Convergence of pseudostate expansions in electron-hydrogen scattering

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A close-coupling calculation using a nine-state pseudostate expansion is performed in the intermediate-energy range for a simplified model of electron-hydrogen scattering. The resulting elastic scattering and excitation cross sections exhibit rather narrow structure below pseudothresholds. Except for this narrow structure, the cross sections have converged to the exact results and the T-matrix elements have converged to the previously corrected T-matrix elements for a smaller basis set.

In recent work, we performed calculations for a simplified model of electron-hydrogen scattering employing pseudostate expansions of rather different characters.[1] Pseudothreshold structure was found to extend over a broad range of incident energy in the intermediate-energy range. This physically meaningless structure was removed by making a linear least-squares fit to elements of the T matrices using a low-order polynomial in energy. The resulting elastic scattering and excitation cross sections were found to be reasonably accurate. In this work, we employ a larger basis set in order to examine the nature of convergence of the pseudostate expansions.

This calculation was performed with the following motivations. In a practical calculation the infinite number of eigenstates of the target atom are approximately represented by a few judiciously chosen states. This raises the question of the completeness of the finite expansion basis set. Another problem is that of the broad pseudoresonances for small basis sets.[1,2] Does a larger basis set alleviate this problem as is suggested schematically by Burke, Berrington, and Sukumar[3] for a somewhat similar situation? That is, does a calculation with a larger basis set result in relatively narrow pseudoresonances thereby reducing the range of incident energy over which unreliable cross sections are found? The answers to these questions should apply to real problems as well as to the model problem examined here. The model considered here is that of a hydrogen atom which has only s states and where the total angular momentum during the collision is considered to be zero.

We construct the orthonormal set of target functions R_i as a linear combination of Slater orbitals η_j.

$$R_i(r)=\sum_{j=1}^{m} c_j{}^i \eta_j(r) \quad , \tag{1}$$

where

$$\eta_j(r)=r^{n_j}e^{-\xi_j r} \quad . \tag{2}$$

The choice of n_j and ξ_j uniquely determines the expansion coefficients $c_j{}^i$ by simultaneous diagonalization of the Hamiltonian and overlap matrices constructed on the basis of R_i. We also obtain the energy eigenvalues E_i in this process.

It was found in our previous work that the best results for this model were obtained with the shortest-range basis set (set B of Ref. 1). In this work we augmented that basis set by including three more orbitals to account for the exact $3s$ eigenstate of the hydrogen atom and one more relatively short-range orbital. The parameters for the basis set and the resulting spectrum of energy eigenvalues are given in Table I. The highest pseudostate resides at a high eigenvalue of 13.22 Ry in the continuum. It appears that this basis set would represent short-range projectile-target electron correlation better than any set in the previous work on this model.

The scattering calculations were performed using the alge-

TABLE I. Parameters and energies of the basis set.

j	n_j	ξ_j	E_i
1	0	1.0	−1.0
2	0	0.5	−0.25
3	1	0.5	−0.1111
4	0	$\frac{1}{3}$	−0.060 58
5	1	$\frac{1}{3}$	0.2034×10^{-3}
6	2	$\frac{1}{3}$	0.1713
7	0	1.5	0.6682
8	1	1.0	2.3929
9	2	0.75	13.2170

TABLE II. Numerical values of cross sections for ^1S in units of $\pi a_0{}^2$.

	$\sigma(1s\rightarrow 1s)$			
Energy	5s(uncorrected)[a]	5s(corrected)[a]	Exact[b]	9s(present)
1.21	0.2501	0.2465	0.2469	0.2477
1.44	0.1926	0.1967	0.1944	0.1955
1.70	0.1724	0.1592	0.1581	0.1602
2.00	0.1340	0.1305	0.1314	0.1310
2.25	0.1131	0.1139	0.1159	0.1180
3.00	0.0866	0.0862		0.0887
		$\sigma(1s\rightarrow 2s)$		
1.30	0.0247	0.0311	0.0323	0.0333
1.70	0.0149	0.0219	0.0220	0.0207
2.00	0.0147	0.0163	0.0168	0.0171
2.50	0.0123	0.0111	0.0113	0.0118
3.00	0.0083	0.0087	0.0080	0.0078

[a]Reference 1. [b]Reference 5.

