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Variational Calculations on Electron-Helium Scattering*

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Calculations have been made on the elastic scattering of low-energy electrons by helium using a variational procedure which takes polarization and correlation effects into account by means of continuum Bethe–Goldstone equations. The convergence of the results is examined using two methods to obtain a complete set of basis functions. Results for the s, p, d, and f waves are presented. The width of the ^2S closed-channel resonance below the $n=2$ threshold is found to be 0.015 eV, in comparison with the 0.015–0.020-eV estimates of Andrick and Ehrhardt from experiment and the 0.01-eV estimate of Simpson and Fano.

I. INTRODUCTION

Interest in the application of variational methods to scattering problems has recently been revived by Harris and collaborators[1] and Nesbet.[2] The advantage of the algebraic expansion method lies in the ease with which polarization and correlation effects can be taken into account. However, as the approach is based mainly on representing the trial wave function as a linear expansion over basis functions, it is important to check that these functions form a complete set and that the results are convergent. The problem has been investigated by Schwartz[3] in his pioneering work on electron-hydrogen collision, using the Hylleraas type of function for H$^-$ to describe the closed-channel part of the scattering. The choice is indeed very good as might be anticipated, because it is well known that the corresponding Hylleraas function of He gives a good description of the correlation effect. For atomic systems with more than two electrons it is much more difficult to obtain the wave functions with the Hylleraas method and it is usually better to use the configuration-interaction method. However, it has long been recognized that, to obtain the same degree of accuracy with the configuration-interaction method, many more terms are needed in the expansion over basis functions. It is therefore important that, if the variational approach is to be applied to the study of electron scattering by targets other than hydrogen, the problem of convergence should be further investigated.

The aim of the present work is twofold: first, to study the convergence of the calculations using two methods to obtain a complete set of basis functions; and second, to examine the contribution of polarization and correlation effects in electron-atom scattering using the Bethe–Goldstone method to describe these interactions. The plan of this paper is as follows. In Sec. II we discuss briefly the theory of electron-atom scattering using the variational approach. Section III describes an investigation of the convergence of the calculations using two methods to choose sets of basis functions. The results of the calculations on electron-helium scattering are given in Sec. IV, and we summarize our conclusions in Sec. V. The present work extends variational calculations previously reported by Michels *et al.*[1] by carrying the orbital expansion to practical completeness and by including f-wave results.

II. THEORY

The scattering of an electron by an N-electron atom is described by a stationary-state wave function

$$\Psi=\sum_p \mathfrak{A}\Theta_p\psi_p+\sum_\mu \Phi_\mu c_\mu . \qquad (1)$$

Here Θ_p is a normalized N-electron wave function for the electronic stationary state of the target atom corresponding to scattering channel p; ψ_p is the one-electron channel wave function for an open channel with angular momentum l_p and wave-vector magnitude k_p (kinetic energy $\frac{1}{2}k_p^2$ in Hartree atomic units); Φ_μ is one of an assumed orthonormal set of $(N+1)$-particle Slater determinants that constitute the Hilbert-space component of Ψ. The operator $\mathfrak{A}$ antisymmetrizes $\Theta_p\psi_p$ and includes the factor $(N+1)^{-1/2}$ required to give the antisymmetrized function the same relative normalization as an $(N+1)$-electron Slater determinant.

The Slater determinants, defined in terms of an N-electron reference-state determinant Φ_0, are exemplified by

$$\Phi^a=\det\phi_1(1)\cdots\phi_i(i)\cdots\phi_j(j)\cdots\phi_N(N)\phi_a(N+1).$$

$$\Phi_i^{ab}=\det\phi_1(1)\cdots\phi_a(i)\cdots\phi_j(j)\cdots\phi_N(N)\phi_b(N+1), \quad (2)$$

$$\Phi_{ij}^{abc}=\det\phi_1(1)\cdots\phi_a(i)\cdots\phi_b(j)\cdots\phi_N(N)\phi_c(N+1),$$

where an assumed denumerable set of one-electron orbital functions is subdivided into orbitals ϕ_i, ϕ_j, ... occupied in Φ_0, and orbitals ϕ_a, ϕ_b, ... that are orthogonal to the occupied set; det means antisymmetrization and normalization appropriate to the number of electrons. The orbitals are quadratically integrable functions of space and spin variables, normalized to unity. An assumed Hilbert space of orbitals and assumed reference state Φ_0 generate a uniquely defined $(N+1)$-electron Hilbert space $\{\Phi_\mu\}$ through Eq. (2) if indices are ordered by the convention

$$i<j<\cdots\leq N<a<b\cdots . \tag{3}$$

The general computational procedure of successive variational calculations using nested subspaces in a lattice decomposition of the Hilbert space $\{\phi_\mu\}$ has been described elsewhere.[4] The computational procedure is equivalent to variational solution of a hierarchy of continuum Bethe–Goldstone equations.[5] The use of the Bethe–Goldstone formalism in electron-atom scattering was originally proposed by Mittleman.[6]

