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Electron-He$^+$ *P*-wave elastic scattering and photoabsorption in two-electron systems

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In a previous paper [A. K. Bhatia, Phys. Rev. A **69**, 032714 (2004)], electron-hydrogen *P*-wave scattering phase shifts were calculated using the optical potential approach based on the Feshbach projection operator formalism. This method is now extended to the singlet and triplet electron-He$^+$ *P*-wave scattering in the elastic region. Phase shifts are calculated using Hylleraas-type correlation functions with up to 220 terms. Results are rigorous lower bounds to the exact phase shifts, and they are compared to phase shifts obtained from the method of polarized orbitals and close-coupling calculations. The continuum functions calculated here are used to calculate photoabsorption cross sections. Photoionization cross sections of He and photodetachment cross sections of H$^-$ are calculated in the elastic region—i.e., leaving He$^+$ and H in their respective ground states—and compared with previous calculations. Radiative attachment rates are also calculated.

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INTRODUCTION

Benchmark results are useful to compare results obtained using different approaches. For this reason, scattering by single-electron systems is always of interest because the wave function of the target is known exactly. Various approximations have been employed to take into account distortion produced in the target. Among them are the method of polarized orbitals [1], perturbation theory [2], the pseudostate close-coupling method [3], and the Harris-Nesbet method [4]. Recently, electron-hydrogen (*e*-H) and electron-He$^+$ (*e*-He$^+$) scattering in the elastic region have been studied [5–7] using the Feshbach projection operator formalism [8]. In this approach, the usual Hartree-Fock and exchange potentials are augmented by an optical potential and the resulting phase shifts, being lower bounds, are in general agreement with those of Schwartz [9], Armstead [10], and close-coupling results [11]. Now this optical potential approach is being applied to the *e*-He$^+$ system to obtain accurate results in the elastic region for *P*-wave scattering. The optical potential is constructed using Hylleraas-type correlations with up to 220 terms. The present results are rigorous lower bounds on the phase shifts, provided the total energy of the system is less than all the resonance positions [12].

In the study of resonances, electron impact of He$^+$ and photoionization of helium atoms continuum functions are required [13]. The optical potential approach has been employed to calculate such functions by a number of authors (cf., e.g., Ref. [14] for H$^-$). Similarly, the *R*-matrix approach has been used to calculate such functions [15,16]. The region of interest in the present paper is the elastic region. The present approach can be generalized to the inelastic region provided appropriate projection operators are used to project out all the lower hydrogenic states.

The total spatial function for the *e*-He$^+$ for the *L*th partial wave is written as

$$\Psi_L(\mathbf{r}_1,\mathbf{r}_2)=\frac{u_L(r_1)}{r_1}Y_{L0}(\hat{r}_1)\phi_{10}(\mathbf{r}_2)\pm(1\leftrightarrow 2)+\Phi_L(\mathbf{r}_1,\mathbf{r}_2), \tag{1}$$

where the target function is given by

$$\phi_{10}(\mathbf{r}_2)=\sqrt{\frac{Z^3}{\pi}}\exp(-Zr_2). \tag{2}$$

The upper and lower signs correspond to singlet and triplet states, respectively. The first two terms containing u_L explicitly give rise to the exchange approximation, and the function Φ_L is the correlation function. For arbitrary L this function is most efficiently written in terms of symmetric Euler angles [17]:

$$\Phi_L=\sum_{\kappa}[f_L^{\kappa,+1}(r_1,r_2,r_{12})\mathcal{D}_L^{\kappa,+1}(\theta,\phi,\psi)+f_L^{\kappa,-1}(r_1,r_2,r_{12})\mathcal{D}_L^{\kappa,-1}(\theta,\phi,\psi)]. \tag{3}$$

