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Few-Body Systems

Scattering of Heavy Charged Particles on Hydrogen Atoms*

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Abstract. Low-energy scattering of heavy positively charged particles on hydrogen atoms (H) is investigated by solving Faddeev equations in configuration space. A resonant value of the pH scattering length, $a = 750 \pm 5$ a.u., in the *pp* antisymmetric state was found. This large value indicates the existence of a first excited state with a binding energy $B = 1.14 \times 10^{-9}$ a.u. below the H ground state. Resonances for non-zero angular-momenta states are predicted.

1 Introduction

The scattering of heavy charged particles (X^+) on atoms at kinetic energies smaller than the inelastic thresholds is dramatically influenced by the presence of atomic electrons. Their virtual excitations in presence of the incoming charged particle result into long-range attractive forces which dominate the low-energy scattering. These states were proposed as a possible source of metastability in the $\bar{p}$He system [1] and were found to play a determinant role in the low-energy $\bar{p}$H annihilation [2]. A full solution of these problems is however made extremely difficult by the presence of annihilation channels and only approximate solutions were achieved. We present in what follows a rigorous solution for the simplest problem of scattering on hydrogen atoms.

A simple two-body approximation is first discussed in Sect. 2. Sect. 3 is devoted to the solution of the three-body ($X^+ e^- p^+$) problem, obtained by solving the Faddeev equations in configuration space. We treat with special care the *p*H case, for it exhibits the more interesting properties and constitutes moreover a realistic experimental challenge. Some final remarks about the present calculations and plans for future work are given in the conclusion. We use all along the paper electronic atomic units ($m_e = e^2 = \hbar = 1$).

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2 Two-Body Approach

To get a first qualitative insight into the underlying physics, it is interesting to consider a simple two-body X^+H problem. The H atom is supposed to be point-like and to interact with the incoming particle via a central potential

$$V(r) = \frac{1}{2}\frac{\alpha(r)}{r^4}. \tag{1}$$

$\alpha(r)$ tends to the H dipole polarizability ($\alpha_d = \frac{9}{2}$) for large values of r and regularizes the $1/r^4$ singularity at $r = 0$. Its precise form is given in ref. [3].

We have displayed in Fig. 1 the binding energies of the π^+H bound states with interaction (1). One can see a large number of states with angular-momentum values up to $L = 7$. Some of them are very close to the dissociation threshold. The elastic μ^+H cross section in the momentum range $k \in [0.48, 0.64]$ has been plotted in Fig. 2 with the most relevant partial-wave contributions shown separately. The $L = 5$, 6, 7 states display a clear resonant behaviour also visible in the total cross section. A direct calculation of their position and width – using the complex rotation method [4] – provides the values $E_5 = (7.9 - 1.4i)10^{-4}$, $E_6 = (1.1 - 0.25i)10^{-3}$, $E_7 = 1.0 \times 10^{-3} - 1.3i \times 10^{-7}$, respectively [5]. These resonances concern all high angular-momentum states, involving large centrifugal

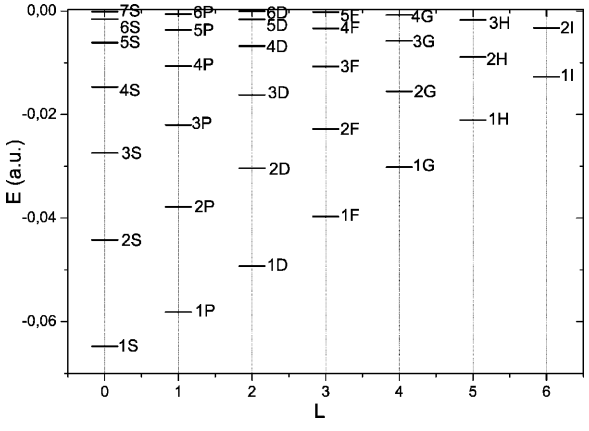

Fig. 1. Discrete spectrum for πH in the two-body approach

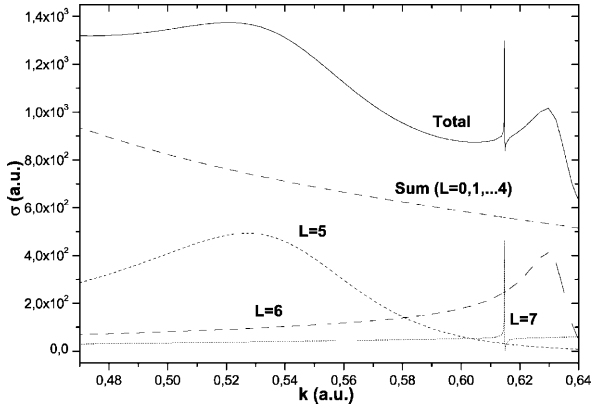

Fig. 2. Elastic μH cross section for several partial waves displaying resonant behaviour

barriers and relatively large energies. It is worth noticing, however, that they can be found even for $L=1$ and at extremely small energy values. In the π^+H case one has, e.g., $E_1=(4.9-1.4i)\times 10^{-7}$. The examples shown in Figs. 1 and 2 illustrate well the kind of physics governed by the polarization forces. An extensive work as a function of the projectile mass has been done [6] showing a very rich spectrum of bound and resonant states, with a complexity increasing as a function of the projectile mass.