The channel wave function is of the form

$$\psi_p=f_p(r)Y^{m_{lp}}_{l_p}(\theta,\ \phi)v_{m_{sp}}, \tag{4}$$

where f_p satisfies the usual bound-state boundary condition at $r=0$, is orthogonal (by construction) to all radial functions for Hilbert-space orbitals $\{\phi_i;\ \phi_a\}$ with the same angular and spin quantum numbers, and has the asymptotic form

$$f_p(r)\sim k_p^{-1/2}r^{-1}\sin(k_pr-\tfrac{1}{2}l_p\pi+\delta_p). \tag{5}$$

Here Y^m_l is a normalized spherical harmonic and v is an elementary spin function. Equation (5) can be written in the form[2]

$$f_p=\alpha_{0p}S_p+\alpha_{1p}C_p, \tag{6}$$

where

$$\begin{aligned} S_p&\sim k_p^{-1/2}r^{-1}\sin(k_pr-\tfrac{1}{2}l_p\pi),\\ C_p&\sim k_p^{-1/2}r^{-1}\cos(k_pr-\tfrac{1}{2}l_p\pi). \end{aligned} \tag{7}$$

The functions are constructed to satisfy the same boundary and orthogonality conditions as f_p.

The target-atom wave function Θ_p is expressed as

$$\Theta_p=\textstyle\sum_\sigma\Phi_\sigma c^p_\sigma, \tag{8}$$

where each Φ_σ is a normalized N-electron Slater determinant constructed from the orbital functions $\{\phi_i;\ \phi_a\}$. The coefficients c^p_σ are obtained as a normalized eigenvector of the N-electron configuration interaction matrix $H_{\sigma\sigma'}$, corresponding to energy eigenvalue E_p. If E is the total energy of the system, an open-channel k value is defined by

$$\tfrac{1}{2}k_p^2=E-E_p, \tag{9}$$

for energies in Hartree atomic units, if $E-E_p$ is non-negative. The operator H is the nonrelativistic Schrödinger Hamiltonian, either for N or for $N+1$ electrons, according to context here.

In the present procedure both the target wave functions and the closed-channel part of the continuum functions with the same symmetry are constructed from the same sets of basis orbitals.

Let us consider, for example, the d-wave elastic scattering of electrons by helium, which is described in the calculation by sets of s, p, d, and f orbitals. In the static-exchange calculation the channel taken into account is $1s^2\tilde{d}$, where the tilde indicates the continuum function. In the Bethe–Goldstone calculation with the virtual excitation of one electron from the ground state, the following additional channels are included:

$$1s2p\begin{Bmatrix}\tilde{p}\\ \tilde{f}\end{Bmatrix},\quad 1s\bar{p}\begin{Bmatrix}\tilde{p}\\ \tilde{f}\end{Bmatrix},\quad 1s\bar{d}\tilde{s},\ \text{etc.},$$

where the bar over the character denotes a pseudostate. In this way, not only excited states of the target are allowed for, but polarization can be taken into account too by including the corresponding pseudostates in the sets of basis orbitals. Moreover, as the coefficients in the expansion on the trial wave function over basis orbitals are energy dependent [see Eqs. (8)–(12)], the procedure describes polarization and correlation in a dynamic form.

The linearity of the Schrödinger equation makes it possible to express Eq. (1) in the form

$$\Psi=\sum_I\sum_p\alpha_{Ip}\Big(\sum_\sigma\Phi^{Ip}_\sigma c^p_\sigma+\sum_\mu\Phi_\mu c^{Ip}_\mu\Big), \tag{10}$$

where the coefficients α_{Ip}, with $I=0$, 1, are defined in Eq. (7), and the coefficients c^p_σ are the target-state eigenvector coefficients of Eq. (8). The coefficients c_μ of Eq. (1), which are to be determined by the variational scattering calculation, are expanded as[2,3]

$$c_\mu=\sum_p(\alpha_{0p}c^{0p}_\mu+\alpha_{1p}c^{1p}_\mu). \tag{11}$$

The unnormalized $(N+1)$-electron Slater determinants Φ^{Ip}_σ are defined by

$$\Phi^{0p}_\sigma=\mathfrak{a}\Phi_\sigma S_p,\quad \Phi^{1p}_\sigma=\mathfrak{a}\Phi_\sigma C_p. \tag{12}$$

