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# Total and ionization cross sections in a simplified model of electron-hydrogen scattering

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The total cross section (inclusive of all scattering) is calculated as a function of energy for a simplified model of electron-hydrogen scattering in which all terms involving nonzero angular momenta are neglected. Only the $^1S$ state is considered. The two-body Schrödinger equation is integrated numerically, and the optical theorem is used to determine the total cross section. The results agree rather well with those obtained from a pseudostate expansion. High and low bounds are given for the ionization cross section, and these are compared with estimates of ionization obtained from a pseudostate expansion.

## I. INTRODUCTION

We consider in this paper a simplified model of electron-hydrogen scattering in which the actual Coulomb interaction between electrons, $e^2/|\vec{r}_1-\vec{r}_2|$, is replaced by the leading term in a multipole expansion of this quantity, $e^2/r_>$ (where $r_>$ is the greater of $r_1$ and $r_2$). This model ignores much of the essential physics of the real hydrogen atom, in particular, the degeneracy of the states of the same $n$ but different $l$. All angular dependence of the wave function is suppressed. However, there still are an infinite number of discrete bound states and an ionization continuum. We believe that the model retains enough complexity to be both interesting in its own right, and useful as a test case in which calculational methods intended to be applied to more realistic problems can be tested. Our calculation here will concern the $^1S$ state of the two-electron system. This state is interesting in that the short-range correlation between the two electrons is extremely important. No angular momentum barrier is present. Also, essentially exact results are available for some scattering processes from other authors (see below). Our technique could be readily adapted to the $^3S$ state, but here the Pauli principle prevents the close approach of two electrons, and the scattering is predominately elastic.

The study of this model was initiated by Temkin *et al.*[1–3] The two-body Schrödinger equation for this model is simply a partial differential equation in the two radial variables $r_1$ and $r_2$. Temkin *et al.* attempted to solve this equation directly, by expansion in a complete set of elementary solutions. We use a related procedure here, although our numerical methods are very different in detail. Burke and Mitchell[4] studied the application of a pseudostate basis in a close-coupling calculation of bound-state excitation, and uncovered complications due to pseudoresonances. We have recently shown that it is possible to obtain rather good results for excitation cross sections by averaging over pseudoresonances.[5]

This model has also been studied by Poet[6–8] who has obtained essentially exact results for the cross sections for elastic scattering and for the excitation of the 2*s* state up to an incident energy of 3 Ry. We are concerned here with the extension of Poet's methods to calculate the total cross section for all scattering processes and the ionization cross section. We shall compare our results for these quantities with corresponding results obtained from several pseudostate expansions.

## II. COMPUTATIONAL METHODS

The symmetry of the two-electron-configuration space implies that we can restrict our attention to the open triangle $r_2 \le r_1$. The two-body Schrödinger equation has the form given below within this triangle (see Fig. 1)

$$\frac{\partial^2}{\partial r_1^2}\psi(r_1,r_2)+\frac{\partial^2}{\partial r_2^2}\psi(r_1,r_2)+\left[\frac{2}{r_2}-E\right]\psi(r_1,r_2)=0,\quad r_2\le r_1 \tag{1}$$

in which $E$ is the total energy. Atomic units with energies in rydbergs are used, and the quantity we denote by $\psi$ is actually $r_1 r_2$ times the wave function. Equation (1) is separable, but the problem is saved from triviality by the fact that the boundary conditions on the line $r_1=r_2$ are not separable. They are

$$\begin{aligned}&\psi(r,r)=0\quad(\text{triplet})\,,\\&\frac{\partial\psi}{\partial r_1}=\frac{\partial\psi}{\partial r_2}\quad\text{when } r_1=r_2\quad(\text{singlet})\,.\end{aligned} \tag{2}$$

We shall solve the differential equation using an efficient algorithm due to Poet.[7] Only the essential features of this procedure will be discussed here. For further details consult Refs. 7 and 9.

Suppose that we consider a square grid of points denoted $(i,j)$ (where $i$ refers to $r_1$ and $j$ to $r_2$). A (nonsquare) matrix $D_{j,j'}^{(i)}$ is introduced which relates the wave function at grid points on two successive vertical lines (see Fig. 1),

$$\psi(i,j)=\sum_{j'=1}^{i+1} D_{jj'}^{(i)}\psi(i+1,j')\ . \tag{3}$$

The matrix $D^{(i)}$ can be calculated by a straightforward procedure described in Ref. 7. The advantage of working

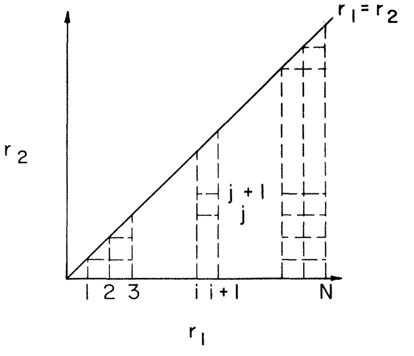

FIG. 1. Configuration space for the two-electron system.

with $D^{(i)}$ is that the most time consuming step in its computation is the inversion of a related matrix of order $(i \times i)$, a process which must be repeated for each value of $i$. This gives a time of order of $(i)^4$ to obtain $D^{(i)}$, starting from the origin, whereas many other noniterative approaches would require times of the order $(i)^6$.

