

# Hybrid theory of electron-hydrogenic systems elastic scattering

A. K. Bhatia

NASA/Goddard Space Flight Center, Greenbelt, Maryland 20771 USA

## Introduction

Accurate electron-hydrogen and electron-hydrogenic cross sections are required to interpret fusion experiments, laboratory plasma physics and properties of the solar and astrophysical plasmas.

The advantage of working with hydrogenic targets is that the wave function is known exactly which allows us to test any new theories on scattering of the simplest three-body systems. The incident electron produces a distortion of the target orbital and various methods have been used to take into account this distortion producing a long-range potential. Among them is the method of polarized orbitals [1]. In spite of the fact that this method includes the essential physics by modifying the target wave function suitably in the presence of the incident electron, the results obtained for the phase shifts do not obey any bound principles. In spite of this shortcoming, this method has been used extensively on electron scattering from atoms [1] and molecules [2].

In spite of singularities in his calculations, Schwartz [3] used the Kohn variational principle to obtain accurate phase shifts for electron-hydrogen scattering. More recently, scattering from hydrogenic systems has been carried out by using the Feshbach projection operator formalism [4]. In these calculations [5, 6, 7], the short-range correlations could be included explicitly by introducing separate correlation functions and then amalgamating them into the scattering equation via an optical potential, thus replacing the many- particle Schrodinger equation with a single-particle equation. The results obtained for the phase shifts are very accurate and they have an important property namely that they have the rigorous lower bounds to the exact phase shifts. That is the exact phase shifts are always higher than the calculated phase shifts. In this way, we obtained accurate *S*-wave and *P*-wave phase shifts for electron-hydrogenic systems. This approach also helps us to get very accurate scattering wave functions for *S* and *P* states in  $\text{He}^+$  ion and H atoms. Very accurate cross sections for photoionization of He and photodetachment cross sections of  $\text{H}^-$  ion were obtained along with radiative

attachment cross sections [8]. A detailed account of these methods and calculations has been given in [9].

In these calculations [5, 6, 7, 8], the short-range correlations could be included explicitly but not the long-range correlations at the same time. In this article, we present an approach which includes the long-range correlations as well as short-range correlations explicitly at the same time [10]. Also, we do not use the projection operator formalism of Feshbach [4]. Let us write the wave function for an angular momentum  $\mathbf{L}$  in the form

$$\Psi_L(\vec{r}_1, \vec{r}_2) = \frac{u_L(r_1)}{r_1} Y_{L0}(\Omega_1) \phi_0(r_2) \pm (1 \leftrightarrow 2) + \sum_{\lambda} C_{\lambda} \Phi^{\lambda}_L(\vec{r}_1, \vec{r}_2). \quad (1)$$

The summation index  $\lambda$  takes values from 1 to the number of terms  $N$  in the wave function  $\Phi$ , the correlation function. The target function is given by

$$\phi(r_2) = \sqrt{\frac{Z^3}{\pi}} e^{-Zr_2}. \quad (2)$$

$Z$  is the nuclear charge of the target. The  $(\pm)$  above in Eq. (1) refers to singlet (upper sign) or triplet (lower sign) scattering, respectively. The first term represents the static approximation. Beyond the first term are the terms giving rise to the exchange approximation [11]. The function  $\Phi_L$  is the correlation function which for arbitrary  $\mathbf{L}$  can be written in terms of symmetric Euler angles [12]:

$$\Phi_L = \sum_{\kappa} [f_L^{\kappa,+1}(r_1, r_2, r_{12}) D_L^{\kappa,+1}(\vartheta, \varphi, \psi) + f_L^{\kappa,-1}(r_1, r_2, r_{12}) D_L^{\kappa,-1}(\vartheta, \varphi, \psi)] \quad (3)$$

The  $\mathbf{D}$  functions have been called *rotational harmonics* and  $\theta$ ,  $\varphi$  and  $\psi$  are the Euler angles. The  $\mathbf{f}$ 's above are the generalized 'radial functions' which depend on the three residual coordinates which are required to define the two vectors  $\mathbf{r}_1$  and  $\mathbf{r}_2$ . The radial functions have to be defined for each angular momentum  $\mathbf{L}$  [12].

The Euler angles under *exchange* are given by

$$\vartheta \rightarrow \pi - \theta, \varphi \rightarrow \pi + \varphi, \Psi \rightarrow 2\pi - \Psi \quad (4)$$

The Hamiltonian in Rydberg units can be written as

$$H = -\nabla_1^2 - \nabla_2^2 - \frac{2Z}{r_1} - \frac{2Z}{r_2} + \frac{2}{r_{12}}, \quad (5)$$

and the total energy is given by  $E = k^2 - Z^2$ , where  $k^2$  is the kinetic energy of the incident electron.