It is convenient to define the $(N+1)$-electron unnormalized functions as

$$\Theta^{Ip}=\sum_\sigma\Phi^{Ip}_\sigma c^p_\sigma. \tag{13}$$

These definitions make it possible to apply the multichannel variational method[2] to the general wave function given by Eq. (1) or (10). The present calculations use a modified version of the multichannel Kohn variational method, to be described in detail elsewhere.[7] This modified method is referred to as the "optimized anomaly-free" (OAF) method. The asymptotic normalization indicated in Eq. (5) is appropriate to this method. The principal computational step in this method is construction of the auxiliary matrix m^{pq}_{ij}, from which K-matrix elements are determined. This matrix is defined by

$$m^{pq}_{ij}=M^{pq}_{IJ}-\sum_\mu\sum_\nu M^p_{I\mu}(M^{-1})_{\mu\nu}M^q_{\nu J}, \tag{14}$$

where $i=I$, $j=J$ with values 0, 1 as in Eq. (10), and p, q are open-channel indices. Here M denotes $H-E$, where H is the $(N+1)$-electron Hamiltonian. The matrices combined in Eq. (14) are the bound-bound matrix (Hermitian)

$$M_{\mu\nu} = H_{\mu\nu} - E\delta_{\mu\nu}, \tag{15}$$

where

$$H_{\mu\nu} = (\Phi_\mu, H\Phi_\nu), \tag{16}$$

the bound-free matrix (Hermitian)

$$M^{p}_{\mu I} = (\Phi_\mu, (H-E)\Theta^{Ip}), \tag{17}$$

and the free-free matrix (non-Hermitian)

$$M^{pq}_{IJ} = (\Theta^{Ip}, (H-E)\Theta^{Jq}). \tag{18}$$

III. CHOICE OF BASIS FUNCTIONS

A serious shortcoming of the variational procedure is that the approach does not satisfy minimum principles[8,9] and this may lead to serious difficulties. There is no rigorous way for choosing the set of basis functions used for linear expansion of the trial wave function except by trying different sets to find the stationary value of the phase shift. Consequently, care must be taken to ensure that the basis functions used form a complete set and that the results are convergent. Moreover, it is important to check that anomalous or completely erroneous results are not obtained.[3]

We now describe the procedure we have adopted in choosing the set of basis functions and consider the $e^-+\mathrm{He}$ s-wave elastic scattering as a test case. Let the one-electron orbital be represented in the form

$$\Phi_i = Nr^n e^{-\alpha r} Y_{lm}(\hat{r}). \tag{19}$$

To test the convergence of the results, we have tried two methods of choosing the set of basis functions: (a) a sequence of exponents α *decreasing* in geometric progression for a fixed order n, together with a sequence of exponents α *increasing* in arithmetic progression for the same order n; (b) a sequence of exponents α *increasing* in geometric progression for a fixed order n, together with a sequence of a *constant* exponent α with *increasing* higher orders of n.

It has been shown by Muntz[10] that a set of basis functions with only the exponents α in increasing geometric progression for a fixed order n does not form a complete set. For this reason, we have chosen the methods mentioned above to choose the basis functions[11] and it can be shown that both methods would give a complete set. The results are first checked that they converge with the geometric sequence before superimposing the arithmetic sequence in the case (a), or the sequence of higher powers of n in the case (b). The rate of convergence is examined by increasing the number of the basis functions used for different l states at the same time. Moreover, we choose functions that have maximum values at the same R_0 defined by

$$R_0 = \frac{n}{\alpha}\;;\quad \frac{d\phi_i}{dr} = 0 \quad \text{at } r = R_0$$

for different values of the quantum number l. The target states of the He atom are taken into account to the zeroth order by adding to the set (a) or (b) the orbitals $n=1$, $\alpha=2.0$, for the ground state; $n=2$, $\alpha=0.5$ for the $2s$ state; $n=2$, $\alpha=0.5$, 2.0 for the $2p$ and the pseudostate $2\bar{p}$; and $n=3$, $\alpha=2.0$ for the pseudostate $3\bar{p}$. It should be noted also that if, when adding the basis functions, the values are close to those of the target states, they are replaced by the corresponding exponents in the next-higher power of n. It is to be noted that all basis orbitals of given l are combined in each computed function.

