

Approximating the target wave function in positronium-helium scattering

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We consider the effect of using necessarily inexact target wave functions in a Kohn variational calculation of the Ps—He scattering length. We use the simplest closed-shell or one-term Hylleraas function in the static-exchange approximation and examine two plausible ways of handling such an inexact function. Both of these methods have been employed in the past, and our results are compared with these previous calculations. Significant differences are found which may persist in more elaborate calculations.

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I. INTRODUCTION

Positronium-helium (Ps-He) elastic scattering has been of interest for a long time, and it has been a difficult problem from both the theoretical and the experimental viewpoints. Even what should be the simplest theoretical question—computing the scattering length—has generated a wide variety of estimates and approximations [1]. Table II of Ref. [1] displays a variety of experimental and theoretical values for the scattering length, varying from $a=0.81a_0$ to $a=1.81a_0$. Some of the experimental values come from measurements of scattering extrapolated to zero energy and some are from analyses of the behavior of Ps in bulk helium. The theories include Kohn variational and other calculations, some more fundamental than others, which employed model exchange potentials. But as far as we know, all of these need to calculate separately an approximate form for the wave function of the target helium atom and must also choose a method of dealing with the inexactness of this function. Even the diffusion Monte Carlo calculation reported in [1] needs to calculate a target function separately, for both its asymptotic form and its use in the importance function. That method gives a scattering length $a=1.4046(6)a_0$, which appears to be a definitive result.

In this paper we look at the differences between Kohn variational scattering length calculations in which the inexact target wave function is treated in two different ways: In the first method one simply calculates the stationary expression including the explicit form of the target wave function. In the second method we treat the target wave function as if it were exact, letting the helium Hamiltonian act as if the function is an exact eigenfunction, and finally inserting the explicit approximate form. These two methods (neither of which is known to be more correct) should converge as the target wave function approaches the exact form. These two variants have been discussed previously for the electron-atom case [2]. Similar investigations, for positron-atom scattering where there is no exchange, have also been carried out [3]. A static-exchange calculation for Ps-Xe done using the first variant [4] proved to be unstable, but the second variant was satisfactory [5].

In this paper we will calculate the Ps—He scattering length using both variants and applying the Kohn variational principle. We will use the simplest helium wave function, the closed-shell exponential (or one-term Hylleraas), and will evaluate the scattering length in the Born and static-exchange approximations. We find significant but not large differences between the two variants, larger in the Born approximation than in the static-exchange approximation, and in the course of our calculations we have clarified certain historically obscure results.

II. FORMULATION OF THE METHOD

The system consists of three electrons, one positron, and a helium nucleus, taken as fixed at the origin of coordinates. The nonrelativistic Hamiltonian in Rydberg atomic units is

$$H = -\nabla_x^2 + \frac{4}{x} - \sum_{i=1}^3 \left(\nabla_i^2 + \frac{4}{r_i} + \frac{2}{\rho_i} \right) + 2 \left(\frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \right), \quad (1)$$

where \vec{x} and \vec{r}_i describe the positions of the positron and the electrons, respectively, $\vec{\rho}_i = \vec{x} - \vec{r}_i$, and $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$. We are interested in obtaining a variationally correct estimate [a] of the scattering length for Ps-He, using the Kohn variational principle at zero energy:

$$[a] = a + \frac{1}{2\pi} \int d\tau \Psi(H - E)\Psi. \quad (2)$$

Here a is the explicit scattering length appearing in the asymptotic form of the trial function Ψ . We will use the static-exchange form of the trial function:

$$\Psi = \frac{1}{\sqrt{3}} [F(R_1)\phi(\rho_1)\psi(r_2, r_3)\alpha_1 s_{23} + F(R_2)\phi(\rho_2)\psi(r_3, r_1)\alpha_2 s_{31} + F(R_3)\phi(\rho_3)\psi(r_1, r_2)\alpha_3 s_{12}], \quad (3)$$

