should be noted that due to the presence of these overt effects a spin-orbit coupling constant deduced from a single multiplet that follows the Lande interval rule need not be representative of the entire configuration.

When the parameters are derived from a least-squares method it is impossible to distinguish the contributions to the spin-orbit coupling constant that arise from the effects of electrostatically correlated interactions with other configurations and those that arise from the spin-orbit interactions within the configuration. Likewise, in empirical determinations of the spin-other-orbit interactions for a configuration, it is impossible to decide whether the derived spin-other-orbit parameters represent a real spin-other-orbit interaction within the configuration or whether they are attributable to a pseudo-spin-other-orbit interaction that arises out of the effects of electrostatically correlated spin-orbit interactions.

Electrostatically correlated spin-orbit interactions are by no means the only possible correlated interactions that couple configurations. In fact, these interactions are probably of lesser significance than the electrostatically correlated two-particle orbit-orbit, spin-spin, and spin-other-orbit interactions between configurations. The properties of these interactions will be taken up in a later paper.

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Nonadiabatic Theory of Inelastic Electron-Hydrogen Scattering*

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The nonadiabatic theory is applied to the inelastic S-wave scattering of low-energy electrons from atomic hydrogen. The zeroth-order (angle-independent) approximation for excitation of the $2s$ level from the ground state is described by the same equation used to describe elastic scattering below the $2s$ threshold, but with more complicated boundary conditions. The solution has been effected by expanding the wave function in terms of separable solutions. With the assumption of reciprocity it is also possible to obtain the $2s-2s$ cross sections. The elastic $(1s-1s)$ cross sections are within 1% of the close-coupling results in the triplet case, but are about 20% greater in the singlet case. The inelastic $(1s-2s)$ cross sections are reduced about 20% in the triplet case and 20 to 40% in the singlet case, relative to the close-coupling results.

I. INTRODUCTION

In previous papers[1] a nonadiabatic theory of elastic scattering has been developed and applied, among other things, to the low-energy scattering of electrons from atomic hydrogen. At present the theory is being extended to cover inelastic S-wave scattering, and hence obtain the scattering cross sections σ_{1s-1s} and σ_{1s-2s} above the $2s$ excitation threshold. This paper deals with the solution of the zeroth-order (angle-independent or relative s wave) problem described in Sec. II of this paper. Only a brief review of the nonadiabatic theory is given since a full description is to be found in I. As pointed out in Sec. III, the elastic scattering cross section σ_{2s-2s} may also be found from our calculation if it is assumed that the reciprocity condition is fulfilled.

The accuracy of the solution is discussed in Secs. IV and V. In Sec. VI the nonadiabatic results are presented and compared with the results from the $1s-2s$ close-coupling expansion.[2–5] The latter has been shown to be a variational approximate solution of the zeroth-order problem.[1] Finally, the implication of our results for both the experimental and theoretical determination of the total inelastic cross section, σ_{1s-2s} is discussed in Sec. VII.

II. ZEROTH-ORDER NONADIABATIC THEORY

It will be recalled from I that the nonadiabatic theory starts with a decomposition of the S-wave function

$$\Psi(r_1r_2\theta_{12})=1/r_1r_2\sum_{l=0}(2l+1)^{1/2}\Phi_l(r_1r_2)P_l(\cos\theta_{12})\,, \quad (I2.3)$$

from which by substitution into the Schrödinger equa-

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[1] A. Temkin, Phys. Rev. Letters **4**, 566 (1960); Phys. Rev. **126**, 130 (1962). The latter paper will be referred to as I in the text. Equations referring to it will be prefixed by a I.

[2] R. Marriott, Proc. Phys. Soc. (London) **72**, 121 (1958).

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

[4] K. Omidvar, in *Proceedings of the Third International Conference on the Physics of Electronic and Atomic Collisions* (North-Holland Publishing Company, Amsterdam, to be published). Dr. Omidvar has kindly calculated for us the $1s$–$2s$ close-coupling results just above threshold. Cf. also, K. Omidvar, Phys. Rev. **133**, A970 (1964).

[5] R. Damburg and R. Peterkop, Proc. Phys. Soc. (London) **80**, 1073 (1962).

tion an infinite set of coupled two-dimensional differential equations results. One defines a zeroth-order problem by neglecting the coupling terms of the $l=0$ equation:

$$(\Delta_{12}+2/r_2+E)\Phi_0^{(0)}(r_1r_2)=0 \quad (r_1>r_2)\,, \qquad \text{(I3.3)}$$

where

$$\Delta_{12}=\partial^2/\partial r_1^2+\partial^2/\partial r_2.$$

Our units are lengths in Bohr radii and energy in Rydbergs.

Equation (I3.3) can describe only relative s states and is therefore also called the relative s problem. In this paper we will consider incident electrons with energies greater than 10.2 eV. In such cases the target atom may be excited to the $2s$ state by collision. Hence the zeroth-order wave function $\Phi_0^{(0)}$ will be required to have the asymptotic form

$$\lim_{r_1\to\infty}\Phi_0^{(0)}(r_1r_2)=[(A/k_1)\sin k_1r_1+ae^{ik_1r_1}]\times R_{1s}(r_2)+be^{ik_2r_1}R_{2s}(r_2)\,. \qquad (2.1)$$

For incident electron energies greater than 12.09 eV higher s states may be excited and for completeness should be included in (2.1). However since each new term added to the right-hand side of (2.1) adds greatly to the complexity of the problem, only the $(1s)$ and $(2s)$ channels are included in our calculation.

