922250       | 0.000000590       | 0.000000000       |
| 70  | 0     | 0.0008816009      | 0.0000003338      | 0.000000000       |
|     | 1     | 0.0007769888      | 0.0000000260      | 0.000000000       |
|     | 2     | 0.000694041       | 0.000000199       | 0.000000000       |
| 71  | 0     | 0.0006344935      | 0.0000000999      | 0.000000000       |
|     | 1     | 0.0005759509      | 0.000000073       | 0.000000000       |
|     | 2     | 0.0005303019      | 0.000000054       | 0.000000000       |
| 72  | 0     | 0.0004741116      | 0.000000020       | 0.000000000       |
|     | 1     | 0.000447914       | 0.000000014       | 0.000000000       |
|     | 2     | 0.0004272         | 0.000000010       | 0.000000000       |
| 73  | 0     | 0.000394          | 0.000000002       | 0.000000000       |
Table V shows contrasting behaviors for the probabilities $P_{L\nu}(K)$ of vibrational excited states. The $K = 0$ probabilities are not shown as they always remain close to 1. For $K = 1$, the probabilities decrease when $\nu$ increases. For $K = 2$, they increase for $L < 66$ and decrease for $L > 66$. For $K = 3$, they always increase with $\nu$. The dependence of $P_{L0}(K)$ on $L$ is illustrated in Fig. 3. All probabilities decrease monotonically with increasing $L$. They also decrease with $K$. The $K = 2$ probabilities are smaller than $10^{-4}$. The $K = 3$ probabilities become smaller than $10^{-11}$ beyond $L = 68$. They explain why this component does not affect the energies in this range. The smallness of the $K > 0$ probabilities implies that $P_{L\nu}(0)$ is always close to unity. Its smallest value, near 0.92, is for $L = 56$.

![Figure 3. Probabilities of the $K > 0$ components as a function of $L$ for $\nu = 0$.](image)

IV. DISCUSSION

Some high $L$ levels of antiprotonic helium have long lifetimes (see Ref. [12] and references therein). The spontaneous emission of an electron is strongly hindered in these states [5] because the electron can only be emitted with a rather high orbital momentum $l$ [27]. This Auger electron emission (or autodetachment) is then a slow process.

The same effect explains that the dissociation widths of the quasibound levels of $p\bar{p}e$ can be very small [14]. The states from $L = 60$ to 73 have long lifetimes with respect to the channels $p\bar{p} + e$. Indeed, the orbital momentum $l$ carried out by the emitted electron is at least 3 beyond $L = 56$. The electron emission energies $E_{L0} - E_{p\bar{p}}^{L-l}$, where $E_{p\bar{p}}^{L-l}$ is the highest $p\bar{p}$ threshold energy below $E_{L0}$ corresponding to the lowest orbital momentum $l$ of the emitted electron, are displayed in Fig. 4 as a function of $L$. The points are labeled with
the value of this minimal orbital momentum \( l \) (denoted as \( l_0 \) in Table II of Ref. [14]). One observes that this energy is very small at \( L = 59 \), which may explain why the search for optimal parameters was very difficult in that case. It is also quite small for \( L = 56 \) and 61. These energies tend to more constant values at high \( L \).

![Figure 4](image)

Figure 4. Electron emission energy \( E_{L0} - E_{pp}^{L-l} \) for the lowest electron orbital momentum \( l \) as a function of \( L \), where \( E_{pp}^{L-l} \) is the energy of the highest open threshold below \( E_{L0} \).

The quantum number \( \nu \) is interpreted here as representing a vibrational excitation. In order to deepen this interpretation, we now perform a comparison with the Born-Oppenheimer picture as used in Ref. [14]. To this end, we solve the Born-Oppenheimer equation

\[
\left( -\frac{1}{2} \Delta - \frac{1}{r_{pe}} + \frac{1}{r_{pe}} - \frac{1}{R} \right) \chi_{nm}(r_{pe}, R) = E_{nm}(R) \chi_{nm}(r_{pe}, R),
\]

where \( R \equiv r_{pp} \) is fixed and the Laplacian \( \Delta \) corresponds to the proton-electron coordinate \( r_{pe} \). The energies depend on the parameter \( R \) and on the magnetic quantum number \( m \). They are labeled by the excitation quantum number \( n \) starting from 0. This equation is separable in confocal elliptic coordinates (or prolate spheroidal coordinates) [28]. Here, we solve it for \( m = 0 \) with the Lagrange-mesh method as explained in Ref. [29].

