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Research Article

Hybrid Theory of Scattering of Positrons from Helium Atoms

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Abstract. Hybrid theory of L-wave scattering of positrons from helium atoms is developed. Phase shifts are calculated for the incident positron momentum from 0.1 to 1.2 for $L = 0,1,2,3$ before the onset of excitation, and positronium formation. The phase shifts are compared with phase shifts obtained by Drachman, and by Campeanu and Humberston.

Keywords. Positrons, Scattering, Hybrid theory

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1. Introduction

Scattering of electrons and positrons from hydrogenic systems are important because the target wave functions are known exactly. This helps to judge the importance of various formulations. We formulated a hybrid theory of one-electron systems earlier (Bhatia [3]) to calculate phase shifts of scattering of electrons from hydrogen atoms. We applied the same approach to the scattering of electrons from He^+ and Li^{2+} (Bhatia [1]). This formulation included short-range, and long-range correlations at the same time. It is variationally correct, that is, the calculated phase shifts approach the correct phase shifts as the number of bases is increased. In addition to scattering, photoabsorption and recombination cross sections of two-electrons systems were also calculated (Bhatia [2]). Phase shifts and cross sections agreed with those obtained using the close-coupling and the R-matrix formulations, which are known to provide very accurate results. The curves for the photoionization of the helium atom obtained using the hybrid theory and

R-matrix approach overlapped. We applied the hybrid theory to positron-hydrogen scattering, annihilation, and positronium formation (Bhatia [4]), requiring fewer terms than used in previous calculations.

The hybrid theory is based on the method of polarized orbitals (Temkin [7]). In the present approach, we use the closed-shell wave function because this provides a simple orbital for each target electron. A correlated wave function for the target does not provide orbital for each electron to be usable in the method of polarized orbitals (Temkin [7]). The closed-shell wave function of the target is given by $\phi(r_2)\phi(r_3)$, where

$$\phi(r_2) = \sqrt{\frac{z^3}{\pi}} e^{-zr_2}, \tag{1.1}$$

$$\phi(r_3) = \sqrt{\frac{z^3}{\pi}} e^{-zr_3}. \tag{1.2}$$

In equations (1.1) and (1.2), r_2 and r_3 represent the target electrons coordinates and $z = 2-5/16$, 2 being the charge of He. The distorted orbit is given by

$$\phi^{pol}(r_1;r_2,r_3) = \left[\phi(r_2) + \frac{u_{1s\to p}(r_2)}{r_2}\cos(\theta_{12})/\sqrt{\pi z + (2\to 3)}\right], \tag{1.3}$$

$$u_{1s\to p}(r) = e^{-zr_2}(0.5zr^3 + r^2). \tag{1.4}$$

The total scattering wave function is given by

$$\psi(\vec{r}_1;r_2,r_3) = u(\vec{r}_1)\phi^{pol}(r_1;r_2,r_3), \tag{1.5}$$

where

$$u(\vec{r}_1) = \frac{u(r_1)}{r_1} Y_{L0}(\Omega_1), \tag{1.6}$$

Y_{L0} is the spherical harmonic of angles Ω_1, and r_1 represents the incident positron.

The scattering function $u(r_1)$ is determined by using the functional

$$\iiint d\Omega_1 d\vec{r}_2 d\vec{r}_3 \phi^{pol}(r_1;r_2,r_3)|H-E|\psi(\vec{r}_1;r_2,r_3) = 0. \tag{1.7}$$

It is important to use $\phi^{pol}(r_1;r_2,r_3)$ on the left rather than $\phi(r_2)\phi(r_3)$ in order to obtain variationally correct phase shifts.

2. Results

Drachman [6] calculated phase shifts using a closed- shell wave for the helium atom. However, it does not give the experimentally determined polarizability $\alpha = 1.376a_0^3$ of the helium atom. He multiplied the $1/r_1^4$ term by 1.2463 to get the correct polarizability, with the result that there is no variational bound on the phase shifts anymore. He obtained phase shift = 0.0385 radians for $k = 0.1$, whereas we have obtained 0.0541 radians for $k = 0.1$. We use Rydberg units: energy is in Rydberg units and the length is in terms of the Bohr radius. He has given results in figures. It is difficult to get accurate values from these figures. We give in Table 1 phase shifts obtained using the hybrid theory and compare them with those obtained by Campeau and Humberston [5]. They have used three correlated helium atom wave functions, getting phase shifts 0.037, 0.031, and 0.0032 radians for $k = 0.1$, a wide variation in values.

Table 1. A comparison of the present phase shifts (radians) for S-wave scattering with those obtained in reference [5]

K	Present phase shifts	Phase shifts [5]
0.0	-0.1271^a	−0.524
0.1	0.05409	0.037
0.2	0.07412	0.051
0.3	0.07061	0.044
0.4	0.05214	0.027
0.5	0.02448	0.001
0.55	0.00843	
0.58	−0.00168	
0.6	−0.08602	−0.031
0.7	−0.04464	−0.066
0.8	−0.08205	−0.098
0.9	−0.11979	−0.133
1.0	−0.15714	−0.167
1.1	−0.19362	
1.2	−0.22899	

^{a} : $k = 0$ represents the scattering length

We have calculated phase shifts for an incident momentum below the onset of excitation and positronium formation. Scattering length is given by

$$k\cot(\eta) = -\frac{1}{a}, \tag{2.1}$$

where η is the phase shift and a is the scattering length. At $R = 225.9562$ for $k = 0.0001$, $\eta = 7.28254 \times 10^{-5}$ radians. Eq. (2.1) gives $a = 0.1271$. However, there is a correction due to the long-polarization potential (Temkin [8]) given by

$$a = a(R) - \alpha\left(\frac{1}{R} - \frac{a}{R^2} + \frac{a^2}{3R^3}\right). \tag{2.2}$$

This does not change the scattering length significantly. The calculated value of a given in Table 1 does not agree with that given by Campeanu and Humberston [5].

In Table 2, we give phase shifts for higher partial waves, $L = 1, 2$, and 3. We find that phase shifts are not very sensitive to the increase of L. There are no results available for comparison for higher partial waves.

Phase shifts for higher partial waves can be obtained from

$$\eta = \frac{\pi\alpha k^2}{(2L-1)(2L+1)(2L+3)}. \tag{2.3}$$

Table 2. Phase shifts (radians) for higher partial waves

K	$L=1$	$L=2$	$L=3$
0.1	0.05379	0.05320	0.05233
0.2	0.07359	0.07253	0.07096
0.3	0.06990	0.06849	0.06639
0.4	0.05129	0.04961	0.04710
0.5	0.02353	0.02163	0.01881
0.6	−0.00963	−0.01169	−0.01476
0.7	−0.04574	−0.04792	−0.05119
0.8	−0.08320	−0.08548	−0.08890
0.9	−0.12197	−0.12333	−0.01269
1.0	−0.15835	−0.16079	−0.01644
1.1	−0.19485	−0.19729	−0.20095
1.2	−0.23017	−0.23263	−0.23631

3. Conclusions

We have developed a hybrid theory for the scattering of positrons from helium atoms. We have not included the short-range correlations because this requires three-particle integrals, calculations of eigenvalues and eigenvectors. This might result not in a very significant increase in the calculated phase shifts, despite of lot of work. Despite the absence of short-range correlations, phase shifts continue to have a variational bound, that is they are always below the exact phase shifts. However, there is a need for another calculation providing definitive results for all partial waves because only Drachman's calculations give results for higher partial waves, which are given in figures only.

Competing Interests

The author declares that he has no competing interests.

Authors' Contributions

The author wrote, read and approved the final manuscript.

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