In (2.1) k_1 is the wave number of the incident electron and $k_2=(k_1^2-0.75)^{1/2}$ is the wave number of an inelastically scattered electron. The function $R_{ns}(r)$ equals r times the nth radial hydrogenic s state. A is an arbitrary normalization of the incident plane wave, while a and b are constants which govern, respectively, the elastic and inelastic scattering cross sections.

The zeroth-order wave function must also obey the additional boundary conditions[1]

$$\begin{aligned}\Phi_0^{(0)}(r_1r_2)|_{r_1=r_2}&=0 \quad \text{triplet},\\ (\partial/\partial n)\Phi_0^{(0)}(r_1r_2)|_{r_1=r_2}&=0 \quad \text{singlet},\end{aligned} \qquad \text{(I2.6)}$$

and

$$\Phi_0^{(0)}(r_1,0)=0. \qquad \text{(I2.7)}$$

Here $(\partial/\partial n)$ is the normal derivative. Equation (I2.6) simply states the spatial symmetry of the wave function:

$$\Phi_0^{(0)}(r_1r_2)=\pm\Phi_0^{(0)}(r_2r_1)\,.$$

The scattering cross sections obtained from (2.1) are

$$\sigma_{1s-1s}=4\pi\frac{|a|^2}{|A|^2} \qquad (2.2)$$

$$\sigma_{1s-2s}=\frac{4\pi k_2}{k_1}\frac{|b|^2}{|A|^2}. \qquad (2.3)$$

In order to ensure conservation of current, the constants A, a, and b are required to obey the relationship

$$\text{Im}(A^*a)=k_1|a|^2+k_2|b|^2. \qquad (2.4)$$

To facilitate the solution of certain nonlinear equations which appear in the problem, we let[6]

$$\text{case (i)} \quad A=k_1(1-ia)\,,$$

and

$$\begin{aligned}a&=x+iz^2\\ b&=(k_1/k_2)^{1/2}ze^{i\delta}.\end{aligned} \qquad (2.5)$$

As a check on the calculations the singlet case was also solved with[7]

$$\text{case (ii)} \quad A=k_1,$$

and

$$\begin{aligned}a&=(xe^{2i\delta_1}-1)/2i\\ b&=\tfrac{1}{2}[(k_1/k_2)(1-x^2)]^{1/2}e^{i(\delta_1+\delta_2)}.\end{aligned} \qquad (2.6)$$

In both cases the form of b is so chosen that Eq. (2.4) was automatically satisfied. Hence the complex numbers a and b are fully determined by the real numbers Re(a), Im(a), and Arg(b). The method of solution of Eq. (I3.3) follows that used in I: $\Phi_0^{(0)}$ is expanded in a series consisting of separable eigenfunctions of (I3.3):

$$\Phi_0^{(0)}(r_1r_2)=\left(\frac{A}{k_1}\sin k_1r_1+ae^{ik_1r_1}\right)\times R_{1s}(r_2)+be^{ik_2r_1}R_{2s}(r_2)+\left(\sum_n+\int dp\right)C_ne^{-\kappa_nr_1}R_{ns}(r_2)\,. \qquad (2.7)$$

The sum plus integral means, as usual, that the continuum s states of hydrogen in addition to the discrete states must be included. For the discrete states

$$\kappa_n=(1-n^{-2}-k_1^2)^{1/2}, \qquad (2.8)$$

and for the continuum

$$\kappa_p=(1+p^2-k_1^2)^{1/2}. \qquad (2.9)$$

With this relationship each term of (2.7) is an exact solution of (I3.3)

The expansion (2.7) automatically satisfies two of the boundary conditions (2.1) and (I2.7) but not the third (I2.6). In order to satisfy (I2.6) we determine a, b, and C_n by the variational conditions[1]

$$\left.\begin{aligned}\partial I_S/\partial\chi_j&=0\\ \partial I_T/\partial\chi_j&=0\end{aligned}\right\} \quad \chi_j=a,\ \text{Arg}(b), C_n \quad n=3,\cdots,N+2. \qquad (2.10)$$

N is the number of terms, beyond the first two, included in the expansion (2.7) and

$$\begin{aligned}I_T&=\int_0^\infty|\Phi_0^{(0)}(r_1=r_2)|^2dr\\ I_S&=\int_0^\infty\left|\frac{\partial}{\partial n}\Phi_0^{(0)}(r_1r_2)\right|^2_{r_1=r_2}dr.\end{aligned} \qquad (2.11)$$

[6] H. S. Massey and B. L. Moiseiwitsch, Proc. Phys. Soc. (London) **A66**, 406 (1953). Our case (i) asymptotic wave form was suggested by this paper.

[7] R. Karplus and L. S. Rodberg, Phys. Rev. **115**, 1058 (1959). Our case (ii) asymptotic form was taken from this paper.