Taking  $N=1$ , for illustration, calculate the functional (arising in the Kohn variational principle)

$$I = \langle \psi_L(\mathbf{r}_1, \mathbf{r}_2) | H - E | \psi_L(\mathbf{r}_1, \mathbf{r}_2) \rangle, \quad (6)$$

which can be written as

$$I = A + C_1 B + C_1^2 D, \quad (7)$$

where

$$A = \langle [\varphi_0(r_2)u(r_1) \pm (1 \leftrightarrow 2)] | H - E | \varphi_0(r_2)u(r_1) \pm (1 \leftrightarrow 2) \rangle \quad (8)$$

and

$$\begin{aligned} B &= 2 \langle \Phi_L^{(1)}(r_1, r_2) | H - E | \varphi_0(r_2)u(\vec{r}_1) \pm (1 \leftrightarrow 2) \rangle \\ &= 4 \langle V_1(\vec{r}_1)u(\vec{r}_1) \rangle \end{aligned} \quad (9)$$

In the above equation,

$$V_1(\vec{r}_1) = \langle \Phi_L^{(1)}(\vec{r}_1, \vec{r}_2) | H - E | \varphi_0(\vec{r}_2) \rangle. \quad (10)$$

In Eq. (7)

$$D = \langle \Phi_L^{(1)}(\vec{r}_1, \vec{r}_2) | H - E | \Phi_L^{(1)}(\vec{r}_1, \vec{r}_2) \rangle = \varepsilon_1 - E, \quad (11)$$

where  $\varepsilon_1$  is the expectation value of  $H$

$$\langle \Phi_L^{(1)} | H | \Phi_L^{(1)} \rangle = \varepsilon_1. \quad (12)$$

The wave function  $\Phi_L^{(1)}$  is normalized to unity. Now we determine the eigenvector  $C_1$ . The variation with respect to  $C_1$  in Eq. (7) is

$$\frac{\partial I}{\partial C_1} = 0, \quad (13)$$

Implies

$$B + 2C_1D = 0. \quad (14)$$

This gives

$$\begin{aligned} C_1 &= -\frac{B}{2D} = \frac{2 \langle \Phi_L^{(1)}(\vec{r}_1, \vec{r}_2) | H - E | \varphi_0(\vec{r}_2) u_L(\vec{r}_1) \rangle}{E - \varepsilon_1} \\ &= \frac{2 \langle V_1(\vec{r}_1) u_L(\vec{r}_1) \rangle}{E - \varepsilon_1} \end{aligned} \quad (15)$$

Now the correlation term in Eq.(1) is known. Thus the variational principle reduces to

$$\langle \varphi_0(\vec{r}_2) | \mathbf{H} - \mathbf{E} | \psi_L \rangle = 0, \quad (16)$$

which can be simplified to

$$\langle \varphi_0(\vec{r}_2) | H - E | [\varphi_0(\vec{r}_2) u(\vec{r}_1) \pm (1 \leftrightarrow 2)] \rangle + C_1 V_1(\vec{r}_1) = 0. \quad (17)$$

Where  $V_1(\vec{r}_1)$  is given in Eq. (10). Substitution of  $C_1$  from Eq. (15) into Eq. (17) gives the equation

$$\langle \varphi_0(\vec{r}_2) | H - E | [\varphi_0(\vec{r}_2) u(\vec{r}_1) \pm (1 \leftrightarrow 2)] \rangle + \frac{2V_1(\vec{r}_1) \langle V_1(\vec{r}) u(\vec{r}) \rangle}{E - \varepsilon_1} = 0 \quad (18)$$

Now the resulting equation for  $u_L(\vec{r})$ , letting  $\vec{r}_1 = \vec{r}$ , can be written in the form

$$\left[ \frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + V_d \pm V_{ex} - V_{op} + k^2 \right] u_L = 0, \quad (19)$$

where

$$V_{op} u_L = 2r \sum_{\lambda=1}^N \frac{V_{\lambda}(\vec{r}) \langle V_{\lambda}(\vec{r}_1) u_L(\vec{r}_1) \rangle}{E - \varepsilon_1}. \quad (20)$$

The above equation also holds when  $\lambda$  ranges from 1 to  $N$ , the number of terms in the correlation function (3). The potentials  $V_d$  is the direct potential and  $V_{ex}$  is the exchange potential. The optical potential has been obtained without the use of the Feshbach projection operator formalism and hence is independent of the projection operators  $\mathbf{P}$  and  $\mathbf{Q}$  [4]. The phase shifts obtained by two approaches are the same within the numerical accuracy.

### Optical potential with polarization

To take into account the long range correlations, we replace  $\phi_0(r_2)$  in Eq.(1) by

$$\Phi^{pol}(r_1, r_2) = \phi(r_2) - \frac{\varepsilon(r_1, r_2)}{r_1^2} \frac{u_{is \rightarrow p}(r_2)}{r_2} \frac{\cos(\theta_{12})}{\sqrt{Z\pi}}, \quad (21)$$

where

$$u_{is \rightarrow p}(r_2) = e^{-Zr_2} \left( \frac{Zr_2^3}{2} + r_2^2 \right), \quad (22)$$

which is the dipole part of the polarized orbital and  $\theta_{12}$  is the angle between  $r_1$  and  $r_2$ . Temkin [1] introduces the function

