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Hybrid theory of P-wave electron-hydrogen elastic scattering

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We report on a study of electron-hydrogen scattering, using a combination of a modified method of polarized orbitals and the optical potential formalism. The calculation is restricted to P waves in the elastic region, where the correlation functions are of Hylleraas type. It is found that the phase shifts are not significantly affected by the modification of the target function by a method similar to the method of polarized orbitals and, except at the very lowest energies, they are close to the phase shifts calculated earlier by Bhatia [A. K. Bhatia, Phys. Rev. A **69**, 032714 (2004)]. This indicates that the correlation function is general enough to include the target distortion (polarization) in the presence of the incident electron. The important fact is that in the present calculation, to obtain similar results only a 35-term correlation function is needed in the wave function compared to the 220-term wave function required in the above-mentioned previous calculation. Results for the phase shifts, obtained in the present hybrid formalism, are rigorous lower bounds to the exact phase shifts. Accurate values for the effective range parameters are also calculated.

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I. INTRODUCTION

Scattering of electrons by hydrogenic systems is always of interest because the target function is known exactly, allowing us to test the various methods of calculation. At low incident energies, the distortion of the target produced by the incident electron is important. One of the methods used to take into account this distortion is the method of polarized orbitals [1], which includes the effect of polarization and essential physics in the ansatz for the scattering wave function. Various other approximations have been used: Kohn-Feshbach variational method [2], Kohn variational method [3], R-matrix method [4], and the finite-element method [5]. In previous papers [6,7], the P-wave e-H and e-He$^+$ scattering phase shifts were calculated by using the Feshbach projection operator formalism [8]. The results obtained are accurate and are variational lower bounds to the exact phase shifts. However, it has not been possible to take into account in the Feshbach formalism the distortion produced by the incident electron which results in a direct $-1/\mathrm{r}^4$ potential in the scattering equation.

In Ref. [9], the S-wave electron-hydrogen scattering phase shifts were calculated by using a hybrid method in which both long-range potential proportional to $-1/\mathrm{r}^4$ and short-range correlations via an optical potential were included in the scattering equation at the same time. We did not use any projection operators in this calculation [9] but the important property, namely, that the phase shifts are rigorous lower bounds to the exact phase shifts, is retained [10]. We follow the same procedure in the present calculation on P-wave scattering as in Ref. [9]. We use Rydberg units: energy in Rydbergs and length in Bohr radius a_0. The phase shifts, throughout, are in radians.

II. THEORY

The total spatial wave function for the e-H partial wave (denoted by L) problem is written as

$$\Psi_L(\vec{r}_1,\vec{r}_2) = \frac{u_L(r_1)}{r_1} Y_{L0}(\hat{r}_1)\phi_0(\vec{r}_2) \pm (1 \leftrightarrow 2) + \sum_{\lambda}^{N} C_\lambda \Phi_L^\lambda(\vec{r}_1,\vec{r}_2). \tag{1}$$

N is the number of terms in the expansion. The target wave function is given by

$$\phi_0(\vec{r}_2) = (Z^3/\pi)^{0.5} e^{-Zr_2} Y_{00}, \tag{2}$$

where Z is the charge of the nucleus. The $(\pm)$ above refers to singlet (upper sign) or triplet (lower sign) scattering, respectively. Beyond the terms containing u_L explicitly (those are the terms giving rise to the exchange approximation), the functions Φ_L are the correlation functions. These functions include all the many-body effects and the resulting scattering equation is a single-particle equation. For an arbitrary L, this function is most efficiently written in terms of the Euler angles [11]:

$$\Phi_L^\lambda = \big[f_L^{\kappa+}(r_1,r_2,r_{12}) D_L^{\kappa+}(\vartheta,\phi,\psi) + f_L^{\kappa-}(r_1,r_2,r_{12}) D_L^{\kappa-}(\vartheta,\phi,\psi) \big]. \tag{3}$$