TABLE I. Satisfaction of the diagonal boundary condition $I_S=I_T=0$ at various incident momenta k_1.

k_1 (atomic units)	0.8662	0.9	0.94		0.95	1.0	1.1	1.2	1.5
I_S	1×10^{-5}	3×10^{-6}	2×10^{-5}	3s	1×10^{-3}	5×10^{-3}	2×10^{-2}	4×10^{-2}	1×10^{-1}
I_T	3×10^{-5}	2×10^{-5}	3×10^{-5}	threshold	1×10^{-4}	1×10^{-3}	2×10^{-3}	4×10^{-3}	1×10^{-2}

Since a and the (C_n) are complex, $2N+3$ real equations result from (2.10). These equations are linear in the C_n, hence $2N$ of them may be solved immediately to obtain the (C_n) in terms of $\text{Re}(a)$, $\text{Im}(a)$, and $\text{Arg}(b)$. The procedure followed is analogous to that outlined in part four of I, although some of the integrals involved are slightly different in form. The integrals were obtained in analytic form and were checked by numerical integration. However, in the singlet case due to the difficulty of the numerical integrations the analytic results were in some cases only checked to one or two significant figures. In order to obtain sufficient accuracy it was necessary to solve for the C_n using double precision arithmetic; i.e. 16 significant figures were retained in the calculations. The remaining three equations are highly nonlinear in $\text{Re}(a)$, $\text{Im}(a)$, and $\text{Arg}(b)$ and were therefore solved numerically. All calculations were done on the IBM 7094 computer of the Theoretical Division of the Goddard Space Flight Center.

III. THE SCATTERING MATRIX

If an exact solution were obtained for the zeroth-order Eq. (I3.3), then the reciprocity condition[8] should be fulfilled and the scattering cross sections σ_{2s-2s} and σ_{2s-1s} could also be obtained from this same calculation. Although we have no direct check on how closely the reciprocity condition is fulfilled, it is expected that when I_S and I_T are small enough, reciprocity is satisfied to an accurate degree of approximation. The cross section σ_{2s-1s} follows immediately from the reciprocity condition, one form of which is

$$\sigma_{2s-1s}=(k_1/k_2)^2\sigma_{1s-2s}.$$

It is however necessary to introduce the scattering matrix S in order to obtain σ_{2s-2s}.

Many forms of the asymptotic boundary condition, Eq. (2.1), have been introduced by various authors. Two of the more common variations are of the following types:

$$\lim_{r_1\to\infty}\Phi_0^{(0)}(r_1r_2)=(\sin k_1r_1+T_{11}e^{ik_1r_1})R_{1s}(r_2)+(k_2/k_1)^{1/2}T_{12}e^{ik_2r_1}R_{2s}(r_2)\,, \quad (3.1)$$

$$\lim_{r_1\to\infty}\Phi_0^{(0)}=(e^{-ik_1r_1}-S_{11}e^{ik_2r_1})R_{1s}(r_2)-(k_2/k_1)^{1/2}S_{12}e^{ik_2r_1}R_{2s}(r_2)\,. \quad (3.2)$$

In (3.1) the T_{ij} are elements of the transmission matrix T while in (3.2) the S_{ij} are the elements of the scattering matrix S. The coefficient $(k_2/k_1)^{1/2}$ multiplying T_{12} and S_{12} is introduced so that T_{ij} and S_{ij} will be symmetric.

Equations (2.1) and (3.1) are related in the following way:

$$T_{11}=k_1aA^*/|A|^2, \quad (3.3)$$

$$T_{12}=k_1(k_1/k_2)^{1/2}bA^*/|A|^2. \quad (3.4)$$

The S and T matrices defined by (3.1) and (3.2) are related by

$$S=1+2iT. \quad (3.5)$$

Here 1 is the unit matrix.

If the S matrix is required to conserve probability current, then it will be unitary:

$$SS^\dagger=1. \quad (3.6)$$

If the reciprocity condition also holds, then the S matrix will be symmetric:

$$S_{12}=S_{21}. \quad (3.7)$$

From (3.6) S_{22} may be found to be

$$S_{22}=-S_{11}^*S_{12}S_{21}/|S_{12}|^2. \quad (3.8)$$

Finally, the reaction cross sections are given by the formula

$$\sigma_{is\to js}=\pi|\delta_{ij}-S_{ij}|^2/k_i^2, \quad (3.9)$$

where δ_{ij} is the Kronecker delta function. The σ_{2s-2s} thus obtained are listed in Table VI.

IV. INTERNAL CONSISTENCY OF THE SOLUTION

The integrals I_S and I_T, Eq. (2.11), should ideally be zero. Presumably if enough terms could be taken in the wave-function expansion, (2.7), this should occur to an arbitrary precision, however, for $N>8$ the determinant of the C_j, $(j=1, N)$, was generally too small for accurate results to be obtained. By trial and error sets of terms in the expansion were chosen which minimized I_S and I_T. The confidence we have in our results depends both on the smallness of I_S and I_T, and on the consistency of the cross sections obtained by choosing different sets of virtual eigenstates. The magnitude of the obtainable I_S and I_T are shown in Table I. As can be seen I_S and I_T are both quite small for energies less than that required to excite the 3s level of hydrogen. As soon as the 3s threshold is passed, there is a marked increase in the size of the diagonal integrals (particularly in the singlet case). The size of the diagonal integral continues to

[8] A derivation of the reciprocity theorem as it applies to scattering matrices is given by J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1952), p. 528.

