S-wave collisions of positrons with helium

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Received 22 June 1976

Abstract. S-wave elastic collisions of positrons with helium have been studied using the method of models in an optical-potential formulation that gives lower bounds to the phaseshifts within the accuracy of the helium-atom model. Four simple approximations to the helium ground-state wavefunction are used in a trial function with up to 84 correlation terms. The annihilation rate calculated from what is considered to be the best model treated (of analytic Hartree-Fock type with the correct polarizability) is in good agreement with the most recent experiment. The scattering results are compared with those of other recent calculations.

In a related calculation involving the eigenvalues of the correct positron–helium Hamiltonian in the basis of the correlation functions, a stabilized eigenvalue, which may suggest a resonance, is found in the inelastic region (above the positronium formation threshold and just below the first singlet excited state of helium).

1. Introduction

There is considerable current interest in the positron–helium scattering problem, both experimentally and theoretically. In theoretical work for targets other than hydrogen, an approximate target wavefunction must of necessity be employed. Peterkop and Rabik (1971) and Houston (1973) in Kohn-method calculations of scattering lengths found that violently different results could be obtained by using inexact target wavefunctions. Wardle (1973) and Ho et al (1975) considered positron–helium non-zero-energy scattering using the (inadequate) coupled static approximation, and found that the phaseshifting could be quite different from model to model (in fact for one model considered in this approximation, the simplest Hylleraas approximation—HY1 below—it may be inferred that the scattering length lies somewhat below the lower bound calculated by Hahn and Spruch 1974).

In order to preserve the applicability of a bound theorem, Drachman (1972) suggested the method of models in which the target Hamiltonian is replaced by a model Hamiltonian and the calculation then proceeds as exactly as practicable. Houston and Drachman (1971) in a positron–helium scattering calculation used this method together with Kohn’s method to calculate the scattering length and used the Harris method for non-zero-energy calculations. Humberston (1973) employed the method

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of models and Kohn's method using a five-parameter Hylleraas target wavefunction. The scattering lengths that these authors obtained are upper bounds within the reliability of the model helium wavefunctions. However, the bound property does not apply to their phaseshifts. It is the purpose of this work to apply the method of models to an S-wave positron–helium elastic scattering calculation, using the correlation method. It is also interesting to compare results from a rather simple helium wavefunction with those obtained from a more elaborate one such as H5 from Humberston (1973). Both scattering lengths and phaseshifts obtained here obey the bound principle for a given target wavefunction. It should be noted that the most rigorous elastic $e^+–H$ (the hydrogen wavefunction being of course exactly known) non-zero-energy scattering results have been obtained by Bhatia et al (1971) using the correlation method.

2. Formulation

The Schrödinger equation for the positron–helium system is

$$ (H - E)\Psi = \left(-\nabla_p^2 + \frac{4}{r_p} - \frac{2}{r_{1p}} - \frac{2}{r_{2p}} + H_{\text{He}} - E\right)\Psi(r_1, r_2, r_p) = 0 \tag{1} $$

where $r_i$ and $r_p$ are the position vectors of the electrons and the positron and $r_{ip} = |r_i - r_p|$ with $i = 1, 2$. Atomic units in which $\hbar = 2m = \frac{1}{2}e^2 = 1$ are used in this work. The unit of length is $a_0$, the Bohr radius, and the energies are in rydbergs ($\approx 13.6 \text{ eV}$). The total energy $E$ of the system is $E = E_{\text{He}} + k^2$, where $k^2$ is the kinetic energy of the incident positron; $H_{\text{He}}$ and $E_{\text{He}}$ are the Hamiltonian and energy of the helium atom respectively.

The trial wavefunction is of the form, for $l = 0$ scattering,

$$ \Psi^l(r_1, r_2, r_p) = \psi_{\text{He}}(r_1, r_2)F(r_p) + \sum C_i\chi_i \tag{2} $$

where $\psi_{\text{He}}(r_1, r_2)$ is the ground-state wavefunction and $\chi_i$ are so-called short-range correlation terms which represent the closed part of the trial wavefunction. Explicitly we take

$$ \chi_i = r_p^{l_i}e^{-\gamma r_p}(r_1^{m_{1i}}r_2^{m_{2i}}e^{-\beta r_1} - \beta r_2 + r_2^{m_{1i}}r_1^{m_{2i}}e^{-\beta r_2} - \beta r_1) \tag{3} $$