The $D^{\kappa,\varepsilon}$ functions ($\varepsilon = +1,-1$) are called *rotational harmonics* [11] and are functions of the Euler angles θ,ϕ,ψ. The f's above are generalized "radial" functions which depend on the three residual coordinates that are required (beyond the Euler angles) to define the two vectors $\mathbf{r}_1$ and $\mathbf{r}_2$. The distance between two electrons is given by $r_{12} = |\vec{r}_1 - \vec{r}_2|$. The radial functions are defined as follows:

$$f_1^{1+} = \cos(\theta_{12}/2)\,[f_\lambda(r_1,r_2,r_{12}) \pm f_\lambda(r_2,r_1,r_{12})]\,, \tag{4}$$

$$f_1^{1-} = \sin(\theta_{12}/2)\,[f_\lambda(r_1,r_2,r_{12}) \mp f_\lambda(r_2,r_1,r_{12})]. \tag{5}$$

θ_{12} is the angle between $\vec{r}_1$ and $\vec{r}_2$, and

$$f_\lambda(r_1,r_2,r_{12}) = \sum_{lmn}^{N} C_{lmn}^\lambda\, r_1^l r_2^m r_{12}^n\, e^{-\gamma r_1 - \delta r_2}. \tag{6}$$

The minimum value of l is equal to 1 while that of m and n is 0. The number of terms in this function is equal to N. The number of eigenvalues is also equal to N, therefore, λ takes the values from 1 to N. First, we derive the wave function of the scattered electron *without the long-range correlations* and it is given implicitly by

$$\int [Y_{10}^{*}(\Omega_1)\phi_0^{*}(\vec{r}_2)(H-E)\Psi_L]d\vec{r}_2 = 0. \tag{7}$$

H is the Hamiltonian and E is the total energy of the e-H scattering system:

$$H = -\nabla_1^2 - \nabla_2^2 - \frac{2Z}{r_1} - \frac{2Z}{r_2} + \frac{2}{r_{12}}, \tag{8}$$

$$E = k^2 - Z^2, \tag{9}$$

where k^2 is the kinetic energy of the incident electron and Z is the nuclear charge which is equal to1 in the present calculation (electron-hydrogen scattering).

In order to derive Eq. (7) for the scattering function $u(r_1) \equiv u_L(r_1)$, the coefficients C_λ must be known. Following the procedure given in Ref. [9], it can be shown that the resulting equation for the scattering function for $u(r)$ is given by

$$\left[\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + V_d \pm V_{\rm ex} - V_{\rm op} + k^2\right]u_L(r) = 0, \tag{10}$$

where

$$V_{\rm op}u_L = 2r\sum_{\lambda=1}^{N}\frac{V_\lambda(r)\langle V_\lambda(r_1)u(r_1)\rangle}{E-\varepsilon_\lambda}, \tag{11}$$

where

$$V_\lambda(r_1) = \left\langle \Phi_L^{(\lambda)}(\vec{r}_1,\vec{r}_2)\middle| H - E|\varphi_0(\vec{r}_2)Y_{10}(\Omega_1)\right\rangle. \tag{12}$$

In Refs. [6,7], the optical potential of the type given in Eq. (11) was derived by using the Feshbach projection operator formalism [8] based on projection operators ***P*** and ***Q***. The present formalism is independent of the projection operators ***P*** and ***Q***.

In the above formalism [6,7], those terms coming from the correlation function are such that they take into account only the short-range correlations and there is no direct long-range potential proportional to $1/r^4$ in the scattering equation satisfied by $u(r)$.

