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Applications of the hybrid theory to the scattering of electrons from He^{+} and Li^{2+} and resonances in these systems

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The hybrid theory of electron-hydrogen elastic scattering [Phys. Rev. A **75**, 032713 (2007)] is applied to the S-wave scattering of electrons from He^{+} and Li^{2+}. In this method, both short-range and long-range correlations are included in the Schrödinger equation at the same time. Phase shifts obtained in this calculation have rigorous lower bounds to the exact phase shifts and they are compared with those obtained using the Feshbach projection operator formalism [Phys. Rev. A **66**, 064702 (2002)], the close-coupling approach [J. Phys. B **2**, 44 (1969)], and the Harris-Nesbet method [J. Phys. B **35**, 4475 (2002); J. Phys. B **36**, 2291 (2003)]. The agreement among all the calculations is very good. These systems have doubly excited or Feshbach resonances embedded in the continuum. The resonance parameters for the lowest ^{1}S resonances in He and Li^{+} are calculated and they are compared with the results obtained using the Feshbach projection operator formalism [Phys. Rev. A **11**, 2018 (1975); Phys. Rev. A **15**, 131 (1977)]. It is concluded that accurate resonance parameters can be obtained by the present method, which has the advantage of including corrections due to neighboring resonances and the continuum in which these resonances are embedded.

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I. INTRODUCTION

Testing of various scattering theories is important. Scattering by single-electron systems provides such means of testing because the wave function of the target is known exactly. In a previous paper [1] on the scattering of electrons from hydrogen atoms, we showed that it is possible to include long-range polarization potential [2] and short-range correlations [3] in the Schrödinger equation at the same time. The phase shifts obtained in this calculation have rigorous lower bounds to the exact phase shifts. The phase shifts obtained by the close-coupling approach also has this property while those obtained from the Kohn variational principle, and other methods closely related to it, do not have any bounds except at zero incident energy. In [3], we compared the results obtained by the Feshbach projection operator formalism with those obtained using the method of polarized orbitals which gives reasonably accurate phase shifts but does not provide any bounds on the phase shifts but they do contain the dominant correlations [3].

Now we apply the formalism given in [1] to the S-wave elastic scattering of electrons from Coulombic targets He^{+} and Li^{2+}. Phase shifts obtained are compared with the results of other calculations. We also show that the same formalism can be used to calculate ^{1}S and ^{3}S parameters as well of resonances in electron+target systems. Resonances are exhibited, at an appropriate energy, when the incident electron excites the target electron and itself gets attached to the excited target for a finite duration of time. These resonances have been investigated extensively by the use of the Feshbach projection operator formalism [4], close-coupling approach [5], complex rotation method [6], etc.

II. THEORY AND CALCULATIONS

Below we recapitulate very briefly the formalism presented in [1]. In order to replace the many-particle Schrödinger equation with a single-particle integrodifferential equation, we write the wave function for any angular momentum L in the form

$$\Psi_L(\mathbf{r}_1,\mathbf{r}_2) = \left[\frac{u_L(r_1)}{r_1}Y_{L0}(\hat{r}_1)\Phi^{\text{pol}}(\mathbf{r}_1,\mathbf{r}_2) \pm (1 \leftrightarrow 2)\right] + \sum_{\lambda=1}^{N} C_\lambda \Phi_L^\lambda(\mathbf{r}_1,\mathbf{r}_2), \quad (1)$$

where C_λ are the unknown coefficients, the upper sign refers to the singlet states, and the lower sign to the triplet states. The effective target wave function in the presence of the incident electron r_1 is

$$\Phi^{\text{pol}}(\mathbf{r}_1,\mathbf{r}_2) = \phi_0(\mathbf{r}_2) - \frac{\chi_{ST}(r_1)}{r_1^2}\frac{u_{1s\to p}(r_2)}{r_2}\frac{\cos(\theta_{12})}{\sqrt{Z\pi}}, \quad (2)$$

where the unperturbed target function is

$$\phi_0(r_2) = \sqrt{\frac{Z^3}{\pi}}e^{-Zr_2}, \quad (3)$$

and the second term in Eq. (2) is of the same type as derived by Temkin [2], except for the cutoff function, using the first order perturbation theory. The function $u_{1s\to p}$ is given by