where $\alpha$, $\beta$ and $\gamma$ are positive constants and $l_i + m_i + n_i \leq w$ with $w = 1, 2, 3, 4, 5, 6$ which correspond respectively to a total number $(N)$ of correlation terms $N = 4, 10, 20, 35, 56, 84$. The asymptotic behaviour of $F(r_p)$ is as follows:

$$ r_pF(r_p) \sim 0 \tag{4a} $$

$$ r_pF(r_p) \sim \sin kr_p + (\tan \eta_0)\cos kr_p \tag{4b} $$

where $\eta_0$ is the S-wave phaseshift. By projecting the ‘Schrödinger equation’ for $\Psi^l$ onto $\psi_{\text{He}}$ and the $\chi_j$, we may construct the optical potential. From

$$ \langle \psi_{\text{He}}|H - E|\psi_{\text{He}}F + \sum C_i\chi_i \rangle = 0 \tag{5a} $$

$$ \langle \chi_j|H - E|\psi_{\text{He}}F + \sum C_i\chi_i \rangle = 0 \tag{5b} $$
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we obtain an integro-differential equation, with \( f(r_p) = r_p F(r_p) \),

\[
\left( \frac{d^2}{dr_p^2} + k^2 \right) f(r_p) = U(r_p) f(r_p) + \int U_{\text{opt}}(r_p, r'_p) f(r_p) \, dr'_p
\]

where \( U(r_p) \) is the mean static potential and \( U_{\text{opt}} \) is the optical potential:

\[
U_{\text{opt}}(r_p, r'_p) = \sum_x V'(r_p) V_x'(r'_p)/(E - E').
\]

\( U_{\text{opt}} \) is constructed as follows.

We first solved the eigenvalue equation

\[
\sum_j H_{ij} a_j^k = \epsilon^k \sum_j N_{ij} a_j^k \tag{8}
\]

where \( H_{ij} = H_{ji} = \langle \chi_i | H | \chi_j \rangle \) and \( N_{ij} = N_{ji} = \langle \chi_i | \chi_j \rangle \). \( V^x \) is then given by

\[
V^x(r_p) = \sum_j a_j^x V_j(r_p) \tag{9}
\]

where the \( a_j \) are such that

\[
\sum_{i,j} a_i^x N_{ij} a_j^{x'} = \delta_{xx'}
\]

with

\[
V_j(r_p) = r_p \langle \psi_{He} | H - E | \chi_j \rangle. \tag{10}
\]

Following the proof of Gailitis (1965), if \( \psi_{He} \) is the exact ground state of the helium atom and \( E \) is below the lowest eigenvalue of \( QHQ \) (\( Q = 1 - P = 1 - |\psi_{He}\rangle\langle\psi_{He}| \)), then the phaseshifts obtained are lower bounds to the exact ones. Furthermore, Burke and Taylor (1966) pointed out that the \( \chi_i \) need not be made orthogonal to the open-channel space; as long as they vanish asymptotically and do not affect the asymptotic behaviour of \( F(r_p) \), the bound theorem is retained. No attempt has been made to compute \( QHQ \) eigenvalues; the lowest eigenvalue probably lies close to the first excitation threshold, as is the case in hydrogen (Bhatia et al. 1971).

The argument so far is valid if the target wavefunction is exact. Therefore, if we apply the method of models of Drachman (1972) we must replace \( H_{He} \) and \( E_{He} \) of the above equations by \( H_{He}^M \) and \( E_{He}^M \) respectively, such that \( H_{He}^M \psi_{He} = E_{He}^M \psi_{He} \), the phaseshifts then obtained are lower bounds to the exact phaseshifts for the modified target (the scattering lengths are upper bounds). The results clearly depend on the target wavefunction. By improving the target wavefunction the scattering parameters obtained will be closer to the exact ones. However, in a method-of-models \( e^+ - H \) scattering calculation, Ho and Fraser (1975) pointed out that results could be unrealistic if the target wavefunction is, in particular, over-polarizable. Furthermore, they confirmed that the target being correctly polarizable is an important consideration in low-energy scattering, as emphasized particularly by Drachman (1968) and Houston and Drachman (1971).