Several geometric ratios have been tried to determine the one which gives the best convergence for the geometric sequence. An extremely small ratio is usually avoided, because it would give no effect at all because of the incompleteness of the geometric sequence. For method (a), the ratio is found to be 0.5 and the series for the s orbitals is $n=1$, $\alpha=1.0$, 0.5, 0.25, 0.125, 0.0625; for the p orbital $n=2$, $\alpha=1.0$, 0.25, 0.125, 0.0625 and $n=3$, $\alpha=0.75$. (Since for $n=2$, $\alpha=0.5$ is already used to describe the target $2p$ state, we take the term into account by including the corresponding term in the $3p$ state.) For the arithmetic sequence, we have used several arithmetic differences λ. For example, for $\lambda=0.6$, the arithmetic series for the s orbitals is $n=1$, $\alpha=0.7$, 1.3, 2.7, ..., and $n=2$, $\alpha=2.0$. (The orbital $n=1$, $\alpha=2.0$ is already included, so we use the corresponding value of $n=2$ and $\alpha=4.0$.) The corresponding arithmetic sequence for the p orbital is $n=2$, $\alpha=1.4$, 2.6, 4.0, 5.4, ... We show in Figs. 1 and 2 the s-wave results for $k=0.1$ and

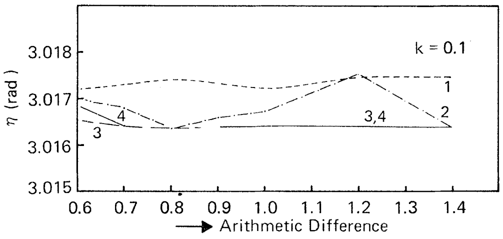

FIG. 1. Variation of the phase shift for s-wave scattering with the number of terms used in the arithmetic sequence of given arithmetic difference λ. The number of terms is indicated on the graphs. The geometric sequence included is given in text.

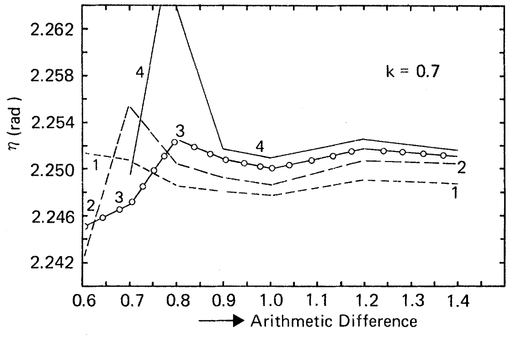

FIG. 2. Variation of the phase shift for s-wave scattering with the number of terms used in the arithmetic sequence of given arithmetic difference λ. The number of terms is indicated on the graphs. The geometric sequence included is given in text.

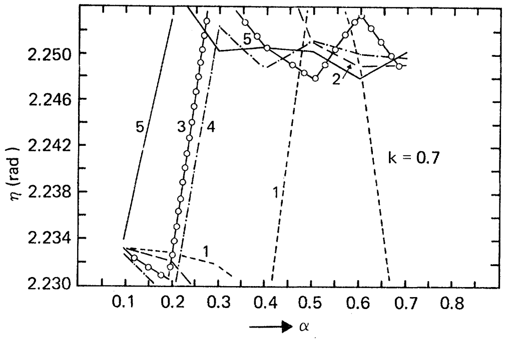

FIG. 4. Variation of the phase shift for s-wave scattering with the number of terms used in the r^n sequence with a fixed exponent α. The number of terms used is indicated on the graphs, starting with $n=2$ for both s and p orbitals. The arithmetic sequence included is given in text.

0.7, respectively. It is seen that the phase shifts are quite stationary as a function of λ. However, for $k=0.7$ anomalous results occur for $\lambda < 0.9$.

For method (b), the geometric ratio used is 2.0 and the geometric sequence for the s orbital is $n=1$, $\alpha=0.9$, 3.6, 7.2, and $n=2$, $\alpha=3.6$ (the function $n=1$, $\alpha=1.8$ is replaced by the corresponding $n=2$, $\alpha=3.6$ because the ground-state term $n=1$, $\alpha=2.0$ is already used); and for the p orbital the sequence is $n=2$, $\alpha=7.2$, 14.4, and $n=3$, $\alpha=2.7$. The results converge rapidly since large exponents are used, i.e., very-short-range functions. To complete the set of basis functions, we use a sequence of a constant exponent α with increasing higher powers of n with $n=3$, 4, 5, ... for both s and p orbitals. We show in Figs. 3 and 4 the convergence of the calculations with the same number of terms used in the sequence for s and p orbitals. A comparison of the results indicates that although the "stationary" values of the phase shifts obtained with methods (a) and (b) agree to the third significant figure, the first method gives more consistent results, and it is the method we have adopted for choosing the basis functions in the subsequent calculations.

