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Application of P-wave hybrid theory to the scattering of electrons from He$^+$ and resonances in He and H$^-$

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The P-wave hybrid theory of electron-hydrogen elastic scattering [Bhatia, Phys. Rev. A **85**, 052708 (2012)] is applied to the P-wave scattering from He ion. In this method, both short-range and long-range correlations are included in the Schrödinger equation at the same time, by using a combination of a modified method of polarized orbitals and the optical potential formalism. The short-range-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 they are close to the phase shifts calculated earlier by 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 20-term correlation function is needed in the wave function compared to the 220-term wave function required in the above-mentioned calculation. Results for the phase shifts, obtained in the present hybrid formalism, are rigorous lower bounds to the exact phase shifts. The lowest P-wave resonances in He atom and hydrogen ion have also been calculated and compared with the results obtained using the Feshbach projection operator formalism [Bhatia and Temkin, Phys. Rev. A **11**, 2018 (1975)] and also with the results of other calculations. 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, bound states, and the continuum in which these resonances are embedded.

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I. INTRODUCTION

There are a number of scattering theories and it is important to test them. Scattering of electrons and positrons by hydrogenic systems provides such a test because the target function is known exactly, allowing us to compare and test the various methods of calculations. At low incident energies, the distortion of the target produced by the incident electron is important. In previous papers [1–3] on scattering, we showed that it is possible to include a long-range polarization potential proportional to $-1/r^4$ and short-range correlations via an optical potential in the Schrödinger equation at the same time. One of the methods used to take into account this distortion is the method of polarized orbitals [4], which includes the effect of polarization in the ansatz for the wave function for the scattering. In previous papers [1–3], scattering phase shifts were calculated by using this hybrid method. In [5], the P-wave calculation was based on the Feshbach projection operator formalism [6]. We do not use any projection operators in the present calculation but the important property, namely, that the phase shifts are rigorous lower bounds to the exact phase shifts, is retained. The phase shifts obtained by the close-coupling approach also have this property while those obtained from the Kohn variational principle, and other methods closely related to this principle, do not have any bounds except at zero incident energy. We use Rydberg units: energy in rydbergs and length in Bohr radius a_0. The phase shifts, throughout, are in radians.

Now we apply the formalism given in [3] to the P-wave elastic scattering of electrons from a Coulombic He$^+$ target. Phase shifts obtained are compared with other calculations. We show that the same formalism can be used to calculate ^1P and ^3P resonance parameters in electron plus target systems. Resonances are exhibited, at appropriate energies, 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 [6], close-coupling approach [7], complex-rotation method [8], etc.

II. THEORY

Below we describe very briefly the formalism presented in [3]. 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

$$\Psi_L(\vec{r}_1,\vec{r}_2) = \left[\frac{u(r_1)}{r_1} Y_{L0}(\hat{r}_1)\Phi^{\text{pol}}(r_1,r_2) \pm (1 \leftrightarrow 2)\right] + \sum_\lambda C_\lambda \Phi_L^\lambda(\vec{r}_1,\vec{r}_2), \tag{1}$$

where C_λ are the unknown coefficients. The ($\pm$) above refers to singlet (upper sign) or triplet (lower sign) scattering, respectively. The summation over λ is from 1 to N, the number of terms in the expansion. The effective target wave function can be written as

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

where

$$\phi_0(\vec{r}_2) = \sqrt{\frac{Z^3}{\pi}} e^{-Zr_2}, \tag{3}$$

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

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 [4] by a smooth cutoff function $\chi_\beta(r_1)$ which is of the form

$$\chi_\beta(r_1) = (1 - e^{-\beta r_1})^n, \tag{5}$$

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. (2) is valid throughout the range. This is unlike the step function $\varepsilon(r_1,r_2)$ used by Temkin [4] which ensures that the polarization takes place when the scattered electron r_1 is outside the orbital electron r_2. Furthermore, the function in Eq. (5) gives us another parameter β, which is a function of k, the incident electron momentum. 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.