In this work we have used four kinds of simple helium wavefunction, namely HY1, HY2, HF1 and HF2; HY and HF represent Hylleraas and analytic Hartree–Fock-type wavefunctions respectively. The index '1' denotes the minimum variational energy wavefunctions and the index '2' indicates the wavefunctions with the correct
polarizability \( \alpha \) (for reasons discussed elsewhere \( \text{Ho et al. 1975} \) we take \( \alpha = 1.376 a_0^3 \)). They are described as follows:

\[
\begin{align*}
\text{HY1} &= \psi_{\text{He}} = N_1 e^{-\mu_1(r_1 + r_2)} \\
\mu_1 &= 1.6875 \\
\text{HY2} &= \psi_{\text{He}} = N_2 e^{-\mu_2(r_1 + r_2)} \\
\mu_2 &= 1.5992
\end{align*}
\] (11a)

\[
\begin{align*}
\text{HF1} &= \psi_{\text{He}} = N_3(e^{-a_1 r_1} + C_1 e^{-2a_1 r_1})(e^{-a_1 r_2} + C_1 e^{-2a_1 r_2}) \\
a_1 &= 1.455799 \\
C_1 &= 0.6 \\
\text{HF2} &= \psi_{\text{He}} = N_4(e^{-a_2 r_1} + C_2 e^{-2a_2 r_1})(e^{-a_2 r_2} + C_2 e^{-2a_2 r_2}) \\
a_2 &= 1.481102 \\
C_2 &= 0.6.
\end{align*}
\] (11b)

The method used to obtain the wavefunction HF2 and some physical parameters of these helium wavefunctions are described by Ho et al. (1975).

3. Method of solution

The integro-differential equation is first converted into an integral equation by the use of Green's function:

\[
f(r_p) = \sin kr_p + \int G(r_p, r_p') U(r_p') f(r_p') \, dr_p' + \int \int G(r_p, r_p', r_p'') U_{opt}(r_p', r_p'') f(r_p'') \, dr_p' \, dr_p''
\] (12)

where

\[
G(r_p, r_p') = \begin{cases} \\
-\frac{\sin kr_p \cos kr_p'}{k} & \text{if } r_p \leq r_p' \\
-\frac{\cos kr_p \sin kr_p'}{k} & \text{if } r_p' \leq r_p
\end{cases}
\] (13a)

The functional values of \( f(r_p) \) were determined at 40 Gaussian integration points by solving a system of approximating algebraic equations. We use 16 Gauss–Legendre points to cover the range from the origin to \( r_p = R \), and 24 Gauss–Laguerre points to cover the remaining region which extended to \((81.5 + R) a_0 \) approximately. The value of \( R \) ranged from \( 4 a_0 \) to \( 6 a_0 \). Also in approximating the integral numerically due note was taken of the discontinuities of the slope of the Green's functions.

Once \( f(r_p) \) is determined, scattering parameters (phaseshifts or scattering lengths) can be obtained by examining the asymptotic behaviour of \( f(r_p) \). Furthermore the \( C_i \) in equation (2) can be calculated and the solution can be applied to evaluate (for the S-state considered here) parameters such as \( Z_{\text{eff}}, \psi_{1p} \) and \( P_n \) defined and described below:

\[
Z_{\text{eff}} = 2 \int |\Psi(r_1, r_2, r_p)|^2 \delta(r_1 - r_p) \, dr_1 \, dr_2 \, dr_p
\] (14)

\[
\psi_{1p} = \frac{\langle \Psi | \delta(r_1 - r_p) \partial / \partial r_1 \Psi \rangle}{\langle \Psi | \delta(r_1 - r_p) \Psi \rangle}
\] (15)

and

\[
P_n = \frac{\int dr_p |\int dr_2 \phi_n^*(r_2) \Psi(r_p, r_2, r_p)|^2}{\langle \Psi | \delta(r_1 - r_p) \Psi \rangle}.
\] (16)
$Z_{\text{eff}}$ is the effective charge of the target atom for annihilation felt by the incoming positron, and measures the annihilation rate. $v_{1p}$ is an average electron–positron cusp value (this is equal to $-0.5 \alpha_0^2$ everywhere for an exact wavefunction). This parameter, whose use has been emphasized by Schrader and his co-workers (e.g. Lebeda and Schrader 1969), probes the accuracy of the trial wavefunction near the region of coalescence of positron and electron. Finally, $P_n$ is the probability of finding the residual ion $\text{He}^+$ in state $n$ after annihilation (Drachman 1966b).