III. OPTICAL POTENTIAL WITH POLARIZATION

This long-range potential is due to the polarization of the target produced in the presence of the incident electron. This can be taken into account by the method of polarized orbitals. Temkin [12] has shown, using the adiabatic approximation in the first-order theory and using the dipole part of the resulting perturbed wave function, that in the presence of the incident electron r_1, the effective target wave function can be written as

$$\Phi^{\rm pol}(\vec{r}_1,\vec{r}_2) = \phi_0(\vec{r}_2) - \frac{\chi_\beta(r_1)}{r_1^2}\frac{u_{1s\to p}(r_2)}{r_2}\frac{\cos(\theta_{12})}{\sqrt{Z\pi}}, \tag{13}$$

where

$$u_{1s\to p}(r_2) = e^{-Zr_2}\left(\frac{Z}{2}r_2^3 + r_2^2\right), \tag{14}$$

and ϑ_{12} is the angle between $\vec{r}_1$ and $\vec{r}_2$. We have replaced the step function $\varepsilon(r_1,r_2)$ used by Temkin [12] by a smooth cutoff function $\chi_\beta(r_1)$ which is of the form

$$\chi_\beta(r_1) = (1 - e^{-\beta r_1})^n, \tag{15}$$

where $n \geqslant 3$. Now the polarization takes place whether the scattered electron is inside or outside the orbital electron. The polarization function given in Eq. (13) is valid throughout the range. This is unlike the step function $\varepsilon(r_1,r_2)$ used by Temkin [12] which ensures that the polarization takes place when the incident electron r_1 is outside the orbital electron r_2. Furthermore, the function in Eq. (15) gives us another nonlinear parameter β, which is a function of k, the incident electron momentum, along with the exponent n. This term guarantees that $\chi_\beta(r_1)/r_1^2 \to 0$ when $r_1 \to 0$ and it also contributes to the short-range correlations in addition to those obtained from the correlation function Φ_L, and therefore, is useful to optimize the results. Now the electron-target wave function can be written as

$$\Psi_L(\vec{r}_1,\vec{r}_2) = \frac{u_L(r_1)}{r_1}Y_{L0}(\Omega_1)\Phi^{\rm pol}(\vec{r}_1,\vec{r}_2) \pm (1 \leftrightarrow 2) + \sum_\lambda C_\lambda\Phi_L^\lambda(\vec{r}_1,\vec{r}_2). \tag{16}$$

We arrive at the same form of the scattering equation as Eq. (10), when we replace $\phi_0(\vec{r}_2)$ by $\Phi^{\rm pol}(\vec{r}_1,\vec{r}_2)$ given in Eq. (13). We further restrict ourselves to $L = 1$ and we can write the final scattering equation in the form

$$\left[D(r)\frac{d^2}{dr^2} + k^2 + \frac{2}{r^2} + V_d + V_d^{\rm pol} \pm\left(V_{\rm ex} + V_{\rm ex}^{\rm pol}\right) - V_{\rm op}^{\rm pol}\right]u(r) = 0. \tag{17}$$

We give below various quantities:

$$D(r) = 1 + \frac{43}{8Z^6}\left[\frac{\chi_\beta(r)}{r^2}\right]^2. \tag{18}$$

The direct potentials are given by

$$V_d = \frac{2(Z-1)}{r} + 2e^{-2Zr}\left(Z + \frac{1}{r}\right), \tag{19}$$

and

$$V_d^{\rm pol} = (x_1 + x_3) + x_2\frac{d}{dr}. \tag{20}$$

We give only x_1 below to show its dependence on the polarizability $\alpha(r)$ of the target

$$x_1 = 2\frac{\chi_\beta(r)}{(Zr)^4}\alpha(r), \tag{21}$$

$$\alpha(r) = \frac{9}{2} - e^{-2Zr}\left[(Zr)^4 + 5(Zr)^3 + 9(Zr)^2 + 9(Zr) + \frac{9}{2}\right]. \tag{22}$$

The quantities x_2 and x_3 are fairly complicated and they are not given here. The exchange terms are given by

$$V_{\mathrm{ex}}u(r) = -\frac{8Z^3}{3}e^{-Zr}\left[\frac{1}{r}\int_0^r dx e^{-Zx}x^2u(x) + r^2\int_r^\infty dx\frac{e^{-Zx}}{x^2}u(x)\right]. \tag{23}$$

The exchange polarization terms are too detailed and are also not given here. The optical potential is now given by

$$V_{\mathrm{op}}^{\mathrm{pol}}u(r) = r\sum_s^N \frac{\langle Y_{10}^*(\Omega_1)\Phi^{\mathrm{pol}}(\vec{r}_1,\vec{r}_2)|H-E|\Psi_0'\rangle}{E-\varepsilon_s}, \tag{24}$$

where Ψ_0' is the wave function Ψ_0 given in Eq. (16) without the correlation term Φ_L. This optical potential includes the effects of polarization. The right-hand side of Eq. (24) has not been given explicitly because it contains a large number of terms.