$$u_{1s\to p}(r_2) = e^{-Zr_2}\left(\frac{Z}{2}r_2^3 + r_2^2\right). \quad (4)$$

The pseudostate $2\bar{p}$ later derived by Damburg and Karule [7], to account for the polarizability of the target, is based on the method of polarized orbitals and is of the same form as $u_{1s\to p}$, except for the normalization constant. The angle between r_1 and r_2 is θ_{12} and the cutoff function χ_{ST} [8] is given by

$$\chi_{ST}(r_1) = 1 - e^{-2Zr_1}\left[\frac{1}{3}(Zr_1)^4 + \frac{4}{3}(Zr_1)^3 + 2(Zr_1)^2 + 2Zr_1 + 1\right], \tag{5}$$

which guarantees that $\chi_{ST}(r_1)/r_1^2 \to 0$ when $r_1 \to 0$. This cutoff function allows the polarization of the target to take place whether the scattered electron is inside or outside the target electron. This is unlike the cutoff function introduced by Temkin [2]. In that case the polarization takes place only when the scattered electron is outside the target. A more flexible cutoff function [1] is given by

$$\chi_\beta = (1 - e^{-\beta r_1})^n, \tag{6}$$

where the exponent $n \geq 3$ and β is a function of k, but it is easier to use χ_{ST} and the results are not too different when χ_β is used [1]. The function Φ_L^λ is the correlation function and for each λ and for any L it is given by

$$\Phi_L = \sum_\kappa [f_L^{\kappa,+1}(r_1,r_2,r_{12})\mathcal{D}_L^{\kappa,+1}(\theta,\phi,\psi) + f_L^{\kappa,-1}(r_2,r_1,r_{12})\mathcal{D}_L^{\kappa,-1}(\theta,\phi,\psi)]. \tag{7}$$

The $\mathcal{D}^{\kappa,\epsilon}$ functions ($\epsilon = +1,-1$) are called rotational harmonics [9]. The fs are the generalized "radial" functions, which depend on the three residual coordinates to define the two vectors $\mathbf{r}_1$ and $\mathbf{r}_2$, in addition to the Euler angles [9]. We restrict ourselves to $L=0$, and we take Φ_0 of the Hylleraas form,

$$\Phi_{L=0}(\mathbf{r}_1,\mathbf{r}_2) = \sum_{lmn}^{N(\omega)} C_{lmn}[e^{-\gamma r_1 - \delta r_2} r_1^l r_2^m r_{12}^n \pm (1 \leftrightarrow 2)], \tag{8}$$

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

The nonrelativistic Hamiltonian, in Rydberg units, is given by

$$H = -\nabla_1^2 - \nabla_2^2 - \frac{2Z}{r_1} - \frac{2Z}{r_2} + \frac{2}{r_{12}}, \tag{9}$$

where Z is the nuclear charge of the target. Use of the variational principle in the Schrödinger equation

$$H\Psi(\mathbf{r}_1,\mathbf{r}_2) = E\Psi(\mathbf{r}_1,\mathbf{r}_2) \tag{10}$$

results in the integrodifferential equation [1] for the scattering function $u(r_1)$ for $L=0$, and letting $r_1 = r$,

$$\left[D(r)\frac{d^2}{dr^2} + k^2 + V_d + V_d^{\mathrm{pol}} \pm (V_{ex} + V_{ex}^{\mathrm{pol}}) - \mathcal{V}_{\mathrm{op}}^{\mathrm{pol}}\right]u(r) = 0, \tag{11}$$

where

$$D(r) = 1 + \frac{43}{8Z^6}\left(\frac{\chi_{ST}}{r^2}\right)^2. \tag{12}$$

TABLE I. Comparison of the presently calculated ^1S and ^3S phase shifts (rad) for the scattering of electrons from He$^+$ ions with those obtained from using the Feshbach projection operator formalism (OP) [3], with those obtained by close-coupling and correlations [10], and with those obtained by Gien from the Harris-Nesbet method [12].