TABLE II. Investigation of the internal consistency of the singlet nonadiabatic calculations. This table is discussed in Sec. IV.

k_1 Atomic units	I_S Case (i)	I_S Case (ii)	σ_{1s-2s} Case (i)	σ_{1s-2s} Case (ii)	σ_{1s-1s} Case (i)	σ_{1s-1s} Case (ii)	Virtual states Discrete	Virtual states Continuum
0.9	3×10^{-6}	1×10^{-6}	0.0339	0.0338	0.4674	0.4674	3,4	0.05, 0.3, 0.6, 0.9, 1.1
0.9	1×10^{-5}	7×10^{-6}	0.0339	0.0339	0.4674	0.4674	3	0.05, 0.3, 0.5, 0.7, 0.9, 1.1
0.9	1×10^{-4}	5×10^{-5}	0.0334	0.0335	0.4676	0.4676	4	0.05, 0.3, 0.5, 0.7, 0.9, 1.1
0.9	5×10^{-4}	3×10^{-4}	0.0309	0.0310	0.4680	0.4684	...	0.05, 0.3, 0.5, 0.7, 0.9, 1.1, 1.3
0.9	8×10^{-4}	7×10^{-4}	0.0289	0.0291	0.4672	0.4680	...	0.2, 0.4, 0.6, 0.75, 0.9, 1.05
1.0	5×10^{-3}	3×10^{-3}	0.0469	0.0488	0.3263	0.3290	...	0.05, 0.25, 0.45, 0.65, 0.85, 1.0, 1.15, 1.30
1.0	7×10^{-3}	4×10^{-3}	0.0463	0.0481	0.3283	0.3319	...	0.05, 0.3, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6
1.5	1×10^{-1}	8×10^{-2}	0.0131	0.0196	0.0958	0.1126	...	1.15, 1.23, 1.33, 1.43, 1.53, 1.63

increase out to 30.6 eV. At these higher energies there is also a marked decrease in the agreement of the cross sections obtained by choosing different sets of virtual continuum states. Again this was most bothersome in the singlet case.

For the singlet case this behavior is illustrated in Table II by the two top entries for $k_1=0.9$ and the entries for $k_1=1.0$ and $k_1=1.5$. These entries represent some of the better runs obtained at these energies. The uncertainty in the singlet results can be gauged by comparing case (i) and case (ii) results. [In Table II the cross sections are in units of πa_0^2 and the statistical weight $\frac{1}{4}$ is included. The columns labeled Discrete and Continuum virtual states refer to the n and p included in (2.7).] At the higher energies the triplet results seem to be quite a bit more accurate than the singlet results.

It should be remarked that it is an assumption that the zeroth-order Eq. (I3.3) can be exactly satisfied subject to the more limited asymptotic boundary condition (2.1) in an energy domain in which we know that the $3s$ state, for example, is accessible. The above disparity in the quality of results on the two sides of the $3s$ threshold may tend to indicate that this assumption is in fact incorrect. However, it is our opinion that the chief difficulty above the $3s$ threshold is not in the boundary condition (2.1) but in the loss of flexibility in the wave function in the region of interaction caused by the absence of the $3s$ state. Partial confirmation of this can be found in the last four $k_1=0.9$ entries in Table II which illustrate the effect of omitting various low energy discrete virtual states from the expansion. Nevertheless because there is a provision for including a flexible choice of continuum states, we feel that any theoretical incompleteness in our expansion above 12.1 eV can be largely compensated for.

A more relevant question is how these cross sections will change by virtue of the redistribution of current when the totality of open channels is included. Clearly the present calculation cannot answer that question, although in some sense the assumption must be made that their effect is small. For if it were not, then the calculation of scattering in the ionization region would be a complete impossibility, because their inclusion would entail a wave function containing not only a discrete infinity of bound excited states but a dense infinity of ionized states as well. It is our opinion therefore that in close coupling, for example, when additional states are added at an energy where they may be excited their main effect arises from the increased flexibility they allow the wave function in the region of interaction rather than in the opening of the channels that they afford. Thus the present method, which places virtually no restriction on the number of terms that can describe the wave function in the region of interaction, is expected to contain most of the effects on the $1s$ and $2s$ channels of a close-coupling expansion with a similar number of terms.

V. EFFECTIVE RANGE EXPANSION ABOUT THE 2S THRESHOLD

A final check was made to insure that our calculation was compatible with previous nonadiabatic (NA) calculations below the $2s$ threshold. Ross and Shaw[9] have recently developed a multichannel effective-range theory. This is an extension of the ordinary (single channel) effective-range theory which can in principle describe all channels of a reaction both above and below the threshold for a new channel. The correlation is accomplished in terms of an M matrix whose elements around threshold may be expanded in a power series in the energy. The first two of these coefficients reduce essentially to the scattering length and effective range in the one channel case. The M matrix has been used by Damburg and Peterkop[5] to extrapolate the results of $1s-2s$ close-coupling calculations immediately above the $2s$ threshold to infer the elastic scattering below threshold. In the same spirit we have extrapolated our present NA results to below threshold. In this case, however, the extrapolation was in the nature of a check as the NA results below threshold have already been calculated.[10] For compatibility the extrapolated values

[9] M. H. Ross and G. L. Shaw, Ann. Phys. (N. Y.) **13**, 147 (1961).