The $\mathcal{D}^{\kappa,\epsilon}$ ($\epsilon=+1,-1$) are the modified spherical harmonics which depend upon the Euler angles [17]. The *f*'s above are radial functions, which depend on the three residual coordinates r_1, r_2, and r_{12}. The wave function of the scattered electron is determined by

$$\int[\phi_{10}^*(\mathbf{r}_2)(H-E)\Psi_L]d\mathbf{r}_2=0, \tag{4}$$

where H is the Hamiltonian and E is the total energy of (*e*-He$^+$). We have, in Rydberg units,

$$H=-\nabla_1^2-\nabla_2^2-\frac{2Z}{r_1}-\frac{2Z}{r_2}+\frac{2}{r_{12}} \tag{5}$$

and

$$E=k^2-Z^2, \tag{6}$$

where k^2 is the kinetic energy of the incident electron and Z is the nuclear charge which is equal to 2 in the present calculation. Carrying out the integration leads to an integro-differential equation for the scattering function $u_L(r_1)$ and letting $r_1=r$,

TABLE I. Convergence [the phase shifts (in radians) have been optimized with respect to γ and δ for each $N(\omega)$] of the P-wave phase shift as a function of $N(\omega)$ for $k=0.8$.

^1P				^3P			
$N(\omega)$	γ	δ	$\eta^{(+)}$	$N(\omega)$	γ	δ	$\eta^{(-)}$
EA[a]			−0.079 627	EA[a]			0.205 41
4(1)	1.60	1.60	−0.045 082	4(1)	1.60	1.97	0.234 33
10(2)	1.16	1.55	−0.043 302	10(2)	1.10	1.87	0.236 33
20(3)	1.34	1.80	−0.042 807	20(3)	1.10	2.07	0.236 82
35(4)	1.60	1.90	−0.042 662	35(4)	1.10	1.57	0.237 27
56(5)	1.40	1.40	−0.042 503	56(5)	1.10	1.57	0.237 31
84(6)	1.40	1.40	−0.042 448	84(6)	1.10	1.57	0.237 39
120(7)	1.40	1.40	−0.042 423	120(7)	1.10	1.57	0.237 41
165(8)	1.40	1.40	−0.042 389	165(8)	1.10	1.57	0.237 43
220(9)	1.40	1.40	−0.042 383	220(9)	1.10	1.57	0.237 44

[a] EA are the well-known exchange approximation phase shifts [18]; they correspond to no correlation terms [$N(\omega)=0 \rightarrow \mathcal{V}_{op}=0$ in Eq. (7)].

$$\left[-\frac{d^2}{dr^2}-\frac{L(L+1)}{r^2}+V_d \pm V_{ex}+\mathcal{V}_{op}-k^2\right]u_L=0, \qquad (7)$$

where V_d and V_{ex} are the well-known direct and exchange potentials of the "exchange approximation" [18]. The latter are nonlocal potentials. The optical potential acting on $u_L(r)$ is

$$\mathcal{V}_{op}u_L = r\left\langle Y_{L0}^{*}PHQ\frac{1}{E-QHQ}QHP\Psi_L\right\rangle. \qquad (8)$$

The details are given in [7] and are not repeated here. The integro-differential Eq. (7) is solved noniteratively. The solution is unique (up to an arbitrary normalization) with asymptotic form

$$\lim_{r\to\infty} u_L(r) \propto \sin\left[kr - L\frac{\pi}{2}+\frac{Z-1}{k}\ln(2kr) + \arg\Gamma\left(L+1-\frac{i(Z-1)}{k}\right)+\eta\right]. \qquad (9)$$

Since the Coulomb field extends very far, Eq. (7) has to be integrated to large distance especially for small values of k. From $u_L(r)$ and its derivative the phase shift η, deviation from the pure Coulomb field of $(Z-1)$ is readily extracted, provided higher terms in the asymptotic expansion of Coulomb functions F_1 and G_1 [19] are retained in the scattering function $u_L(r)$:

$$u_L(r) = A[F_1(r)+\tan(\eta)G_1(r)], \qquad (10)$$

where F_1 is the regular Coulomb wave function, G_1 is the irregular Coulomb wave function, and η is the required phase shift for the Lth partial wave. Examples demonstrating the convergence of η for $k=0.8$ as a function of N_ω are given in Table I. By virtue of the fact that η's are rigorous lower bounds on the phase shift [12], the convergence then becomes a good indication of the accuracy of the result. The number of terms for a particular ω is also indicated in Table I for ^1P as well as ^3P in the expansion given in Eq. (15) of Ref. [7]. It should be noticed that phase shifts always increase as the number of terms increases in the optical potential. In the singlet case, the exchange approximation results are negative and there is a lot of cancellation with the contribution to the phase shifts from the optical potential, unlike in the triplet case where the exchange approximation results are always positive. Phase shifts as a function of k are given in Tables II and III for ^1P and ^3P, respectively.