For the coordinate \( \xi = (r_{pe} + r_{pe})/R - 1 \) defined in the interval \((0, \infty)\), a Lagrange-Laguerre mesh with \( N_\xi \) points and a scale parameter \( h \) is employed. For the coordinate \( \eta = (r_{pe} - r_{pe})/R \) defined in the interval \((-1, 1)\), a Lagrange-Legendre mesh with \( N_\eta \) points is used. For \( m = 0 \), the azimutal angle \( \varphi \) of \( r_{pe} \) does not play a role. Since the calculation is very fast, a rough optimization is sufficient. We use \( N_\xi = 30 \) and \( N_\eta = 20 \). The scale parameter is given by \( h = \max(6/R - 1, 2/R) \). The lowest energies \( E_{00}(R) \) correspond to those labeled \((0,0,0)\) in Refs. [14, 28]. The first excited ones \( E_{10}(R) \) correspond to those
labeled (1,0,0) in these references. These energies are obtained with at least nine stable decimal digits. When rounded at the fifth decimal digit, they perfectly agree with the results of Ref. [28].

Table VI. Born-Oppenheimer energies $E_{L}^{BO}$ and mean distances $\langle R \rangle_{L}$ of the lowest vibrational states as a function of $L$.

| $L$ | $E_{L0}^{BO}$ | $\langle R \rangle_{L0}$ | $E_{L1}^{BO}$ | $\langle R \rangle_{L1}$ | $E_{L2}^{BO}$ | $\langle R \rangle_{L2}$ |
|-----|----------------|--------------------------|----------------|--------------------------|----------------|--------------------------|
| 58  | -0.1439567     | 4.5952                   | -0.1417104     | 4.9849                   | -0.1397098     | 5.4040                   |
| 59  | -0.1409907     | 4.8804                   | -0.1390290     | 5.3055                   | -0.1372899     | 5.7638                   |
| 60  | -0.1383227     | 5.1987                   | -0.1366258     | 5.6654                   | -0.1351293     | 6.1703                   |
| 61  | -0.1359388     | 5.5575                   | -0.1344874     | 6.0739                   | -0.1332150     | 6.6349                   |
| 62  | -0.1338256     | 5.9669                   | -0.1326009     | 6.5440                   | -0.1315350     | 7.1736                   |
| 63  | -0.1319704     | 6.4413                   | -0.1309544     | 7.0937                   | -0.1300774     | 7.8091                   |
| 64  | -0.1303614     | 7.0012                   | -0.1295362     | 7.7496                   | -0.1288310     | 8.5753                   |
| 65  | -0.1289873     | 7.6779                   | -0.1283352     | 8.5528                   | -0.1277847     | 9.5246                   |
| 66  | -0.1278375     | 8.5217                   | -0.1273408     | 9.5701                   | -0.1269278     | 10.7438                  |
| 67  | -0.1269017     | 9.6198                   | -0.1265423     | 10.9188                  | -0.1262493     | 12.3869                  |
| 68  | -0.1261701     | 11.1386                  | -0.1259291     | 12.8271                  | -0.1257375     | 14.7552                  |
| 69  | -0.1256327     | 13.4434                  | -0.1254894     | 15.7992                  | -0.1253790     | 18.5175                  |
| 70  | -0.1252778     | 17.5009                  | -0.1252083     | 21.1596                  | -0.1251568     | 25.4150                  |
| 71  | -0.1250861     | 26.4883                  | -0.1250624     | 33.1343                  | -0.1250453     | 40.9531                  |
| 72  | -0.1250152     | 52.0999                  | -0.1250103     | 67.2742                  | -0.1250067     | 80.5372                  |

