PHYSICAL REVIEW A VOLUME 9, NUMBER 5 MAY 1974

Scattering of electrons by hydrogen atoms at intermediate energies*

Joseph Callaway and John W. Wooten
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803

(Received 27 November 1973)

The algebraic variational method has been applied to the scattering of electrons by hydrogen atoms at intermediate energies. The atom was represented by an eleven-state expansion, including exact 1*s*, 2*s*, 2*p*, and 3*d* states plus seven pseudostates. The pseudochannels are allowed to be open. Results are presented for 1*s*-2*s* and 1*s*-2*p* excitations for energies between 10 and 12 eV, and for 1*s*-1*s* elastic scattering from 10 to 30 eV.

I. INTRODUCTION

The scattering of electrons by atoms at intermediate energies is a topic of much interest at present. This work is an application of the algebraic variational method[1,2] to electron-hydrogen scattering in the energy range 10–30 eV. The atomic states are described in terms of pseudostates[3,4] and the pseudochannels are allowed to be open. The general theory of this approach has been outlined elsewhere,[5] and some preliminary results have been reported.[6]

Previous pseudostate calculations for the electron-hydrogen system have emphasized the low-energy region below the $n=2$ threshold at 10.2 eV,[4,7] and the region between the $n=2$ and $n=3$ excitation thresholds.[8] In these calculations all pseudochannels are closed. Two studies have been reported in which pseudochannels are open.[9,10] In the first of these calculations,[9] the excitation of the 2*s* and 2*p* levels was studied using the three-state close-coupling expansion, supplemented by an *s* and a *p* pseudostate with energies of 13.6 eV. The second calculation of this nature[10] employed three *s*-type pseudostates in addition to the exact 1*s* and 2*s* atomic states in an investigation of the convergence of the pseudostate expansion for states with $L=0$ and $S=0$.

In the present work, the exact 1*s*, 2*s*, 2*p*, and 3*d* states are supplemented by three additional *s*-type pseudostates, three additional *p*-type pseudostates, and a single *d* pseudostate, giving an eleven-state expansion. The parameters of the pseudostates are varied in order to avoid the unphysical pseudoresonances which may exist below the pseudostate thresholds.[10]

II. PROCEDURE

Let us denote the channels relevant to the electron-atom scattering problem by the symbol Γ_i. The quantum numbers which specify Γ_i include the conserved quantum numbers describing the total orbital angular momentum, spin, and parity; the orbital angular momentum of the atomic state and of the scattered electron; and all other numbers (γ_a) required to determine the atomic state. Insofar as is convenient, we will use the notation of Burke.[11] The total wave function is expressed as

$$\Psi(\Gamma_j, x_1, x_2) = (2)^{-1/2}(1-P_{12}) \sum_{\Gamma_i} \psi(\Gamma_i, \vec{x}_1, \hat{r}_2, \sigma_2) F_{ij}(r_2) \tag{1}$$

in which $\vec{x}_i$ denotes the space and spin coordinates $(\vec{r}_i, \sigma_i)$ of particle *i*; the function ψ is formed from the radial atomic function $R(l_a, \gamma_a, \vec{r})$, combined with spin and angular momentum functions for both electrons so as to form a state of quantum numbers Γ_i. The incident channel is specified by Γ_j. The operator P_{12} interchanges coordinates and spins of both electrons. The radial function F_{ij} describes channel *i* when an electron is incident in channel *j* and obeys the specified boundary conditions

$$F_{ij}(r) \xrightarrow[r\to 0]{} a_{ij}\, r^{l_i}\ , \tag{2a}$$

$$rF_{ij} \xrightarrow[r\to\infty]{} k_i^{-1/2}(\sin\theta_i\, \delta_{ij} + \cos\theta_i\, K_{ij}) \quad (k_i^2 > 0)\,, \tag{2b}$$

$$rF_{ij} \xrightarrow[r\to\infty]{} N_{ij}\, e^{-|k_i| r} \quad (k_i^2 < 0)\,, \tag{2c}$$

with

$$\theta_i = k_i r - l_i \pi/2\,. \tag{2d}$$

The stated form of the boundary conditions is appropriate only if the atom in the final state is neutral; that is, if no explicit account is taken of the possibility of ionization. The *K* matrix is real and symmetric, and is related to the *S* matrix by

$$S = (1 + iK)/(1 - iK)\,. \tag{3}$$

Cross sections are computed from the elements of *S* by standard procedures.