In the S-wave scattering [5], the phase shift converged when the maximum number of terms in the wave function was 84. The P-wave phase shifts are found to converge slowly compared to the S-wave results [5]. Therefore, the computation has to be carried up to 220 terms. In principle,

TABLE II. Phase shifts of ^1P for various k for $N=220$.

k	γ	δ	η	η(PO)[a]	η(Oza)[a]	η(Gien)[c]
0.1	1.10	1.90	−0.038 311		−0.039 38	
0.2	1.10	1.90	−0.038 958	−0.0404	−0.040 02	−0.0407
0.3	1.20	1.60	−0.039 911		−0.040 95	
0.4	1.30	1.70	−0.040 971	−0.0428	−0.043 04	−0.0428
0.5	1.40	1.80	−0.041 951		−0.042 03	
0.6	1.40	1.80	−0.042 633	−0.0450	−0.043 81	−0.0447
0.7	1.50	1.80	−0.042 834		−0.044 16	
0.8	1.40	1.40	−0.042 383	−0.0457	−0.043 91	−0.0446
0.9	1.75	1.35	−0.041 158		−0.042 89	
1.0	1.80	1.40	−0.039 036	−0.0436	−0.040 98	−0.0414
1.1	1.30	1.60	−0.035 948			
1.2	1.30	1.60	−0.031 838	−0.0384		
1.3	1.50	1.60	−0.026 592			
1.4	1.50	1.50	−0.019 982	−0.0301		

[a] Phase shifts obtained by Sloan [1] using the polarized orbital method.

[b] Close-coupling results of Oza [3].

[c] Harris-Nesbet method, Gien [4].

TABLE III. Phase shifts of ^3P for various k for $N=220$.

k	γ	δ	η	η(PO)[a]	η(Oza)[b]	η(Gien)[c]
0.1	0.85	1.94	0.215 16		0.2148	
0.2	1.00	1.82	0.216 81	0.2232	0.2165	0.217
0.3	1.45	1.85	0.219 44		0.2192	0.219
0.4	1.25	1.80	0.222 83	0.2290	0.2226	0.223
0.5	1.40	1.90	0.226 61		0.2263	
0.6	1.55	1.95	0.230 48	0.2364	0.2302	0.230
0.7	1.60	1.60	0.234 15		0.2337	
0.8	1.10	1.57	0.237 44	0.2429	0.2368	0.237
0.9	1.20	1.60	0.240 08		0.2393	0.240
1.0	1.25	1.50	0.242 02	0.2469	0.2412	0.242
1.1	2.05	1.80	0.243 22			
1.2	1.40	1.65	0.243 78	0.2479		
1.3	1.45	1.65	0.243 70			
1.4	1.88	1.75	0.243 20	0.2317		

[a] Phase shifts obtained by Sloan [1] using the polarized orbital method.

[b] Close-coupling results of Oza [3].

[c] Harris-Nesbet method, Gien [4].

the number of terms can be increased further but then too much computer time is required. The convergence of the results suggests that they are accurate to one or two units in the fourth significant place after the decimal point, and we have given five significant digits because to that accuracy they are rigorous lower bounds. The phase shifts are compared to the polarized orbital results of Sloan [1], the pseudostate close-coupling results of Oza [3], and the results of Gien obtained using the Harris-Nesbet method [4]. In general, the agreement is good. The presently calculated phase shifts are higher than most of the results obtained in various calculations. It should be noted that the phase shifts decrease as a function of k up to $k=0.8$ and then they increase up to $k=1.4$ for the singlet case while the phase shifts for the triplet case increase continuously as a function of k up to $k=1.4$. This behavior indicates the importance of spatial correlations in the singlet case and of less importance in the triplet case where the spatial function is antisymmetric. The phase shifts obtained by Sloan [1], including the exchange polarization terms, are also given in Tables II and III for ^1P and ^3P, respectively. The polarized orbital method does not provide any bound on the phase shifts but they are seen to contain the dominant part of the correlation enhancement over the exchange approximation (cf. Tables II and III). The results given by Gien [4] are only up to three decimal places and therefore are not as accurate as calculated presently.