Target	k	^1S (present)	^1S (OP)	^1S (CC)	^1S (Gien)
He$^+$	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	0.3774	0.3721
	1.4	0.38158	0.38560		0.3786
	1.5	0.39802			0.4014
	1.6	0.34480			

V_d and V_{ex} are the well known direct and exchange potentials, V_d^{pol} and V_{ex}^{pol} are the direct and exchange polarization potentials. Expressions for various quantities are rather lengthy. They are given in [1] and are not repeated here. It should be pointed out that the potential $-V_d^{\mathrm{pol}}$ has a term which is equal to $-4.5/(Zr)^4$ for $r \to \infty$. This is the attractive long-range potential [2] with the correct polarizabilty $4.5/Z^4$. The optical potential $\mathcal{V}_{\mathrm{op}}^{\mathrm{pol}}$ takes into account the short-range correlations [1]. The total energy in Rydberg units is given by

$$E = k^2 - Z^2, \tag{13}$$

where k^2 is the incident electron energy.

The integrodifferential equation is solved by using the noniterative method. Since we are dealing with the Coulombic systems, this equation has to be solved up to large distances, especially for low k. The solution is unique (up to an arbitrary normalization) with asymptotic form

$$\lim_{r\to\infty} u(r) \propto \sin\left[kr + \frac{Z-1}{k}\ln(2kr) + \arg\Gamma\left(1 - \frac{i(Z-1)}{k}\right) + \eta\right]. \tag{14}$$

Phase shifts presently calculated for e-He$^+$ in ^1S and ^3S states are given in Tables I and II. They are also given at very low values of the incident energy. The phase shifts are compared with those obtained from including only the optical potential obtained by use of the Feshbach projection operator formalism. In the present hybrid approach [1], we do not use any projection operators to construct the optical potential $\mathcal{V}_{\mathrm{op}}^{\mathrm{pol}}$. A comparison indicates that the inclusion of the perturbed target wave function in the variational principle has given results which are slightly higher but not too different from

TABLE II. Comparison of the presently calculated ^3S phase shifts (rad) for the scattering of electrons from He$^+$ ions with those obtained from using the Feshbach projection operator formalism (OP) [3], with those obtained by close-coupling and correlations [10], and with those obtained by Gien using the Harris-Nesbet method [12].

Target	k	^3S (present)	^3S (OP)	^3S (CC)	(Gien)
He$^+$	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

TABLE III. Comparison of the presently calculated ^1S and ^3S phase shifts (rad) for the scattering of electrons from Li^{2+} with those obtained by Gien [14] by using the Harris-Nesbet method.

Target	k	^1S (present)	^1S (Gien)	^3S (present)	^3S (Gien)
Li^{2+}	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

those obtained in the Feshbach formalism. Nevertheless, they include the short-range and long-range correlations and have rigorous lower bounds to the exact phase shifts, as in [3]. The same conclusion was arrived at in [1], namely that the correlation functions by themselves include some effects of the long-range forces. The phase shifts are also compared to the interpolated close coupling (CC) with correlation results of Burke and Taylor [10]. Their results have been obtained by using $1s$, $2s$, and $2p$ target states and 16 correlation terms of the Hylleraas type. This calculation is akin to the present approach in the sense that it takes into account the short-range and long-range correlations, except that the polarizability depends upon the number of target states included in the calculation.

Shimamura [11] and Gien [12] have carried out calculations by using the Harris-Nesbet method. Gien has used various combination of target states in his calculations but he obtained improved results labeled (E4S), considered to be most accurate among his various versions, by using $1s$, $2s$, $2p$ states of the target along with a $2\bar{\bar{p}}$ pseudostate [13] and correlations. The pseudostate is given by

$$2\bar{\bar{p}} = Z^{\sqrt{5/2}}\left[0.340r^2e^{-Zr/2} - 0.966r^2e^{-Zr}\left(1+\frac{Z}{2}r\right)\right]. \quad (15)$$

This state has been formed as linear combination of target $2p$ state and $u_{1s\rightarrow p}$ with a constant factor such that it ($2\bar{\bar{p}}$ state) is normalized and is orthogonal to the $2p$ state. The inclusion of the pseudostate helps to give the exact polarizablity of the target. The singlet and triplet S-phase shifts have been calculated at irregular energy points, obtained from the diagonalization of the Hamiltonian with correlation terms for a particular value of the nonlinear parameter, and his results could be fitted to

$$\eta = A + BE + CE^2 + DE^3 + F\,\exp[aE], \quad (16)$$

where $E=k^2$ is the incident energy, A, B, C, D, F, and a are the fitting parameters. The phase shifts obtained by Gien are fairly accurate, however, they suffer from the disadvantage of not having lower bounds. His results along with the presently calculated phase shifts are shown in Tables I and II. The agreement among all four calculations is very good. There are a number of other calculations (see references in [12]) but no attempt has been made to compare with all of them.