To what extent the results of this simple approach are reliable? Answering this question was the main motivation of this work. A definite answer will only appear by letting the electron dynamics in H play its full role, that is by considering the $(X^+p^+e^-)$ three-body problem. And this is the aim of the next section.

3 Three-Body Calculations

The three-body $(X^+p^+e^-)$ calculations are performed using Faddeev equations in configuration space. The standard Faddeev equations provide satisfactory solutions for bound states but are not suitable for scattering Coulomb problems. The reason is that their right-hand sides do not decrease fast enough to ensure the decoupling of Faddeev amplitudes in the asymptotic region and to allow unambiguous implementation of boundary conditions. In order to circumvent this problem, Merkuriev [7] proposed to split the Coulomb potential V into two parts, $V=V^s+V^l$, by means of some arbitrary cut-off function χ:

$$V^s(x,y)=V(x)\chi(x,y), \qquad V^l(x,y)=V(x)[1-\chi(x,y)]. \tag{2}$$

One is then left with a system of equivalent equations

$$(E-H_0-W_\alpha-V^s_\alpha)\Psi_\alpha=V^s_\alpha\sum_{\alpha\neq\beta}\Psi_\beta, \qquad W_\alpha=V^l_\alpha+V^l_\beta+V^l_\gamma, \tag{3}$$

the right-hand side containing only short-range contributions (V_s) and with some three-body potential (W_α) which incorporates the long-range parts. This approach was found to be very efficient in calculating the e^+Ps and e^+H cross sections [8, 9].

Eqs. (3) were solved by expanding Ψ_i in the bipolar harmonics basis and their components $\varphi_{i\alpha_i}$ in the basis of two-dimensional splines.

Binding energies for the lower three-body π^+H and μ^+H bound states are plotted in Fig. 5. They are compared to the results of the two-body approach (1). One can see that, although there is a qualitative agreement, two-body energies are systematically underestimated. These results can be used to improve the short-range part of the two-body potential.

Some interesting features of the three-body Coulomb system can be learned from Fig. 3, where the zero-energy X^+H cross section as a function of the projectile mass m_X is displayed. Each peak corresponds to the appearance of a new S-wave bound state. The critical mass values m_i at which they occur, would enable to generalize the ground-state stability triangle [10] to higher excitations. A zoom in the region of physical interest, μ^+ and π^+, is shown in Fig. 4. The calculated values are, respectively, $a_{\mu\mathrm{H}}=69.1$ and $a_{\pi\mathrm{H}}=24.4$. Some care has to be taken in extracting the scattering observables especially at zero energy, from the asymptotic solution at finite distance. The long-range polarization force makes the

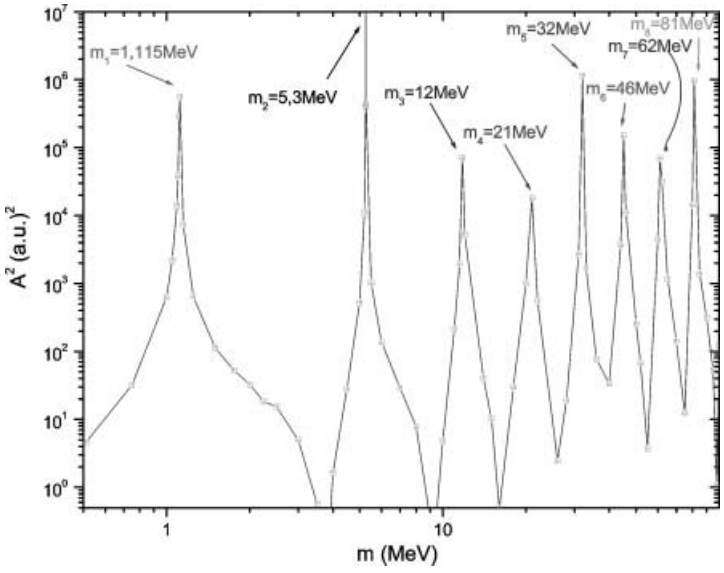

Fig. 3. Three-body zero-energy X^+H cross section as a function of the projectile mass m_X