The effects of polarization and other long-range potentials could be significant. Since such terms are not included in the calculation, no attempt has been made to extrapolate the calculated results. Moreover, the inclusion of such effects in any approximate manner results in a loss of the bound property, an important feature of this calculation.

The problem to calculate phase shifts is not a new one, but it is expected that the present results, because of their accuracy and the rigorous lower bounds, will be useful to test other theoretical methods for scattering problems.

PHOTOABSORPTION IN He AND H$^-$

Photoionization and photodetachment cross sections are useful in many ways: They are required to calculate rediative attachment cross sections, to probe the electron interactions with the atomic structure, and to study reactions in upper atmosphere and planetary nebulae. Atomic He is of interest due to its high relative abundance in astrophysical plasmas.

In the above calculation, continuum functions for the scattering of electrons from He$^+$ have been calculated while calculating the phase shifts for $L=1$, and improvements have been obtained over the exchange approximation results. These functions can be used now to calculate photionization cross sections. The cross sections (in length form and in units of a_0^2) for a transition from the initial state i to the final state f are given by

$$\sigma = 4\pi\alpha k\omega|\langle\Psi_f|z_1+z_2|\Phi_i\rangle|^2, \tag{11}$$

where α is the fine-structure constant, k is the momentum of the outgoing electron, and ω is the energy of the incident photon:

$$\omega = I + k^2, \tag{12}$$

where I, the ionization potential of the atom, and k^2, the energy of the ejected electron, are in Rydberg units. Φ_i, the ground-state wave function of the (^1S) state of the helium atom, is of the Hylleraas form and is given by

$$\Phi_i = \frac{1}{\sqrt{8\pi^2}}\sum_{lmn}^{N_\omega} C'_{lmn}[e^{-ar_1-br_2}r_1^l r_2^m + (1\leftrightarrow 2)]r_{12}^n. \tag{13}$$

The final-state wave function [20] is given by

$$\Psi_f = P\Psi_L + Q\Psi_L, \tag{14}$$

where (for singlet states)

$$P\Psi_L = \frac{1}{\sqrt{(2)}}\left[\frac{u_L(r_1)}{r_1}Y_{L0}(\hat{r}_1)\phi_{10}(\mathbf{r}_2) + (1\leftrightarrow 2)\right] \tag{15}$$

and

$$Q\Psi_L = \sum_s \frac{Q|\Phi_L^s\rangle\langle Q\Phi_L^s|QHP|P\Psi_L\rangle}{E-\mathcal{E}_s}. \tag{16}$$

Note that the angular part in Ψ_L, Eq. (1), is $Y_{L0}(\hat{r}_1)$ and not $P_L(\hat{r}_1)$. We can write the matrix element in Eq. (11) as

$$\langle\Psi_f|z_1+z_2|\Phi_i\rangle = \langle P\Psi_L|z_1+z_2|\Phi_i\rangle + \langle Q\Psi_L|z_1+z_2|\Phi_i\rangle, \tag{17}$$

where the first term represents the contribution from the exchange approximation and the second term represents the contribution from the closed channels. Most of the contribution to the cross section comes from the first term in the matrix element. The bound-state wave functions for the He ground state have been obtained up to 220 terms. The eigen-

TABLE IV. Convergence of photoionization cross sections (Mb) for the ground state of He with outgoing electron with momentum $k=0.8$.

