

On the dynamical origin of H^- and Ps^- binding

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Abstract . It is demonstrated that extended polarization potential plays a crucial role in the binding of H^- and Ps^- ions. The conclusion is based on a scattering theoretic approach to the problem.

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In the H^- ion two like particles (e^-, e^-) undergo correlated motion in the central field of massive proton. On the other hand, the Ps^- ion is much harder to visualize since it consists of three particles of equal mass (e^-, e^+, e^-) tumbling about their centre of mass in some complicated fashion. In many respects, these two systems differ [1]. Despite that, the binding energy of Ps^- (0.012005 a.u.) in the ground state is approximately one half the corresponding value (0.027750 a.u.) for H^- . Further, it has been found [2] that the photodetachment cross section of Ps^- parallels that of H^- . Apparently, no simple explanation is known for the observed scaling in energies and parallelism in the photodetachment cross sections. These facts, however, tend to point out that there must be common dynamical origin for binding an electron either to hydrogen or to positronium although the few-particle correlations in the two systems are entirely different. The present work is an attempt to disclose this by using physically founded assumptions. Relatively recent studies [3] indicate that H^- is formed when an incoming electron is trapped by a potential well created between the incident electron and hydrogen atom. It can be hoped that a similar conjecture may also be true for the positronium negative (Ps^-) ion since detailed three-body calculations [4] conclude that Ps^- can be adequately represented as a positronium core with an extra loosely bound and nearly uncorrelated electron. In view of this, we regard H^- and Ps^- ions as the reaction products of appropriate e^- -atom low-energy scattering processes and postulate that the systems are so weakly bound that the effective-range parametrization of the binding energy is a useful tool to search for the law of interaction responsible for ionic binding.

For short-range potentials, the scattering phase shifts $\delta_l(k)$ are odd functions of k which are regular at the point $k = 0$. In this case, the quantity $k^{-1} \tan \delta_l(k)$ can be expanded as

a series in k^2 , the first few coefficients of which completely determine the scattering at low energies. In particular, for s -wave scattering the effective-range expansion

$$k \cot \delta(k) = -\frac{1}{a} + \frac{1}{2} r_e k^2 \quad (1)$$

is always a good approximation. In writing (1) we have omitted the subscript $l = 0$ and shall follow this convention throughout. Further, we shall work in Hartree atomic units in which the energy $E = k^2/2$. Here a is the scattering length and r_e , the effective range. The physical significance of these quantities can be found in any standard text on nuclear physics. In a pioneering work, O'Malley *et al* [5] considered modification of the effective-range theory for scattering on long-range potentials. We shall refer to this modification wherever necessary. Meanwhile, we note that the expansion in (1) has been sought about $k = 0$. If there exists a shallow bound state with energy $F_1 = E_b$, it is then more convenient to look for expansion about E_b rather than $E = 0$. In this case, (1) takes the form [6]

$$k_b = \frac{1}{a} + \frac{1}{2} k_b^2 r_e, \quad (2)$$

where k_b is the wave number corresponding to the bound-state energy E_b . For values of a and r_e corresponding to a prescribed law of interaction between the projectile and target, k_b can be computed from (2) to determine the binding energy via $E_b = \frac{k_b^2}{2}$ if the scattering reaction ends up in forming a bound state.

The interaction potential $V(r)$ for e^- -atom scattering is complicated enough to permit analytical solution even at the zero energy. Thus to deal with the present problem, one must look for an uncomplicated numerical method to compute the effective-range parameters. Fortunately, the phase-function method [7] provides a basis for that. In this method the values for scattering length a and effective range r_e is computed by solving the differential equations

$$a'(r) = V(r) [r - a(r)]^2, \quad (3)$$

and

$$b'(r) = 2V(r) [r - a(r)] b(r) - r^2 V(r) \left[a^2(r) - \frac{4}{3} r a(r) + \frac{1}{3} r^2 \right] \quad (4)$$

with the initial conditions $a(0) = 0$, and $b(0) = 0$ for the interpolating functions $a(r)$ and $b(r)$. Here, prime denotes differentiation with respect to r . The quantities a and r_e are obtained from

$$a = \text{Lt}_{r \rightarrow \infty} a(r), \quad (5)$$

and

$$r_e = \text{Lt}_{r \rightarrow \infty} 2b(r) / a^2(r). \quad (6)$$

The eqs. in (3) and (4) work only if $V(r)$ does not support any bound state. Otherwise at some point r_1 at which the potential has a level, the functions $a(r)$ and $b(r)$ become infinite. In such cases, it is necessary to renormalize the equation to avoid the unwanted singularity [8] and this is achieved by setting