$$\begin{aligned} \varepsilon(r_1, r_2) &= 1, & r_1 > r_2 \\ &= 0, & r_1 < r_2, \end{aligned} \quad (23)$$

which ensures that the polarization takes place when the scattered electron is outside the orbital electron. Now we want the polarization function in Eq. (21) to be valid through out the range, rather than only just for  $r_1 > r_2$ . We, therefore, replace the function  $\varepsilon(r_1, r_2)$  by a cut off function and in order to avoid discontinuity at  $r_1 = r_2$  we choose it of the form

$$\chi_\beta(r_1) = (1 - e^{-\beta r_1})^n, \quad (24)$$

where the exponent  $n \geq 3$ . The nonlinear parameter  $\beta$ , which is function of  $k$ , can be used to optimize the results. This function vanishes at large values of  $r_1$ , it also contributes to the short-range correlations in addition to those obtained from the correlation function  $\Phi_L$ . Another form of the cutoff has been proposed by Shertzer and Temkin [13]

$$\chi_{ST} = \frac{1}{N} \int d^3 r_2 \phi_0(\vec{r}_2) \frac{u_{1s \rightarrow p}(r_2)}{r_2} \frac{\varepsilon(r_1, r_2)}{r_1^2}, \quad (25)$$

where  $N$  denotes the normalization and is given by

$$N = \int d^3 r_2 \phi_0(r_2) \frac{u_{1s \rightarrow p}(r_2)}{r_2} \frac{1}{r_1^2}. \quad (26)$$

In the above equations the integrations are from 0 to infinity. This gives

$$\chi_{ST}(r_1) = 1 - e^{-2Zr_1} \left[ \frac{1}{3}(Zr_1)^4 + \frac{4}{3}(Zr_1)^3 + 2(Zr_1)^2 + 2Zr_1 + 1 \right], \quad (27)$$

which guarantees that  $\chi(r_1)/r_1^2$  approaches 0 when  $r_1$  approaches 0. Now the scattering wave function can be written as

$$\Psi_L(\vec{r}_1, \vec{r}_2) = \frac{u_L(r_1)}{r_1} Y_{L0}(\Omega_1) \Phi^{pol}(r_1, r_2) \pm (1 \leftrightarrow 2) + \sum_\lambda C_\lambda \Phi_L^\lambda(\vec{r}_1, \vec{r}_2), \quad (28)$$

where the target function with polarization is given by

$$\Phi^{pol}(r_1, r_2) = \phi(r_2) - \frac{\chi(r_1)}{r_1^2} \frac{u_{is \rightarrow p}(r_2)}{r_2} \frac{\cos(\theta_{12})}{\sqrt{Z\pi}}. \quad (29)$$

The cutoff function  $\chi$  can be of either form given in Eq. (24) or Eq. (27). We arrive at the same form of Eq. (18) by replacing  $\phi_0$  by  $\Phi^{pol}(\vec{r}_1, \vec{r}_2)$  in Eqs. (6)-(20). We restrict ourselves to  $L=0$  and we can write the final equation in the form

$$[D(r)\frac{d^2}{dr^2} + k^2 + V_d + V^{pol} \pm (V_{ex} + V_{ex}^{pol}) - V_{op}^{pol}]u(r) = 0 \quad (30)$$

The various quantities are given below:

$$D(r) = 1 + \frac{43}{8Z^6} \left( \frac{\chi(r)}{r^2} \right)^2. \quad (31)$$

The direct potential is given by

$$V_d = \frac{2(Z-1)}{r} + 2e^{-2Zr} \left( Z + \frac{1}{r} \right) \quad (32)$$

and

$$V_d^{pol} = (x_1 + x_3) + x_2 \frac{d}{dr}. \quad (33)$$

$$x_1 = \frac{43}{8Z^6} \left( \frac{2Z}{r} - \frac{2}{r^2} + k^2 \right) \left( \frac{\chi(r)}{r^2} \right)^2. \quad (34)$$

$$x_2 = B_1(r) \frac{43}{8Z^6} \left( \frac{\chi(r)}{r^2} \right), \quad (35)$$

$$x_3 = B_2(r) \frac{43}{8Z^6} \left( \frac{\chi(r)}{r^2} \right) + \frac{2\alpha(r)}{(Zr)^4} \chi(r) - \frac{4.5\chi(r)^2}{(Zr)^4} - \frac{8}{3Z} d(r) \left( \frac{\chi(r)}{r^2} \right)^2. \quad (36)$$

$$B_1(r) = \frac{1}{r^2} \left[ -2Z\chi(r) + 2Z - \frac{2}{r} + e^{-2Zr} \left( -\frac{2}{3}Z^4r^3 - \frac{4}{3}Z^3r^2 + 2Z + \frac{2}{r} \right) \right], \quad (37)$$

$$B_2(r) = -2ZB_1(r) - \frac{4Z}{r^3} + \frac{6}{r^4} + e^{-2Zr} \left( \frac{4}{3}Z^5r + 2Z^4 - \frac{4Z^2}{r^2} - \frac{8Z}{r^3} - \frac{6}{r^4} \right). \quad (38)$$