[10] A. Temkin and R. Pohle, Phys. Rev. Letters **10**, 22 (1963). It should be emphasized that only results of the zeroth-order or relative s-wave problem of this reference are being considered and these show only one resonance. On the other hand, the inclusion of higher relative partial waves introduced more resonances. Cf. the erratum to the above, Phys. Rev. Letters **10**, 268 (1963); A. Temkin, NASA Tech. Note D-1720 (unpublished); A. Temkin, in *Proceedings of the Third International Conference on the Physics of Electronic and Atomic Collisions* (North-Holland Publishing Company, Amsterdam, to be published); and Ref. 12.

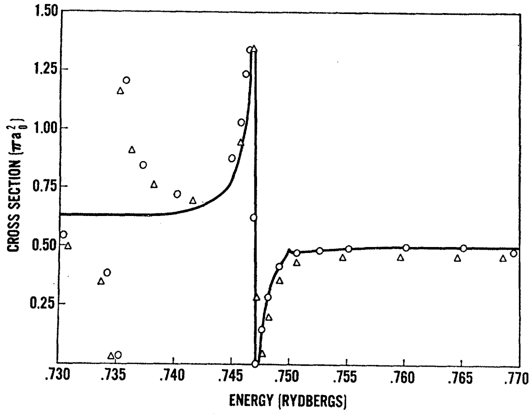

FIG. 1. Comparison of the singlet nonadiabatic ($1s-1s$) cross section (solid line) near the $2s$ threshold with effective-range extrapolations. Circles are the nonadiabatic effective-range extrapolation. Triangles are the ($1s-2s$) close-coupling effective-range extrapolation of Damburg and Peterkop.

of σ_{1s-1s} should then closely match the computed zeroth-order NA σ_{1s-1s} below threshold. The usefulness of this check was brought home in our present calculations, when the values which had been computed at an earlier stage gave an extrapolated singlet σ_{1s-1s} that was not compatible with the explicitly calculated values below threshold. This helped lead to the discovery of a machine programming error which had caused earlier singlet results to indicate a spuriously high peak in σ_{1s-2s} cross section just above the $2s$ threshold.[11]

The T and M matrices are related for relative s-wave scattering by the equation[9]

$$T=k^{1/2}(M-ik)k^{1/2}. \quad (5.1)$$

In this equation k is considered to be a diagonal matrix with diagonal elements k_i. The elastic scattering is then given by

$$\sigma_{1s-1s}=4\pi(M_{22}^2+k_2^2)/|(M_{11}-ik_1)\times(M_{22}-ik_2)-M_{12}M_{21}|^2. \quad (5.2)$$

TABLE III. The first two coefficients in the expansion of the M matrix elements at the $2s$ threshold, Eq. (5.3).

	NA = nonadiabatic Singlet		CC = close coupling[a] Triplet	
	NA	CC	NA	CC
$M_{11}(0)$	1.0610	1.300	0.0293	0.0301
$M_{21}(0)$	−0.0569	−0.0629	−0.0017	−0.0017
$M_{22}(0)$	−0.0368	−0.0356	0.1208	0.1206
R_{11}	4.2267	4.82	1.1373	1.20
R_{12}	−3.9292	−4.32	0.0642	−0.06
R_{22}	11.489	11.54	5.1528	5.14

[a] Close-coupling coefficients taken from Damburg and Peterkop (Ref. 5).

[11] H. L. Kyle and A. Temkin, in *Proceedings of the Third International Conference on the Physics of Electronic and Atomic Collisions* (North-Holland Publishing Company, Amsterdam, to be published).

Expanding the elements of M_{ij} about a reference incident-electron energy E_0, we obtain

$$M_{ij}(E)=M_{ij}(E_0)+\tfrac{1}{2}R_{ij}(E-E_0)+\cdots. \quad (5.3)$$

In the effective range approximation the series is cut off after the second term. We take E_0 to be 10.2 eV, the energy required to excite hydrogen from the $1s$ to the $2s$ state. The expansion is valid for $E<10.2$ eV, but in this case we must put $k_2=i\kappa_2$ in Eqs. (5.1) and (5.2).

In the triplet case the expansion (5.3) is valid over a fairly long range, however in the singlet case the presence of a resonance just below the $2s$ threshold sharply limits the applicability of the expansion. According to the analysis of Ross and Shaw,[9] the effective range approximate formalism can describe only one narrow resonance below threshold. Below this resonance the formalism will not accurately predict the true scattering cross section.