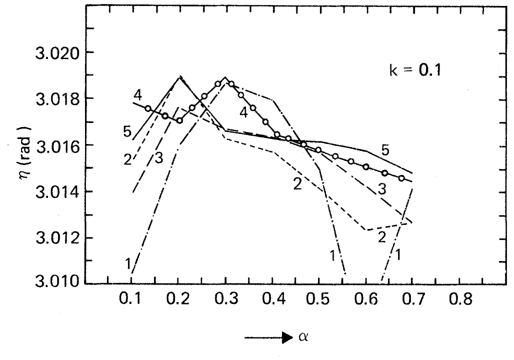

FIG. 3. Variation of the phase shift for s-wave scattering with the number of terms used in the r^n sequence with a fixed exponent α. The number of terms used is indicated on the graphs, starting with $n=2$ for both s and p orbitals. The arithmetic sequence included is given in text.

IV. RESULTS

A. Elastic Scattering from the Ground-State Atom

Extensive calculations have been made on the elastic scattering of low-energy electrons by helium for the s, p, d, and f waves. Table I shows the sets of basis functions used, and Table II the results of the calculations.

We compare in Fig. 5 our results for the s wave with previous calculations. Our results for the static-exchange calculations agree quite well with those of Burke, Cooper, and Ormonde,[12] who solved

TABLE I. Basis sets of orbitals of given l used for the different partial-wave scattering. Every orbital is of the form $\phi_i = N r^n e^{-\alpha r} Y_{lm}(\hat{r})$.

s wave	s	$n=1$, $\alpha=2.0$, 1.0, 0.5, 0.125, 0.0625, 1.3, 2.5, 3.7; $n=2$, $\alpha=0.5$
	p	$n=2$, $\alpha=0.5$, 2.0, 1.0, 0.25, 0.125, 0.0625, 2.6, 5.0, 7.4; $n=3$, $\alpha=2.0$, 0.75
p wave	s	$n=1$, $\alpha=2.0$, 1.0, 0.5, 0.25, 0.125, 0.0625, 0.7, 1.3; $n=2$, $\alpha=0.5$
	p	$n=2$, $\alpha=0.5$, 2.0, 1.0, 0.25, 0.125, 1.4, 2.6; $n=3$, $\alpha=2.0$, 0.75
	d	$n=3$, $\alpha=0.333$, 1.5, 0.75, 0.1875, 2.1, 3.9; $n=4$, $\alpha=0.5$
d wave	s	$n=1$, $\alpha=2.0$, 1.0, 0.5, 0.25, 0.125, 0.0625; $n=2$, $\alpha=0.5$
	p	$n=2$, $\alpha=0.5$, 2.0, 1.0, 0.25, 0.125, 0.7, 1.4; $n=2$, $\alpha=2.0$
	d	$n=3$, $\alpha=0.333$, 1.5, 0.1875, 1.05, 2.1; $n=4$, $\alpha=0.5$
	f	$n=4$, $\alpha=2.0$, 1.0, 0.5, 0.25, 0.125
f wave	s	$n=1$, $\alpha=2.0$, 1.0, 0.5; $n=2$, $\alpha=0.5$
	p	$n=2$, $\alpha=0.5$, 2.0, 1.0, 0.25, 0.125, 0.0625; $n=3$, $\alpha=2.0$
	d	$n=3$, $\alpha=0.5$, 1.5, 0.75, 0.1875, 0.09375; $n=4$, $\alpha=0.5$
	f	$n=4$, $\alpha=0.333$, 2.0, 1.0, 0.5, 0.25, 0.125; $n=5$, $\alpha=0.333$
	g	$n=5$, $\alpha=0.125$; $n=6$, $\alpha=0.125$

TABLE II. Partial phase shifts for *s*-, *p*-, *d*-, and *f*-wave scattering.

	η_0		η_1		η_2		η_3	
k(a.u.)	(i)[a]	(ii)[a]	(i)	(ii)	(i)	(ii)	(i)	(ii)
0.1	2.9936	3.0164	0.0061	0.0032	0.29-4[b]	0.42-3[b]	0.13-8[b]	0.13-3[b]
0.2	2.8473	2.8822	0.0035	0.0129	0.60-4	0.0016	0.10-6	0.31-3
0.3	2.7037	2.7459	0.0108	0.0297	0.15-3	0.0036	0.12-5	0.52-3
0.4	2.5675	2.6142	0.0239	0.0539	0.41-3	0.0064	0.70-5	0.95-3
0.5	2.4325	2.4836	0.0426	0.0847	0.0010	0.0097	0.28-4	0.0015
0.6	2.3107	2.3638	0.0671	0.1200	0.0021	0.0141	0.86-4	0.0023
0.7	2.1963	2.2518	0.0947	0.1567	0.0040	0.0197	0.21-3	0.0032
0.8	2.0956	2.1338	0.1248	0.1947	0.0066	0.0258	0.45-3	0.0043
0.9	1.9808	2.0426	0.1552	0.2311	0.0101	0.0322	0.84-3	0.0057
1.0	1.8900	1.9550	0.1844	0.2646	0.0143	0.0393	0.0014	0.0076
1.1	1.8055	1.8765	0.2103	0.2927	0.0191	0.0473	0.0022	0.0098

[a] (i) Static-exchange results. (ii) Results of static exchange with Bethe–Goldstone virtual excitation from the 1*s* state.