The polarizability of the target as a function of  $r$  is given by

$$\alpha(r)/Z^4, \quad (39)$$

where

$$\alpha(r) = 4.5 - \frac{2}{3} e^{-2Zr} \left( \frac{3}{2} (Zr)^4 + 7.5 (Zr)^3 + 13.5 (Zr)^2 + 13.5 (Zr) + 6.75 \right). \quad (40)$$

and

$$d(r) = \frac{129}{32Z^5} \frac{1}{r} + \frac{18}{Z^7} \frac{1}{r^3} - e^{-2Zr} \left( \frac{3}{16} r^4 + \frac{27}{16Z} r^3 + \frac{54}{8Z^2} r^2 + \frac{135}{8Z^3} r + \frac{975}{32Z^4} + \frac{1281}{32Z^5} \frac{1}{r} + \frac{36}{Z^6} \frac{1}{r^2} + \frac{18}{Z^7} \frac{1}{r^3} \right). \quad (41)$$

$$x_3 \rightarrow \frac{9}{2Z^4 r^4}, \quad r \rightarrow \text{infinity}$$

In the above expression  $9/(2Z^4)$  is the dipole polarizability of the target with nuclear charge  $Z$ . The direct polarization potential has also terms proportional to  $1/r^2$  and  $1/r^3$  which go to zero for  $r \rightarrow 0$ .

For completeness, we give other terms in the Eq. (30). The exchange terms are given by

$$V_{ex} u(r) = 4Z^3 e^{-Zr} [(k^2 + Z^2) r \int_0^\infty dx e^{-Zx} x u(x) - 2 \int_0^r dx e^{-Zx} u(x) - 2r \int_r^\infty dx e^{-Zx} u(x)], \quad (42)$$

$$V_{ex}^{pol} u(r) = J_2 u(r) + J_3 u(r) + J_4 u(r), \quad (43)$$

where

$$J_2 u(r) = \frac{8Z}{3} \frac{u_{1s \rightarrow p}(r)}{r} \left[ \frac{1}{r} \int_0^r dx e^{-Zx} \chi(x) u(x) + r^2 \int_r^\infty dx e^{-Zx} \chi(x) \frac{u(x)}{x^3} \right], \quad (44)$$

$$J_3 u(r) = \frac{8Ze^{-Zr} \chi(r)}{3r^2} \left[ \frac{1}{r} \int_0^r dx u_{1s \rightarrow p}(x) x u(x) + r^2 \int_r^\infty dx u_{1s \rightarrow p}(x) x u(x) + r^2 \int_r^\infty dx u_{1s \rightarrow p}(x) \frac{u(x)}{x^2} \right], \quad (45)$$

and

$$J_4 u(r) = -\frac{8Ze^{-Zr} \chi(r)}{3} \left[ \int_0^\infty dx u_{1s \rightarrow p}(x) \frac{u(x)}{x^2} \chi(x) \right] + G_2 u(r) + G_3 u(r). \quad (46)$$



Now we will write below the expressions for  $G_2u$  and  $G_3u$ .

$$G_2u(r) = \frac{4\chi(r)u_{1s \rightarrow p}(r)}{3Zr^2} \int_0^\infty dx e^{-Zx} \left[ \frac{Z^3 x^3}{2} - 2Z^2 x^2 - Zx + 2 + \left( \frac{Zx^3}{2} + x^2 \right) \left( \frac{2Z}{x} - \frac{2}{x^2} + k^2 \right) \right] \frac{\chi(x)u(x)}{x^2} \quad (47)$$

$$G_3u(r) = -\frac{8\chi(r)u_{1s \rightarrow p}(r)}{8Zr^2} \left[ \frac{1}{r} \int_0^r dx \frac{u_{1s \rightarrow p}(x)}{x^2} \chi(x)u(x) + \int_r^\infty dx \frac{u_{1s \rightarrow p}(x)}{x^3} \chi(x)u(x) + \frac{2}{5}Gu(r) \right] \quad (48)$$

$$Gu(r) = \frac{1}{r^3} \int_0^r dx u_{1s \rightarrow p}(x) \chi(x)u(x) + r^2 \int_r^\infty dx \frac{u_{1s \rightarrow p}(x)}{x^5} \chi(x)u(x) \quad (48a)$$

The polarization term in Eq. (21) gives rise to terms in equations (33 - 41) and equations (43-48). These terms make the calculations much more intricate compared to the calculations without these term.

The optical appearing in Eq. (30) is given by

$$V_{op}^{pol}u(r_1) = r_1 \sum_s \frac{\langle Y_{00}^*(\Omega_1) \Phi^{pol}(\vec{r}_1, \vec{r}_2) | H - E | \Phi_0^{(s)} \rangle \langle \Phi_0^{(s)} | H - E | \Psi_0' \rangle}{E - \varepsilon_s}, \quad (49)$$

It should be noted that in the above expression, we have  $\Psi_0'$  instead of  $\Psi_0$  given in Eq. (1). The function  $\Psi_0'$  is the wave function without the correlation terms in Eq. (1). This is very clear in the projection operator - formalism of Feshbach [4] used in [5, 6, 7, 8] to obtain the scattering equations. There the function  $\Psi_0$  is written as  $\mathbf{P}\Psi_0 + \mathbf{Q}\Psi_0$  and the function  $\mathbf{P}\Psi_0$  only occurs on the right hand side of the formulation. It should be pointed out that  $\mathbf{P} + \mathbf{Q} = 1$ . Now, we have given most of the quantities occurring in Eq. (30).