IV. CALCULATION AND RESULTS

Equation (17) is solved for the continuum function $u(r)$ by the noniterative method of Omidvar [13] and the phase shift η is obtained from the value of the function at a large distance:

$$\lim_{r\to\infty} u_l(r) \propto j_1(kr) - \tan(\eta)n_l(kr), \tag{25}$$

where j_1 and n_1 are the spherical Bessel and Neumann functions, respectively.

In order to obtain phase shifts which can be compared to those obtained by the method of polarized orbitals, we exclude the correlation terms Φ_L in Eq. (1). Also, the present cutoff function χ_β given in Eq. (15), which allows optimization with respect to β to get the best results, is replaced by the cutoff function obtained by Shertzer and Temkin [14]:

$$\chi_{\mathrm{ST}} = 1 - e^{(-2Zr)}\left[\frac{(Zr)^4}{3} + \frac{4(Zr)^3}{3} + 2(Zr)^2 + 2(Zr) + 1\right]. \tag{26}$$

Now the calculation should be similar to that carried out by the method of polarized orbitals. The results obtained by the use of two cutoffs, Eqs. (15) and (26), are not very different. The phase shifts obtained, using this cutoff of Shertzer and Temkin [14], for ^1P and ^3P are given in Table I and compared with those obtained by Sloan [15]. These results include contributions from the exchange polarization terms. The present results have variational bounds, i.e., they are always lower than the exact phase shifts. We see that phase shifts, obtained using the polarized orbital method which is not variational, are always higher than the present ones.

TABLE I. Comparison of phase shifts η without correlations with those obtained in Ref. [15].

	^1P		^3P	
k	Present η	η_{PO}	Present η	η_{PO}
0.1	0.0057	0.0067	0.0094	0.0109
0.2	0.0110	0.0171	0.0384	0.0486
0.3	0.0006	0.0210	0.0867	0.1151
0.4	– 0.0090	0.0163	0.0148	0.2005
0.5	– 0.0295	0.0064	0.2100	0.2867
0.6	– 0.0495	– 0.0039	0.2625	0.3574
0.7	– 0.0646	– 0.0100	0.2999	0.4063
0.8	– 0.0721	– 0.0095	0.3225	0.4351

TABLE II. Convergence of ^1P phase shifts η for $k = 0.1$ with the number of terms.

N	β	γ	δ	η
0	0.47			0.0060892
4	0.27	0.42	0.99	0.0062066
10	0.21	0.30	0.99	0.0063271
20	0.34	0.33	0.84	0.0063444
35	0.34	0.30	0.87	0.0063508

In Table II, we give the convergence of ^1P phase shifts for $k = 0.1$ with increasing number of terms in the correlation function. We use the cutoff function given in Eq. (15). The results have been optimized with respect to the nonlinear parameters β, γ, and δ, with $n = 3$, the optimum value. The nonlinear parameters are also given in the table. We see that we do not need more than 35 terms to get results comparable in accuracy to those obtained in Ref. [6] without the use of the polarization term in the target wave function and using the Feshbach formalism of projection operators, where it is not possible to modify the formulation in such a way as to produce a direct polarization potential proportional to 1/r^4 in the scattering equation.

Gailitis [16] has shown that as the number of terms in the correlation function is increased the optical potential becomes more attractive. Consequently, phase shifts increase as the number of terms is increased. We see from the results given in Table II that this holds true.