Beyond the terms containing $u(r)$ explicitly (those are the terms giving rise to the exchange approximation), the function Φ_L is the correlation function. For arbitrary L this function is most efficiently written in terms of the Euler angles [9]:

$$\Phi_L = \big[f_L^{1+}(r_1,r_2,r_{12})D_L^{1+}(\vartheta,\phi,\psi) + f_L^{1-}(r_1,r_2,r_{12})D_L^{1-}(\vartheta,\phi,\psi)\big]. \tag{6}$$

The $D^{1\pm}$ functions are called *rotational harmonics* [9]. The f's above are the 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 the two electrons is given by $r_{12} = |\vec{r}_1 - \vec{r}_2|$.

The radial functions $f_1^{1\pm}$ for $L = 1$ are defined as follows:

$$f_1^{1+} = \cos(\theta_{12}/2)[f(r_1,r_2,r_{12}) \pm f(r_2,r_1,r_{12})], \tag{7}$$

$$f_1^{1-} = \sin(\theta_{12}/2)[f(r_1,r_2,r_{12}) \mp f(r_2,r_1,r_{12})], \tag{8}$$

and

$$f(r_1,r_2,r_{12}) = \sum_{lmn} C_{lmn} r_1^l r_2^m r_{12}^n e^{-\gamma r_1 - \delta r_2}. \tag{9}$$

The upper sign in Eqs. (7), (8) refers to the singlet state and the lower sign refers to the triplet state. The minimum value of l is equal to 1 while that of m and n is 0. The wave function of the scattered electron is given implicitly by

$$\int [Y_{L0}(\Omega_1)\Phi^{\text{pol}}(\vec{r}_1,\vec{r}_2)(H-E)\Psi_L]d\vec{r}_2 = 0, \tag{10}$$

where H is the Hamiltonian and E is the total energy of the electron-target system. We have, in Rydberg units,

$$H = -\nabla_1^2 - \nabla_2^2 - \frac{2Z}{r_1} - \frac{2Z}{r_2} + \frac{2}{r_{12}}, \tag{11}$$

$$E = k^2 - Z^2, \tag{12}$$

where k^2 is the kinetic energy of the incident electron and Z is the nuclear charge which is 2 for He$^+$.

We can write the final scattering equation in the form

$$\left[D(r)\frac{d^2}{dr^2} + k^2 + \frac{2}{r^2} + V_d + V^{\text{pol}} \pm \left(V_{\text{ex}} + V_{\text{ex}}^{\text{pol}}\right) - V_{\text{op}}^{\text{pol}}\right]u(r) = 0. \tag{13}$$

We give below a few of the quantities:

$$D(r) = 1 + \frac{43}{8Z^6}\left[\frac{\chi_\beta(r)}{r^2}\right]^2. \tag{14}$$

The direct potentials are given by

$$V_d = \frac{2(Z-1)}{r} + 2e^{-2Zr}\left(Z + \frac{1}{r}\right), \tag{15}$$

and

$$V_d^{\text{pol}} = (x_1 + x_3) + x_2\frac{d}{dr}. \tag{16}$$

We give x_1 below:

$$x_1 = 2\frac{\chi_\beta(r)}{(Zr)^4}\alpha(r), \tag{17}$$

$$\alpha(r) = \tfrac{9}{2} - e^{-2Zr}\big[(Zr)^4 + 5(Zr)^3 + 9(Zr)^2 + 9(Zr) + \tfrac{9}{2}\big]. \tag{18}$$

All other quantities are fairly complicated and they are not given here. It can be seen from the detailed expressions that $(x_1 + x_3)$ has a term $\frac{9}{2Z^4r^4}$, where $9/(2Z^4)$ is the dipole polarizability of the target with nuclear charge Z. The exchange term is given by

$$V_{\text{ex}}u(r) = -\frac{8Z^3}{3}e^{-Zr}\left[\frac{1}{r}\int_0^r dx e^{-Zx}x^2u(x) + r^2\int_r^\infty dx\frac{e^{-Zx}}{x^2}u(x)\right]. \tag{19}$$

