Further examination of a simplified model for positronium-helium scattering

J DiRienzi[1] and Richard J Drachman[2]

[1]Notre Dame of Maryland University, Baltimore, MD 21210 USA
[2]NASA Goddard Space Flight Centre, Greenbelt, MD 20771 USA

Abstract. While carrying out investigations on Ps-He scattering we realized that it would be possible to improve the results of a previous work on zero-energy scattering of ortho-positronium by helium atoms. The previous work used a model to account for exchange and also attempted to include the effect of short-range Coulomb interactions in the close-coupling approximation. The 3 terms that were then included did not produce a well-converged result but served to give some justification to the model. Now we improve the calculation by using a simple variational wave function, and derive a much better value of the scattering length. The new result is compared with other computed values, and when an approximate correction due to the van der Waals potential is included the total is consistent with an earlier conjecture.

1. Introduction

The positronium-helium system at low energy has been of interest for a long time, from both the experimental and theoretical points of view. Some surprising recent experimental results have shown an unexpected similarity between scattering of electrons and Ps from a series of different targets [1]. Low- and zero-energy scattering calculations and measurements have been quite difficult as documented in Table II of reference [2]. There 17 theoretical and 4 experimental values for the Ps-He scattering length are listed, spanning a very wide range from 0.8 to 2.2 in units of a_0 . Finally, an apparently definitive calculation of the scattering length has appeared, giving a value of 1.4046(6) and based on the diffusion Monte Carlo method (DMC) [3]. However, this method is relatively complicated, and it is still worthwhile to consider simpler and more physical models of this system.

This is the third in a series of papers examining the consequences of a particular model that attempts to describe low-energy scattering of positronium atoms (Ps) by helium atoms (He). The basic simplification is to treat the electron in the Ps atom as distinguishable, but to account for exchange by adding an empirically determined local, repulsive potential. In the first paper of the series [4] it was also assumed that the exchange potential was by far the most important part of the Hamiltonian, and effects due to the local Coulomb interaction were omitted. In addition, the helium atom was assumed to remain unperturbed in its ground state. Because of this target-elastic approximation the long-range van der Waals interaction was also neglected, and the authors of [4] suggested that the effect of these two interactions might approximately cancel. In spite of these approximations the result “shows an uncannily good agreement with the DMC estimate” [3].

In the second paper [5] we attempted to account for the short-range Coulomb effect with a three-term close-coupling approximation. Although the result was not well converged it did indicate that the original assumption (or hope) that exchange was dominant could not be quantitatively supported. In the present work the program of [5] is more efficiently carried out using a short-range correlation function variationally. Although the van der Waals potential is still

not properly accounted for its effects can be estimated from the early work of Barker and Bransden [6], and the two effects do seem to cancel, at least approximately.

The model is based on the following Hamiltonian:

$$H = H_0 - \tfrac{1}{2}\nabla_R^2 + V + V_{\text{int}}$$
$$H_0 = -2\nabla_\rho^2 - \frac{2}{\rho} + H(\vec{r}_2, \vec{r}_3). \tag{1}$$

Here H_0 contains the non-relativistic Hamiltonians of the projectile positronium atom and the target helium atom, respectively, V is the "exchange potential" and has the form $V = V_0 \exp\left(-\alpha\left|\vec{\mathrm{R}} + \tfrac{1}{2}\vec{\rho}\right|\right)$, where V_0=39 and α=2.9 which give good agreement with the static exchange results. The interaction potential between the Ps and helium atoms is

$$\mathrm{V}_{\text{int}} = \frac{4}{x} - \frac{4}{r_1} + \sum_{i=2}^{3}\left[\frac{2}{|\vec{r}_1 - \vec{r}_i|} - \frac{2}{|\vec{x} - \vec{r}_i|}\right]. \tag{2}$$