$$a(r) = \tan \alpha(r), \quad (7)$$

$$b(r) = \beta(r) \cos^{-2} \alpha(r). \quad (8)$$

The functions $\alpha(r)$ and $\beta(r)$ satisfy

$$\alpha'(r) = V(r) [r \cos \alpha(r) - \sin \alpha(r)]^2; \alpha(0) = 0, \quad (9)$$

and

$$\beta'(r) = -2\beta(r) V(r) [r \cos \alpha(r) - \sin \alpha(r)] [\cos \alpha(r) + r \sin \alpha(r)] - \frac{1}{3} r^2 V(r) [r^2 \cos^2 \alpha(r) - 4r \sin \alpha(r) \cos \alpha(r) + 3 \sin^2 \alpha(r)]; \beta(0) = 0. \quad (10)$$

In the present case,

$$a = \text{Lt}_{r \rightarrow \infty} \tan \alpha(r), \quad (11)$$

$$r_e = \text{Lt}_{r \rightarrow \infty} 2\beta(r) / \sin \alpha(r). \quad (12)$$

We now follow the above view point to calculate the binding energies of H^- and Ps^- from some postulated laws of interaction one thereby derive a pedagogical realisation for the dynamical origin of their binding.

The interaction which contributes in e^-H scattering consists of three basic ingredients. The first one is the so-called static potential (short range) in which the incident electron feels only the mean field of the undistorted atom and the second one goes by the name polarization potential (long range) resulting from the distortion of the atom by the charged projectile. Both of these potentials are local. In addition, there is a highly nonlocal potential that gives us the possibility that the incident electron is captured and the atomic electron ejected. This potential accounting for the electron exchange distinguishes between the singlet and triplet scattering [9]. Here, we assume that there is only one singlet bound state of H^- and proceed accordingly.

We note that the nonlinear equations in (3) and (4) relate to scattering on local potentials and can not be applied directly in the presence of a nonlocal interaction [7]. We, therefore, constructed an equivalent local potential by following a prescription given by one of us [10]. We have also seen that the effect of nonlocality can be simulated by an appropriate change in the strength of the static potential to fit the low-energy scattering phase shift [9]. This equivalent local potential was then combined with the usual static potential and the extended polarisation potential of Callaway *et al* [11] to construct the effective interaction for the electron-hydrogen atom singlet scattering.

First we solved the eq. (3) for the static potential only and found $a = -9.447$ a.u. in agreement with the result given in Mott and Massey [9]. This shows that the algorithms presented above do not introduce numerical inaccuracy. We then attempted to solve the same equation in presence of the polarization potential and found that the function $a(r)$ exhibits singularity. Thus, the attractive polarisation potential plays key role in forming a hydrogen negative ion. We computed the scattering length for the full potential by using (9) and (11) and found $a = 4.3150$ a.u.. It is unfortunate that we were unable to calculate the value of effective range by using (10) and (12) because $b(r)$ was found to exhibit a singularity. This is not unexpected in view of an early observation by O'Malley *et al* [5] who explicitly demonstrated that the presence of long-range ($\sim r^{-4}$) potential, the effective-range theory needs a radical modification. However, it was also found by these authors that for loosely-bound states the

binding energy (E_b) can be reliably calculated from the knowledge of the scattering length only by using

$$E_b = \frac{1}{2a^2} \text{ (a. u.)}. \quad (13)$$

From (13) our value E_b of H^- comes out to be 0.0268 (a.u.). Interestingly, this number is not far off from the so-called exact result quoted earlier. We followed the same procedure to calculate the binding energy of Ps^- . The dipole polarizability of the Ps -atom is taken eight times as that of hydrogen. For electron scattering by positronium atom, the static potential is zero. The polarisation potential is the only interaction that contributes to Ps^- binding. Our result for a is 6.482 (a.u.) with the corresponding binding energy $E_b = 0.0119$ (a.u.).

In the recent past, many variational and nonvariational calculations [1, 4, 12] have been reported giving more accurate values for the binding energies of the Ps^- . It was not our intention to contest these numbers with regard to numerical accuracies. On the other hand, we tried to present a physico-mathematical analysis that tends to clarify the dynamical origin of H^- and Ps^- binding. In particular, we found the polarisation potential play a crucial role in the dynamics.

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