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

$$V_{\text{op}}^{\text{pol}}u(r) = r\sum\nolimits_s^N \frac{\langle Y_{10}^*(\Omega_1)\Phi^{\text{pol}}(\vec{r}_1,\vec{r}_2)|H-E|\Psi_0'\rangle}{E-\varepsilon_s}, \tag{20}$$

where Ψ_0' is the wave function Ψ_0 given in Eq. (1) without the correlation term Φ_L. The eigenvalues ε_s are given by

$$\left\langle \Phi_L^\lambda \middle| H \middle| \Phi_L^\lambda \right\rangle = \varepsilon_\lambda. \tag{21}$$

The functions Φ_L^λ are normalized to 1. The summation over s in Eq. (20) is from 1 to N, the number of terms in the expansion. This optical potential includes the effects of polarization of the target. The right-hand side of Eq. (20) has not been given explicitly because it contains a large number of terms. Provided the total energy $E < \varepsilon_s$, the optical potential given in Eq. (20) is negative definite and therefore corresponds to an attractive potential. Gailitis [10] has shown that as the number of terms in the correlation function is increased, the optical potential becomes more negative. Consequently, phase shifts increase as the number of terms is increased.

In order to derive the equation for the scattering function $u(r)$, the coefficients C_λ must be known. The detailed derivation is given in [1] and is not repeated here. In [5], the optical potential of the type given in Eq. (20), in the absence of long-range potential, was derived by using the Feshbach projection operator formalism based on projection operators $\boldsymbol{P}$ and $\boldsymbol{Q}$ [6]. In [5], the correlation function is such that it takes 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 $u(r)$. The present formalism is independent of the projection operators $\boldsymbol{P}$ and $\boldsymbol{Q}$.

III. CALCULATIONS AND RESULTS

Equation (13) is solved for the continuum function $u(r)$ by the noniterative method of Omidvar [11] and the phase shift η is obtained from the value of the function at a large distance:

$$\lim_{r\to\infty} u(r) \propto \sin\left\{kr - L\frac{\pi}{2} + \frac{Z-1}{k}\ln(2kr) + \arg\Gamma\left[L+1-\frac{i(Z-1)}{k}\right] + \eta\right\}. \tag{22}$$

Since the Coulomb field extends very far, Eq. (13) has to be integrated to a large distance, especially for small values of k. From $u(r)$ and its derivative, the phase shift η, the deviation from the pure Coulomb field of $(Z–1)$ is readily extracted, provided the higher terms in the expansion of Coulomb functions F_1 and G_1 [12] are retained in the scattering function $u(r)$:

$$u(r) = A\,[F_1(r) + \tan(\eta)G_1(r)]\,, \tag{23}$$

where F_1 is the regular Coulomb wave function and $G_1(r)$ is the irregular Coulomb wave function, and η is the required phase shift for the $L = 1$ partial wave.

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). The phase shifts, optimized with respect to the nonlinear parameter β, obtained for ^1P and ^3P, are given in Table I and compared with those obtained by Sloan [13]. These results include contributions from the exchange polarization term. 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.

In Table II, we give convergence of ^1P phase shifts for $k = 0.1$ with increasing number of terms in the correlation function. 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. It is seen from the table that we do not need more than 20 terms to get results comparable in accuracy to those obtained with 220 terms in [5] without the use of the polarization term in the target wave function and using the projection operator formalism of Feshbach, where it is not possible to modify the formulism in such a way as to produce a direct polarization potential proportional to $1/r^4$ in the scattering equation for $u(r)$.

TABLE I. Comparison of phase shifts η (radians) without correlations with those obtained by the method of polarized orbitals [13].

	^1P		^3P	
k	Present η	η_{PO}	Present η	η_{PO}
0.2	– 0.047405	– 0.0394	0.20143	0.2232
0.4	– 0.050130	– 0.0404	0.20715	0.2290
0.6	– 0.053033	– 0.0428	0.21448	0.2364
0.8	– 0.054106	– 0.0450	0.22119	0.2429
1.0	– 0.053466	– 0.0436	0.22582	0.2469
1.2	– 0.049405	– 0.0384	0.22779	0.2479
1.4	– 0.042442	– 0.0301	0.22726	0.2462
1.6	– 0.032978	– 0.0193	0.22474	0.2425
1.8	– 0.021577	– 0.0068	0.22141	0.2375
2.0	– 0.009349	+ 0.0066	0.21699	0.2317

TABLE II. Convergence of ^1P phase shifts (radians) for electron-helium ion for $k = 0.1$.