4. Results

Throughout this work, up to 84 correlation terms were used. The first step is to optimize the non-linear parameters $\alpha, \beta, \gamma$ of equation (3). Guided by the bound theorem, the non-linear parameters were chosen such that the calculation gave the highest phaseshifts (or the lowest scattering length for zero energy). The results should in principle be optimized for each $k$ and each $N$ for each helium model. However this is economically impractical; therefore we have used two sets of non-linear parameters for each model. They are shown in table 1. Further, with the large number of linear parameters eventually used, the results will not be sensitive to the precise values of the non-linear parameters. The first set is applied to the energy region $k \leq 0.1$ and the second set is applied to $k > 0.1$ up to $k = 1.0$. The optimization was carried out at $N = 10$ terms and $k = 0.0$ and 0.2 respectively.

| Table 1. Non-linear parameters for different models (optimized at $N = 10$). |
|---|---|---|---|---|---|
| Model | $\alpha$ | $\beta$ | $\gamma$ |
|     | I    | II   | I    | II   | I    | II   |
| HY1  | 1.395 | 1.402 | 1.702 | 1.705 | 0.5195 | 0.660 |
| HY2  | 1.322 | 1.320 | 1.614 | 1.617 | 0.503  | 0.606 |
| HF1  | 1.212 | 1.225 | 1.675 | 1.679 | 0.488  | 0.622 |
| HF2  | 1.220 | 1.243 | 1.705 | 1.708 | 0.503  | 0.627 |

I: applied to $k \leq 0.1$, optimized at $k = 0.0$.
II: applied to $k > 0.1$, optimized at $k = 0.2$.

The method of calculating the matrix elements $H_{ij}$ and $N_{ij}$ of equation (8) are those of Perkins (1968). The integrals necessary to construct the optical potential (equation (7)) have been discussed by Ho and Page (1975), in whose work some numerical examples have been presented.

In table 2 we present the convergence behaviour for model HF2, which is typical of the other cases. It is found that the monotonicity theorem is indeed obeyed. In figure 1, we present results ($N = 84$) for the four models. The best result of this work is considered to be that from HF2, a Hartree–Fock-type wavefunction with the correct polarizability ($\alpha = 1.376 \alpha_0^2$). The result of HF2 is shown in figure 2 and table 3 together with the results of other authors. Column 4 shows those of Houston and Drachman (1971) (their model B is model HY2 in this work). The result of Humberston's model H5 (Humberston 1973) is shown in column 5. This is also a method-of-models calculation with a five-parameter Hylleraas helium function which bears essentially the correct polarizability. However, for other than zero energy, the Kohn algebraic method used by Humberston is not a bound calculation. Also shown in figure 2 are the results of Aulenkamp et al (1974) who used variant I.
Table 2. Convergence behaviour of phaseshifts from model HF2. Phaseshifts are in radians; the $k = 0$ entry is the scattering length.

<table>
<thead>
<tr>
<th>$k$</th>
<th>4</th>
<th>10</th>
<th>20</th>
<th>35</th>
<th>56</th>
<th>84</th>
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<td>-0.3371</td>
<td>-0.4032</td>
<td>-0.4295</td>
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<td>0.007518</td>
<td>0.01629</td>
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<td>0.02038</td>
<td>0.02088</td>
<td>0.02106</td>
</tr>
<tr>
<td>0.1</td>
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<td>0.02944</td>
<td>0.03398</td>
<td>0.03536</td>
<td>0.03573</td>
<td>0.03583</td>
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<tr>
<td>0.15</td>
<td>0.01702</td>
<td>0.03777</td>
<td>0.04212</td>
<td>0.04364</td>
<td>0.04382</td>
<td>0.04388</td>
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<tr>
<td>0.2</td>
<td>0.01701</td>
<td>0.04121</td>
<td>0.04504</td>
<td>0.04613</td>
<td>0.04637</td>
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<tr>
<td>0.25</td>
<td>0.01324</td>
<td>0.03946</td>
<td>0.04293</td>
<td>0.04399</td>
<td>0.04455</td>
<td>0.04471</td>
</tr>
<tr>
<td>0.3</td>
<td>0.008752</td>
<td>0.03322</td>
<td>0.03704</td>
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<td>-0.1731</td>
<td>-0.1703</td>
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</tr>
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</table>

(so termed by Peterkop and Rabik 1971) in which the true Hamiltonian and the variational energy of the helium model were employed. In figures 1 and 2 we also show the cross correlation limits of Jaduszliwer and Paul (1974)

$$\eta_0 = \Delta - 0.34k$$

where $\Delta$ is 0.14 and 0.18 for the lower and upper limits respectively.