Our expansion parameters $M_{ij}(E_0)$ and R_{ij} were obtained by fitting a two-term polynomial of the form (5.3) to the computed values of M_{ij} in the range $0<k_2{}^2\leq1.5\times10^{-3}$. They are given in atomic units in Table III together with the coefficients obtained from the $1s-2s$ close-coupling values by Damburg and Peterkop.[5] In Fig. 1 the computed NA elastic cross section is compared with our effective range extrapolation. As can be seen the extrapolation quite accurately reproduces the resonance near $k_1^2=0.797$. The second peak at $k_1^2=0.735$ is spurious in the present zeroth-order problem but more resonances are actually present when relative p waves are included in the calculation.[10,12]

VI. RESULTS

The results obtained for the spherically symmetric portion of the $L=0$ scattering cross sections σ_{1s-1s}, σ_{1s-2s}, σ_{2s-2s} are shown in Tables IV to VI and in Figs. 1 to 3. For comparison purposes the ($1s-2s$) close coupling results are also given. As previously

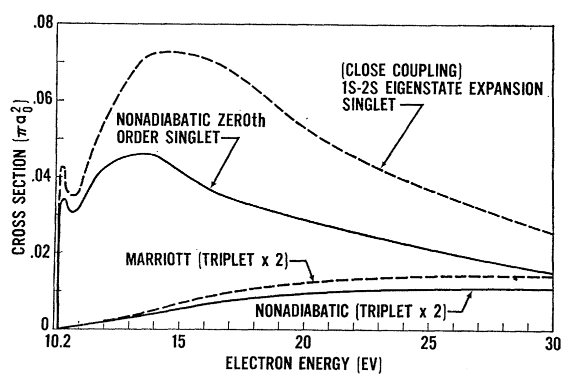

FIG. 2. Comparison of zeroth-order nonadiabatic $1s-2s$ excitation cross section with the close-coupling $1s-2s$ expansion.

[12] M. Gailitis and R. Damburg, Proc. Phys. Soc. (London) **82**, 192 (1963).

TABLE IV. The spherically symmetric portion of the $L=0$ elastic $(1s-1s)$ cross section for the scattering of electrons by atomic hydrogen in units of πa_0^2. NA=nonadiabatic[a]; CC=close coupling $1s-2s$.[b]

		Singlet			Triplet		Sum	
k_1 (au)	Energy (eV)	NA		CC	NA	CC	NA	CC
0.810	10.061	0.635						
0.863	10.132	0.760						
0.864	10.155	1.20						
0.86429	10.163	1.337						
0.8645	10.169	0.0						
0.865	10.179	0.2925						
0.8654	10.189	0.3893						
0.8656	10.194	0.4255						
0.8658	10.198	0.4465						
0.866	10.203	0.4743						
0.86601	10.2033	0.4768						
0.86602	10.2036	0.4795						
0.866025		case (i)	case (ii)			Threshold		
0.86604	10.2040	0.4790	0.4789					
0.8661	10.2055	0.4755	0.4754	0.4244	3.995	3.995	4.470	4.4194
0.8662	10.2085	0.4742	0.4740	0.4235	3.994	3.993	4.468	4.4165
0.870	10.298		0.4955	0.4541	3.958	3.957	4.454	4.4111
0.880	10.536	0.4955	0.4954	0.4568	3.864	3.864	4.359	4.3208
0.89	10.777	0.4826	0.4825	0.4454	3.773	3.772	4.256	4.2174
0.90	11.02	0.4674	0.4673	0.4324	3.684	3.684	4.151	4.1164
0.94	12.02	0.399	0.399		3.349		3.748	
1.0	13.605	0.327	0.330	0.2824	2.905	2.903	3.233	3.1854
1.1	16.46	0.239	0.250	0.1865	2.300	2.297	2.550	2.4835
1.2	19.6	0.175	0.190	0.1397	1.833	1.829	2.023	1.9687
1.5	30.6	0.095	0.113	0.0905	0.974	0.9716	1.087	1.0621

[a] The statistical factors $\frac{1}{4}$ and $\frac{3}{4}$ are included in the cross sections. When available case (ii) results were used to find the total scattering cross sections.
[b] All close-coupling results were computed by K. Omidvar, Ref. 4.

stated this latter calculation is a variational approximate solution of the zeroth-order problem.[1] The internal consistency of our calculations has already been extensively examined in Sec. IV. For the nonadiabatic entries in Tables IV–VI the number of significant figures given indicates the internal consistency of the calculation with the last significant figure being in doubt. For the singlet entries at $k_1=1.5$ even the first significant figure is uncertain. The NA singlet-case (i) cross sections are the ones which are plotted in those figures, however the case (ii) calculations are of equal weight.

In Fig. 2 the nonadiabatic σ_{1s-2s} cross sections are compared with the close-coupling expansion with the $1s$ and $2s$ channels open. The close-coupling results just above threshold were kindly computed for us by Dr. Omidvar of the Theoretical Division of the Goddard Space Flight Center. They appear to be in good agreement with those of Damburg and Peterkop.[5] The other close-coupling results were obtained from Marriott[2] and Omidvar,[4] which in turn are in good agreement with those of Smith and his co-workers.[3,13] The nonadiabatic results are about 40% lower than those of the close-coupling calculation. In fact the case (i) nonadiabatic σ_{1s-2s} cross sections agree quite well with the variational calculation of Massey and Moiseiwitsch.[6]

Figure 3 shows the zeroth-order nonadiabatic elastic singlet cross section in the neighborhood of the threshold (10.203 eV) and out to 30 eV. A definite Wigner cusp is indicated at threshold. The close-coupling results, dashed line, also indicate a cusp at threshold. Above 30 eV the case (ii) nonadiabatic σ_{1s-1s} remains 20% larger than the close-coupling results and as such are larger than the plotted case (i) results which at these energies are within 5% of the close-coupling values.