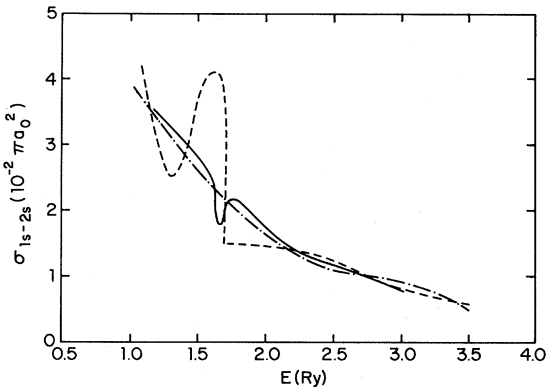

FIG. 1. Cross sections for the $1s \rightarrow 2s$ transition in the ^1S state. The solid curve is the present nine-state result; the dashed curve is the result of a five-state expansion (Ref. 1); the chain curve is the result of the T-matrix fitting procedure for the five-state expansion (Ref. 1).

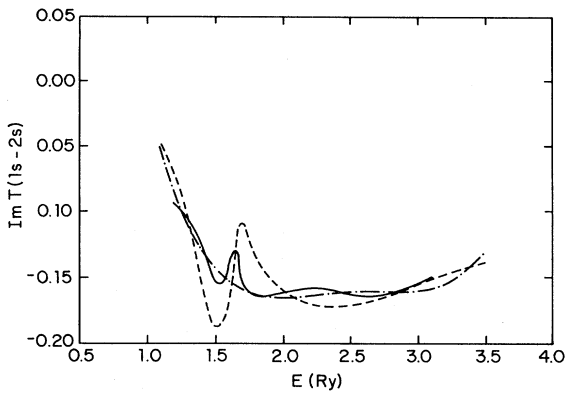

FIG. 3. Imaginary part of the T matrix for the $1s \rightarrow 2s$ transition in the ^1S state. Curves have the same significance as in Fig. 2.

braic variational method which is described in detail by Callaway.[4]

In the triplet case, the convergence was achieved in our previous work,[1] even with the five-state expansion, to a remarkable degree. The present results are identical and hence not repeated here.

The cross sections for elastic scattering and excitation to the $2s$ state are given in Table II at the same representative values of energies as in Ref. 1 for the ^1S case. The five-state results and the exact results of Poet[5] are also included in the table. The elastic scattering cross section for the nine-state expansion at 1.21 Ry is quite accurate although there is a pseudothreshold at 1.171 Ry indicating rather narrow pseudostructure. The elastic scattering and excitation cross sections ($1s \rightarrow 2s$) are reasonably accurate at 1.7 Ry with another pseudothreshold at 1.669 Ry. At other incident energies the present results are satisfactory.

The excitation cross section for the nine-state calculation is shown in Fig. 1 as a function of incident energy. It can be compared with the results of the five-state calculation.[1] The broad structure (~ 1.0 Ry) of the five-state calculation is reduced to a very narrow structure (~ 0.2 Ry). Further, the structure is not as pronounced. Apart from this very narrow structure, the agreement is quite good with the previously corrected results.

The elements of T matrix give a more stringent test than the cross section. In Figs. 2 and 3, we display the real and imaginary parts of the T_{12} elements, respectively. The structure in these quantities is narrower and less pronounced in the nine-state case than in the five-state case. Furthermore, it is quite remarkable that the nine-state values approximately converge to the previously corrected T-matrix elements by the fitting procedure.

The corresponding scattering information for the elastic scattering is displayed in Figs. 4–6. The not-too-prominent structure in the cross section for the five-state calculation is dramatically reduced further for the nine-state calculation. The remarks made for T-matrix elements for excitation also hold for elastic scattering.