N	β	γ	δ	η
0	1.10			– 0.04657765
4	1.00	1.75	2.00	– 0.04047531
10	0.85	1.40	2.00	– 0.03839231
20	0.75	1.50	2.40	– 0.03830765
35	0.75	1.50	2.40	– 0.03812654

In Table III, we give ^1P phase shifts for various values of the incident momentum for 20 terms and compare them with those obtained in [5] with 220 terms in the correlation function, but without the polarization term. We find that the results are comparable in accuracy to those obtained in [5] with longer expansions in the correlation function. This indicates that very long expansions do give fairly accurate results. We compare the present results with the pseudostate close-coupling results of Oza [14] and the results of Gien [15] obtained using the Harris-Nesbet method.

In Table IV, we give the convergence of ^3P phase shifts for $k = 0.1$ with the number of terms in the correlation function. 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 from the table that we do not need more than 20 terms to get results comparable in accuracy to those obtained in [5] without the use of the polarization term in the target wave function.

In Table V, we give ^3P phase shifts for various values of incident momentum for 20 terms and compare them with those

TABLE III. Phase shifts (radians) of ^1P for various k for $N = 20$.

k	Present η	η_{PQ}	η(Oza)[a]	η(Gien)[b]
0.1	– 0.038308	– 0.038311	– 0.03938	
0.2	– 0.038956	– 0.038958	– 0.04002	– 0.0407
0.3	– 0.039873	– 0.039911	– 0.04095	
0.4	– 0.040902	– 0.040971	– 0.04304	
0.5	– 0.041469	– 0.041951	– 0.04203	– 0.0428
0.6	– 0.041641	– 0.042633	– 0.04381	
0.7	– 0.041438	– 0.042834	– 0.04416	– 0.0447
0.8	– 0.039927	– 0.042383	– 0.04391	
1.0	– 0.037132	– 0.039036	– 0.04098	
1.1	– 0.035430	– 0.035948		– 0.0414
1.3	– 0.026419	– 0.026592		
1.4	– 0.020773	– 0.019982		

[a] Close-coupling results of Oza [14].

[b] Harris-Nesbet method, Gien [15].

TABLE IV. Convergence of ^3P phase shifts (radians) for electron-helium ion for $k = 0.1$.

N	β	γ	δ	η
0	0.90			0.19981
4	1.20	1.65	1.94	0.21332
10	1.80	1.65	1.84	0.21500
20	1.30	1.75	1.94	0.21511
35	1.30	1.75	1.94	0.21516

obtained in [5] with 220 terms in the correlation function, but without polarization term. Again, we find that the results are comparable to those obtained in [5] with longer expansions in the correlation function. This indicates that very long expansions do give fairly accurate results. We compare the present results with the pseudostate close-coupling results of Oza [14] and the results of Gien [15] obtained using the Harris-Nesbet method.

Fairly accurate results have been obtained by 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, especially when it is necessary to carry out the calculations in quadruple precision to obtain accurate results. The main purpose of the variation of the nonlinear parameters is to obtain the largest value of the phase shift.

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

The main aim of the 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.

TABLE V. ^3P phase shifts η (radians) for electron-helium ion, $N = 20$.

k	Present η	η_{PQ}	η(Oza)[a]	η(Gien)[b]
0.1	0.21516	0.21516	0.2148	
0.2	0.21683	0.21681	0.2165	0.217
0.3	0.21945	0.21944	0.2192	0.219
0.4	0.22283	0.22283	0.2226	0.223
0.5	0.22662	0.22661	0.2263	
0.6	0.23088	0.23048	0.2302	0.230
0.7	0.23417	0.23415	0.2337	
0.8	0.23753	0.23744	0.2368	0.237
0.9	0.24038	0.24008	0.2393	0.240
1.0	0.24205	0.24202	0.2412	0.242
1.1	0.24323	0.24322		
1.2	0.24379	0.24378		
1.3	0.24370	0.24370		
1.5	0.24261			

[a] Close-coupling results of Oza [14].

[b] Harris-Nesbet method, Gien [15].