The atomic function $R(\gamma_a, l_a, r)$ is determined as follows: For fixed l_a, choose a set of component functions, here assumed to be Slater-type orbitals of the form

$$\eta_b(r) = r^{n_b} e^{-\zeta_b r} \tag{4}$$

and diagonalize the Hamiltonian for an isolated hydrogen atom on this basis. The resulting eigenfunctions are

$$R(\gamma_a, l_a, r) = \sum_b c_b^{(a)} \eta_b(r) . \tag{5}$$

If the basis set η_b includes all the components making up a particular exact hydrogen-atom wave function, that eigenfunction will be obtained from the diagonalization. It is convenient to choose the expansion so that some of the low-lying states of greatest interest are included exactly. The other states will be called pseudostates.

The possible results of the scattering calculation are determined by the choice of pseudostates, and at present it is necessary to proceed mainly by trial and error. One hopes to find a set such that the scattering cross sections of interest will converge to the correct results. We have experimented with several sets of pseudostates. The criteria employed in the choice of pseudostates and the results of this experimentation will be discussed in Sec. III.

The calculation proceeds in a rather straightforward manner after the pseudostates have been determined. The matrix variational technique of Nesbet[1] was employed. The results of three-state close-coupling (CC) calculations using this method have been reported previously,[12] and we will only outline our procedure here.

The function F_{ij} of Eq. (1) is represented as follows:

$$F_{ij}(r) = \alpha_{0i} S_0(k_i, r) + \alpha_{1i} S_1(k_i, r) + \Phi_{ij}(r) , \tag{6}$$

where the S are functions having a specified asymptotic form and Φ_{ij} is a normalizable function. The coefficients α are in accord with Eq. (2b),

$$\alpha_{0i} = k_i^{-1/2} \delta_{ij} , \tag{7a}$$

$$\alpha_{1i} = k_i^{-1/2} K_{ij} . \tag{7b}$$

The specific forms of the functions S employed here are

$$S_0(k_i, r) = (1 - e^{-\gamma r})^{n_i} k_i \bar{j}_{l_i}(k_i r) , \tag{8a}$$

$$S_1(k_i, r) = (1 - e^{-\gamma r})^{n_i} k_i \bar{n}_{l_i}(k_i r) . \tag{8b}$$

If channel i involves the 1s atomic state, $\bar{j}_{l_i}$ and $\bar{n}_{l_i}$ are the usual spherical Bessel and Neumann functions. For other states, these functions are obtained from the ordinary spherical Bessel and Neumann functions by deleting all terms decreasing more rapidly than r^{-2}. Thus, except for the 1s state,

$$(kr)\bar{j}_l(k, r) = \sin(kr - \tfrac{1}{2} l \pi) + [l(l+1)/2kr] \cos(kr - \tfrac{1}{2} l \pi) , \tag{9a}$$

$$(kr)\bar{n}_l(kr) = -\cos(kr - \tfrac{1}{2} l \pi) + [l(l+1)/2kr] \sin(kr - \tfrac{1}{2} l \pi) . \tag{9b}$$

The functions $\bar{j}_l$ and $\bar{n}_l$ coincide with the usual functions for $l = 0, 1$, but differ for higher l. The exponent n_i in (8) is chosen so that as $r \to 0$, $S_1 \sim r^{l_i + 1}$. Hence,

$$\begin{aligned} n_i &= l_i + 2, \quad l_i > 0 \\ n_i &= 1, \quad l_i = 0 . \end{aligned} \tag{10}$$

This truncation of the asymptotic function has the practical advantage of reducing the time required for the computation of "free-free" integrals (our major limiting factor). The computation of integrals with large negative powers of r and correspondingly large powers (n_i) of the cutoff function is quite time consuming, and may involve large errors of cancellation. Hence, from a practical point of view, it is highly desirable to eliminate these terms. Moreover, in the case of electron-hydrogen scattering, as opposed to scattering problems involving only short-range interactions, the correct asymptotic functions are not simply spherical Bessel and Neumann functions, but are modified because of the long-range off-diagonal potentials connecting degenerate channels.[13] Equation (2b) is, however, still valid. One must rely on the square-integrable function Φ to supply the required correction to the square-integrable part of the asymptotic functions. Hence, we incorporate relatively long-range, oscillatory functions in the set in which Φ_{ij} is expanded. Use of the truncated functions j and n does not produce any loss of accuracy.