The σ_{1s-1s} curve is shown as varying smoothly above the $2s$ threshold. Actually tentative results indicate that there is probably a slight ripple in the elastic cross section just below the $3s$ excitation threshold. The magnitude of this ripple appears to be only a few percent of the total cross section and it is difficult to separate

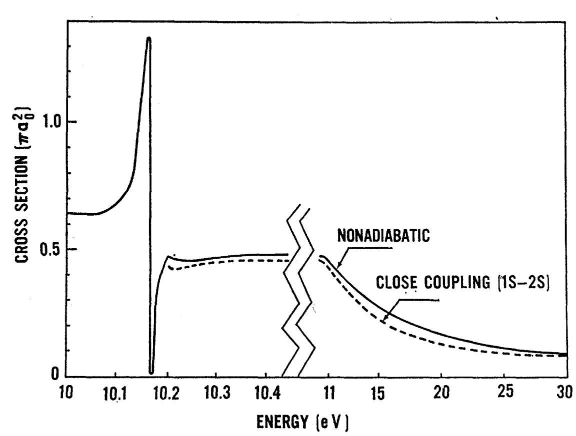

FIG. 3. Comparison of the zeroth-order nonadiabatic elastic scattering cross section with the close-coupling $1s-2s$ expansion.

[13] P. G. Burke and K. Smith, Rev. Mod. Phys. 34, 458 (1962).

TABLE V. The spherically symmetric portion of the $L=0$ $(1s-2s)$ cross section for the excitation of atomic hydrogen by electrons in units πa_0^2. NA = nonadiabatic[a] and CC = close coupling $1s-2s$.

		Singlet NA			Triplet		Sum	
k_1 (au)	Energy (eV)	Case (i)	Case (ii)	CC	NA	CC	NA	CC
0.86604	10.2004	0.0066	0.0066				0.0066	
0.8661	10.20176	0.0142	0.0142	0.0168	9.9×10^{-6}	9×10^{-6}	0.0142	0.0168
0.8662	10.2041	0.0204	0.0204	0.0266	1.5×10^{-5}	1.6×10^{-5}	0.0204	0.0266
0.870	10.294		0.0354	0.0420	7.8×10^{-5}	8.3×10^{-5}	0.0355	0.0420
0.880	10.536	0.0313	0.0314	0.0356	1.8×10^{-4}	1.9×10^{-4}	0.0316	0.0358
0.890	10.776	0.0318	0.0319	0.0355	2.7×10^{-4}	2.9×10^{-4}	0.0322	0.0322
0.90	11.02	0.0339	0.0338	0.0375	3.8×10^{-4}	4×10^{-4}	0.0342	0.0379
0.94	12.02	0.0448	0.0448		9.1×10^{-4}		0.0457	
1.0	13.605	0.046	0.048	0.0725	1.9×10^{-3}	2.1×10^{-3}	0.050	0.0746
1.1	16.46	0.035	0.040	0.0701	3.3×10^{-3}	4.4×10^{-3}	0.043	0.0745
1.2	19.59	0.031	0.039	0.0547	4.7×10^{-3}	6.1×10^{-3}	0.044	0.0608
1.5	30.61	0.013	0.019	0.0241	5.6×10^{-3}	7.3×10^{-3}	0.025	0.0314

[a] See Table IV footnotes.

TABLE VI. The spherically symmetric portion of the $(L=0)2s-2s$ cross section for the scattering of electrons by atomic hydrogen in units of πa_0^2. NA = nonadiabatic[a]; CC = close coupling $1s-2s$.

		Singlet NA			Triplet sum			
k_2 (au)	Energy (eV)	Case (i)	Case (ii)	CC	NA	CC	NA	CC
0.00503	0.0003	654	654					
0.0114	0.0018	622	622	650.3	205		827	
0.0174	0.0041	579	579	602	204	206.8	783	808.8
0.0831	0.094		137	135.55	170.6	172.3	307.6	307.85
0.1562	0.332	19.6	19.6	19.36	110.4	110.5	130	129.86
0.2052	0.573	3.69	3.68	3.515	71.21	71.20	74.89	74.715
0.245	0.819	0.441	0.441	0.3303	45.99	45.94	46.531	46.27
0.365	1.82	0.43	0.41		7.37		7.78	
0.500	3.40	1.8	1.9	1.532	0.02	0.2102	1.92	1.7422
0.678	6.26	1.8	1.8	1.115	1.37	1.36	3.17	2.475
0.831	9.39	1.3	1.3	0.8980	2.45	2.112	3.75	3.010
1.225	20.41	0.60	0.55	0.5702	1.94	1.811	2.49	2.3812

[a] See Table IV footnotes.