where $\vec{R}_i = (\vec{x} + \vec{r}_i)/2$, $\phi = \exp(-\rho/2)/\sqrt{8\pi}$ is the ground-state wave function of the Ps atom, and ψ is the spatial part of the helium atom wave function, symmetric in the two electronic

coordinates. The spinor α denotes up spin, and because of the antisymmetry of the singlet helium spin function s , the entire wave function is antisymmetric under interchange of any two of the electrons. For the present purposes, we choose a very simple form for the scattering function:

$$F(R) = 1 - \frac{a}{R}(1 - e^{-\varepsilon R}), \quad (4)$$

where a and ε will serve as variational parameters. (Our experience with this type of trial function shows that it is very effective in dealing with short-range potentials.) With this form of Ψ the variational scattering length becomes $[a] = C_0 + C_1(\varepsilon)a + C_2(\varepsilon)a^2$. We will be interested here in two different choices of a : setting $a=0$ gives the Born approximation $[a]_{\text{Born}} = C_0$ and minimizing $[a]$ as a function of a gives

$$[a]_{\text{min}} = C_0 - \frac{C_1^2(\varepsilon)}{4C_2(\varepsilon)}, \quad (5)$$

where

$$a_{\text{min}} = -\frac{C_1(\varepsilon)}{2C_2(\varepsilon)}.$$

So the solution of the problem involves calculating the integrals leading to the three coefficients $C_j(\varepsilon)$.

After carrying out the spin algebra and without loss of generality because of the symmetrical form, we rewrite the Kohn expression (2) in the following explicit form:

$$[a] = a + \frac{1}{2\pi} \int d\tau [F(R_1)\phi(\rho_1)\psi(r_2, r_3) - F(R_2)\phi(\rho_2)\psi(r_1, r_3)] \left[H_0(\rho_1) - E_{Ps} + H_0(r_2, r_3) - E_{He} - \frac{1}{2}\nabla_{R_1}^2 + V_1 \right] F(R_1)\phi(\rho_1)\psi(r_2, r_3), \quad (6)$$

where

$$H_0(\rho_1) = -2\nabla_{\rho}^2 - \frac{2}{\rho_1},$$

$$H_0(r_2, r_3) = -\sum_{j=2}^3 \left(\nabla_{r_j}^2 + \frac{4}{r_j} \right) + \frac{2}{r_{23}},$$

and

$$V_1 = 4 \left(\frac{1}{x} - \frac{1}{r_1} \right) + 2 \sum_{j=2}^3 \left(\frac{1}{r_{1j}} - \frac{1}{\rho_j} \right).$$

The two terms in the first factor of the integral generate the direct and exchange parts of the scattering length, respectively. The volume element $d\tau = d^3x d^3r_1 d^3r_2 d^3r_3$; all the coordinates are independent and run over all space. In this paper we will be using the simplest helium wave function $\psi_V(r_3, r_3) = (Z^3/\pi) \exp[-Z(r_2 + r_3)]$, with $Z = 27/16$, which corresponds to a variational energy $E_V = -2Z^2 = -5.6953125$; this differs from the best variational energy

value by about 2%. There are two reasonable ways to handle the inexactness of this wave function in Eq. (6).

A. Variant 1

In this method we simply carry out the indicated operations on the approximate wave function and insert the value of E_V in place of E_{He} in Eq. (6). That is,

$$[H_0(r_2, r_3) - E_V]\psi_V(r_2, r_3) = \left[\frac{2}{r_{23}} + (2Z - 4) \left(\frac{1}{r_2} + \frac{1}{r_3} \right) \right] \times \psi_V(r_2, r_3) \equiv Q(2, 3)\psi_V(r_2, r_3). \quad (7)$$

In the first term in Eq. (6) this expression vanishes because it is equivalent to the helium energy variational calculation itself, but it does not vanish in the second term, where the coordinates 1 and 2 are exchanged.

B. Variant 2

Instead, we can treat the helium wave function as if it is exact until it is necessary to insert an explicit form for it. That is, we simply recognize the Schrödinger equation satisfied by the exact wave function:

$$[H_0(r_2, r_3) - E_{He}]\psi_{He}(r_2, r_3) = 0. \quad (8)$$

Of course, this simplifies some of the mathematical operations that must be carried out, but it also expresses the idea that one should go as far as possible with the exact computation before inserting the inevitable approximations.