For  $S$ -waves (i.e.,  $L=0$ ),  $\mathbf{D}_L = \text{constant}$  in Eq. (3) and the correlation function is a function of “radial” coordinates. We take  $\Phi_0$  of Hylleraas form

$$\Phi_{L=0}(\vec{r}_1, \vec{r}_2) = \sum_{lmn}^{N_\omega} C_{lmn} [e^{-\gamma r_1 - \delta r_2} r_1^l r_2^m r_{12}^n \pm (1 \leftrightarrow 2)], \quad (50)$$

The sum includes all values of  $l$ ,  $m$  and  $n$  such that  $l+m+n=\omega$  and  $\omega$  is equal to 0, 1, 2, 3, ..., 8. The total number of terms  $N_\omega$  depends on spin and whether  $\gamma=\delta$  or not. There are 95 terms for  $^1S$  state and 84 terms for  $^3S$  state for  $N_\omega=8$  in these calculations. Solutions of the integrodifferential equations have been carried by the noniterative method [see Appendix A] and by using quadruple precision. We present results for the  $^1S$  and  $^3S$  states in Table I and II in three approximations:

A. Phase shifts calculated using optical potential obtained by using the projection operator formalism [4].

B. Phase shifts calculated using optical potential obtained without using the projection operator formalism [4], Eq. (19).

C. Phase shifts calculated using optical potential without using the projection operator formalism but including the effects of polarization, Eq. (30).

Table I. Phase shifts (radians) of  $^1S$  state for various  $k$ .

	Ref. 5		C	C	Ref. 3	Ref. 15
$k$	A	B	$\chi_{ST}$	$\chi_\beta$	$\eta_{\text{Schwartz}}$	$\eta_{\text{SSB}}$
0.0 <sup>a</sup>		6.05327	6.00092	5.99567	5.965	
0.1	2.55358	2.55158	2.55372	2.55370	2.553	2.550
0.2	2.06678	2.06644	2.06699	2.06717	2.0673	2.062
0.3	1.69816	1.69640	1.69853	1.69684	1.6964	1.691
0.4	1.41540	1.41783	1.41561	1.41554	1.4146	1.410
0.5	1.20094	1.20084	1.20112	1.20195	1.202	1.196
0.6	1.04083	1.04074	1.04110	1.04191	1.041	1.035
0.7	0.93111	0.93105	0.93094	0.93084	0.930	0.925
0.8	0.88718	0.88717	0.88768	0.88802	0.886	

<sup>a</sup> $k=0$  results represent scattering lengths.

The scattering length  $a$  is defined by

$$\lim_{k \rightarrow 0} k \cot \eta = -1/a \quad (51)$$

It should be noted that the phase shifts given above have the rigorous lower bounds to the exact phase shifts while the scattering lengths have the rigorous upper bounds to the exact scattering lengths.

Temkin [14] has shown that the scattering length is significantly affected by the long-range polarization. The scattering length obtained at a short distance  $\mathbf{R}$  can be corrected by the following formula

$$a = a(\mathbf{R}) - \alpha \left( \frac{1}{\mathbf{R}} - \frac{\alpha}{\mathbf{R}^2} + \frac{1}{3} \frac{\alpha^2}{\mathbf{R}^3} \right), \quad (52)$$

where  $\mathbf{a}$  is the true scattering length. The scattering length  $\mathbf{a}(\mathbf{R})$  for  $^1S$  state obtained using  $\chi_\beta$  is 5.99567 at  $\mathbf{R}=146.0782$  for  $N=95$  terms. Using the formula (52), we get  $\mathbf{a}=5.96611$  which agrees well with the value  $\mathbf{a}=5.965 \pm 0.0003$  given by Schwartz [3]. He also included long-range polarization in his zero-energy calculation. The scattering lengths are rigorous upper bounds to the exact scattering results.

We find that the phase shifts obtained with the Feshbach formalism [4] are fairly close to the present results. That indicates that the short-range correlations do try to assimilate the effect of the long-range correlations to some extent. The present phase shifts have rigorous lower bounds to the exact results. We compare our results with those of Schwartz [3]. His calculation was carried out using the Kohn variational principle. But his calculations do not provide any bounds on the phase shifts though the Kohn variational principle does provide a bound on the scattering length.

In Table II, we give the results for the  $^3S$  state. The  $^3S$  scattering length for  $N=84$  with  $\chi_\beta$ ,  $\beta=0.6$  and  $n=4$  is  $\mathbf{a}(\mathbf{R})=1.7681542$  at  $\mathbf{R}=349.0831$ . The corrected value, using formula (52), is 1.76815 is a little lower compared to the Schwartz value  $1.7686 \pm 0.0002$ . The formula (52) certainly gives a good agreement with the Schwartz value. Lower scattering lengths are consistent with the rigorous upper bounds, as state earlier.