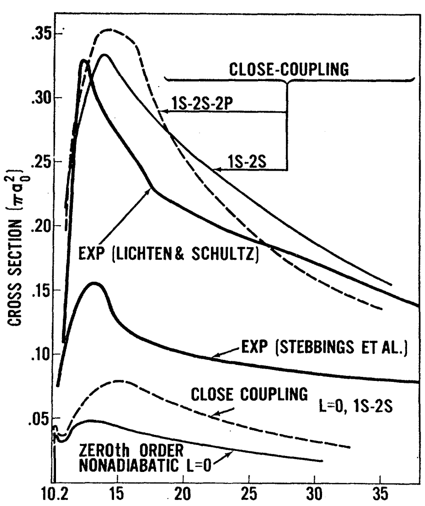

FIG. 4. The top four curves represent the total close-coupling theoretical and the experimental cross sections for the $1s-2s$ excitation of H by electron impact. The two bottom curves give the $L=0$, angle independent portion of this cross section.

it from the ordinary scatter in the calculated cross section at this point. This effect also occurs in the $(1s-2s)$ and $(2s-2s)$ channels, and it may be analogous to the resonance in σ_{1s-1s} below the $2s$ threshold but much reduced in scale.

Our triplet elastic cross sections agree with the close-coupling results to better than 1%. Since the triplet cross sections dominate in this region, the total non-adiabatic elastic cross section $(\sigma_s+\sigma_t)$ lies within 2% of the close-coupling result.

It would be of interest to be able to solve the zeroth-order Eq. (I3.3) exactly by numerical means. A continuing effort is being made to do this with the non-iterative method which has already been used in the triplet case below threshold.[14] So far the results have been unsatisfactory. This is at least partly due to the large effective interaction radius between the $2s$ state of hydrogen and the scattered electron.

[14] A. Temkin and E. Sullivan, Phys. Rev. **129**, 1250 (1963).

VII. DISCUSSION

Figure 4 compares the spherically symmetric portion of the inelastic cross section with the total close-coupling theoretical cross section and with the total experimental cross sections obtained by Stebbings *et al.*[15] and Lichten and Schultz.[16] Examination of the graph indicates that the nonadiabatic $L=0$, $1s-2s$ cross section is reduced from the $1s-2s$ close-coupling (CC) results by about the same percentage as the Lichten and Schultz cross section is reduced from the $1s-2s-2p$ CC results around the region of maximum cross section (15 eV) or as the Stebbings *et al.* are from the Lichten *et al.* results over most of the energy range. Thus this calculation reinforces what one would be tempted to believe on looking at the $1s-2s-2p$ results in comparison with the experimental results: a more exact theoretical calculation will reduce the theoretical cross section toward the experimental results.

As to the amount of this decrease one must be infinitely more circumspect in guessing. In the language of the nonadiabatic theory the $L=0$ part of the $1s-2s-2p$ calculation refers to the relative $s+p$ wave problem whereas the $1s-2s$ calculation refers to only the relative s-wave problem. From that point of view, the latter appears to be a better approximation relative to its complete solution (to which the present paper is addressed) than the former is to its complete solution. In either case, it might seem ridiculous to try to approximate by two or three terms what in principle is described by a singly or doubly (discrete plus continuous) infinite set of functions. Here, however, one must recall what Seaton[17] long ago emphasized, that the explicit (anti) symmetrization of the wave function in fact doubles the number of terms and goes a long way in including the effects of the continuum in these calculations. Secondly, with regard to the $1s-2s-2p$ calculation, the singlet $L=0$ gives only the second largest contribution to σ_{1s-2s}. The largest contribution comes from the triplet $L=1$ state. Experience thus far indicates that the close-coupling approximation is much more accurate in triplet as opposed to singlet states.

Thus it is very difficult at this time to infer the correct normalization of the experimental result. In view of the many competing elements which are either included or left out of the close-coupling calculation, our own opinion is that the correct normalization of the experimental result is between those of Lichten *et al.* and Stebbings *et al.* and closer to the latter, very close, in fact, to that curve where the error bars of the respective experiments overlap.[11,18] This conclusion is supported by a recent $(1s-2s-2p-3s-3p)$ close-coupling calculation by Taylor and Burke[19] which produced more than a 30% decrease in σ_{1s-2s} at 16.5 eV from the close-coupling $(1s-2s-2p)$ calculation.[3,4]

Our results and those of Damburg and Peterkop[5] also show that one must be very cautious in naively extrapolating cross sections to threshold using the Wigner threshold behavior law.[20] The present results, Table V, indicate that the law's range can be exceedingly small. When the $2p$ state is included in the calculation the $2s$ and $2p$ states are degenerate and Wigner's threshold laws no longer necessarily apply.[12]

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[16] W. Lichten and S. Schultz, Phys. Rev. **116**, 1132 (1959).

[17] M. J. Seaton, Phil. Trans. Royal Soc. London **A245**, 469 (1953).

[18] D. G. Hummer and M. J. Seaton, Phys. Rev. Letters **6**, 471 (1961).

[19] A. J. Taylor and P. G. Burke, in *Proceedings of the Third International Conference on the Physics of Electronic and Atomic Collisions* (North-Holland Publishing Company, Amsterdam, to be published).

[20] E. P. Wigner, Phys. Rev. **73**, 1002 (1948).