The expansion employed for Φ_{ij} is

$$\Phi_{ij}(r) = \sum_\mu c_{i,\mu}^{(j)} \eta_{l_i,\mu}(r) + \sum_{\rho=1}^{2} d_{i,\rho}^{(j)} s_{i\rho}(r) . \tag{11}$$

The functions $n_{l_i,\mu}$ are taken to be Slater-type orbitals

$$\eta_{l,\mu} = \left(\frac{(2\zeta_\mu)^{2l+3}}{\Gamma(2l+3)} \right)^{1/2} r^l e^{-\zeta_\mu r} . \tag{12a}$$

Thus, the exponential part of Φ is a combination of functions all containing the same power of r, but of differing exponential dependence. The exponents ζ_μ are selected to give as good a representation of the scattering wave function as is possible. The functions S_{il} are

$$\begin{aligned} s_{i1}(r) &= (1 - e^{-\gamma r})^{l+2} \sin k_i r / r^2 , \\ s_{i2}(r) &= (1 - e^{-\gamma r})^{l+2} \cos k_i r / r^2 . \end{aligned} \tag{12b}$$

The slow oscillatory decay of Φ at large distances, which is caused by the long-range dipole coupling, is difficult to represent if only exponential functions are used in the expansion. Hence, we have included functions of the form (12b) in the basis set to represent this oscillatory behavior, although this makes the basis set energy dependent.

The central part of the algebraic variational method is the determination of a matrix whose elements are denoted $\mathfrak{M}_{st}^{ij}$, with i and j being channel indices and $s, t\,(=0, 1)$ specifying asymptotic forms according to Eqs. (8a) and (8b). This matrix can be expressed as

$$\mathfrak{M}_{st}^{ij} = N_{st}^{ij} + \sum_{m\mu, n\nu} M_{s\mu}^{im} (M^{-1})_{\mu\nu}^{mn} M_{\nu t}^{nj} \ . \tag{13}$$

The terms appearing in (13) are specified below.

(i) Free-free integrals:

$$N_{st}^{ij} = (\psi(\Gamma_i) S_s(k_i) \,|\, (H-E)(1-P_{12}) \,|\, \psi(\Gamma_j) S_t(k_j)) \ . \tag{14}$$

The functions $\psi(\Gamma_i)$ are the combinations of atomic functions and spin and angular functions for the scattering electron which appear in Eq. (1), while the S_t are defined by Eq. (8). The operator H is the complete Hamiltonian for the two-electron system, and E is the total energy of the system. The computation of these integrals is the most time consuming portion of our calculation. Analytic methods are employed; the procedure involved in the particularly troublesome exchange part has been described in detail elsewhere.[14]

(ii) Bound-free integrals:

$$M_{s\mu}^{im} = (\psi(\Gamma_i) S_s(k_i) \,|\, (H-E)(1-P_{12}) \,|\, \psi(\Gamma_m) b_\mu) \tag{15}$$

in which b_μ is either a Slater-type orbital $(b_\mu = n_{l,\mu})$ given by Eq. (12a), or a function of the form $s_{l\rho}$ as given by Eq. (12b). The computation by analytic methods is straightforward if b_μ is a Slater-type orbital.[15] The required integrals were obtained from the free-free integral program when b_μ is a harmonic function $(b_\mu = S_{l\rho})$.

(iii) Bound-bound integrals:

$$M_{\mu\nu}^{mn} = (\psi(\Gamma_m) b_\mu \,|\, (H-E)(1 \pm P_{12}) \,|\, \psi(\Gamma_n) b_\nu) \ . \tag{16}$$

The functions b_μ and b_ν are as specified in the preceding paragraph. When both b's are Slater-type orbitals, very simple analytic formulas may be employed; the other integrals are obtained from either the bound-free or free-free integral programs.

Four procedures based on the Kohn variational principle are available for extracting the K matrix from $\mathfrak{M}$. These are the Kohn and inverse-Kohn methods,[1] and variants employing a preliminary orthogonal transformation of $\mathfrak{M}$: the "optimized minimum norm" (OMN) and "optimized anomaly-free" (OAF) methods.[16] The reader is referred to Refs. 1 and 16 for derivation and description of the specific procedures. Some brief comments follow.