TABLE VI. ^3P and ^1P phase shifts (radians) for electron-helium ion in the resonance region, $N = 20$.

Incident energy	$\eta(^3P)$	Incident energy	$\eta(^1P)$
2.30	0.2426352	2.58	0.0320292
2.32	0.2426888	2.60	0.0902568
2.33	0.2427454	2.605	0.1412791
2.35	0.2426462	2.61	0.3382261
2.38	0.2432013	2.613	1.0553706
2.40	0.2435423	2.615	2.2412107
2.41	0.2438905	2.617	2.6999855
2.42	0.2444182	2.619	2.8625805
2.43	0.2454991	2.6195	2.8857529
2.44	0.2470834	2.6197	2.8939338
2.45	0.2493821	2.621	2.9363176
2.46	0.2547154	2.625	3.0017527
2.47	0.2719629	2.63	3.0420385
2.472	0.2813351	2.64	3.0792809
2.474	0.2979640		
2.476	0.3358026		
2.478	0.5025307		
2.479	1.4022793		
2.48	3.0426651		
2.481	3.2177122		
2.482	3.2738246		
2.484	3.309042		
2.486	3.326290		
2.488	3.335755		
2.49	3.3517906		
2.50	3.3830000		

IV. RESONANCES

Doubly excited states or Feshbach resonances or autoionization states have been studied extensively [7,8,16,17]. The resonance parameters can be inferred by calculating phase shifts at energies where a rapid change in phase shifts is observed. The phase shifts for the ^3P and ^1P in the resonance regions are given in Table VI. Here we have used only 20 terms in the correlation function. They are fitted to the Breit-Wigner form to obtain the resonance parameters,

$$\eta_{\text{calc.}}(E) = \eta_0 + AE + \tan^{-1}\frac{0.5\Gamma}{(E_R - E)}, \tag{24}$$

where $E = k^2$ is the incident energy, $\eta_{\text{calc.}}$ are the calculated phase shifts, and η_0, A, Γ, and E_R are the fitting parameters. E_R is the resonance position and Γ is the resonance width. A good way to determine resonance parameters from the phase shifts in the resonance region is to minimize the sum of squares of the difference between the left and right sides of Eq. (24), the difference being calculated at resonance energies given in Table VI. The results of the fit are given in Table VII and they are compared with the previous calculation of Bhatia and Temkin [16,17]. We get for ^3P resonance position at 58.3226 eV with respect to the ground state of the helium atom and width equal to 0.008 317 eV compared to 58.3209 eV for the position [16] and 0.008 90 eV [16] for the width, respectively. The latter results were obtained by using the Feshbach projection operator formalism [6]. The agreement is

TABLE VII. Resonance parameters (eV) of ^3P, ^1P in He atom and of ^3P in hydrogen ion, and comparison with the results of various calculations and experiments.

^3P He		^1P He		^3P H$^-$	
Position	Width	Position	Width	Position	Width
58.3226[a]	0.00832[a]	60.1450[a]	0.03560[a]	9.7399[a]	0.00631[a]
58.3209[b]	0.00890[b]	60.1450[b]	0.0363[b]	9.7385[b]	0.0063[b]
58.3599[c]	0.01064[c]	60.2687[c]	0.04375[c]	9.741[d]	0.0071[d]
58.3209[e]	0.00813[e]	60.1456[f]	0.0371[f]	9.73805[g]	0.005796[g]
		60.1765[h]	0.0382[h]		

[a] Present results; resonances in He are with respect to the ground state of He atom and the resonance in hydrogen ion is with respect to the ground state of the hydrogen atom.
[b] Feshbach formalism [16].
[c] Close-coupling approximation [21].
[d] Close-coupling with correlations [22].
[e] Complex-rotation method [23].
[f] Complex-rotation method [24].
[g] Complex-rotation method [24].
[h] Pseudopotential method [25].

TABLE VIII. ^3P phase shifts for electron hydrogen in the resonance region, $N = 20$.