[b] The final signed integer indicates the power of ten by which the number must be multiplied.

the close-coupling equations using only the target states $n=1$ and $n=2$ of He, and also with those of Burke and Robb,[13] who used the R-matrix method with the $n=1$ target state only. When polarization and correlation effects are taken into account by the inclusion of the virtual excitation from the 1*s* state using the Bethe–Goldstone method, we find that the phase shifts are increased by about 3%. Our results then agree exactly with those of Callaway *et al.*,[14] who used the extended polarized orbital method. It might be of interest to point out that, if the assumed target states of helium had been exact, the calculations of Burke, Cooper, and Ormonde would satisfy the minimum principles and their results would be lower bounds. This would not be the case in the work of Callaway *et al.*, since only the first- or second-order terms were retained in the effective potentials.[15]

Figures 6 and 7 show the results for the p and d waves. Again, our static-exchange results are in close agreement with those of Burke and Robb, and our Bethe–Goldstone results with those of Callaway *et al.* To show the importance of the $l=3$ partial wave in the d-wave scattering, we display in Fig. 8 our results for static-exchange calculations and our Bethe–Goldstone calculations with and without the f orbitals. It will be seen that the inclusion of the f orbitals increases the phase shift appreciably. This results from the external closed-channel orbital of $l=3$ symmetry, required to represent the virtual polarization of the open-channel d wave, as a contribution to the dipole polarization potential. Figure 9 shows the results for the f-wave scattering, and finally Fig. 10 compares our total scatter-

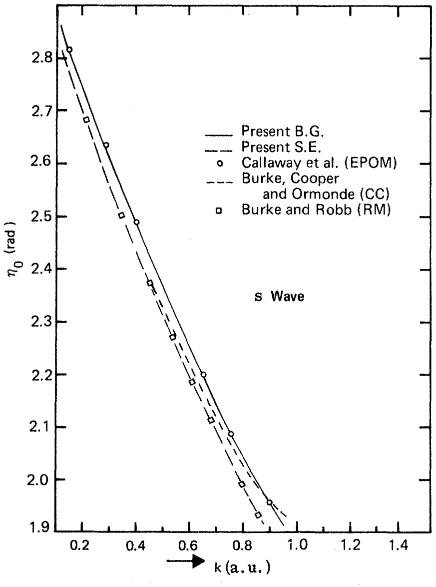

FIG. 5. *s*-wave phase shift.

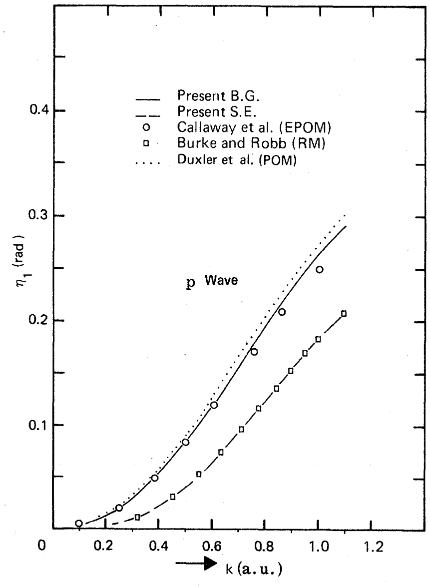

FIG. 6. *p*-wave phase shift.

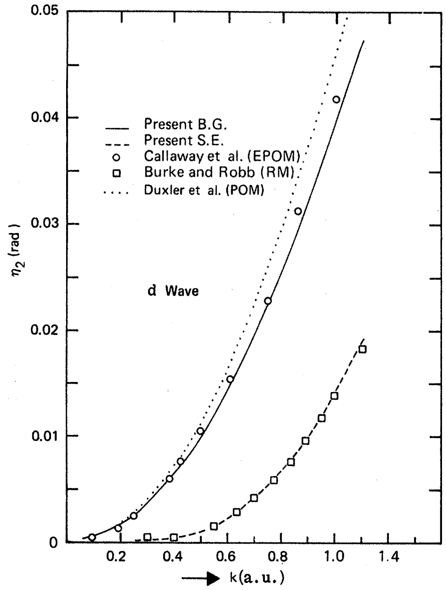

FIG. 7. *d*-wave phase shift.

ing cross sections with previous calculations and with the experiment of Golden and Bandel.[16]

Calculations have recently been made by Duxler, Poe, and LaBahn[17] using the polarized-orbital method (POM). Their results are in agreement with ours for the *s* wave, and are not shown in Fig. 5. Their results for the *p* and *d* waves are shown in Figs. 6 and 7. They are greater by up to 4% for the *p* wave at $k = 1.1$ a.u., and by about 10% for the *d* wave at $k = 1.1$ a.u.