C. Born approximation

As a first (crude) estimate we can set $a=0$ in Eq. (4), which generates the Born approximation for the scattering length $[a]$ and also evaluates the constant C_0 to be used in the full variational expression, Eq. (5). The Born expression reduces to

$$[a]_{\text{Born}}^{(k)} = -\frac{1}{2\pi} \int d\tau W [V_1 + Q(2, 3)\delta_{1k}] = C_0^{(k)}, \quad (9)$$

where $W = \phi(\rho_1)\psi(r_2, r_3)\phi(\rho_2)\psi(r_1, r_3)$ and the index $k=1$ or 2 denotes the variant. In both cases the direct term vanishes: symmetry under interchange $\vec{r}_1 \leftrightarrow \vec{x}$ makes the integral term in V_1 vanish, and the Q integral vanishes as discussed above.

D. Terms depending on ε

The coefficients of linear and quadratic terms in a are dependent in complicated ways on the variational parameter ε , and they also have contributions from both exchange and direct terms in Eq. (6). The coefficients take the following slightly simplified forms:

$$C_1^{(k)}(\varepsilon) = \frac{1}{2\pi} \int d\tau W \left\{ [\bar{F}(R_1) + \bar{F}(R_2)][V_1 + Q(2, 3)\delta_{1k}] + \frac{\varepsilon^2}{2R_1} e^{-\varepsilon R_1} \right\}, \quad (10)$$

$$C_2^{(k)}(\varepsilon) = \frac{\varepsilon}{2} - \frac{1}{2\pi} \int d\tau W \bar{F}(R_2) \left\{ \bar{F}(R_1) [V_1 + Q(2,3) \delta_{1k}] + \frac{\varepsilon^2}{2R_1} e^{-\varepsilon R_1} \right\}, \quad (11)$$

where $\bar{F}(R) = (1 - e^{-\varepsilon R})/R$. In these expressions for C_1 and C_2 we have used the fact that the positronium wave function $\phi(\rho) = (1/\sqrt{8\pi})e^{-\rho/2}$ is an exact eigenfunction, have set all the direct integrals involving the potentials to zero as discussed above, and have carried out the direct kinetic-energy integrals explicitly.

III. RESULTS AND COMPARISONS

We found the evaluation of the necessary integrals to be quite tedious, and we are relegating to the Appendix some discussion of the various methods we applied. In this section we will present our results and will compare them with earlier results to clarify differences appearing in the literature.

The results for the Born approximation are $[a]_{Born}^1 = 5.83751a_0$ and $[a]_{Born}^2 = 4.93799a_0$ for the two variants, respectively. Both of these results are very large, but there is clearly a significant difference stemming from the two treatments of the target. When we include the ε -dependent correlation function the situation changes. The minimum values of the scattering length using the two variants are much smaller than the Born values and are much closer to each other: $[a]_{min}^1 = 1.82a_0$ (at $\varepsilon = 0.6221$) and $[a]_{min}^2 = 1.70a_0$ (at $\varepsilon = 0.6386$). We actually calculated the quantities in Eq. (5) at intervals of $\Delta\varepsilon = 0.125$, with ε going from 0.25 to 1.0, and interpolated to find the minima. The curves are very flat near the minima. These two values of the scattering length are interesting when compared with previously reported static-exchange values. Table I gives a summary of all such values.

Table I shows that there are two sets of values, those near $1.8a_0$ and those near $1.7a_0$. Our two values lie just above the results of Barker and Bransden [7] and Sarkar and Ghosh [9], respectively. The unpublished result of Kraidy [8] is also consistent with variant 2, as it should be, since it used that variant at the request of one of us (R.J.D.). Only the result of Fraser [6] is significantly far from the value we obtained for

TABLE I. Reported values of the scattering length in units of a_0 .