In tables I and II, we have given  $\eta_{\text{SSB}}$  obtained by Scholz, Scott and Burke [15] using the well known  $\mathbf{R}$ -matrix formulation. In these calculations, all the correlations are included in the inner region of a certain radius  $\mathbf{R}$ . The

functions in the two regions are then matched at this radius  $R$ . Their results are fairly close to the presently calculated phase shifts.

Table II. Phase shifts (radians) of  $^3S$  state for various  $k$ .

	Ref. 5		C	C	Ref. 3	Ref. 15
$k$	A	B	$\chi_{ST}$	$\chi_{\chi}$	$\eta_{\text{Schwartz}}$	$\eta_{\text{SSB}}$
0.0 <sup>a</sup>		1.81644	1.78467	1.78154	1.7686	
0.1	2.93853	2.93850	2.93856	2.93856	2.9388	2.939
0.2	2.71741	2.71740	2.71751	2.71751	2.7171	2.717
0.3	2.49975	2.49956	2.49987	2.49987	2.4996	2.500
0.4	2.29408	2.29394	2.29465	2.29457	2.2938	2.294
0.5	2.10454	2.10414	2.10544	2.10574	2.1046	2.105
0.6	1.93272	1.93280	1.93322	1.93336	1.9329	1.933
0.7	1.77950	1.78010	1.77998	1.77998	1.7797	1.780
0.8	1.64379	1.64408	1.64425	1.64444	1.643	

<sup>a</sup> $k=0$  results represent scattering lengths.

We see that the hybrid theory developed here includes both the short-range and long-range forces. The present development is significant even when the present results do not differ significantly from those obtained using the Feshbach formalism.

### Electron-He<sup>+</sup> Scattering

The above approach has been applied to the scattering of electrons from helium ions. Now the phase shifts are given by

$$\lim_{r \rightarrow \infty} u(r) \propto \sin[kr + \frac{Z-1}{k} \ln(2kr) + \arg \Gamma(1 - \frac{i(Z-1)}{k}) + \eta].$$

(53)

Phase shifts obtained for e-He<sup>+</sup> in  $^1S$  and  $^3S$  states are given in Tables III and IV.

They are given at low energies as well and have been compared with the results obtained using the Feshbach projection operator formalism [6]. They are also compared with those obtained in the close-coupling approximation [16] and also obtained using the Harris-Kohn method [17].

Table III. Comparison of the presently obtained  $^1S$  phase shifts in  $e\text{-He}^+$  scattering with other calculations: (OP) Ref. 6, (CC) Ref. 16 and Harris-Kohn Ref. 17.

$k$	Hybrid	(OP)	(CC)	Harris-Kohn
0.1	0.43808			
0.2	0.43550			
0.3	0.43142			0.4300
0.4	0.42608	0.42601		0.4228
0.5	0.41974	0.41964		0.4078
0.6	0.41265	0.41278	0.4111	0.4086
0.7	0.40568	0.40561	0.4046	0.4024
0.8	0.39865	0.39857	0.3974	0.3968
0.9	0.39213	0.39202	0.3906	0.3893
1.0	0.38644	0.38634	0.3850	0.3836
1.1	0.38200	0.38187	0.3805	0.3794
1.2	0.37914	0.37899	0.3780	0.3741
1.3	0.37846	0.37832	0.3744	0.3721
1.4	0.38158	0.38560		0.3786
1.5	0.39802			0.4014
1.6	0.34480			

Phase shifts are higher for triplet states and both  $^1S$  and  $^3S$  phase shifts decrease with increasing incident energy. It is seen that phase shifts start rising after  $k=1.4$ , indicating the existence of a resonance which we will discuss below.

Table IV. Comparison of the presently obtained  $^3S$  phase shifts in  $e\text{-He}^+$  scattering with other calculations: (OP) Ref. 6, (CC) Ref. 16 and Harris-Kohn Ref. 17.

$k$	Hybrid	(OP)	(CC)	Harris-Kohn
0.1	0.93065			
0.2	0.92704			0.9270
0.3	0.92114			0.9210
0.4	0.91302	0.91300		0.9128
0.5	0.90282	0.90275	0.9019	0.9025
0.6	0.89057	0.89050	0.8910	0.8902
0.7	0.87645	0.87640	0.8777	0.8762
0.8	0.86066	0.86069	0.8617	0.8605
0.9	0.84366	0.84356	0.8440	0.8435
1.0	0.82536	0.82531	0.8253	0.8251
1.1	0.80636	0.80625	0.8062	0.8062
1.2	0.78677	0.78666	0.7868	0.7865
1.3	0.76696	0.76684	0.7672	0.7665
1.4	0.74708	0.74697		0.7466
1.5	0.72746			0.7274
1.6	0.70815			0.7095

### Electron- $\text{Li}^{++}$ scattering

A similar calculation has been carried out for  $e\text{-Li}^{++}$  scattering. As in the case of  $\text{He}^+$ , there is a long-range Coulomb potential in addition to the long-range potential due to polarization of the target.