In the Kohn method, the K matrix is obtained from the expression

$$K_{ij} = -\left(\mathfrak{M}_{00}^{ij} - \sum_{nk} (\mathfrak{M}_{10})^{ki} (\mathfrak{M}_{11}^{-1})^{kn} (\mathfrak{M}_{10})^{nj} \right) \Big/ (k_i k_j)^{1/2} \ . \tag{17}$$

Anomalies can occur in the Kohn method near energies for which the submatrix $\mathfrak{M}_{11}$ is singular. A somewhat similar formula, which will be called

TABLE I. Comparison of K matrices from four methods. The elements of the K matrix and the partial cross sections for elastic scattering, $1s$-$2s$, and $1s$-$2p$ excitation are given for $L = 0$, $k^2 = 0.81$ as computed according to the four methods described in the text. $\sum\delta$ is the sum of the eigenphases. The entry det refers to $\det(\mathfrak{M}'_{11})$ for the Kohn procedure, $\det(\mathfrak{M}_{00})$ for inverse Kohn, $\det(\mathfrak{M}'_{11})$ for OMN and $\det(\mathfrak{M}'_{01})$ for OAF.

	$k^2 = 0.81$, $L = 0$							
	Singlet				Triplet			
	Kohn	Inverse Kohn	OMN	OAF	Kohn	Inverse Kohn	OMN	OAF
det	3.114×10^{-3}	0.3698	−5.392	0.9962	-8.458×10^{-4}	-8.743×10^{-4}	0.0223	0.9966
K_{11}	1.715	1.718	1.764	1.721	21.21	21.27	21.30	21.22
K_{12}	1.474	1.480	1.567	1.490	−0.3853	−0.3953	−0.3972	−0.3896
K_{13}	1.692	1.692	1.763	1.694	0.6005	0.5747	0.5728	0.5962
K_{22}	3.517	3.523	3.689	3.557	−0.5030	−0.5000	−0.5047	−0.5053
K_{23}	3.643	3.643	3.777	3.648	0.1972	0.2013	0.1992	0.2001
K_{33}	2.655	2.655	2.758	2.656	1.795	1.805	1.792	1.803
$\sum\delta$	1.621	1.623	1.627	1.631	2.100	2.105	2.098	2.100
σ_{1s-2s}	0.5564	0.5564	0.5569	0.5562	3.692	3.692	3.692	3.692
σ_{1s-2s}	0.0589	0.0587	0.0594	0.0586	0.0012	0.0013	0.0013	0.0012
σ_{1s-2p}	0.0260	0.0261	0.0259	0.0263	0.0006	0.0006	0.0006	0.0006

TABLE II. Parameters of basis states.

$l=0$

		Standard	
b	n_b	ζ_b	E (Ry)
1	0	1.0	−1.0
2	0	0.5	−0.25
3	1	0.5	−0.10932
4	0	0.8	0.03073
5	1	0.2	1.7073

$l=1$

	Standard			Variant 1		
b	n_b	ζ_b	E (Ry)	n_b	ζ_n	E (Ry)
1	1	1.0	−0.25	1	1.0	−0.25
2	1	0.8	−0.10900	1	0.5	−0.10936
3	1	0.5	0.03515	1	0.2	−0.02392
4	1	0.2	1.2413	2	0.5	0.81793

$l=2$

	Standard			Variant 2		
b	n_b	ζ_b	E (Ry)	n_b	ζ_n	E (Ry)
1	2	0.5	−0.11111	2	0.8	−0.11111
2	2	$\frac{1}{3}$	0.00065	2	$\frac{1}{3}$	0.18820

TABLE III. Comparison of phase shifts and eigenphase sums for $L=0, k^2=0.49$ and $L=0$, $k^2=0.81$.

$L=0$, $k^2=0.49$	δ_s	δ_T
Present work	0 917	1.778
Ref. 7	0.917	1.777
Ref. 4	0.881	1.777
Ref. 18	0.930	1.780
$L=0$, $k^2=0.81$	$(\sum\delta)_s$	$(\sum\delta)_T$
Present work	1.623	2.105
Six state CC (Ref. 8)	1.518	2.084
$3\bar{s}3\bar{p}3\bar{d}$ (Ref. 8)	1.559	2.104
Correlation (Ref. 8)	1.618	2.097

the inverse-Kohn method, can be derived for the computation of the inverse matrix K^{-1}:

$$(K^{-1})_{ij}=\Big((\mathfrak{M}_{11})^{ij}-\sum_{kn}\mathfrak{M}_{01}^{ki}(\mathfrak{M}_{00}^{-1})^{kn}(\mathfrak{M}_{01})^{nj}\Big)\Big/(k_i k_j)^{1/2}. \tag{18}$$

The inverse-Kohn formula may yield anomalous results in the neighborhood of energies for which $\mathfrak{M}_{00}$ is singular.