IMAX[a]	JMAX[b]=84	120	165	220
Exchange	4.5076	4.5079	4.5083	4.5085
4	4.6574	4.6578	4.6582	4.6584
10	4.6711	4.6715	4.6719	4.6721
20	4.6461	4.6465	4.6469	4.6470
35	4.6399	4.6403	4.6407	4.6409
56	4.5147	4.5151	4.5155	4.5157
84	4.4971	4.4975	4.4979	4.4981
E_0^c (Ry)	−5.807 447 809	−5.807 448 501	−5.807 448 659	−5.807 448 723

[a] IMAX is the number of terms in the optical potential.
[b] JMAX is the number of terms in the bound-state wave function.
[c] Ground-state energy of the ^1S state of He.

value for 220 terms is −5.807 448 723 Ry, converged up to at least seven decimal places. The convergence of the photoionization cross section, given in Table IV, with respect to the number terms in the bound-state wave function Φ_i is fairly rapid but not with respect to the number of terms in the optical potential. This is rather surprising because the phase shifts converge fairly rapidly as the number of terms in the optical potential is increased. In spite of electron correlations in the initial and final states, expectations to get definitive results were not borne out. For this reason, results for the cross section are presented in Table V for up to 84 terms in the optical potential, although phase shifts are calculated up to 220 terms. There are a number of calculations on this process but the present results are only compared to the method of polarized orbitals results of Bell and Kingston [21], the close-coupling results of Burke and McVicar [13], and the experimental results of West and Marr [22]. The agreement is good.

It is known that the stellar opacity is due to photoabsorption in the H$^-$ ion. The bound-state wave functions of the ground-state of H$^-$ have been calculated up to 560 terms. The eigenvalue for 560 terms is −1.055 502 029 Ry, converged up to at least seven decimal places. There have been a number of calculations on photodetachment, the oldest among them is due to Chandrasekhar [23]. The detachment cross sections have been calculated by Bell and Kingston [24] by using continuum functions obtained by the method of polarized orbitals and a 70-term wave function for the ground state of H$^-$. A recent calculation is due to Ajmera and Chung [14] who used the Kohn-Feshbach variational method to obtain continuum functions. Phase shifts for e-H were calculated in Ref. [7]. The accompanying continuum functions have been used to calculate the photodetachment of H$^-$, and the cross sections are presented in Table VI. Convergence with respect to the H$^-$ wave functions is very rapid. Again definitive results could not be obtained and the cross sections

TABLE V. Photoionization cross sections (Mb) for the ground state of He with outgoing electron with momentum k.

k	JMAX=120	165	220	Bell and Kingston[a]	Burke and McVicar[b]	West and Marr[c]
0.1	7.844 37	7.842 93	7.842 34	7.560		7.51
0.2	7.652 78	7.651 40	7.650 88	7.386		7.28
0.3	7.163 86	7.162 68	7.162 28	7.083		6.93
0.4	6.788 78	6.787 89	6.787 66	6.685		6.49
0.5	6.262 91	6.262 41	6.262 37	6.220	5.598	5.99
0.6	5.755 89	5.755 79	5.755 89	5.713	5.449	5.46
0.7	5.152 42	5.512 63	5.512 82	5.185	5.103	4.92
0.8	4.497 55	4.497 91	4.498 09	4.651	4.570	4.38
0.9	3.869 22	3.868 77	3.869 69	4.127	4.005	3.87
1.0	3.302 78	3.303 04	3.303 07	3.614	3.511	3.38
1.1	3.051 14	3.051 26	3.051 24	3.152	3.021	2.93
1.2	2.648 82	2.648 83	2.648 78	2.721	2.627	2.52
1.3	2.241 42	2.241 36	2.241 32	2.335	2.293	2.17
1.4	1.928 78	1.928 71	1.928 69	2.002	2.010	1.87

[a] Interpolated, Ref. [20].
[b] Interpolated, Ref. [13].
[c] Interpolated, Ref. [21].