Gien [18] has carried out calculations by using Harris-Nesbet method and has used various combinations of target states in his calculations. We have given results which are labeled (E4S) in his paper. He used  $1s$ ,  $2s$ ,  $2p$  states of the target along with a  $2\bar{p}$  pseudostate [19] and correlations. The pseudostate is given by

$$2\bar{p} = Z^{\sqrt{5/2}} [0.340r^2 e^{-0.5Zr} - 0.966r^2 e^{-Zr} (1 + 0.5Zr)]. \quad (54)$$

This state has been formed as a linear combination of target  $2p$  state and  $u_{1s \rightarrow p}$  with a constant factor such that it is normalized and orthogonal to the  $2p$  state. The inclusion of the pseudostate gives the exact polarizability of the target.

Table V. Comparison of the presently calculated  $^1S$  and  $^3S$  phase shifts in  $e\text{-Li}^{++}$  scattering with those obtained by Gien [18].

$k$	$^1S(\text{Hybrid})$	$^1S(\text{Gien})$	$^3S(\text{Hybrid})$	$^3S(\text{Gien})$
0.1	0.23188		0.56084	
0.2	0.23176		0.56020	
0.3	0.23148		0.55869	
0.4	0.23109		0.55678	
0.5	0.23064	0.2273	0.55435	0.5526
0.6	0.23012	0.2264	0.55142	0.5499
0.7	0.22960	0.2265	0.54799	0.5467
0.8	0.22906	0.2272	0.54413	0.5430
0.9	0.22855	0.2277	0.53925	0.5390
1.0	0.22807	0.2275	0.53514	0.5345
1.1	0.22769	0.2262	0.53000	0.5296
1.2	0.22740	0.2250	0.52456	0.5244
1.3	0.22724	0.2258	0.51880	0.5189
1.4	0.22724	0.2328	0.51276	0.5131
1.5	0.22742	0.2521	0.50646	0.5069
1.6	0.22782		0.49997	0.5005

Gien [17, 18] obtained phase shifts at irregular energy points, obtained from the diagonalization of the Hamiltonian. His results could be fitted to

$$\eta = A + BE + CE^2 + DE^3 + F \exp[aE]. \quad (55)$$

In the above equation  $E=k^2$  is the incident energy and  $A, B, C, D, E, F$  and  $a$  are the fitting parameters.

## Resonances

The first time, a resonance was calculated, was in 1962 by Burke and Schey [20]. This was in electron-hydrogen scattering. They used the close-coupling approximation and found that the resonance was centered at 9.61 eV.

Resonances have been known by many names: autoionization states, doubly excited states and Feshbach resonances. It is observed that there is a rapid change of phase shift in the resonance region. This phase shift can be fitted to the Breit-Wigner form to obtain the resonance parameters,

$$\eta_{calc.}(E) = \eta_0 + AE + \tan^{-1} \frac{0.5\Gamma}{(E_R - E)}, \quad (56)$$

where  $E=k^2$  is the incident energy,  $\eta_{calc.}$  are the calculated phase shifts,  $\eta_0$ ,  $A$ ,  $\Gamma$ , and  $E_R$  are the fitting parameters.  $E_R$  and  $\Gamma$  are the resonance position and resonance width. We would like to calculate the resonance position and width of the lowest  $^1S$  resonance in He (below the  $n=2$  threshold of  $\text{He}^+$ ). In Table VI, we give phase shifts for 70 terms in the correlation function in the resonance region.

Table VI. Phase shifts in the resonance region for the lowest  $^1S$  resonance in He and  $\text{Li}^+$ .

Target	$k$	$\eta$	Target	$k$	$\eta$
$\text{He}^+$	1.555	0.5483195	$\text{Li}^{++}$	2.282	-0.090487
	1.558	0.6398967		2.2825	-0.058190
	1.560	0.7803777		2.283	-0.031793
	1.562	1.177147		2.2835	-0.009842
	1.5634	1.938293		2.284	0.008626
	1.56345	1.972649		2.2845	0.02451
	1.565	2.776815		2.285	0.038199
	1.5655	-3.372919			
	1.566	-3.276240			
	1.567	-3.148991			

We calculate the square of the difference between the left and right side of Eq. (57). The difference is being calculated at the energies given in Table



VI. Minimize the sum of the squares for various fitting parameters. We find  $\eta_0=0.3761$ ,  $A=0$ ,  $E_R=2.4426$  Ry with respect to  $\text{He}^+$  and  $\Gamma=0.00906$  Ry when the minimized sum is  $1.57 \times 10^{-7}$ . This gives resonance position  $E_R=57.8481$  eV with respect to the ground state of He and width  $\Gamma=0.1233$  eV. This agrees very well with  $E_R=57.8435$  eV and  $\Gamma=0.125$  eV, obtained using the Feshbach formalism [21]. These resonance parameters, calculated now, include the contribution from the long-range and short-range correlations. But these parameters do not have any rigorous bounds although the calculated phase shifts do have rigorous lower bounds. This is the disadvantage of fitting to the Breit-Wigner form Eq. (56).