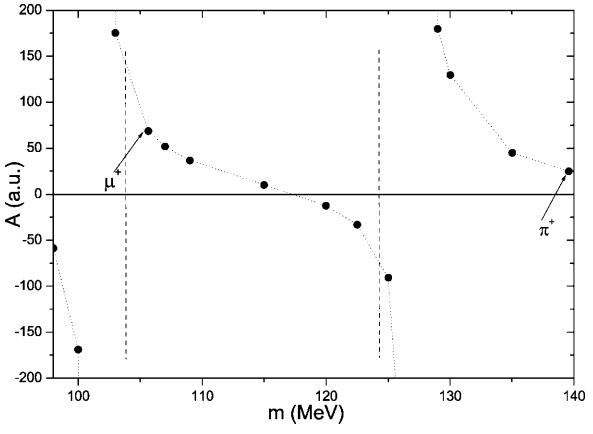

Fig. 4. Scattering length as a function of m_X, in the region of μ and π

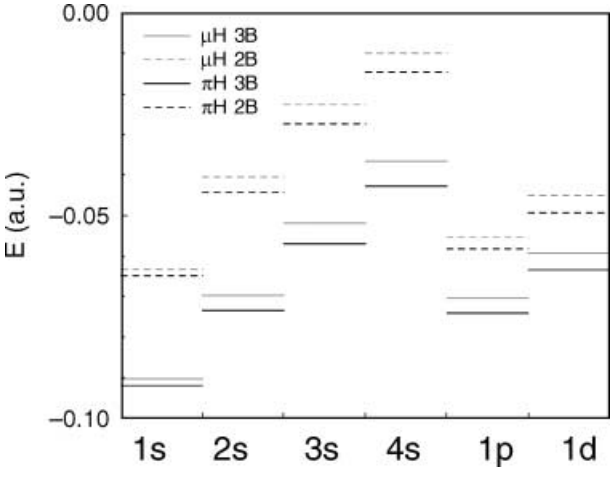

Fig. 5. Energies for lower πH and μH bound states compared to two-body results (1)

convergence of the observables as a function of the X^+-H distance very slow and requires an appropriate extrapolation procedure [6].

pH scattering deserves special comments. The three-body wave function has to be antisymmetric with respect to the p exchange. This can be realized in two different ways following the proton-spin coupling. For the case when the two proton spins are antiparallel (singlet) the spatial part of the wave function is symmetric, while for the parallel case (triplet) it is antisymmetric. In the two-body approach, these two cases give rise to completely different potentials.

The singlet case has a broad attractive well which supports a great number of bound states. They have been calculated since the first days of quantum mechanics and they are presently known with a very high precision (see, e.g., refs. [11, 12] and references therein). Our three-body calculations cannot reach this kind of accuracy for bound states but are in good agreement for the lower excitations. They provide furthermore the first result for the pH scattering length $a_s = -29.3$. We notice that the zero-energy scattering wave function shows 20 nodes in y_1-direction, indicating the existence of 20 $L=0$ σ_g energy levels for H_2^+.

The triplet case – modeled by Landau [14] – is dominated by the Pauli repulsion between the two protons, overbalanced at $r \sim 10$ by the attractive polarization forces. Our three-body calculations give a scattering length of $a_t = 750 \pm 5$. The nodal structure of the Faddeev amplitudes indicates that such a big value is due to the existence of a first excited $L=0$ state with extremely small binding energy. By using the modified effective-range theory [15] we are able to determine its value $B = (1.135 \pm 0.035) \times 10^{-9}$ below the H ground state. To our knowledge, this is the weakest bond ever predicted, three times smaller than the ^{4}He atomic dimer [13]. The existence of $L=0$ and $L=1$ ground states is well known and their binding energies have been very precisely calculated [11, 12]. These authors were, however, not able to conclude about the existence of a second S-wave bound state.

It is interesting to compare three-body calculations with those provided by the simple Landau two-body potential. S-wave cross sections are plotted in Fig. 6.

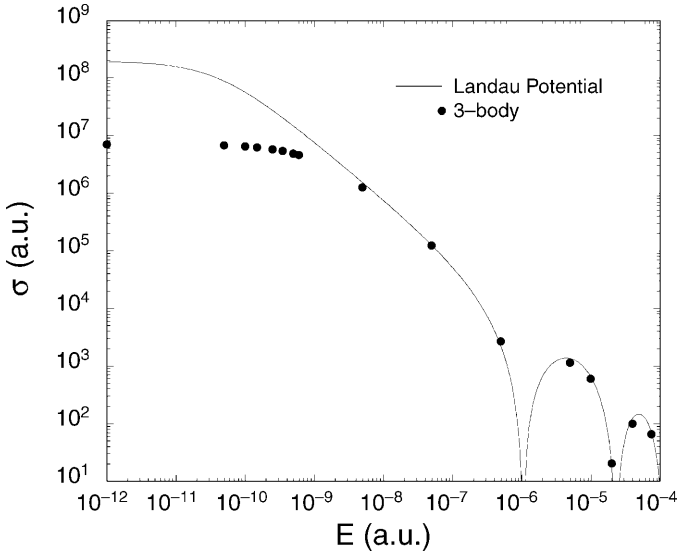

Fig. 6. Zero energy pH in the pp triplet state, compared to the results of the Landau potential