Phase shifts are higher for triplet states and both ^1S and ^3S phase shifts decrease with increasing incident energy. It is seen that the phase shifts for ^1S start rising after $k=1.4$, indicating that we are now in the resonance region.

A similar calculation has been carried out for e-Li^{2+} scattering in the singlet and triplet S states. In this case, the polarizablity of the target is small compared to that of the He$^+$ ion which implies that the effect of the second term in Eq. (2) should be less significant. Phase shifts decrease with increasing incident energy. The presently calculated phase shifts are compared in Table III with those obtained by Gien [14], labeled (E4S), by using $1s$, $2s$, $2p$ states of the target along with a $2\bar{\bar{p}}$ pseudostate [13] and correlations. Gien has various versions in his calculations but the results labeled (E4S) are considered to be most accurate. His results for e-Li^{2+} again could be fitted using Eq. (16). The agreement between the two calculations is good but as pointed out earlier Gien's results do not have any bounds.

TABLE IV. Resonance parameters[a] for the lowest ^1S resonance in He and Li^+.

System	N	E_R	Γ	System	E_R	Γ
He	22	57.85087	0.12994	Li^+	70.5884	0.1570
	34	57.84896	0.12545		70.5898	0.1615
	50	57.84815	0.12395		70.5897	0.1659
	70	57.84805	0.12326		70.5904	0.1657

[a] Resonance position in He is with respect to the ground state of He while that in Li^+ is with respect to the ground states of Li^{2+}.

TABLE V. Phase shifts (rad) for the lowest ^1S resonance states in He and Li^+ for various k in the resonance region obtained using 70 terms in the wave function.

Target	k	η	Target	k	η
He^+	1.555	0.5483195	Li^{++}	2.282	−0.09048750
	1.558	0.6398967		2.2825	−0.05819017
	1.560	0.7803777		2.283	−0.03179365
	1.562	1.177147		2.2835	−0.009842305
	1.5634	1.938293		2.284	0.008682685
	1.56345	1.972649		2.2845	0.02451586
	1.565	2.776815		2.285	0.03819930
	1.5655	−3.372919			
	1.566	−3.276240			
	1.567	−3.148991			

Calculations have not been carried out at the incident energy $k=0$ to calculate scattering lengths as in $e-\mathrm{H}$ system [1]. The scattering length becomes an undefined quantity because the Coulomb field extends to infinity for the scattering of electrons from Coulombic systems. The maximum number of terms in the singlet case for $\gamma=\delta$ is $N(\omega)=70(7)$ and $N(\omega)=84(6)$ for triplet states where $\gamma\neq\delta$.

III. RESONANCES

Doubly excited states or Feshbach resonances have been studied extensively [4–6]. These states are also known as autoionization states. In the evaluation of phase shifts from Eq. (11), expectation values of $\langle\Phi_0|H|\Phi_0\rangle$, occurring in the denominator of $\mathcal{V}_{\mathrm{op}}^{\mathrm{pol}}$, Eq. (55) of [1], are calculated giving a whole range of eigenvalues. But it is not possible to distinguish resonance positions from other pseudoresonances. It is therefore necessary to calculate phase shifts at those incident energies where a rapid change of phase shifts is observed. Then those phase shifts obtained in this approach are fitted to the Breit-Wigner form to obtain the resonance parameters for any resonance,

$$\eta_{\mathrm{calc.}}(E)=\eta_0+AE+\tan^{-1}\frac{0.5\Gamma}{(E_R-E)}, \tag{17}$$

where $E=k^2$ is the incident energy, $\eta_{\mathrm{calc.}}$ are the calculated phase shifts, η_0, A, Γ, and E_R are the fitting parameters. E_R and Γ represent the resonance position and resonance width.

We have calculated the lowest resonance position and width of the ^1S state (below the $n=2$ threshold of He^+) in He by obtaining the phase shifts in the resonance region. In Table IV, we give the resonance position with respect to the ground state of He and width in eV obtained for various number of terms ($N=22$, 34, 50, 70) in the trial wave function given in Eq. (8), while in Table V we give the phase shifts in the resonance region only for $N=70$.