Nesbet originally proposed to select the Kohn formula if $|\det(\mathfrak{M}_{11})\geq\det(\mathfrak{M}_{00})|$; the inverse-Kohn formula if not.[1] In practice, we find excellent agreement between the Kohn and inverse-Kohn results for energies lower than the $n=2$ threshold, so that the question of choice does not arise in this energy range. The agreement is not so good above this threshold, and a decision must in fact be made between the results of (16) and (17). Since the proposed criterion will lead to differing choices as a function of energy, it is possible that artificial discontinuities will occur in the predicted K matrix. We do not believe that this problem is particularly serious when a relatively coarse grid of energies is used, but we are more concerned with the possibility that the energies at which singularities of $\mathfrak{M}_{00}$ and $\mathfrak{M}_{11}$ occur may not be greatly different, so that it may be quite difficult to obtain reliable results in some energy regions.

Therefore, there is considerable interest in the alternate approaches furnished by the OMN and OAF methods, both of which introduce a preliminary orthogonal transformation of the matrix $\mathfrak{M}$.[16] In the OMN method, this transformation is constructed from the eigenvalues and eigenvectors of a symmetric approximate K matrix, which in turn is constructed from the N eigenvectors corresponding to the N smallest eigenvalues of the $2N\times 2N$ matrix $\mathfrak{M}^T\mathfrak{M}$. The OMN procedure appears to give good results, except near energies where the transformed submatrix $\mathfrak{M}'_{11}$ is singular. The OAF method introduces an orthogonal transformation which converts the matrix $\mathfrak{M}$ to upper triangular form.[17] The K matrix is determined in the transformed coordinate system in a form that should have no singularities, and then transformed back to the physical system.

The results of all four methods appear to be of comparable accuracy except near an anomaly.

TABLE IV. Eigenphase sums for $L=0$, 1, 2 and $k^2=0.76$, 0.78, 0.81, 0.83, and 0.85.

	Singlet			Triplet		
k^2	$L=0$	$L=1$	$L=2$	$L=0$	$L=1$	$L=2$
0.76	−0.473	−1.189	−0.261	1.010	−0.440	0.839
0.78	1.677	0.658	−0.778	2.938	1.462	0.425
0.81	1.623	−0.359	−1.323	2.105	0.658	0.179
0.83	1.622	−0.757	1.687	1.710	0.403	0.139
0.85	1.621	−0.970	1.727	1.386	0.333	0.074

TABLE V. Exponents of Slater-type orbitals [Eq. (12a)].

4.0	2.5	1.5	0.9	0.6	0.4	0.2	0.1	0.05

This is illustrated in Table I, where the computed K matrices and cross sections are exhibited for $L=0$, $k^2=0.81$, using our standard set of psuedostates (see Sec. III). It will be seen that there is a reasonable degree of agreement among the methods, except that in the singlet state, the OMN procedure has given a K matrix whose elements are noticeably larger than the three other methods described. Studies of the calculation of the K matrix in the three-state close-coupling approximation show that there is no strong reason to prefer any one of the four methods on grounds of consistently closer agreement with published K matrices based on numerical integration of the coupled equations. We have not relied on a single method in the computation of cross sections reported in Sec. IV, but have, in the case of disagreement between methods, selected an apparently "best" value on the basis of criteria of internal consistency and continuity.

III. CHOICE OF PSEUDOSTATES

The choice of pseudostates to be employed is a central problem of the present calculation. Ideally, one should increase the number of pseudostates until adequate convergence is demonstrated; however, limitations of the computing facilities available to us prevent a thorough investigation of this point. Some evidence of reasonable convergence for states with $L=0$ is furnished by comparison of the results obtained here with those obtained by extrapolation from complex energies (see Sec. IV below) and with our previous results employing a smaller set of states.[6]

Our present calculations have been performed using a set of eleven states: five of s type, four p type, and two d type, with 1s, 2s, 2p, and 3d exact hydrogenic states contained in this set. Some results have been reported from a preliminary calculation using eight states (including exact 1s, 2s, and 2p).[6] The formal expansion for these states is given in Eqs. (4) and (5). The states are defined for given l by the choice of orbital exponents ζ_b and power n_b. Several sets of pseudostates were studied for $L=0$ with $k^2=0.49$ and $k^2=0.81$, where the computations are relatively simple. However, for the reasons specified below, we have found it undesirable to employ only a single set of pseudostates.