A similar calculation has been carried out for the lowest  $^1\text{S}$  state in  $\text{Li}^+$ . The phase shifts in the resonance region for 70 terms in the correlation function are given in Table VI. By fitting, we obtain  $E_R=70.5904$  eV with respect to ground state of  $\text{Li}^{++}$  and  $\Gamma=0.1657$  eV which compares very well with  $E_R=70.5837$  eV and  $\Gamma=0.157$  eV [22]. In the Feshbach formalism, the resonance parameters, position and width, are defined as

$$E_R = \langle \Phi | Q H Q | \Phi \rangle + \Delta = \varepsilon_R + \Delta \quad (57)$$

$$\Gamma = 2k \langle \psi | P H Q | \Phi \rangle \quad (58)$$

It should be noted in the projection operator formalism of Feshbach, the contribution  $\Delta$  to the position of the resonance from the continuum and nearby resonance has to be calculated separately. This contribution is already included in the present calculation which is a great advantage.

## Conclusions

We have developed a method in which the short-range and long-range correlations can be included at the same time in the scattering equations. The phase shifts have rigorous lower bounds and the scattering lengths have rigorous upper bounds. The phase shifts in the resonance region can be used to calculate very accurately the resonance parameters.

## Appendix A

We will briefly describe the non-iterative method for solving integrodifferential equations [23]. Consider the equation for the scattering function  $u(r)$  given by

$$\left[\frac{d^2}{dr^2} + V(r) + k^2\right]u(r) = g(r)\int_0^\infty f(x)u(x)dx \quad (\text{A1})$$

Let

$$u(r) = u_0(r) + Cu_1(r) \quad (\text{A2})$$

The constant  $C$  represents the definite integral in the Eq. (A1).

Substituting  $u(r)$  in Eq. (A1), we get two equations

$$\left[\frac{d^2}{dr^2} + V(r) + k^2\right]u_0(r) = 0 \quad (\text{A3})$$

$$\left[\frac{d^2}{dr^2} + V(r) + k^2\right]u_1(r) = g(r) \quad (\text{A4})$$

These two equations can be solved easily. The substitution of (A2) in  $C$  gives

$$C = \int_0^\infty f(x)u_0(x)dx + C\int_0^\infty f(x)u_1(x)dx = I_0 + CI_1 \quad (\text{A5})$$

Having calculated  $u_0$  and  $u_1$ ,  $I_0$  and  $I_1$  can be calculated. From the above equation, we can now solve for  $C$ . We get

$$C = \frac{I_0}{(1 - I_1)} \quad (\text{A6})$$

The Eq. (A1) can now be written as

$$\left[\frac{d^2}{dr^2} + V(r) + k^2\right]u(r) = Cg(r) \quad (\text{A7})$$

Now the right-hand side is known and this equation can be solved for  $u(r)$ . This method can be generalized to any number of definite integrals.

## References

1. A. Temkin, Phys. Rev. **107**, 1004 (1957).
2. K. V. Vasavada and A. Temkin, Phys. Rev. **160**, 109 (1967).
3. C. Schwartz, Phys. Rev. **124**, 1468 (1968).
4. H. Feshbach, Ann. Phys. **19**, 287 (1962).
5. A. K. Bhatia and A. Temkin, Phys. Rev. **64**, 032709 (2001).
6. A. K. Bhatia, Phys. Rev. A, **66**, 064702 (2002).
7. A. K. Bhatia, Phys. Rev. A, **69**, 032714 (2004).
8. A. K. Bhatia, Phys. Rev. A, **73**, 012705 (2006).
9. A. K. Bhatia in the book 'Atomic Structure and Collision Processes,' published by Narosa Publishing House, edited by Man Mohan, pages 87-103, (2010).
10. A. K. Bhatia, Phys. Rev. A, **75**, 032713 (2007).
11. P. M. Morse and W. P. Allis, Phys. Rev., **44**, 269 (1933).
12. A. K. Bhatia and A. Temkin, Rev. Mod. Phys. **36**, 1050 (1964).
13. J. Shertzer and A. Temkin, Phys. Rev. A **74**, 052701 (2006).
14. A. Temkin, Phys. Rev. Lett. **6**, 354 (1961).
15. T. Scholz, P. Scott and P. G. Burke, J. Phys. B **21**, L139 (1988).
16. P. G. Burke and A. J. Taylor, J. Phys. B **2**, 44(1969).

17. T. T. Gien, J. Phys. B **35**, 4475(2002).
18. T. T. Gien, J. Phys. B **36**, 2291(2003).
19. P. G. Burke, D. F. Gallaher and S. Geltman, J. Phys. B **2**, 1142 (1969).
20. P. G. Burke and H. M. Schey, Phys. Rev. **126**, 147 (1962).
21. A. K. Bhatia and A. Temkin, Phys. Rev. A **11**, 2018 (1975).
22. A. K. Bhatia, Phys. Rev. A **15**, 1315 (1977).
23. K. Omidvar, Phys. Rev. **133**, A970 (1964).