The Ps ground-state wave function is $\phi(\rho) = \exp(-\rho/2)/(8\pi)^{1/2}$, and we approximate the helium wave function as $\psi(r_2, r_3) = Z^3 \exp(-Z[r_2 + r_3])/\pi$. The coordinate $\vec{\rho} = \vec{r}_1 - \vec{x}$ is the internal coordinate of the Ps atom, whose center of mass position is $\vec{R} = (\vec{x} + \vec{r}_1)/2$. (The origin of coordinates is at the helium nucleus, taken to be infinitely massive, and $\vec{x}$ is the position of the positron.) The variational trial scattering function has the same form as in [4]:

$$\Psi = \left[\chi(R) + F(R)G(\vec{R}, \vec{\rho})\right]\phi(\rho)\psi(r_2, r_3), \tag{3}$$

where

$$G(\vec{R}, \vec{\rho}) = \mathrm{g}(\vec{R}, \vec{\rho}) - \left\langle \mathrm{g}(\vec{R}, \vec{\rho}) \right\rangle \text{ and } \mathrm{g}(\vec{R}, \vec{\rho}) = \mathrm{e}^{-\gamma\left|\vec{\mathrm{R}} + \vec{\rho}/2\right|}. \tag{4}$$

Here the bracket notation is defined as $\langle f \rangle \equiv \int \mathrm{d}\vec{\rho}\,\phi(\rho)\, f\, \phi(\rho)$.

At this point the calculation looks exactly the same as that in [4], but in that case the Coulomb interaction potential V_{int} was omitted. In the next section this omission will be corrected, and the details of the calculation will be described.

2. Details of the calculation

The variational principle to be employed is the following:

$$\delta J = 0, \text{ where } J = \int \mathrm{d}\vec{\mathrm{R}}\,\mathrm{d}\vec{\rho}\,\mathrm{d}\vec{\mathrm{r}}_2\,\mathrm{d}\vec{\mathrm{r}}_3\,\Psi\,(H - E)\Psi, \tag{5}$$

and the variation is with respect to the two functions, χ and F. Since the coordinates of the helium wave function appear in Eq.(3) in separable form the integration over them can be performed immediately. Integration of V_{int} over $\mathrm{d}\vec{r}_2\mathrm{d}\vec{r}_3$ gives rise to the following simple potential:

$$U = U(x) - U(r_1). \tag{6}$$

where $U(y) = 4e^{-2Zy}\left(\frac{1}{y} + Z\right)$, and $\mathrm{Z} = \frac{27}{16}$. Following the work in [4] we obtain the two zero-energy coupled differential equations for χ and F :

$$\left[-\tfrac{1}{2}\nabla_R^2 + U_1\right]\chi + U_2 F = 0$$
$$\left[-\tfrac{1}{2}N\nabla_R^2 + W + U_N\frac{\mathrm{d}}{\mathrm{d}R} + U_3 + Q\right]F + U_2\chi = 0. \tag{7}$$

The definitions of the various quantities appearing in (7) are almost the same as in [4], with the addition of the direct potential U where appropriate:

$$U_1 = \langle V \rangle, \quad U_2 = \langle G(V+U) \rangle, \quad U_3 = \langle G^2(V+U) \rangle$$
$$N = \langle G^2 \rangle, \quad W = -\tfrac{1}{2} \langle G \nabla_R^2 G \rangle \tag{8}$$
$$U_N = -\tfrac{1}{2} \frac{\mathrm{d}N}{\mathrm{dR}}, \quad Q = \langle G[H_0, G] \rangle$$

(Notice that U does not appear in the definition of U_1 due to its odd symmetry.) Some of the integrals appearing in (8) involve only the electron coordinate r_1, and they can be easily integrated using the Fourier technique described in Appendix B of [5]. Others involve mixed coordinates (r_1 and x), and we have treated these numerically.

In the conventional way, we rewrite the coupled differential equations in (8) by using the definitions $\chi = u/R$ and $F = v/R$:

$$-\tfrac{1}{2} u'' + U_1 u + U_2 v = 0$$
$$-\tfrac{1}{2} N v'' + U_N v' + (W + U_3 + Q - U_N/R) v + U_2 u = 0. \tag{9}$$

Two linearly independent solutions, $[u_1, v_1]$ and $[u_2, v_2]$, are obtained numerically by starting the integration with either zero or finite slope. Choosing a linear combination of these two solutions that gives a vanishing value for v as $R \to \infty$ leads to the appropriate form for u from which the scattering length a can be obtained: $u \propto (R - a)$.