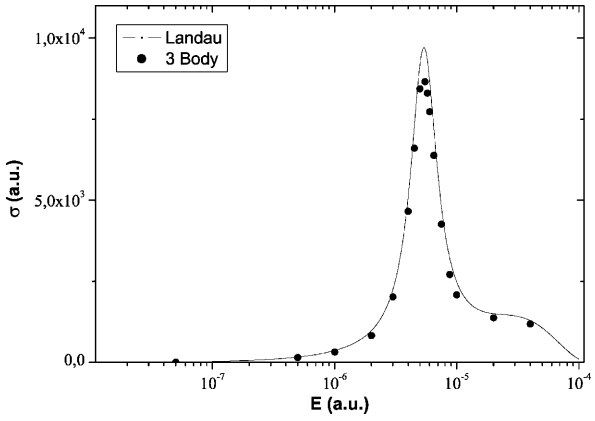

Fig. 7. pH elastic cross section for $L=3$ in the pp spin triplet state

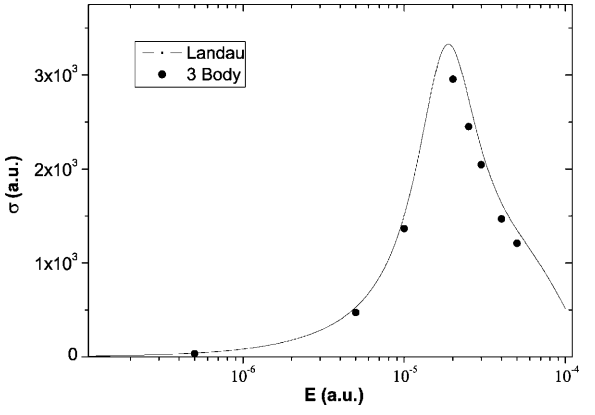

Fig. 8. pH elastic cross section for $L=4$ in the pp spin triplet state

At zero energy, both calculations differ by two orders of magnitude while at energies $E \sim 10^{-6}$ they are already in quite a good agreement, despite the simplicity of the two-body approach. This is due to the fact that the effective interaction is highly repulsive at short distances, what prevents the incoming proton to penetrate inside the H atom and minimizes the effect of the three-body dynamics.

The pH cross sections for higher partial waves have also been calculated. They exhibit some narrow resonances in several partial waves. Figs. 7 and 8 show the elastic cross section for the $L=3$, 4 states. They are compared to the results of the Landau potential. We can see that their agreement in this energy region is rather good. The three-body resonances are a little bit shifted to the lower energy region and have smaller widths. The same effect is seen in the bound-state calculations where the two-body results are always slightly underbound. The position and width of these resonances were estimated to $E=(5.13-1.61i)\times 10^{-6}$ for $L=3$ and $E=(1.56-0.94i)\times 10^{-5}$ for $L=4$.

4 Conclusions

By solving Faddeev equations in configuration space, we calculated the bound and scattering states for the $(X^+p^+e^-)$ system. Long-range polarization forces generate a rich spectrum of bound and resonant states with increasing complexity as

m_X increases. Predictions for the physical cases $X^+ = \mu^+, \pi^+, K^+$ are obtained, with the scattering-length values $a_{\pi^+\mathrm{H}} = 24.4$ and $a_{\mu^+\mathrm{H}} = 69.1$ a.u.

Of special interest is the pH system in the pp spin-triplet state. We predict a second S-wave bound state with binding energy $B = 1.14 \times 10^{-9}$ a.u. below the H ground state. This constitutes the weakest bond ever predicted, even smaller than the ^{4}He atomic dimer.

The existence of such a near threshold state dominates the low-energy pH scattering and results into a scattering length of $a_t = 750 \pm 5$ a.u. A low-energy proton approaching an H atom will behave like colliding with a large nanoscopic object. Several resonances occurring in different partial waves, but visible in the total cross section, are also predicted. The experimental confirmation of these results would be very interesting.

Present calculations were performed using non-relativistic dynamics with Coulomb pair-wise interactions. In this framework, they are parameter-free with the only input of particle masses and charges. Perturbations induced by strong X^+-p interactions or higher electromagnetic corrections have not been included.

In view of the extreme sensibility of the pH results, it is necessary to quantify both relativistic and strong-interaction effects. A direct measurement of the pH cross section at very low energy seems unlikely. One can, however, access the low-energy pH continuum in the final state of the H_2^+ photodissociation cross section. Work is in progress in these two directions.

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