Electron-hydrogen *P*-wave elastic scattering

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In previous papers [A. K. Bhatia and A. Temkin, Phys. Rev. A **64**, 032709 (2001); A. K. Bhatia, *ibid.* **66**, 064702 (2002)], electron-hydrogen and electron-He$^+$ *S*-wave scattering phase shifts were calculated using the optical potential approach. This method is now extended to the singlet and triplet electron-hydrogen *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 previous calculations.

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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], Kohn-Feshbach variational method [2], Kohn variational method [3], *R*-matrix method [4], and the finite element method [5]. Recently, electron-hydrogen (*e*-H) and electron-He$^+$ (*e*-He$^+$) scattering in the elastic region has been studied [6,7] 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] and the close-coupling results [10]. Now this optical potential approach is being applied to the *e*-H system to obtain accurate results in the eleastic 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 those of all the resonance positions [11].

In the study of resonances and photodetachment of negative hydrogen ion continuum functions are required. The optical potential approach has been employed to calculate such functions by Ajmera and Chung [12].

The total spatial function for the *e*-H for the *L*th partial wave is written as

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

The upper and lower signs correspond to singlet and triplet scatterings, 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]:

$$\Phi_L = \sum_\kappa [f_L^{\kappa,+1}(r_1,r_2,r_{12})\mathcal{D}_L^{\kappa,+1}(\theta,\phi,\psi) + f_L^{\kappa,-1}(r_2,r_1,r_{12})\mathcal{D}_L^{\kappa,-1}(\theta,\phi,\psi)]. \tag{2}$$

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

$$\int [\phi_{10}^*(\mathbf{r_2})(H-E)\Psi_L]d\mathbf{r}_2 = 0, \tag{3}$$

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

$$H = -\nabla_1^2 - \nabla_2^2 - \frac{2Z}{r_1} - \frac{2Z}{r_2} + \frac{2}{r_{12}} \tag{4}$$

and

$$E = k^2 - Z^2, \tag{5}$$

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

$$\left[-\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + V_d \pm V_{ex} + \mathcal{V}_{op} - k^2\right]u_L = 0. \tag{6}$$

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

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

In defining the optical potential we have used the Feshbach approach [8], involving projection operators P and Q, which for the hydrogenic (i.e., one-electron) target can be written explicitly [11] as

$$P = P_1 + P_2 - P_1P_2, \tag{8}$$

$$Q = 1 - P, \tag{9}$$

where the spatial projectors are

TABLE I. Convergence [the phase shifts (in radians) have been optimized with respect to γ and δ for each $N(\omega)$] of 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]			−0.11537	EA[a]			0.32044
4(1)	0.77	0.75	−0.017394	4(1)	0.85	0.90	0.41331
10(2)	1.03	0.67	−0.011054	10(2)	0.65	0.90	0.42007
20(3)	0.81	0.67	−0.0079118	20(3)	0.65	0.73	0.42274
35(4)	0.70	0.67	−0.0066112	35(4)	0.65	0.81	0.42575
56(5)	0.70	0.66	−0.0059357	56(5)	0.65	0.65	0.42623
84(6)	0.72	0.76	−0.0053672	84(6)	0.73	0.81	0.42686
120(7)	0.72	0.76	−0.0051894	120(7)	0.73	0.81	0.42698
165(8)	0.72	0.76	−0.0049455	165(8)	0.73	0.81	0.42725
220(9)	0.77	0.75	−0.0048524	220(9)	0.73	0.81	0.42730

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

$$P_i = |\sqrt{4Z^3}e^{-Zr_i}Y_{00}(\hat{\mathbf{r}}_i)\rangle\langle\sqrt{4Z^3}e^{-Zr_i}Y_{00}(\hat{\mathbf{r}}_i)| \,. \qquad (10)$$

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 P-wave (i.e., $L=1$) elastic-scattering phase shifts. The correlation functions f_L^{κ} in Eq. (2) are given by

$$f_{L=1}^{\kappa=1}=\cos\frac{\theta_{12}}{2}[f(r_1,r_2,r_{12})\pm\tilde{f}(r_1,r_2,r_{12})] \qquad (13)$$

and

$$f_{L=1}^{\kappa=-1}=\sin\frac{\theta_{12}}{2}[f(r_1,r_2,r_{12})\mp\tilde{f}(r_1,r_2,r_{12})], \qquad (14)$$

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

$$f(r_1,r_2,r_{12})=e^{-\gamma r_1-\delta r_2}r_1\sum_{lmn}^{N_\omega}C_{lmn}r_1^l r_2^m r_{12}^n \qquad (15)$$

and

$$\tilde{f}(r_1,r_2,r_{12})=f(r_2,r_1,r_{12}), \qquad (16)$$

where the sum includes all triples such that $l+m+n=\omega$ and $\omega=0,1,2,\ldots,7,8,9$. The number of terms for each ω is given in Table I. Since the electron with coordinate r_1 has angular momentum equal to one, the minimum power of r_1 should be equal to one in the expansion given in Eq. (15).

To summarize the calculation, the QHQ problem is solved (for a given γ, 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 integrodifferential equation (6) is solved noniteratively. The solution is unique (up to an arbitrary normalization) with asymptotic form

$$\lim_{r\to\infty}u(r)\propto\sin\left(kr-L\frac{\pi}{2}+\eta\right), \qquad (17)$$

where 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 [11], 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). Phase shifts as a function of k are given in Tables II and III for ^1P and ^3P phase shifts, respectively.