TABLE VI. Photodetachment cross sections (Mb) for the ground state of H$^-$ with outgoing electron with momentum k.

k	JMAX[a]=364	455	560	Bell and Kingston [22]	Ajmera and Chung [14]
0.1	15.400	15.497	15.549	12.34	15.314
0.2	39.411	39.326	39.297	40.48	38.625
0.3	36.639	36.687	36.694	36.40	35.322
0.4	25.296	25.273	25.270	24.47	24.631
0.5	16.473	16.482	16.487	16.43	
0.6	11.601	11.601	11.598	11.29	10.941
0.7	7.587	7.586	7.587		7.690
0.8	6.456	6.457	6.459	5.31	5.838
E_0^b (Ry)	−1.055501996	−1.055502022	−1.055502029		

[a] JMAX is the number of terms in the bound-state wave function.

[b] Ground-state energy of the ^1S state of H$^-$.

are presented for 84 terms in the optical potential and not for a higher number of terms because of the lack of convergence. The present results are compared with those of Bell and Kingston [24] and Ajmera and Chung [14]. The agreement is reasonable. The experimental results of Smith and Burch [25] are between $k=0.12$ and 0.39. Interpolation of their results gives the ratio of the cross sections at $k=0.2$ and $k=0.3$ as 1.086 compared to the calculated value 1.071, in good agreement.

RADIATIVE ATTACHMENT

Along with the dielectronic recombination, the process of radiative attachment of electrons to He$^+$ and H is important in astrophysical plasmas:

$$e(k^2) + \mathrm{He}^+ \rightarrow \mathrm{He} + h\nu, \tag{18}$$

$$e(k^2) + \mathrm{H} \rightarrow \mathrm{H}^- + h\nu. \tag{19}$$

These are the inverse processes of photoabsorption. Knowing the absorption cross section σ, the attachment cross sections σ_a can be obtained by the principle of detailed balance. The radiative attachment rate averaged over the Maxwellian distribution is given by

$$\alpha_{\mathrm{R}} = \langle v\sigma_a\rangle = \sqrt{\frac{2}{\pi}}\frac{1}{[mk_BT_e\ (\mathrm{K})]^{1.5}}\frac{g_f}{g_i}\int dE\frac{(I+E)^2}{c^2}\sigma(E) \times \exp[-E/k_BT_e\ (\mathrm{K})], \tag{20}$$

where g_i and g_f are the weight factors in the initial and final states. Here $g_i=4$ and $g_f=2$, k_B is the Boltzmann constant, T_e is in kelvin, and $E=mv^2/2$ is the incident electron energy. In Ry units, $E=k^2$ and α_R is then in the units of cm^3/s. With σ in Mb, given in Tables V and VI, we have

$$\alpha_{\mathrm{R}} = \frac{7.249\times 10^{10}}{(T_e)^{1.5}}\int dk^2(I+k^2)^2\sigma\exp(-k^2/k_BT_e). \tag{21}$$

The integration over k^2 is from zero to infinity. Only the first few energy points contribute to the integrand. Therefore, in spite of the fact that cross sections have not been calculated throughout the energy range, the results given in Table VII for a few electron temperatures should be fairly accurate. The attachment rates for hydrogen are in qualitative agreement with those of Dalgarno and Kingston [26], given in graphic form only. The radiative recombination rates at the temperatures given in the table appear not to be too temperature dependent.

In conclusion, very accurate singlet and triplet P-wave phase shifts have been obtained for scattering of electrons from He$^+$ but photoabsorption cross sections are found to be sensitive to the continuum functions.

TABLE VII. Radiative attachment rates (cm^3/sec) at a few electron temperatures T_e.

T_e	α_R(He)	α_R(H$^-$)
1000	3.63(−15)[a]	3.06(−16)
2000	4.69(−15)	7.45(−16)
5000	6.15(−15)	1.66(−15)
7000	6.45(−15)	1.96(−15)
10000	6.63(−15)	2.20(−15)
12000	6.67(−15)	2.29(−15)
15000	6.69(−15)	2.36(−15)
17000	6.69(−15)	2.38(−15)
20000	6.67(−15)	2.38(−15)
22000	6.65(−15)	2.37(−15)
25000	6.61(−15)	2.34(−15)

[a] $a(b)$ represents $a\times 10^b$.

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