In Table III, we give ^1P phase shifts for values of the incident momentum from $k = 0.1$ to 0.8 for 35 terms and compare them with those obtained in Ref. [6] with 220 terms in the correlation function, but without the polarization term. We see that in most cases the results are comparable in accuracy to those obtained previously [6] with longer expansions in the correlation function. This indicates that very long expansions do give fairly accurate results. We also compare the present results with the variational results of Ajmera and Chung [17], R-matrix results of Scholz *et al.* [4], and the finite-element results of Botero and Shertzer [5]. Most of the results are comparable but the results obtained in the calculations [4,5,17] for $k = 0.4$ to 0.8 are rather too low compared to the present results. The phase shifts obtained in the above-mentioned calculations do not have any variational bounds. It should be noted that the phase shifts increase up to $k = 0.3$ and then start decreasing up to $k = 0.7$ and increase again.

In Table IV, we give the convergence of ^3P phase shifts for $k = 0.1$ with the number of terms in the correlation function. Again, we use the cutoff function given in Eq. (15). The results have been optimized with respect to the nonlinear parameters β, γ, and δ, with $n = 3$, the optimum value. We again see that we do not need more than 35 terms to get results comparable in accuracy to those obtained in Ref. [6] without the use of the polarization term in the target wave function and using the Feshbach formalism of projection operators.

TABLE III. Singlet P phase shifts η for various k for $N = 35$.

k	Present η	η_{PQ}[a]	η_{AC}[b]	η_{RM}[c]	η_{FEM}[d]
0.1	0.00635076	0.0063083	0.005782	0.006	0.006
0.2	0.01506556	0.014988	0.01445	0.015	0.0148
0.3	0.01670634	0.016613	0.01550	0.016	0.0160
0.4	0.01015347	0.0099980	0.00846	0.009	0.0090
0.5	–0.00061223	–0.00084017	–0.00287	–0.002	–0.0020
0.6	–0.01009367	–0.010359	–0.013029	–0.012	–0.0117
0.7	–0.01321557	–0.013483	–0.017225	–0.016	–0.0149
0.8	–0.0046818[e]	–0.0048524	–0.009544		–0.0068

[a] Phase shifts obtained using the Feshbach formalism [6].
[b] Variational results of Ajmera and Chung [17].
[c] R-matrix results of Scholz *et al.* [4].
[d] Finite-element method results of Botero and Shertzer [5].
[e] Phase shift for $k = 0.8$ is for 56 terms.

In Table V, we give results of ^3P phase shifts for values of the incident momentum from $k = 0.1$ to 0.8 for 35 terms and compare them with those obtained in Ref. [6] with 220 terms in the correlation function, but without the polarization term. We see that in most cases the results are comparable in accuracy to those obtained previously [6] with longer expansions. This indicates that very long expansions do give fairly accurate results because of completeness in the whole space. We also compare the present results with the Kohn variational results of Armstead [18], R-matrix results of Scholz *et al.* [4], and the finite-element results of Botero and Shertzer [5]. Most of the present results are comparable with the results obtained in Refs. [4,5,18]. It should be noted that the phase shifts for ^3P increase continuously throughout the range from $k = 0.1$ to $k = 0.8$. Although the differences are small, the present $^{1,3}P$ are the *largest* of te lower bound results and therefore are the best.

The results for the phase shifts given in various tables are obtained by optimizing the nonlinear parameters β, γ, and δ, one at a time for $N = 35$. Fairly accurate results have been obtained by carrying out the optimization of the nonlinear parameters only once. However, there is always scope for further improvements of results by repeated variation of these nonlinear parameters, requiring a fair amount of computer time, but then the improvements could be marginal. The whole purpose of the variation of the nonlinear parameters is to obtain the largest value of the phase shift.

The uncertainty in the results can be estimated by looking at the convergence of the results given in Tables II and IV. In the case of the singlet P results, increasing N from 20 to 35, the phase shift changes by six units in the fourth significant figure, while in the triplet case it is by one unit in the fourth significant figure.

TABLE IV. Convergence of triplet P phase shifts η for $k = 0.1$ with the number of terms.