By comparing the present HF2 results with those of Humberston's H5, it is noted that the present results lie somewhat higher. This may suggest that for a more definitive solution a bound calculation (like the present correlation method together with the method of models) with a more accurate helium wavefunction should be worth trying.

![Figure 1. S-wave phaseshifts from four helium models: curve A, HF1; curve B, HF2; curve C, HY1; the circles are from model HY2; U and L represent the upper and lower correlation limits respectively of Jaduszliwer and Paul (1974).](image)
The total cross sections have been calculated by combining our S-wave (HF2) and higher partial waves from other work. The results are sensitive to the higher partial waves used. For example, if we use the lowest P- and D-waves from Drachman (1966a), the total cross section seems to agree with Canter et al (1973). However if we combine our S-wave with the P-wave estimate by Jaduszliwer and Paul (1974), the total cross section seems closer to the measurement by Jaduszliwer and Paul (1974). The P-wave phase has been calculated by Campeanu and Humberston (1975) and if we combine the present HF2 with this latter P-wave the total cross section

Table 3. S-wave phaseshifts. Phaseshifts are in radians; the $k = 0$ entry is the scattering length.

<table>
<thead>
<tr>
<th>$k$</th>
<th>Present†‡ (HF2)</th>
<th>Drachman†‡ (1968) HY2</th>
<th>Houston and Drachman† (1971) HY2</th>
<th>Humberston† (1973)</th>
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<td>-0.524‡</td>
<td>-0.472‡</td>
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<td>0.03583</td>
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<td>0.035</td>
<td>0.031</td>
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<td>0:15</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<td>0.049</td>
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<td>0.04471</td>
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</tr>
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<td>0.039</td>
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<td>0.020</td>
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<td>-0.007</td>
<td>-0.003</td>
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<td>-0.039</td>
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<td>-0.1696</td>
<td>-0.174</td>
<td>-0.177</td>
<td>-0.195</td>
</tr>
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</table>

† 'Method-of-models' calculation.
‡ 'Bound calculation within the helium model.'
is lower than that measured by Canter et al. (1973), even with allowance for the higher partial waves.

The consistency of the experimental cross sections $\sigma$ may be checked by applying the sum rule based on a forward dispersion relation (Bransden and McDowell 1969)

$$a + f_B = -\frac{1}{2\pi} \int_0^\infty \sigma(k) \, dk$$

(18)

where $a$ is the scattering length and $f_B$ is the Born approximation for the direct elastic amplitude in the forward direction ($f_B = -0.791$, see Bransden and McDowell 1969). The left-hand side of equation (18) would become $-1.242$ with $a = -0.451$ of model HF2 employed. The right-hand side has been calculated by Bransden and Hutt (1975) and is equal to $-1.24 \pm 0.05$ in which the cross sections of Canter et al. (1973) and Coleman et al. (1975a) were used. The agreement suggests that our results are consistent with experiments.

The S-wave contribution to the effective charge $Z_{\text{eff}}$ is shown in figures 3 and 4. In figure 3, we present the results of four helium models with $N = 84$. In addition, we also estimate the contributions from undistorted higher partial waves, i.e.

$$Z_{\text{eff}}(l > 0) = 2 - 2 \int \psi_{\text{HF}}^2(r_1, r_2) \left( \frac{\sin kr_1}{kr_1} \right)^2 \, dr_1 \, dr_2.$$  

(19)

It is noted that this estimated contribution is less than 30% for the highest energy we considered. In particular, the result of model HF2 is shown in figure 3, curve D. In figure 4, we compare our results (HF2) with other theoretical calculations and with experiments. The agreement with Roellig and Kelly (1967 private communication, see Fraser 1968) and Coleman et al. (1975a,b) is quite good.
The energy-dependent cusp values have been calculated for the four helium models. There is no bound or variational principle for $v_{1p}$ (or indeed $Z_{\text{eff}}$) in this calculation. For model HF2 at $N = 84$, $v_{1p}$ ranges from $-0.435\ a_0^{-1}$ to $-0.478\ a_0^{-1}$ (we recall the exact value is $-0.5\ a_0^{-1}$), with the former value corresponding to the zero-energy result. This may indicate that for zero energy, dipole-type correlation terms may improve the performance (e.g. Humberston 1973).