E	η
0.700	0.442647
0.710	0.465710
0.713	0.509599
0.714	0.546607
0.715	0.687203
0.7151	0.720258
0.7152	0.762370
0.7153	0.817625
0.7155	0.999264
0.7157	1.398412
0.7159	2.175179
0.7162	2.968384
0.7165	3.217367
0.7167	3.295281
0.718	3.463877
0.719	3.497541
0.720	3.514710
0.722	3.532638
0.724	3.541605
0.725	3.546689
0.726	3.549036
0.729	3.555882
0.730	3.557156
0.735	3.562830

quite good, considering that only 20 terms have been used in the correlation function in the present calculation compared to 84 terms in [16], and corrections due to neighboring resonances, bound states, and the continuum need not be calculated separately in the present calculation. The ^1P results have been determined accurately from photoabsorption experiments [18,19]. The present results for position and width, 60.145 and 0.0356 eV, respectively, are very close to those obtained earlier [16] by using the Feshbach projection operator formalism [6]. The present results are within the range of experimental results [18] which are 60.130 ± 0.015 eV for the position and 0.038 ± 0.004 eV for the width. The line-shape parameter q for a resonance which is the result of the photoabsorption is given by

$$\sigma_a = \sigma_B(q+\varepsilon)^2/(1+\varepsilon^2), \tag{25}$$

where

$$\varepsilon = (E - E_R)/(0.5\Gamma). \tag{26}$$

The quantity σ_B is the background cross section .The line-shape parameter can be determined by noticing where the cross section σ_a goes to zero. This gives us $q = -2.533$ which is within the ranges of the experimental values -2.80 ± 0.004 [18] and -2.55 ± 0.16 [19]. The value obtained for q in [16] is -2.2910. Again, it should be emphasized that this calculation has *only* 20 terms in the correlation function and there is no need to calculate separately the various quantities given in [16,17].

We also calculate the ^3P resonance state in H$^-$. The phase shifts obtained using 20 terms are given in Table VIII. They are fitted to the Breit-Wigner form given in Eq. (24). We obtain, with respect to the ground state of the hydrogen atom, 9.7399 eV for the position of the resonance and 0.006 31 eV for the width. This should be compared to 9.7385 and 0.0063 eV, obtained in [16], where 84 terms were used in the correlation function. The present results are also given in Table VII. This resonance state has been observed by McGowan [20] who gets 9.73 eV for the position and 0.01 eV for the width. The line-shape parameter q obtained in this calculation is -2.62. However, there is no experimental value available for this parameter.

Figures 1 and 2 show the ^3P and ^1P resonances in He and Fig. 3 shows the ^1P resonance in hydrogen negative ion. In all the cases, we see that the phase shifts on either side of the resonance differ by π radians.

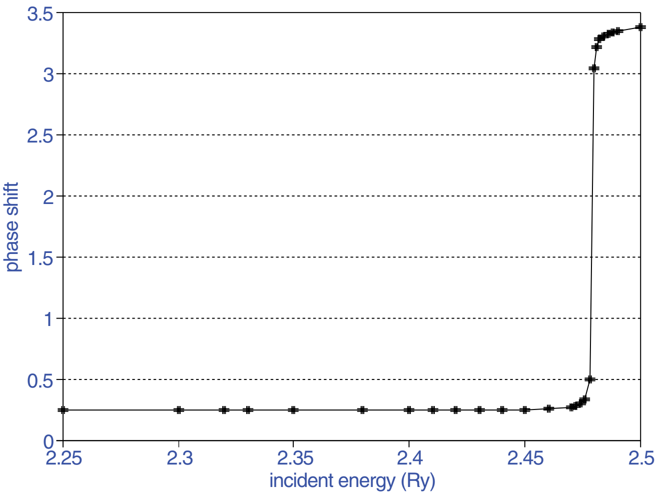

FIG. 1. (Color online) The lowest ^3P resonance state in a helium atom at 58.3226 eV with respect to the ground state of the helium atom. The phase shifts (radians) are for the scattering of an electron from a helium ion.

