Electron-He$^+$ elastic scattering

A. K. Bhatia

Laboratory for Astronomy and Solar Physics, NASA/Goddard Space Flight Center, Greenbelt, Maryland 20771

In a previous paper [Bhatia and Temkin, Phys. Rev. A **64**, 032709-1 (2001)], electron-hydrogen *S*-wave scattering phase shifts were calculated using the optical potential approach. This method is now extended to the singlet and triplet electron-He$^+$ scattering in the elastic region. Phase shifts are calculated using Hylleraas-type correlation functions with up to 95 terms. Results are rigorous lower bounds to the exact phase shifts.

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] and the close-coupling approximation [2]. Recently, electron-hydrogen (*e*-H) scattering in the elastic region has been studied [3] using the Feshbach projection operator formalism [4]. 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 [5]. Now this method is being applied to the *e*-He$^+$ system. Scattering by ionized helium, as for *e*-H, has been studied in the past using the method of polarized orbitals [6] and the close-coupling approximation [2], providing fairly accurate phase shifts. The optical potential approach is applied to the *e*-He$^+$ system to obtain accurate results in the elastic region for *S*-wave scattering. The optical potential is constructed using Hylleraas-type correlations with up to 95 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 [7].

In the study of resonances and electron-impact excitation of He$^+$, continuum functions are required. The optical potential approach has been employed to calculate such functions by a number of authors (cf., e.g., Refs. [8] and [9]). Similarly, the R-matrix approach has been used to calculate such functions (cf., e.g., Refs. [10] and [11]). The recent measurements [12] of the sum of the cross sections for the electron-impact excitation of He$^+$ of the 2^2S and 2^2P states agree very well with those obtained from the close-coupling and *R*-matrix calculations. In all the above-mentioned calculations and other similar calculations, the continuum functions have been calculated at energies much higher than 1.96 Ry. The region of interest in the present paper is the elastic region and therefore there are no results in the above papers that can be compared with the present calculation. The present approach can be generalized to the inelastic region provided appropriate projection operators are used to project out all the lower hydrogenic states. However, in principle, the calculations mentioned above [8–11] could have been carried out in the elastic region as well but they have not been. Therefore, the present calculation complements the above calculations.

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

$$\Psi_L(\mathbf{r_1},\mathbf{r_2}) = \frac{u_L(r_1)}{r_1} Y_{L0}(\hat{r}_1)\phi_{10}(\mathbf{r_2}) \pm (1\leftrightarrow 2) + \Phi_L(\mathbf{r_1},\mathbf{r_2}).$$

(1)

The upper and lower signs correspond to singlet and triplet scattering, 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 [13]:

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

(2)

The $\mathcal{D}^{\kappa,\epsilon}$ ($\epsilon = +1,-1$) are the modified spherical harmonics which depend upon the Euler angles [13]. 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 defined by

$$\int [\phi_{10}^*(\mathbf{r_2})(H-E)\Psi_L]d\mathbf{r_2} = 0,$$

(3)

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

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

(4)

and

$$E = k^2 - Z^2,$$

(5)

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

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

(6)

V_d and V_{ex} are the well known direct and exchange potentials of the "exchange approximation" [14]. The latter are nonlocal potentials. The optical potential acting on u_L(r) is

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

	^1S			^3S		
$N(\omega)$	$\gamma=\delta$	$\eta^{(+)}$	$N(\omega)$	γ	δ	$\eta^{(-)}$
EA [a]		0.33949	EA [a]			0.85195
3(1)	0.93	0.35964	4(1)	1.45	1.65	0.85833
7(2)	1.61	0.39543	10(2)	1.45	1.60	0.85933
13(3)	1.80	0.39719	20(3)	1.35	1.45	0.86040
22(4)	1.40	0.39810	35(4)	1.35	1.20	0.86060
34(5)	1.60	0.39833	56(5)	1.35	1.20	0.86065
50(6)	1.30	0.39844	84(6)	1.35	1.20	0.86069
70(7)	1.45	0.39855				
95(8)	1.30	0.39857				

[a]EA is the well-known exchange approximation phase shifts [14]; it corresponds to no correlation terms [$N(\omega)=0 \to \mathcal{V}_{op}=0$ in Eq. (6)].

$$\mathcal{V}_{op}u_L = r\left\langle Y_{L0}^* PHQ \frac{1}{E-QHQ} QHP\Psi_L \right\rangle, \qquad (7)$$

In defining the optical potential we have used the Feshbach approach [4], involving projection operators P and Q, which for the hydrogenic (i.e., one-electron) target can be written expicitly [7]

$$P = P_1 + P_2 - P_1P_2, \qquad (8)$$

$$Q = 1 - P, \qquad (9)$$

where the spatial projectors are

$$P_i = e^{-Zr_i}Y_{00}(\hat{r}_i)\rangle\langle e^{-Zr_i}Y_{00}(\hat{r}_i). \qquad (10)$$

Note, P_1 and P_2 commute and are each idempotent, hence the complete P and Q operators are idempotent ($P^2=P$; $Q^2=Q$) and orthogonal ($PQ=0$).