It is seen that phase shifts vary very rapidly in the resonance region. A good way to determine resonance parameters from the phase shifts in the resonance region, along with η_0 and A in Eq. (17), is to minimize the sum of squares of the difference between the left and right sides of Eq. (17), the difference being calculated at the energies given in Table V. For the He resonance, parameters for 70 term wave functions are $\eta_0=0.3761$, $A=0$, $E_R=2.444\,26$ Ry with respect to He^+ and $\Gamma=0.009\,06$ Ry when the minimized sum is 1.57×10^{-5}. This gives resonance position $E_R=57.8481$ eV with respect to the ground state of He and width $\Gamma=0.1233$ eV. They agree very well with $E_R=57.8435$ eV and $\Gamma=0.125$ eV, obtained using the Feshbach projection operator formalism [4]. Although the phase shifts obtained here have lower bounds, the resonance position obtained by fitting does not have any bounds. This is a disadvantage of having to determine the resonance position by fitting phase shifts to the Breit-Wigner form Eq. (17).

The position obtained in the Feshbach projection operator formalism also loses the bound because of the corrections applied to the eigenvalue obtained from the $\mathcal{E}_Q=\langle Q\Phi_0|H|Q\Phi_0\rangle=57.8223$ eV, which has an upper bound. The projection operator Q is constructed such that it projects out all the $1s$ states of the target and the states obtained from $\langle Q\Phi_0|H|Q\Phi_0\rangle$ diagonalization have only $2s$ and higher s components [4]. Though these state are really scattering states, the use of the projection operators has reduced the calculation to that of bound states. In this formulation therefore it is easy to find the resonance position by calculating the lowest eigenvalue, the eigenvalue of interest. But this is not the true resonance position which should have been obtained by solving the Schrödinger equation like Eq. (11) in which the optical potential is constructed by using the projection operators Q and $P=1-Q$. Instead of this, expressions for corrections have been obtained by using the first-order perturbation theory. These corrections are interpreted as due to the fact that the resonance is embedded in the continuum and there are other resonance states nearby [4]. This correction is $\Delta=0.021\,12$ eV, giving $E_R=\mathcal{E}_Q+\Delta=57.8435$ eV, given above. On the other hand there are no such corrections when the resonance position is obtained by fitting phase shifts to the Breit-Wigner expression given in Eq. (17).

A similar calculation has been carried out for the lowest ^1S resonance in Li^+. In Table IV, we show the variation of E_R and Γ with the number of terms in the trial wave function given in Eq. (8). The phase shifts in the resonance region are shown in Table V for $N=70$ terms in the wave function only. The resonance position and width obtained by fitting the $N=70$ term phase shifts are $E_R=70.5904$ eV with respect to the $n=1$ state of Li^{2+} and $\Gamma=0.1657$ eV which compare very well with $E_R=70.5837$ eV, which includes contribution Δ

from the nearby resonances and the continuum, and $\Gamma = 0.157$ eV obtained using the Feshbach projection operator formalism [15].

Again the above parameters have been obtained by minimizing the sum of squares of the difference between the left and right sides of Eq. (17), as in He, the difference being calculated at the energies given in Table V. For the Li^+ resonance, parameters for 70 term wave function are $\eta_0 = 2.534$, $A = 0.1585$, $E_R = 5.188\,25$ Ry and $\Gamma = 0.012\,18$ Ry when the minimized sum is 7.96×10^{-6}.

We have calculated all these results for only one value of the nonlinear parameters $\gamma = \delta$. Improved results can be obtained by varying these nonlinear parameters and using a larger number of terms in the trial wave function Eq. (8). Unlike the Feshbach projection operator formalism, where it is easy to search for resonances, phase shifts in this approach need to be calculated for a large number of incident energies at a finer mesh. On the other hand, the present approach does not require any corrections like Δ to the calculated resonance energy.

There is an infinite number of resonances below the $n = 2$ threshold but only one resonance parameters are calculated in each He and Li^+ to demonstrate the capability of this method. The present calculations have been carried out below the $n = 2$ threshold of the target. The calculations can be extended to higher thresholds provided scattering channels from the higher thresholds are included in Eq. (1). Then the problem becomes a multichannel problem including elastic as well as inelastic channels.

In conclusion, we have calculated phase shifts for the scattering of electrons from He^+ and Li^{2+}. These phase shifts have rigorous lower bounds to the exact phase shifts. We have also calculated the lowest ^1S resonances in He and Li^+.

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