We conclude from this work that apart from the pseudostructure, the pseudostate expansions exhibit rapid convergence. The pseudostructure diminishes significantly with increasing number of judiciously chosen basis functions,

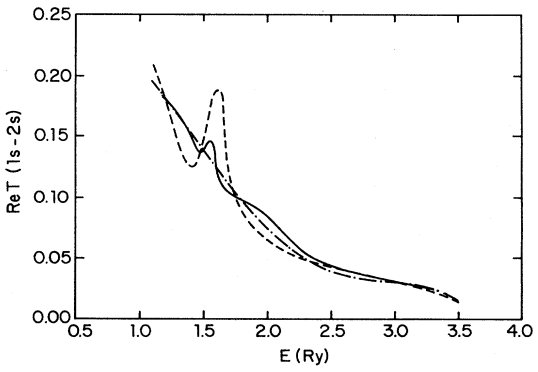

FIG. 2. Real part of the T matrix for the $1s \rightarrow 2s$ transition in the ^1S state: solid curve—present nine-state results; dashed and chain curves—directly calculated values and result of fit, respectively, for the five-state expansion (Ref. 1).

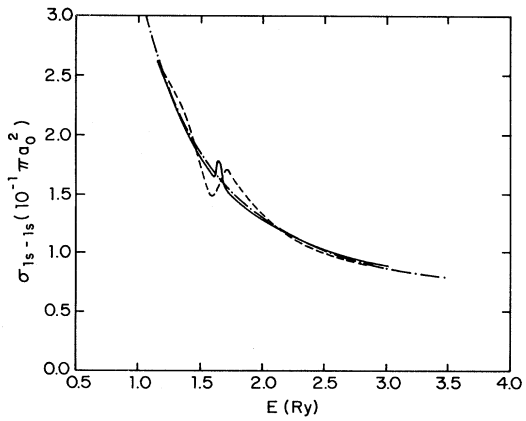

FIG. 4. Cross sections for elastic scattering in the ^1S state. The curves have the same significance as in Fig. 1.

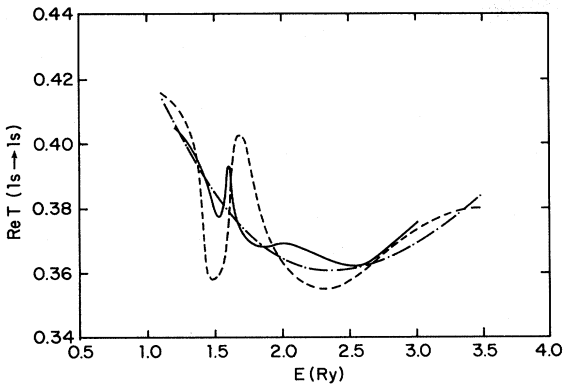

FIG. 5. Real part of the T-matrix element for elastic scattering in the ^1S state. The curves have the same significance as in Fig. 2.

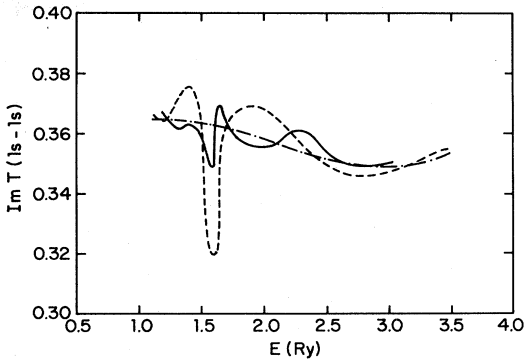

FIG. 6. Imaginary part of the T-matrix element for elastic scattering in the ^1S state. The curves have the same significance as in Fig. 2.

thereby alleviating the problem of pseudoresonance. The convergence property of the T-matrix elements strengthens the validity of the procedure of T-matrix fitting for the removal of meaningless unphysical structure near pseudothresholds.

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