In the S-wave scattering, the phase shift converged when the maximum number of terms in the wave function was 84. The P-wave phase shifts are seen to converge slowly compared to the S-wave results. Therefore, the computation has to be carried up to 220 terms. In principle, the number of terms can be increased further but then too much computer

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

k	γ	δ	η	η_{PO}[a]	η_{Kh}[b]	η_{AC}[c]	η_{RM}[d]	η_{FEM}[e]
0.1	0.36	0.78	0.0063083	0.0067	0.006, 0.007[f]	0.005782	0.006	0.006
0.2	0.50	0.72	0.014988	0.0171	0.0146, 0.0147[f]	0.01445	0.015	0.0148
0.3	0.59	0.80	0.016613	0.0210	0.0163, 0.0170[f]	0.01550	0.016	0.0160
0.4	0.52	0.76	0.0099980	0.0163	0.0096, 0.0100[f]	0.00846	0.009	0.0090
0.5	0.66	0.75	−0.00084017	0.0064	−0.0014, −0.0007[f]	−0.00287	−0.002	−0.0020
0.6	0.55	0.80	−0.010359	−0.0039	−0.010, −0.009[f]	−0.013029	−0.012	−0.0117
0.7	0.64	0.70	−0.013483	−0.0100	−0.014, −0.013[f]	−0.017225	−0.016	−0.0149
0.8	0.77	0.75	−0.0048524	−0.0095	−0.005, −0.004[f]	−0.009544		−0.0068

[a] Phase shifts obtained by Sloan [1] using the polarized orbital method.
[b] Kohn variational results obtained by Armstead [3].
[c] Variational results obtained by Ajmera and Chung [2].
[d] *R*-matrix results of Scholz *et al.* [4].
[e] Finite element method results obtained by Beteroa and Shertzer [5].
[f] Extrapolated phase shifts obtained by Armstead [3].

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 polarized orbital results of Sloan [1], the Kohn variational results of Armstead [3], the variational results of Ajmera and Chung [2], *R*-matrix results of Scholz *et al.* [4], and finite element method of Botero and Shertzer [5]. Armstead [3] has also obtained the most probable values for the phase shifts by extrapolating to $\omega=\infty$. These results have also been included in the tables but they appear to be overestimated in some cases. In general, the agreement is good. The presently calculated phase shifts are higher than most of the results obtained in the calculation of the scattering functions. It should be noted that the phase shifts increase as a function of k up to $k=0.3$ and then they decrease up to $k=0.7$ only to increase again for the singlet case while the phase shifts for the triplet case increase continuously as a function of k up to $k=0.8$. This behavior indicates the importance of spatial correlations in the singlet case and 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. Table I).

In the effective-range theory, it is well known that if only short-range potentials are important $k^{2L+1}\cot\eta$ approaches a constant as k goes to zero. In the presence of long-range potentials such as $1/r^4$, $L\geqslant 1$, it is $k^{2L}\cot\eta$ which approaches a constant as k goes to zero. The scattering lengths A^S and A^T for ^1P and ^3P, respectively, have been calculated by O'Malley *et al.* [15] using phase shifts at $k=0.1$ obtained by the method of polarized orbitals. Using the expression

$$\tan\,\eta/k^2=\pi\alpha/15-Ak, \tag{18}$$

where $\alpha=4.5$, the polarizability of the hydrogen atom, they concluded that $A^S=1.6$ and $A^T=-1.3$. If the presently cal-

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

k	γ	δ	η	η_{PO}[a]	η_{Kh}[b]	η_{RM}[c]	η_{FEM}[d]
0.1	0.35	0.80	0.010382	0.0109	0.0101, 0.0114[e]	0.010	0.0100
0.2	0.35	0.95	0.045345[f]	0.0486	0.0448, 0.0450[e]	0.045	0.0452
0.3	0.62	0.75	0.10679	0.1151	0.1059, 0.1063[e]	0.107	0.1067
0.4	0.55	0.80	0.18730	0.2005	0.1866, 0.1872[e]	0.187	0.1873
0.5	0.68	0.76	0.27058	0.2867	0.2700, 0.2705[e]	0.270	0.2708
0.6	0.77	0.86	0.34128	0.3574	0.3405, 0.3412[e]	0.341	0.3417
0.7	0.89	0.89	0.39257	0.4063	0.3918, 0.3927[e]	0.392	0.3933
0.8	0.73	0.81	0.42730	0.4351	0.425, 0.427[e]		0.4283

[a] Phase shifts obtained by Sloan [1] using the polarized orbital method.
[b] Kohn variational results obtained by Armstead [3].
[c] *R*-matrix results of Scholz *et al.* [4].
[d] Finite element method results obtained by Beteroa and Shertzer [5].
[e] Extrapolated phase shifts obtained by Armstead [3].
[f] The number of terms = 165 instead of 220.

TABLE IV. Phase shifts at lower values of k for $N=84$.

k	$\gamma=\delta$	^1P	$\gamma=\delta$	^3P
0.01	0.20	0.000024321	0.20	0.000029089
0.02	0.20	0.00017003	0.25	0.00020833
0.05	0.25	0.0017060	0.25	0.0021818

culated phase shifts given in Tables II and III are used in the above equation, then least-square fits give $A^S=3.37$ and $A^T=-1.3$. It seems that Hylleraas functions assimilate some of the long-range $1/r^4$ potential, especially when the number of terms is as large as 220. However, if the phase shifts at low k, given in Table IV, are also included then very large positive values for A^S and A^T are obtained. Since these phase shifts are less than $\pi\alpha k^2/15$, omitting this term in the above equation again did not give any meaningful results. Increasing the number of terms to 220 from 84 for these low values of k will not change the phase shifts considerably nor the conclusion that the meaningful results for A^S and A^T cannot be obtained. The only recourse is to add a term proportional to $1/r^2$ [9] to the trial function given in Eq. (15) to assimilate the long-range $1/r^4$ potential. This calculation will be taken up sometime in the future.

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.

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