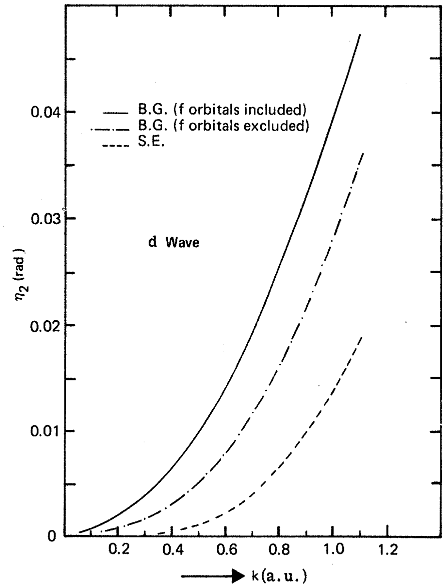

FIG. 8. *d*-wave phase shift for static-exchange calculations, and the Bethe–Goldstone calculations with and without the *f* orbitals.

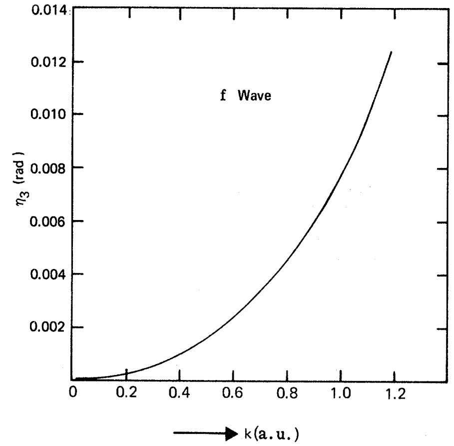

FIG. 9. *f*-wave phase shift.

B. ^2S Resonance

The search procedure for resonances[18] has been used to locate the resonance below the $n = 2$ level of helium. The set of basis functions used is given in Table I.

Our calculation shows a resonance at the energy of 19.4 eV with a width of 0.015 eV, while the close-coupling calculations of Burke, Ormonde, and Cooper[12] predict the resonance at 19.33 eV with a width of 0.039 eV. The exact width of the resonance has never been determined. Simpson and Fano[19] give an estimate of 0.01 eV, and Andrick and Ehrhardt[20] give the estimates of 0.015–0.020 eV from their experiment, while Gibson and Dolder[21] and Golden and Zecca[22] have both measured the width to be 0.008 eV. Our calculation is in closer agreement with the experiment of Andrick and Ehrhardt. Our work is also in quite good agreement with the recent calculation of Temkin *et al.*[23] using the projection-operator formalism of Feshbach. They obtain a width of 0.0144 eV.

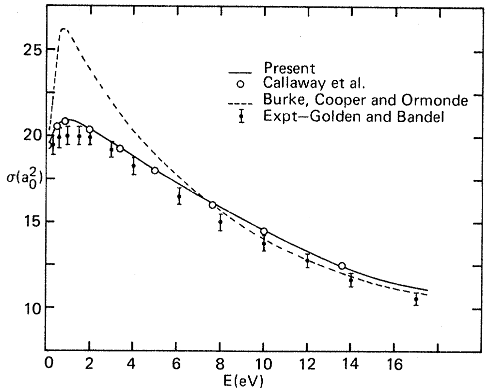

FIG. 10. Total elastic cross section.

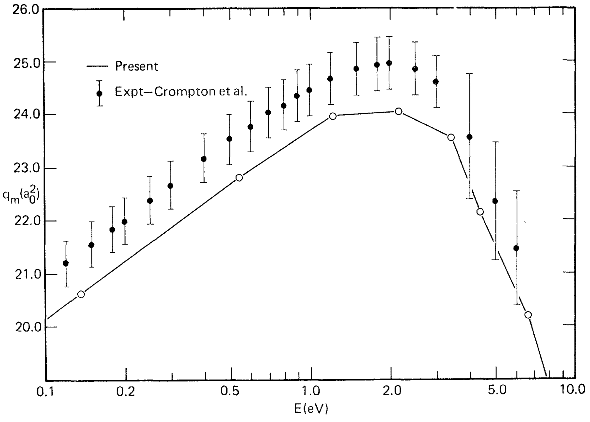

FIG. 11. Momentum-transfer cross section.