The optical potential is expanded in terms of the eigenspectrum of the QHQ problem,

$$\delta\left(\frac{\langle \Phi_L^* QHQ\Phi_L \rangle}{\langle \Phi_L^* Q\Phi_L \rangle} \right) = 0 \qquad (11)$$

This leads to radial eigenfunctions $\Phi_L^{(s)}$ and eigenvalues $\mathcal{E}_s$. Inserting a complete set of the functions obtained from the above equation into Eq. (7), the optical potential can be written as

$$\mathcal{V}_{op}u_L(r_1)$$

$$= r_1 \sum_s^{N\omega} \frac{\left\langle Y_{L0}^*(\hat{r}_1)\phi_{10}(r_2)\frac{2}{r_{12}}Q\Phi_L^{(s)} \right\rangle\left\langle Q\Phi_L^{(s)}\frac{2}{r_{12}}P\Psi_L \right\rangle}{E-\mathcal{E}_s}, \qquad (12)$$

As stated in the beginning, we calculate here only S-wave (i.e., $L=0$) elastic scattering phase shifts. This means, since $\mathcal{D}_L = $const, that the correlation function Φ_L in Eq. (2) is only

a function of the radial coordinates r_1, r_2, and r_{12}. Here Φ_L is taken of the Hylleraas form

$$\Phi_{L=0} = e^{-\gamma r_1 - \delta r_2}\sum_{lmn}^{N_\omega} C_{lmn}r_1^l r_2^m r_{12}^n \pm (1\leftrightarrow 2), \qquad (13)$$

where the sum includes all triples such that $l+m+n=\omega$ and $\omega=0,1,2, \ldots, 8$. The total number of terms N_ω depends on spin and whether $\gamma=\delta$ or not.

To summarize the calculation: the QHQ problem is solved (for a given γ and δ and N_ω). The result is a set of eigenvalues $\mathcal{E}_s(s=1,2,\ldots,N_\omega)$ and associated eigenfunctions $\Phi^{(s)}$. From them the optical potential, Eq. (12) is constructed, and the integro-differential Equation (6) is solved noniteratively. The solution is unique (up to an arbitrary normalization) with asymptotic form

$$\lim_{r\to\infty} u(r) \propto \sin\left[kr + \frac{Z-1}{k}\ln(2kr) \right.$$

$$\left. + \arg\Gamma\left(1 - \frac{i(Z-1)}{k}\right) + \eta \right]. \qquad (14)$$

From $u(r)$ and its derivative the phase shift η, a deviation from the pure Coulomb field of $(Z-1)$, is readily extracted, provided higher terms in the asymptotic expansion of Coulomb functions F_0 and G_0 [15] are retained in the scattering function $u(r)$:

$$u(r) = A[F_0 + \tan(\eta)G_0], \qquad (15)$$

where F_0 is the regular Coulomb wave function and G_0 is the irregular Coulomb wave function.

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 [7], 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 ^1S as well as ^3S in the

TABLE II. Phase shifts of ^1S for various k for $N=95$.

k	$\gamma=\delta$	η	$\eta_{c.c.}$ [a]	$\eta_{P.O.}$ [b]
0.4	1.20	0.42601		0.4301
0.5	1.90	0.41964	0.4169	
0.6	1.30	0.41278	0.4111	0.4153
0.7	1.50	0.40561	0.4046	
0.8	1.30	0.39857	0.3974	0.3986
0.9	1.50	0.39202	0.3906	
1.0	1.65	0.38634	0.3850	0.3823
1.1	1.70	0.38187	0.3805	
1.2	1.30	0.37899	0.3780	0.3685
1.3	1.30	0.37832	0.3774	
1.4	1.40	0.38560		0.3579

TABLE III. Phase shifts of ^3S for various k for $N=84$.