Reference	a
Fraser [6]	1.88
Variant 1	1.82
Barker and Bransden [7]	1.81
Kraidy [8]	1.72
Variant 2	1.70
Sarkar and Ghosh [9]	1.68

variant 1, probably due to numerical difficulties. Both Refs. [6,7] used the same method, numerical solution of an integrodifferential equation; we obviously prefer the result of Ref. [7]. In Ref. [9] the problem was attacked using a momentum-space integral-equation technique, and although it is not obvious from that paper, they seem to have used variant 2. The fact that our results are above the best previous values for each variant is reassuring; since our method is variational and not completely converged, it should give upper bounds on the scattering length.

In conclusion, we have shown the effect, in the static-exchange approximation, of using two different methods in treating the target wave function when it is not exact. The difference is significant but not large, and we suspect that differences of this magnitude might persist in more elaborate variational treatments. Nevertheless, it is interesting and somewhat surprising that the difference between the two variants is so much smaller at the best value of the variational parameters than in the Born approximation.

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Much of the work reported here made essential use of the Mathematica system, Ref. [10].

APPENDIX: DETAILS OF THE CALCULATION

Because our helium function is in the form of a product, it is possible to perform the integral over d^3r_3 analytically, resulting in the following expressions:

$$C_j^{[k]} = \frac{1}{\pi} \int \int \int d^3x d^3r_1 d^3r_2 \{ -\delta_{j0} + [\bar{F}(R_1) + \bar{F}(R_2)] \delta_{j1} - \bar{F}(R_1) \bar{F}(R_2) \delta_{j2} \} \phi(\rho_1) \phi(\rho_2) \psi(r_1, r_2) \left\{ U(x) - U(r_1) + \frac{1}{r_{12}} - \frac{1}{\rho_2} + \frac{1}{2} \left[\frac{Z-1}{r_2} + Z(Z-2) - e^{-2Zr_2} \left(\frac{1}{r_2} + Z \right) \right] \delta_{k1} \right\} + \frac{\varepsilon^2}{2\pi} \int \int \int d^3x d^3r_1 d^3r_2 \{ \delta_{j1} - \bar{F}(R_2) \delta_{j2} \} \frac{e^{-\varepsilon R_1}}{R_1} \phi(\rho_1) \phi(\rho_2) \psi(r_1, r_2) + \frac{\varepsilon}{2} \delta_{j2}, \quad (A1)$$

where $U(r) = 1/r + \exp(-2Zr)(1/r + Z)$. (By the use of Kronecker δ symbols we have constructed a compact expression

that combines all three coefficients and both variants.) Notice that most of the terms appearing here are factorable in terms

of coordinates 1 and 2. For example, the Born approximation involves the coefficient with $j=0$ whose first term can be written as

$$-\frac{4Z^3}{\pi} \int_0^\infty dx x^2 U(x) \left[\int d^3 r \phi(\rho) e^{-Zr} \right]^2. \quad (A2)$$

The integral over r can be performed analytically, and the integral over x can be done easily numerically. Similar separable forms come from other terms, but those involving both R and ρ need to be done numerically. The multidimensional integrals that result have been evaluated in most cases using Gaussian quadrature methods.

The nonseparable terms involving $1/r_{12}$ are more complicated, and we have evaluated them numerically following a Fourier transformation. As an example, we may consider the following Born term:

$$\begin{aligned} &-\frac{1}{\pi} \int \int \int d^3 x d^3 r_1 d^3 r_2 \phi(\rho_1) \phi(\rho_2) \psi(r_1, r_2) \frac{1}{r_{12}} \\ &= -\frac{128Z^5}{\pi^2} \int_0^\infty \frac{p^2 dp}{\left(p^2 + \frac{1}{4}\right)^4} \int_0^\infty dq \frac{(p^2 + q^2 + Z^2)^2 + \frac{4}{3} p^2 q^2}{[(p^2 + q^2 + Z^2)^2 - 4p^2 q^2]^3} \\ &= -\frac{80}{3} \frac{(3 + 36Z + 152Z^2 + 144Z^3 + 48Z^4)}{(1 + 2Z)^6}. \end{aligned} \quad (A3)$$

In passing from the left to the right side of this equation we have inserted the Fourier transforms of all the functions appearing in the integrand, have applied the definition of the δ -function 3 times, and have then carried out the integration over $\mu = \hat{p} \cdot \hat{q}$. The final expression, resulting from the two integrations over p and q , was obtained with the aid of MATHEMATICA.