The fact that our calculation indicates the position of the resonance to be 19.4 eV rather than the experimental value of 19.3 eV is to be attributed to target correlation effects, which are not calculated correctly here. It should not be considered as evidence for a second resonance displaced from 19.3 eV. It has been suggested recently by Golden and Zecca[24] that there may be further structures in this energy region. The essential result of our calculations is that there is a unique resonance, of ^2S symmetry, below the $n = 2$ level. A search for resonances in other partial-wave channels shows none below the ^3S threshold, and furthermore, the calculations using a fine mesh in this energy region fail to indicate any structure apart from the ^2S resonance. A similar conclusion has also been reached by Temkin *et al.* In the opinion of Sanche and Schulz[25] the "observed" structure around 19.5 eV is a spurious one, and they believe it is "an echo of the $1s2s^2$ resonance."

C. Momentum-Transfer Cross Section

The momentum-transfer cross section has been computed from our phase shifts ($l = 0, 1, 2, 3$). Comparison with recent experimental data,[26] shown in Fig. 11, indicates excellent agreement. The small remaining discrepancy may be due to neglect of target-atom electronic correlation in our calculations.

V. CONCLUSION

It is found that the two methods of choosing the basis functions to obtain a complete set give the same stationary values for the phase shifts, but with the first method faster convergence is obtained.

The results for the elastic scattering of electrons by helium indicate that polarization and correlation effects can be taken into account by the use of the Bethe–Goldstone virtual excitation of a single electron from the ground state. With the inclusion of these effects in the calculations, there is better agreement between theory and experiment for the width of the ^2S resonance below the $n = 2$ level of helium. Finally, it is of interest to note that the present calculation is entirely an *ab initio* work, while the calculations of Callaway *et al.* and Duxler *et al.* use an empirical value of the ground-state polarizability of helium.

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Exact Calculation of the Second-Order Born Terms for Proton-Hydrogen Electron-Transfer Collisions*

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The four second-order terms in the Born series for the proton-hydrogen electron-transfer problem are analytically reduced from six-dimensional to three-dimensional integrals. No mass approximations are made. This permits an accurate numerical calculation of the total cross section to second order. Numerical results are given from 0.1 to 2.5 MeV. The complete second-order cross section reduces the first-order results by 30% from 1 to 2.5 MeV. The various first- and second-order Born approximations for this problem are discussed.

I. INTRODUCTION

One of the most basic and widely studied three-body rearrangement processes is that of resonant proton-hydrogen electron-transfer collisions.[1] In an early classical analysis of the problem, Thomas[2] described the collision process as a two-step interaction and found that the total cross section behaved as $E^{-5.5}$ at high energy, where E is the energy of the incident proton. At about the same time, Oppenheimer[3] and Brinkman and Kramers[4] performed a quantum-mechanical calculation leading to a cross section sharply peaked in the forward direction ("pickup" process) with a high-energy behavior of E^{-6}. They used an abbreviated form of the first-order Born approximation which neglected the proton-proton interaction. This neglect is justified in the expected high-energy region of validity of the first-order Born approximation by the large proton-electron mass ratio which allows a classical description of the internuclear motion.

The neglect of the proton-proton interaction was disputed by Bates and Dalgarno[5] and by Jackson and Schiff.[6] The latter have shown that inclusion of this interaction for forward-scattering angles reduces the Brinkman–Kramers cross section at all energies and, in the high-energy limit, by a factor of 0.661. In this approximation, the energy dependence of the cross section remains as E^{-6}.

Mapleton[7] has pointed out that Jackson and Schiff erred in neglecting the contribution to the proton-proton interaction from backward-scattering angles ("knockout" process). Including this, he shows that for resonant systems at high energy the total cross section behaves as E^{-3}. However, due to the small coefficient of the E^{-3} term, the Jackson–Schiff cross section is not in error until around 50 MeV, and the E^{-3} behavior is not approached until well over 100 MeV, a region where relativistic corrections must be considered.[8] It is interesting to note that for the resonant positron-positronium system the E^{-3} behavior is readily apparent at an energy of only 200 eV.[9]

The four second-order terms of the Born approximation were first investigated by Drisko in the high-energy limit.[10] For forward-scattering angles, he found that the first-order proton-proton interaction was cancelled by some of the second-order terms. The total cross section then behaved as $E^{-5.5}$ at high energy as predicted classically by Thomas. However, he did not consider backward scattering, and his arguments need modification in that region. Also, the coefficients of the second-order terms are such that they do not dominate the first-order terms at forward-scattering angles until 50–100 MeV.

The question of the convergence of the Born series for rearrangement collisions has been raised by Aaron *et al.*[11] Their proof of nonconvergence dealt with a divergence of the Green's-