k	γ	δ	η	$\eta_{c.c.}$ [a]	$\eta_{P.O.}$ [b]
0.4	0.70	1.90	0.91300		0.9235
0.5	1.00	1.70	0.90275	0.9019	
0.6	0.80	1.90	0.89050	0.8910	0.9015
0.7	1.00	2.10	0.87640	0.8777	
0.8	1.45	1.60	0.86069	0.8617	0.8723
0.9	1.70	0.90	0.84356	0.8440	
1.0	1.35	1.80	0.82531	0.8253	0.8371
1.1	1.20	2.10	0.80625	0.8062	
1.2	1.21	2.25	0.78666	0.7868	0.7984
1.3	1.90	1.40	0.76684	0.7672	
1.4	2.10	1.50	0.74697		0.7591

[a]Close-coupling plus correlations phase shifts obtained by Burke and Taylor [2].
[b]Phase shifts obtained by Sloan [6] using the polarized orbital method.

[a]Close-coupling plus correlations phase shifts obtained by Burke and Taylor [2].
[b]Phase shifts obtained by Sloan [6] using the polarized orbital method.

expansion given in Eq. (13). Phase shifts as a function of k are given in Tables II and III for ^1S and ^3S, respectively.

The convergence of the results suggests that they are accurate to one or two units in the fourth place after the decimal point. We have given five digits because to that accuracy they are rigorous lower bounds. The phase shifts are compared to the close-coupling (C.C.) results of Burke and Taylor [2] and polarized orbital (P.O.) results of Sloan [6]. The close-coupling results have been obtained by using $1s$, $2s$, and $2p$ target states and 16 correlation terms of the Hyllerras type. These results given as a function of k^2 have been interpolated to obtain phase shifts as a function of k to compare with the present calculations; all the figures in the interpolated numbers might not be accurately given by the interpolation. Only the $k=1.0$ is a common point. There, the ^1S phase shift is higher than the close-coupling result while the results are the same for ^3S phase shifts. In general, the agreement is good. The presently calculated phase shifts are expected to be higher than the close-coupling results [2] because of the larger number of correlations included but they are found to be only slightly higher in the singlet case and

rather slightly lower in the triplet case, except for $k=0.5$. The difference could be due to the explicit inclusion of $2s$ and $2p$ target functions in the calculation of the scattering functions. It should be noted that the phase shifts decrease as a function of k, but at $k=1.4$ the ^1S phase shift has started rising due to the proximity of the lowest resonance which is above the total energy of the e-He$^+$ system. Since the ^3S resonance lies higher than the ^1S resonance, the phase shift at $k=1.4$ in this case is still decreasing as a function of k. The phase shifts obtained by Sloan [6], including the exchange polarization terms are also given in Tables II and III for ^1S and ^3S, 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. Table I).

The effects of polarization and other long-range potentials are expected to be much less than that in e-H scattering. Since they 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.

[1] A. Temkin and J.C. Lamkin, Phys. Rev. **121**, 788 (1961).
[2] P.G. Burke and A.J. Taylor, Proc. Phys. Soc. London **88**, 549 (1966).
[3] A.K. Bhatia and A. Temkin, Phys. Rev. A **64**, 032709 (2001).
[4] H. Feshbach, Ann. Phys. (N.Y.) **19**, 287 (1962).
[5] C. Schwartz, Phys. Rev. **124**, 1468 (1961).
[6] I.H. Sloan, Proc. R. Soc. London, Ser. A **281**, 151 (1964).
[7] Y. Hahn, T.F. O'Malley, and L. Spruch, Phys. Rev. **128**, 932 (1962).
[8] P.G. Burke and A.J. Taylor, J. Phys. B **2**, 44 (1969).
[9] K. Unnikrishnan, J. Callaway, and D.H. Oza, Phys. Rev. A **43**, 5966 (1991).
[10] W.C. Fon, K. Ratnavalu, K.M. Aggerwal, and K.A. Berrington, J. Phys. B **27**, L803 (1994).
[11] K.W. Meyer and C.H. Greens, Phys. Rev. A **52**, 1334 (1995).
[12] A.C.H. Smith, M.E. Bannister, Y-S. Chung, N. Djuric, G.H. Dunn, A. Neau, D. Popovic, M. Stepanovic, and B. Wallbank, J. Phys. B **34**, L571 (2001).
[13] A.K. Bhatia and A. Temkin, Rev. Mod. Phys. **36**, 1050 (1964).
[14] P.M. Morse and W.P. Allis, Phys. Rev. **44**, 269 (1933).
[15] *Handbook of Mathematical Functions*, Natl. Bur. Stand. (U.S.) Appl. Math. Ser. No. 55, edited by M. Abramowitz, and I.A. Stegun (GPO, Washington, D.C., 1964), p. 540.