The energies $E_{10}(R)$ are then used as a proton-antiproton potential in radial Schrödinger equations with reduced mass $\mu = m_p/2$. These equations are solved for $L = 58 - 72$ with the Numerov algorithm. Above $R = 2$, the steps 0.1, 0.05, and 0.02 have been used up to $R = 120$. Below $R = 2$, these high $L$ effective potentials are approximated only by the centrifugal barriers. In fact, the Born-Oppenheimer approximation breaks down below the critical distance $R = 0.639$ but the height of the $L \geq 58$ centrifugal barriers allows the present approximation [14]. The corresponding effective potentials are pictured in Fig. 3 of Ref. [14].
The results are displayed in Table VI for \( h = 0.02 \). The energies \( E_{L\nu}^{BO} \) of the calculations performed with the three different steps 0.1, 0.05, and 0.02 agree within at least 7 decimal digits for the three lowest vibrational states. This accuracy is better than the difference between the present energies and the energies \( E_{BO} \) of the first column of Table II in Ref. [14] which are based on interpolations of the results of Ref. [28]. For the mean proton-antiproton distances, an absolute accuracy better than about \( 10^{-5} \) is obtained with \( h = 0.02 \) for \( \nu = 0 \) and a little less good for \( \nu = 1 \) and 2 up to \( L = 72 \). The poor accuracy of the three-body results for \( L = 73 \) does not allow a precise comparison with the Born-Oppenheimer approach.

In Fig. 5, we display for \( \nu = 0 - 2 \) the differences of the energies \( E_{L\nu}^{BO} \) of Table VI computed with the Born-Oppenheimer approach and the quantal three-body energies \( E_{L\nu} \) of Table III. These differences monotonically decrease. They are positive below \( L = 65 - 66 \) and negative above. They also decrease with increasing \( \nu \). A figure involving the improved Born-Oppenheimer energies of the second column of Table II in Ref. [14] would be hardly different at the present scale. The error of the Born-Oppenheimer approximation is always smaller than \( 4 \times 10^{-4} \) atomic units. This good agreement confirms the interpretation of \( \nu \) as a vibrational quantum number.

With a good accuracy, the three-body binding energies in Fig. 1 present an almost exponential decrease with \( \nu \) for fixed \( L \). For an exponential behavior, the ratios of successive energies must be equal. This is illustrated in Fig. 6 where ratios \( (E_{L\nu} - E_{n=2}^H)/(E_{L\nu+1} - E_{n=2}^H) \) are presented for \( \nu = 0 \) (dots) and 2 (triangles) as a function of \( L = 60 - 72 \). The two sets
of ratios are very similar as expected. The $\nu = 1$ ratios lie between them and are not shown for clarity of the figure. The Born-Oppenheimer approximation offers an explanation of this property. Indeed, for the high centrifugal barriers at $L \geq 60$, the effective Born-Oppenheimer potential is attractive only for large $R$ values where $E_{10}(R)$ behaves as [14]

$$E_{10}(R) \approx -\frac{1}{8} - \frac{3}{R^2}$$ (10)

with a good precision ($< 2\%$ for $R > 85$). For the potential $-3/R^2$, successive energies $\epsilon_{L\nu}$ are related by the constant ratio [30]

$$\frac{\epsilon_{L\nu}}{\epsilon_{L\nu+1}} = \exp \left( 2\pi/\sqrt{6\mu - L(L+1)} - 1/4 \right).$$ (11)

The results of expression (11) are also displayed as squares in Fig. 6. They nicely agree with the numerical three-body results. This interpretation is valid for other three-body systems [26].

![Figure 6](image-url)

**Figure 6.** Ratios $(E_{L\nu} - E_{n=2}^H)/(E_{L\nu+1} - E_{n=2}^H)$ for $\nu = 0$ (black circles) and 2 (blue triangles) as a function of $L$. The $\nu = 1$ ratios (not shown) are located between them. Comparison with approximation $\epsilon_{L\nu}/\epsilon_{L\nu+1}$ of Eq. (11) for a potential $-3/R^2$ (green squares).