2. Results and discussion

We first repeated the static-exchange calculation by solving the first equation in (9) without including U_2 and checked the calculation of [4]. Then we omitted the potential U from (8), solved equations (9), and recovered the correlated result given in [4]. Finally, with U included, we obtained the variationally correct consequences of the target-elastic model. All these results are displayed in Table 1.

It turns out that including the short-range Coulomb potential, which leads to the inclusion of U, does indeed partially cancel the effect of including correlation. What happens is the following. Without correlation the short-range potential U vanishes because of symmetry (as discussed above), and the repulsive exchange potential gives a large value of the scattering length. When the correlation function G is added, as was done in [4], the Ps wave function is distorted to keep the electron further from the target atom than the positron and to allow the Ps to approach closer with a resultant decrease in the scattering length. Finally, when the full model is treated, this distortion allows the short-range Coulomb force to come into play. Since the positron is closer and the electron is further away from the attractive atomic potential the net effect is now repulsive, and the scattering length now increases. All this was qualitatively apparent in [5], but it was necessary in that work to make some fairly large extrapolations; the present calculation makes that unnecessary. From internal considerations of the calculations in [4], we estimate that the present scattering length lies no more than 0.03 above the exact value determined by the model.

To make a realistic estimate of the scattering length of the physical Ps-He system, however, it would be necessary to relax the target-elastic characteristic of the model. The principal effect of allowing distortion of the helium target would be inclusion of the van der Waals potential (vdW) whose long-range asymptotic form is $-C_6/R^6$. An early work [6] attempted to do just that in an adiabatic approximation and found a lowering of the scattering length by 0.19. We may assume that adding the van der Waals potential would lower our result by the same amount, and the total is also shown in the Table. But the value of C_6=19.3 derived in

[6] is apparently about 27% low, compared with the more recent result [7,8] C_6=26.7. If the change in the scattering length is taken to be proportional to this coefficient (which overlooks the short-range parts of the potential) then the scattering length would be lowered by about 0.26. All these estimates are shown in Table 1 with those that are variationally correct upper bounds (for a particular model) indicated.

Table 1. Positronium-helium scattering lengths in units of a_0 in different approximations. Asterisks indicate variational upper bounds. Parentheses contain variant results due to differing treatments of the target wave function in the static-exchange approximation. The "adjusted vdW" entry refers to the more accurate value [7,8] of C_6.

Reference	Scattering length	Description
[9], [4]	(1.80)*, 1.72*	Static exchange
[5]	1.695*	3-state close-coupling
[6]	(1.61), 1.53	Exchange + vdW
	1.573*	Present work
[4]	1.42	
[3]	1.405	DMC "exact"
	1.38	Present + vdW
.	1.31	Present + adjusted vdW

References

[1] Brawley S J, Armitage S, Beale J, Leslie D E, Williams A I and Laricchia G 2010 *Science* **330** 789
[2] Mitroy J and Ivanov IA 2001 *Phys. Rev.* A **65** 012509
[3] Chiesa C, Mella M and Morosi G 2002 *Phys. Rev.* A **66** 042502
[4] Drachman R J and Houston S K 1970 *J. Phys.* B:*Atom. Molec. Phys.* **3** 1657-62
[5] DiRienzi J and Drachman R J 2003 *J. Phys.* B:*Atom. Molec. Phys.* **36** 2409-17
[6] Barker M I and Bransden B H 1968 *J. Phys.* B:*Atom. Molec. Phys.* **1** 1109-14
Barker M I and Bransden B H 1969 *J. Phys.* B:*Atom. Molec. Phys.* **2** 730
[7] Martin D W and Fraser P A 1980 *J. Phys.* B:*Atom. Molec. Phys.* **13** 3383-7
[8] Mitroy J and Bromley M W J 2003 *Phys. Rev.* A **68** 035201
[9] Fraser P A and Kraidy M 1966 *Proc. Phys. Soc.* **89** 533-39
Kraidy M 1969 *private communication*