N	β	γ	δ	Phase shift
0	0.45	0.35	0.80	0.0098336
4	0.45	0.35	0.80	0.0099701
10	0.45	0.35	0.85	0.0103265
20	0.45	0.37	0.85	0.0103714
35	0.38	0.30	0.80	0.0103813

The main aim of this paper has been to show that the inclusion of the long-range polarization term speeds up the convergence of the results and very few terms are needed in the correlation function.

V. LOW-ENERGY SCATTERING

It is known [19] that at low energies $L = 1$ scattering, the long-range correlations contribute most to the phase shift:

$$\tan(\eta)/k^2 = \pi\alpha/15 - Ak, \tag{27}$$

so that

$$\tan\left[\eta(k_1)/k_1^2\right] - \tan\left[\eta(k_2)/k_2^2\right] = -A(k_1 - k_2). \tag{28}$$

The first term in Eq. (27) is due to the long-range potential and the second term has contributions from the short-range correlations of which there are contributions from the cross of Φ^{pol} and Φ_L terms. Thus the values of A of the present calculation do not coincide with values obtained in our previous calculation [6] which included only the short-range correlations. Using phase shifts given in Table VI, we find

$$A^{\mathrm{T}} = -1.002 \quad \text{and} \quad A^{\mathrm{S}} = 2.942. \tag{29}$$

TABLE V. Triplet P phase shifts η for various k for $N = 35$.

k	Present η	η_{PQ}[a]	η_{Kh}[b]	η_{RM}[c]	η_{FEM}[d]
0.1	0.01038234[e]	0.010382	0.0101	0.010	0.0100
0.2	0.04536735	0.045345	0.0448	0.045	0.0452
0.3	0.1069312	0.10679	0.1059	0.107	0.1067
0.4	0.1888873	0.18730	0.1866	0.187	0.1873
0.5	0.2709762	0.27058	0.2700	0.270	0.2708
0.6	0.3416749	0.34128	0.3405	0.341	0.3417
0.7	0.3932100	0.39257	0.3918	0.392	0.3933
0.8	0.4277296[e]	0.42730	0.425		0.4283

[a] Phase shifts obtained using the Feshbach formalism [6].
[b] Kohn variational results obtained by Armstead [18].
[c] R-matrix results of Scholz *et al.* [4].
[d] Finite-element method results of Botero and Shertzer [5].
[e] Phase shifts for $k = 0.1$ and 0.8 are for 56 terms.

TABLE VI. Low-energy P-wave phase shifts for $N = 35$ and values of A from the effective range theory.

State	$k_1 = 0.04$	$k_2 = 0.05$	A
^1P	0.001303692	0.001963464	2.942
^3P	0.001564346	0.002469346	–1.002

O'Malley *et al.* [19] obtained $A(\text{triplet}) \approx -1.3$ and $A(\text{singlet}) \approx 1.6$ by fitting the phase shifts of the original polarized orbitals calculation (e-H) of Temkin and Lamkin [20]. But the latter calculation, although of historical importance, did not give precision results. Thus, I believe, the A values obtained in the present calculation are accurate.

VI. CONCLUSIONS

In conclusion, we have applied the hybrid theory, in the presence of an optical potential, in which the long-range and short-range correlations, as in Eq. (16), can be taken into account at the same time. The close-coupling formalism with short-range correlations is like the present formalism, in the sense that the P states give the polarizability of the lower-lying S state of the target. The P-wave phase shifts are much more sensitive to polarization and short-range correlations than S-wave phase shifts [9]. The present results are calculated variationally and therefore have lower bounds to the exact phase shifts. The present results are very close to those obtained in Ref. [6], using the Feshbach projection operator formalism in which it was not possible to define the projection operators $\boldsymbol{P}$ and $\boldsymbol{Q}$ to modify the target function to include the effect of the distortion produced by the incident electron. Moreover, shorter expansions of the order of *only* 35 terms are needed to get results comparable in accuracy to those obtained in Ref. [6] with 220 terms.

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