The interpretation of $\nu$ as a vibrational quantum number is also confirmed by the ratios of mean distances $\langle R \rangle_{L\nu}$ of Table VI obtained at the Born-Oppenheimer approximation and the quantal mean distances $\langle r_{pb} \rangle_{L\nu}$ of Table IV. The Born-Oppenheimer mean distances are between one and two percent larger than the quantal ones for $L = 60 – 70$. This is true at least for the $\nu = 0 – 2$ values. Beyond $L = 71$, the behavior of these ratios seems to be less regular. At $L = 72$, they start to decrease with $\nu$ from 1.0335. At $L = 73$ where we
could find only one quantal level below the $\bar{p} + H(n = 2)$ threshold, the $\nu = 0$ ratio is much smaller than unity.

Finally, let us mention that we found some evidence around $L = 65$ for other resonances with fewer stable digits and with mean proton-electron distances close to 3. These resonances would correspond to configurations with a hydrogen atom mainly in its ground state. Such structures would contradict the Born-Oppenheimer picture of possible structures discussed in Ref. [14]. Unfortunately, since these resonances should be broader, the present approach is not adequate for confirming their existence and evaluating their properties.

V. CONCLUSION

With an accurate three-body, approximately variational, calculation on a Lagrange mesh, we establish the existence of quasibound states below the $\bar{p} + H(n = 2)$ threshold with extremely small widths for spontaneous dissociation. The existence of these states was predicted in the Born-Oppenheimer study of Ref. [14]. We show that several narrow vibrational states exist over a range of $L$ values. We have studied the six lowest vibrational states between $L = 60$ and 72 and the only obtained such state at $L = 73$. Below $L = 60$, rather narrow resonances still exist but are less well described by the present static study. In all cases, the corresponding configurations are not far from a cylindrical symmetry around the proton-antiproton axis.

This vibrational interpretation is confirmed by a Born-Oppenheimer calculation similar
to the one performed in Ref. [14]. The accuracy of this approximation in the present case is thus determined. It is found to improve with increasing $L$, reaching about $10^{-4}$ atomic units for the energies.

Accurate values are also obtained for the three mean distances between the particles. The mean distances between the proton and electron indicate that the hydrogen-atom-like substructure in the three-body system is in a superposition of excited states, sometimes dominated by the $n = 2$ state assumed in Ref. [14]. The proton-antiproton mean distances increase as expected from the centrifugal effect. They are well described by the Born-Oppenheimer approximation with an overestimation between 1 and 2 percents for $L = 58 - 70$.

The number of stable digits obtained for the energies gives indications about the widths of the quasibound states which are found very small between $L = 60$ and 72. These widths only correspond to spontaneous dissociations into $p\bar{p} + e$ or $\bar{p} + H$. In fact, according to Ref. [14], the main decay channel of these states is radiative: emission of a photon with dissociation into $\bar{p} + H(1s)$. This information is based on a Born-Oppenheimer approach with the restrictive assumption that the hydrogen-atom subsystem is in a specific $n = 2$ state. This assumption is only partly in agreement with our results. A quantal three-body study of radiative transitions from quasibound to unbound states leading to this dissociation as well as of the electromagnetic deexcitations of the vibrational excited states will be the object of a future work.

Predicting precise transition energies is in principle useful for a possible future experimental search. It is however not obvious how such high $L$ states can be accessed. Collisions of antiprotons on atomic hydrogen in its ground state have to excite the $p\bar{p}$ subsystem to high orbital momenta and simultaneously excite the electron. The cross sections for formation of $pp\bar{e}$ in these high $L$ quasibound states might be too small to be practical. Larger cross sections might be obtained in collisions between antiprotons and a beam of metastable excited H($2s$) atoms. Whether such an experiment is possible and efficient is an open question.
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