Each set of pseudostates possesses a series of "false" thresholds corresponding to the opening of some pseudochannel. Broad resonances may be found in the vicinity of these thresholds.[10] We believe it is desirable to avoid these unphysical resonances by shifting the pseudostate parameters so that resonances are not obtained in the energy region in which the calculation is made. We have therefore employed three sets of pseudostates: a "standard set" and two variants. All basis sets employ the same s-like functions. Variant 1 consists of standard s and d states, but the p function $re^{-0.8r}$ is replaced by $r^2e^{-0.5r}$. Variant 2 contains the standard s and p states, while the d function $r^2e^{-0.5r}$ is replaced by $r^2e^{-0.8r}$. These basis sets are shown in Table II.

The standard pseudostates were chosed by an extensive series of tests subject to the following criteria: (1) the set should contain exact 1s, 2s, 2p, and 3d functions; (2) it should give a reasonable approximation to the 3s and 3p energies; (3) the sum of the eigenphases for $L=0$, $k^2=0.81$ should equal or exceed those reported by Geltman and Burke[8]; and (4) the s-wave phase shifts for $L=0$, $k^2=0.49$ should equal or exceed those reported by Matese and Oberoi.[7] Considerable arbitrariness still remains in the choice of pseudostates, and further investigation of different basis function sets is desirable. The results of these comparisons are shown in Table III. It will be seen that the s-wave phase shift, while still below the "exact" result of Schwartz,[18] is still substantially improved with respect to the earlier pseudostate calculation of Burke, Gallaher, and Geltman.[4] In Table IV our eigenphase sums are given for $L=0$, 1, and 2 and $k^2=0.76$, 0.78, 0.81, 0.83 and 0.85.

TABLE VI. 1s→2s excitation cross sections in the range $k^2=0.76$ to $k^2=0.85$ (units of πa_0^2). The contributions labeled "High L" were obtained from Refs. 8 ($L=3$) and 20 ($L>3$).

	Singlet				Triplet				
k^2	$L=0$	$L=1$	$L=2$	High L	$L=0$	$L=1$	$L=2$	High L	Total
0.76	0.037	0.008	0.053	0.000	0.0005	0.037	0.000	0.004	0.140
0.78	0.041	0.003	0.057	0.000	0.0008	0.045	0.000	0.004	0.151
0.81	0.059	0.003	0.061	0.001	0.0013	0.053	0.002	0.013	0.193
0.83	0.062	0.004	0.067	0.002	0.0015	0.057	0.005	0.015	0.214
0.85	0.055	0.006	0.074	0.003	0.0017	0.056	0.006	0.015	0.217

TABLE VII. 1s-2p excitation cross sections in the range $k^2=0.76$ to $k^2=0.85$ (units of πa_0^2). The contributions labeled "High L" were obtained from Refs. 8 ($L=3$) and 20 ($L>3$).

	Singlet				Triplet				
k^2	$L=0$	$L=1$	$L=2$	High L	$L=0$	$L=1$	$L=2$	High L	Total
0.76	0.028	0.066	0.091	0.000	0.0004	0.038	0.000	0.001	0.224
0.78	0.035	0.049	0.091	0.001	0.0004	0.041	0.002	0.012	0.231
0.81	0.026	0.053	0.112	0.004	0.0006	0.047	0.006	0.041	0.290
0.83	0.025	0.059	0.129	0.006	0.0009	0.048	0.009	0.054	0.331.
0.85	0.025	0.066	0.152	0.009	0.0011	0.046	0.012	0.063	0.374

It was apparent from the results of the tests of the pseudostates that the s-wave phase shift below the $n=2$ threshold would be improved by emphasizing short-range pseudostates, which describe short-range correlations. This conclusion is consistent with the results of Matese and Oberoi.[7] However, the eigenphase sum at $k^2=0.81$ is improved by the inclusion of longer-range functions. A compromise is therefore required, and this compromise leads to the standard set employed.

The variants were introduced to avoid encountering pseudostate thresholds at inconvenient energies. Thus, the highest p state of the standard set opens at $k^2=2.24$. This prevents meaningful results from being obtained at $k^2=2.25$. Variant 1 has a lower threshold for the upper p state ($k^2=1.82$) and was used in our calculation for both $k^2=1.96$ and $k^2=2.25$. The second d pseudostate in the standard set opens at $k^2=1.00065$. Variant 2, which displaces this threshold to $k^2=1.19$ was used in calculations for $k^2=1.0$.