We have used both integration methods, Fourier and direct coordinate-space methods, as appropriate in evaluating the various integrals that contribute to the final results. In many cases numerical integration in several dimensions is necessary; this is the limit on the accuracy we can achieve. The most difficult integral we needed to evaluate involves the product of two scattering functions $\bar{F}(R)$ and the troublesome factor $1/r_{12}$:

$$-\frac{1}{\pi} \int \int \int d^3 x d^3 r_1 d^3 r_2 \bar{F}(R_1) \bar{F}(R_2) \phi(\rho_1) \phi(\rho_2) \frac{\psi(r_1, r_2)}{r_{12}}. \quad (A4)$$

This integral taxed our numerical capabilities either in the coordinate or Fourier representation, but we made use of a trick to simplify its evaluation. First, we Fourier transformed the most difficult part of the integrand:

$$\frac{1}{r_{12}} = \frac{1}{2\pi^2} \int d^3 p \frac{e^{i\vec{p} \cdot (\vec{r}_1 - \vec{r}_2)}}{p^2}. \quad (A5)$$

Then Eq. (A4) can be rewritten in a more convenient form

$$-\frac{Z^3}{2\pi^4} \int \int d^3 x \frac{d^3 p}{p^2} |f(\vec{x}, \vec{p})|^2, \quad (A6)$$

where

$$f(\vec{x}, \vec{p}) = \int d^3 r \bar{F}(r) \phi(\rho) e^{-Zr} e^{i\vec{p} \cdot \vec{r}}.$$

If we take \vec{x} along the z axis, then we can write

$$\vec{p} \cdot \vec{r} = pr[\mu_p \mu_r + \sqrt{(1 - \mu_p^2)(1 - \mu_r^2)} \cos(\phi_p - \phi_r)], \quad (A7)$$

where $\mu = \cos \theta$ refers to the polar angle of each vector and ϕ refers to the azimuthal angle. The expression for f becomes the following:

$$\begin{aligned} f(x, p, \mu_p) &= \int_0^\infty dr r^2 e^{-Zr} \int_{-1}^1 d\mu_r \bar{F}(R) \phi(\rho) e^{ipr\mu_p\mu_r} \\ &\quad \times \int_0^{2\pi} d\phi_r e^{ipr\sqrt{(1 - \mu_p^2)(1 - \mu_r^2)} \cos(\phi_p - \phi_r)}. \end{aligned} \quad (A8)$$

The simplification stems from the fact that the ϕ integral above can be written in terms of a Bessel function:

$$\int_0^{2\pi} d\phi e^{iA \cos \phi} = 2\pi J_0(A). \quad (A9)$$

Equation (A8) can be expressed as $f = 2\pi[f_1 + if_2]$, where

$$\begin{aligned} \left\{ \begin{array}{l} f_1 \\ f_2 \end{array} \right\} &= \int_0^\infty dr r^2 e^{-Zr} \int_{-1}^1 d\mu_r \bar{F}(R) \phi(\rho) \times \left\{ \begin{array}{l} \cos(pr\mu_p\mu_r) \\ \sin(pr\mu_p\mu_r) \end{array} \right\} \\ &\quad \times J_0[pr\sqrt{(1 - \mu_p^2)(1 - \mu_r^2)}]. \end{aligned} \quad (A10)$$

Finally, we can write the integral appearing in Eq. (A6) as

$$-16Z^3 \int_0^\infty dx x^2 \int_0^\infty dp \int_{-1}^1 d\mu_p [f_1^2(x, p, \mu_p) + f_2^2(x, p, \mu_p)]. \quad (A11)$$

This is still a high-dimension integration, but it turned out to be tractable, using Mathematica and a standard personal computer.

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