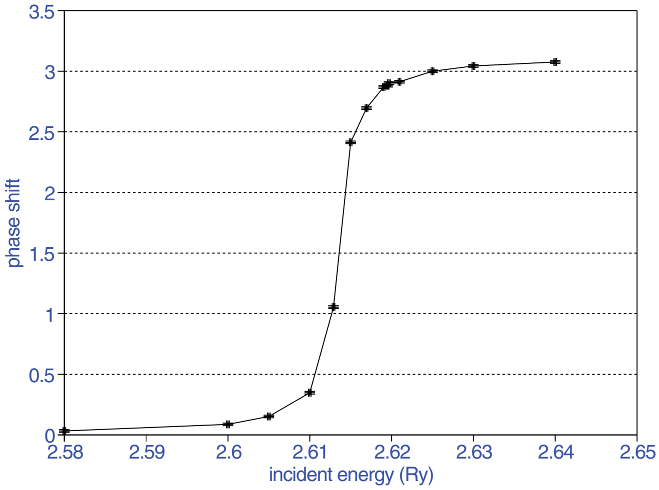

FIG. 2. (Color online) The lowest ^1P resonance state in a helium atom at 60.145 eV with respect to the ground state of the helium atom. The phase shifts (radians) are for the scattering of an electron from a helium ion.

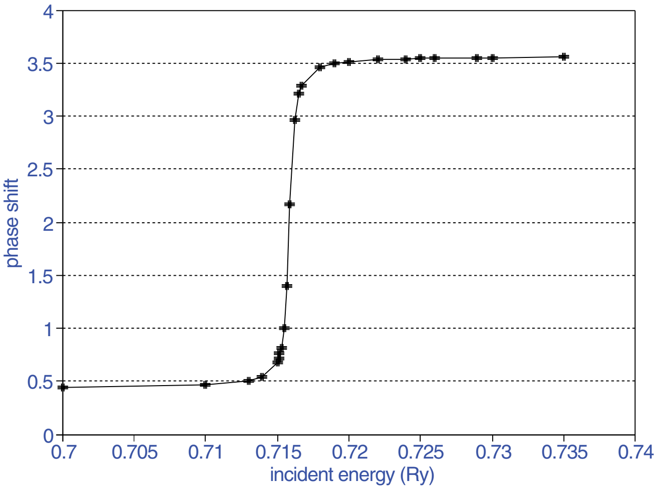

FIG. 3. (Color online) The lowest ^3P resonance in a hydrogen negative ion at 9.7399 eV. The resonance position is with respect to the ground state of the hydrogen atom. The phase shifts (radians) are for the scattering of an electron from a hydrogen atom.

To convert resonance parameters to eV, reduced Rydberg $R_M = 13.603976$ eV is used for resonances produced by photoabsorption while $R_\infty = 13.605\ 826$ eV is used for resonances produced by electron impact on the target; see the Appendix in [16] for details.

We also compare in Table VII the present results with the results obtained from other calculations. Burke and McVicar [21] carried out calculations in the $1s$-$2s$-$2p$ close-coupling approximation. Their results for the ^3P and ^1P resonances in the He atom are much higher compared to the present results as well as compared to the projection-operator results [16]. Calculations have been also been carried out by Ho [23,24] using the complex-rotation method and results obtained are given in Table VII; they are in good agreement with the present results. Martin *et al.* [25] used a pseudopotential method to calculate ^1P resonance in He and their results for the position and width are again much higher than the present results.

The ^3P H$^-$ resonance position and width obtained in the present calculations are compared with those obtained from the projection operator formalism [16], 15-state R-matrix calculation [22], and the complex-rotation method. The agreement between the results obtained from the various approaches is quite good.

V. CONCLUSIONS

In conclusion, we have applied the hybrid theory, in the presence of an optical potential, in which long-range and short-range correlations, Eq. (13), have been taken into account at the same time. The present results have been calculated variationally and therefore have lower bounds to the exact phase shifts, and they are close to those obtained in Ref. [5], using the Feshbach projection operator formalism. In the present calculation, shorter expansions of *only* 20 terms are needed in the correlation function to get results comparable in accuracy to those obtained in [5] with 220 terms. Accurate resonance parameters have also been obtained using short expansions and they agree well with those obtained using the Feshbach formalism, the close-coupling approach, the R-matrix calculation, and the complex-rotation method. The calculation in [16,17] is far more complicated than the present calculation which has the potential to give accurate results.

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