IV. RESULTS

We present results for elastic scattering and excitation of the 2s and 2p states in the region between the $n=2$ and $n=3$ thresholds, and for elastic scattering in the region from the $n=3$ threshold up to $k=2.25$. We have considered states of total angular momentum $L=0,1,2$. The calculations become more lengthy as L increases, as a result of the increasing number and complications of matrix elements, mainly the free-free integrals [Eq. (14)]. The limitation to states of $L \leq 2$ does not permit reliable determination of excitation cross sections above the $n=3$ threshold, since, for example, at $k^2=1.0$, more than $\frac{1}{3}$ of the total 1s $-$ 2p excitation as computed in a three-state close-coupling calculation occurs in states of $L \leq 3$.[19] In contrast, elastic 1s-1s scattering is dominated by ^3S, ^3P, and ^1S states, and for $k^2=2.25$ only 2% of the total cross section involves $L \geq 3$.

Our calculations employed a basis set of nine Slater-type orbitals $\eta_{l,\mu}$ [Eq. (12a)] in each channel (see Table V) as well as two harmonic functions s_{ip} [Eqs. (8a) and (8b)] in each open channel except 1s. The exponents of the $\eta_{l,\mu}$ are listed in Table IV. The bound-bound matrix M [Eq. (15)] had dimension 205×205 in the largest cases, and 18 channels were open.

The partial cross sections for 1s-2s and 1s-2p excitation for the energies calculated are given in

TABLE VIII. 1s-1s elastic-scattering partial and total cross sections in units of πa_0^2. The "High L" contribution is obtained as described in the text.

	Singlet				Triplet				
k^2	$L=0$	$L=1$	$L=2$	High L	$L=0$	$L=1$	$L=2$	High L	Total
0.76	0.645	0.002	0.048	0.010	3.945	2.088	0.121	0.031	6.890
0.78	0.608	0.001	0.056	0.010	3.841	2.042	0.123	0.033	6.714
0.81	0.556	0.001	0.061	0.011	3.692	1.971	0.126	0.034	6.452
0.83	0.527	0.001	0.063	0.011	3.597	1.921	0.127	0.035	6.282
0.85	0.505	0.002	0.062	0.012	3.506	1.870	0.129	0.036	6.122
0.90	0.476	0.004	0.058	0.014	3.292	1.776	0.130	0.039	5.789
0.95	0.417	0.004	0.062	0.015	3.098	1.683	0.134	0.036	5.45
1.00	0.393	0.006	0.056	0.016	2.920	1.588	0.136	0.036	5.15
1.10	0.329	0.008	0.057	0.018	2.606	1.444	0.136	0.038	4.64
1.21	0.288	0.010	0.048	0.021	2.315	1.292	0.139	0.040	4.15
1.30	0.258	0.011	0.045	0.021	2.113	1.192	0.142	0.040	3.82
1.44	0.230	0.013	0.047	0.021	1.846	1.062	0.139	0.040	3.40
1.69	0.186	0.019	0.050	0.018	1.482	0.864	0.136	0.039	2.79
1.96	0.145	0.016	0.045	0.015	1.197	0.705	0.122	0.038	2.28
2.25	0.124	0.024	0.032	0.012	0.975	0.595	0.108	0.036	1.91

TABLE IX. Comparison of the $L = 0$ contribution to the 1s-1s elastic-scattering cross section (units πa_0^2) according to the present calculation, as determined by extropolation from complex energies (Ref. 25).

k^2	$L=0,\ S=0$ Present	Ref. 25	$L=0,\ S=1$ Present	Ref. 25
1.21	0.288	0.296	2.315	2.320
1.44	0.230	0.226	1.846	1.846
1.69	0.186	0.178	1.482	1.485
1.96	0.145	0.146	1.197	1.195
2.25	0.124	0.123	0.975	0.985

Tables VI and VII. The contributions from $L \geqslant 3$ are taken from Refs. 8 and 20. The cross sections are in fairly good agreement with the six-state close-coupling calculation of Ref. 20 and the pseudostate calculation of Ref. 8. However, the present results tend to be a few percent lower than those mentioned. On the whole, the present excitation cross sections are in better agreement with the three-state plus 20 correlation-function calculations of Taylor and Burke.[21] There is good agreement with recent experimental measurements of the 1s-2s excitation cross section[22,23] except for $k^2 = 0.78$, where our values are too low by about 10%. The cross sections for the excitation of the 2p state are uniformly larger than the measured values.[24] This feature is shared by the results of the comparable calculations reported in Refs. 8, 20, and 21. We suggest that it would be desirable to repeat this experiment.