The probability $P_n$ that the residual He$^+$ ion will be in a state $n$ after annihilation has been calculated using equation (16). It is found that the $P_n$ are nearly energy independent (for the energy region we considered here) and approximately 98% of the He$^+$ ions are in the 1S state for model HF2. Moreover, for model HY2, we found that the total probability for a 2P–1S transition after annihilation, in which cascade processes like 5S–4P–3S–2P are included, is about 0.48% compared with 1.2% found by Drachman (1966b) using the same helium model.

5. Related results

Other than the method-of-models calculation, we have also examined different variants of Kohn's variational method which have been investigated by Peterkop and Rabik (1971). If we write the operator $(H - E)$ as

$$H - E = -\nabla_p^2 - \frac{2}{r_{1p}} - \frac{2}{r_{2p}} + \frac{4}{r_p} + C\left(-\nabla_1^2 - \nabla_2^2 + \frac{2}{r_{12}} - \frac{4}{r_1} - \frac{4}{r_2} - E_{\text{He}}\right) - k^2$$

† Complete convergence behaviours of $Z_{\text{eff}}$, $v_{1p}$, and $P_n$ for the four helium models for the energy range considered here have been given by Ho (1975). The results are available upon request.
and characterize equations (5) as
\[
\langle \psi | H - E | \psi F \rangle + \langle \psi | H - E | \sum C_i | \chi_i \rangle = (\text{open-open}) + (\text{open-closed}) = 0
\]
\[
\langle \chi | H - E | \psi F \rangle + \langle \chi | H - E | \sum C_i | \chi_i \rangle = (\text{open-closed}) + (\text{closed-closed}) = 0
\]
we may describe the different variants as follows

**Variant I:** \( C = 1, E_{\text{He}} = E_{\text{av}} \) in (open-closed) and (closed-closed)

**Variant II:** \( C = 0, E_{\text{He}} = E_{\text{av}} \) in (open-closed); \( C = 1, E_{\text{He}} = E_{\text{av}} \) in (closed-closed)

**Variant III:** \( C = 1, E_{\text{He}} = E_{\text{av}} \) in (open-closed) and (closed-closed)

**Variant IV:** \( C = 0, E_{\text{He}} = E_{\text{ex}} \) in (open-closed); \( C = 1, E_{\text{He}} = E_{\text{ex}} \) in (closed-closed).

For the (open-open) terms, \( C = 1 \) and \( E_{\text{He}} = E_{\text{av}} \) is applied to all variants so that the integral exists. \( E_{\text{av}} \) and \( E_{\text{ex}} \) are the variational average energy and the exact energy (Pekeris 1959) of the helium atom respectively.

It should be mentioned that the bound theorem does not apply to these variants, hence it may not be useful to optimize the non-linear parameters. Consequently, we used the same set of non-linear parameters as those which gave optimized values in the method-of-models calculations. It has been found that singularities exist for variant I and III with variant III worst among these variants. The singularity appears earlier than in variant I as \( N \) increases. For simplicity, we only show the convergence behaviour of variant II and IV in table 4 for zero energy. It is also of interest to note that the scattering lengths (phasshifts) from variants II and IV are higher (lower) than those from the corresponding model in the method-of-models calculation.