Our results for the total elastic-scattering (1s → 1s) cross section are given in Table VIII. The contribution from states of $L \geqslant 3$ was estimated as follows: For $k^2 \leqslant 0.90$, the results of Refs. 8 and 20 were employed; at energies larger than this, our estimates were obtained from the three-state close-coupling calculation of Ref. 19. Since we found that, for $L = 2$, our 1s-1s cross sections are larger than those of Ref. 19 by a factor of about 1.5, we have arbitrarily multiplied the partial cross sections for $L \geqslant 3$ contained in Ref. 19 by this factor. We have also interpolated between the published values as necessary. Such procedures are, of course, extremely crude; however the entire contribution from $L \geqslant 3$ is never as large as 3% of the total, and the error introduced by these rough estimates is not significant. The final cross sections we obtain are uniformly larger than those given in Ref. 19 by approximately 15%.

A significant check of the present method is furnished by comparison of the results for elastic scattering at $L = 0$ with those obtained with the method of extrapolation from complex energies by McDonald and Nuttall.[25] This is done in Table IX. The agreement, although not perfect, is rather good and increases confidence in both methods.

Additional tables containing partial cross sections for 1s-2s and 1s-2p excitation from $k^2 = 0.90$ to $k^2 = 2.25$, and K matrices at certain energies can be obtained from the authors or from ASIS/NAPS.*

---

*See NAPS document No. 02330 for 6 pages of supplementary material. Order from ASIS/NAPS c/o Microfiche Publications, 305 E. 46th St., New York, N.Y. 10017. Remit in advance for each NAPS accession number $1.50 for microfiche or $5.00 for photocopies up to 30 pages, 15¢ for each additional page. Make checks payable to Microfiche Publications.

[1] R. K. Nesbet, Phys. Rev. 179, 60 (1969).

[2] F. E. Harris and H. H. Michels, Phys. Rev. Lett. 22, 1036 (1969).

[3] J. F. Perkins, Phys. Rev. 173, 164 (1968).

[4] P. G. Burke, D. F. Gallaher, and S. Geltman, J. Phys. B 2, 1142 (1969).

[5] J. Callaway and J. J. Matese, Int. J. Quantum Chem. 6, 79 (1972).

[6] J. Callaway and J. W. Wooten, Phys. Lett. A 45, 85 (1973).

[7] J. J. Matese and R. S. Oberoi, Phys. Rev. A 4, 569 (1971).

[8] S. Geltman and P. G. Burke, J. Phys. B 3, 1062 (1970).

[9] P. G. Burke and T. G. Webb, J. Phys. B 3, L131 (1970).

[10] P. G. Burke and J. F. B. Mitchell, J. Phys. B 6, 320 (1973).

[11] P. G. Burke, in *Lectures in Theoretical Physics*, edited by S. Geltman, K. T. Mahanthappa, and W. E. Brittin (Gordon and Breach, New York, 1969), Vol. XI-C, p. 1.

[12] G. J. Seiler, R. S. Oberoi, and J. Callaway, Phys. Rev. A 3, 2006 (1971).

[13] E. R. Smith, R. S. Oberoi, and R. J. W. Henry, J. Comput. Phys. 10, 53 (1972).

[14] R. S. Oberoi, J. Callaway, and G. J. Seiler, J. Comput. Phys. 10, 466 (1972).

[15] G. J. Seiler, Ph.D. thesis (Louisiana State University, 1970) (unpublished).

[16] R. K. Nesbet and R. S. Oberoi, Phys. Rev. A 6, 1855 (1972).

[17] J. H. Wilkinson, *The Algebraic Eigenvalue Problem* (Oxford U. P., New York, 1965), Chap. 8.

[18] C. Schwartz, Phys. Rev. 124, 1468 (1961).

[19] P. G. Burke, H. M. Schey, and K. Smith, Phys. Rev. 129, 1258 (1963).

[20] P. G. Burke, S. Ormond, and W. Whitaker, Proc. Phys. Soc. Lond. 92, 319 (1967).

[21] A. J. Taylor and P. G. Burke, Proc. Phys. Soc. Lond. 92, 336 (1967).

[22] A. Oed, Phys. Lett. A 34, 435 (1971).

[23] H. Kochsmeider, V. Raible, and H. Kleinpoppen, Phys. Rev. A 8, 1365 (1973).

[24] J. W. McGowan, J. F. Williams, and E. K. Curley, Phys. Rev. 180, 132 (1969).

[25] F. A. McDonald and J. Nuttall, Phys. Rev. A 4, 1821 (1971).