**Table 4.** Scattering lengths from variants II and IV (Peterkop and Rabik 1971) for different models.

<table>
<thead>
<tr>
<th>Models</th>
<th>( N )</th>
<th>4</th>
<th>10</th>
<th>20</th>
<th>35</th>
<th>56</th>
<th>84</th>
</tr>
</thead>
<tbody>
<tr>
<td>HY1</td>
<td>II</td>
<td>-0.1767</td>
<td>-0.3008</td>
<td>-0.3247</td>
<td>-0.3480</td>
<td>-0.3623</td>
<td>-0.3726</td>
</tr>
<tr>
<td></td>
<td>IV</td>
<td>-0.0852</td>
<td>-0.2443</td>
<td>-0.2915</td>
<td>-0.3201</td>
<td>-0.3329</td>
<td>-0.3435</td>
</tr>
<tr>
<td>HY2</td>
<td>II</td>
<td>-0.2822</td>
<td>-0.3359</td>
<td>-0.3942</td>
<td>-0.4159</td>
<td>-0.4299</td>
<td>-0.4406</td>
</tr>
<tr>
<td></td>
<td>IV</td>
<td>-0.1658</td>
<td>-0.2800</td>
<td>-0.3432</td>
<td>-0.3699</td>
<td>-0.3829</td>
<td>-0.3944</td>
</tr>
<tr>
<td>HF1</td>
<td>II</td>
<td>-0.1372</td>
<td>-0.3163</td>
<td>-0.3756</td>
<td>-0.4080</td>
<td>-0.4249</td>
<td>-0.4333</td>
</tr>
<tr>
<td></td>
<td>IV</td>
<td>-0.1103</td>
<td>-0.2881</td>
<td>-0.3443</td>
<td>-0.3761</td>
<td>-0.3910</td>
<td>-0.4006</td>
</tr>
<tr>
<td>HF2</td>
<td>II</td>
<td>-0.2039</td>
<td>-0.3203</td>
<td>-0.3868</td>
<td>-0.4177</td>
<td>-0.4144</td>
<td>-0.4201</td>
</tr>
<tr>
<td></td>
<td>IV</td>
<td>-0.1737</td>
<td>-0.2900</td>
<td>-0.3534</td>
<td>-0.3789</td>
<td>-0.3922</td>
<td>-0.4074</td>
</tr>
</tbody>
</table>

For the final result of this work, we prefer the results from the method-of-models calculation, since by taking the advantage of the bound property we are able to improve the results systematically. However, judging from the good convergence behaviour of variant IV, we suggest that in calculations on electron–atom scattering where the method of models no longer applies, variant IV type calculations may be worth trying. Also in the \( e^+–\text{He} \) problem it is of interest to see how these variants behave when we use more elaborate helium wavefunctions. Page (1975, 1976a,b) has presented scattering length and phasshift results using a Kohn method with variants

\[ \dagger \] For non-zero energies, the complete convergence behaviour has been calculated by Ho (1975). The results are available upon request.
I and II with more elaborate He models. After all, all four variants and the method of models should lead to the same result as the target wavefunction approaches exactness.

In evaluating the matrix elements $H_{ij}$ for the four variants, we have to employ the true Hamiltonian of the positron–helium system. The eigenvalues of this true Hamiltonian in the $\chi_i$ basis for one set of non-linear parameters ($\alpha = 1.212$, $\beta = 1.6875$, $\gamma = 0.55$) is worth mentioning. The lowest ten eigenvalues which were calculated on increasing the basis by steps of two are shown in figure 5. The fifth eigenvalue seems to be stable in the region of $n = 38$ to 52. Furthermore, it is taken over by the sixth eigenvalue in the region $n = 58$ to 80. In the context of the stabilization method (Hazi and Taylor 1970) this corresponds to a resonance in the $e^+–$He system. If we consider the midpoint of the stabilized region to be the stabilized eigenvalue $E_s$, we have $E_s = -4.3099$ and the resonance position would be $E_s - E_{He} \approx 20.375$ eV. This suggested resonance is located in a region above the positronium formation threshold and just below the first singlet excitation of the helium atom at 20.6 eV. This possible resonance still must be confirmed. Nevertheless, this calculation may provide some reference for future investigation, both experimental and theoretical.

6. Conclusion and discussion

We have performed a bound calculation of S-wave positron–helium scattering based on the correlation method and the method of models. We consider the results from model HF2 (a three-parameter Hartree–Fock-type wavefunction with the correct polarizability) to be the best of the set. Since our phaseshifts do differ from those of Humberston (1973), this may suggest that a more definitive result could be obtained if a bound calculation were performed employing a more accurate helium function.
One stabilized eigenvalue has been observed by examining the eigenvalues of the true Hamiltonian of the e\(^+\)-He system. The possible resonance hence suggested at 20.375 eV deserves future investigation.

Acknowledgments

One of us (YKH) gratefully acknowledges his support through a National Research Council of Canada Scholarship.

The research has been supported by grants from the National Research Council of Canada.

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