The most serious problem encountered is to extract scattering information once $D^{(i)}$ has been determined for the largest value of $i$ considered. To do this, we expand $\psi(r_1,r_2)$ in terms of a complete set of elementary solutions of Eq. (1). These solutions have the form

$$u_{k,q}(r_1,r_2)=e^{ikr_1}f(q,r_2) \ , \tag{4}$$

where $f$ is a Coulomb wave function. Although the $u_{k,q}$ satisfy the differential equation (1) exactly, they do not individually obey the boundary conditions. The complete solution must be represented as a linear combination of these functions. As both bound and continuum solutions must be considered, let us note the following conventions:

$$k^2+q^2=E \ . \tag{5a}$$

For bound states of the hydrogen atom, set

$$q=-i/n \ , \tag{5b}$$

where $n$ is an integer. Then $f$ is a bound (normalized) hydrogen wave function.

In the case of continuum states, $f$ is a continuum hydrogenic function of wave vector $q$. However, we must note that if $q^2 > E$, we should set $k = i\kappa$. We have in such cases an exponentially decaying function along the $r_1$ axis. Furthermore, we will distinguish the channel containing the incident wave by an index $a$; thus $k_a$ is the wave vector of the incident electron. $q_a^2=-1/n_a^2$ is the energy of the hydrogen atom in that state, and $f$ is the corresponding wave function. Then we have

$$\psi(r_1,r_2)=e^{-ik_ar_1}f_a(r_2)+\sum_j c_{ja}u_{k_jq_i}(r_1,r_2) \ . \tag{6}$$

The notation $\sum$ includes both a sum over bound states and an integral over the continuum; the latter includes the close continuum channels. The numerical calculation of the matrix $D$ [Eq. (3)] gives us, in effect, properly symmetrized $\psi(r_1,r_2)$ on a grid. Our problem is to determine the coefficients $c_{ja}$, which contain the scattering information. These are related to the elements of the $S$ matrix for bound-state scattering by

$$S_{ja}=\left[\frac{k_j}{k_a}\right]^{1/2} c_{ja} \ . \tag{7}$$

In principle, the problem of determining the $c_{ja}$ is quite straightforward. It is necessary to substitute (6) into (3), from which one obtains a relation between the $c_{ja}$, the matrix $D$, and the functions $u$ evaluated at the grid points. Actually, the situation is extremely complicated, and in fact the principal difficulty of this calculation is the extraction of the $S$-matrix elements.

The basis of the problem is that Eq. (6) involves an expansion with an infinite number of terms (including an integration over a continuum), whereas $D$ is a finite matrix. We must therefore include only a finite number of functions which should be smaller than the number of points on the line labeled $N$ in Fig. 1. The coefficients $c$ may then be determined by a least-squares procedure as discussed in Ref. 7. Unfortunately, one frequently encounters severe problems of numerical stability.

In the energy range of interest to us (1—4 Ry), we include 5—8 bound states explicitly, and a number of open-channel continuum functions varying from 7 at low incident energy (1.10 Ry) to 23 at 4 Ry. The fit to determine the coefficients was performed generally at $r_1=40$, using a grid spacing of 0.2. These parameters were chosen on the basis of the following considerations: As is discussed below, we estimate the ionization cross section by subtracting bound-state excitation from the total cross section. We found that $r_1 \approx 40$ was needed to obtain convergence for the $3s$ excitation cross section. The grid spacing of 0.2 seemed to be needed to obtain stable results from the least-squares-fitting process. The most time-consuming process is the calculation of $D$; with these parameters, approximately 43 min of CPU (central processing unit) time on an IBM 3033 computer were required for each energy.

There remains a difficulty that while the Coulomb functions $f$ are mutually orthogonal on the infinite interval, they are not on the finite interval $0 \le r_2 \le r_1$. This appears to be the principal source of the numerical problems encountered. We have experimented with several methods of obtaining stable results; including expansion of the coefficients $c_{ja}$ in terms of Legendre polynomials which depend on energy as discussed in Ref. 7. However, the most satisfactory results, in our opinion, were obtained by enforcing orthogonality. The function $f(q,r)$ actually used in the fit are made into an orthogonal set by the Schmidt process. For $r_1 \approx 30$, the $1s$, $2s$, and $3s$ bound-state functions are hardly modified. But higher bound-state and continuum functions are significantly changed. The coefficients $c_{ja}$ for these functions then lose physical significance.

We do obtain reliable results for the cross section for elastic scattering and for the excitation of the $2s$ and $3s$ states. The total cross section is obtained using the optical theorem from the real part of $S_{11}$:

$$\sigma_t=\frac{1}{2k^2}[1-\mathrm{Re}(S_{11})] \ . \tag{8}$$

Our data indicate that $S_{11}$ is stable in phase and in magnitude. We can then obtain the ionization cross section by subtracting from $\sigma_t$ the sum of the elastic cross section plus that for the excitation of the bound states.

There is, of course, some uncertainty in regard to the bound-state cross sections. Let $\sigma_{123}$ be the sum of the elastic cross section and that for excitation of the $2s$ and $3s$ states. We can say with certainty that

$$\sigma_I < \sigma_t - \sigma_{123} \; . \tag{9}$$

At energies sufficiently high for the Born approximation to be valid, the cross section for the excitation of the $n$th $s$ state varies as $n^{-3}$ (this is simply a consequence of the $n$ dependence of the normalization of the bound-state wave functions). Hence, in this limit

$$\sum_{n=4}^{\infty} \sigma_{ns} \approx 27\sigma_{3s} \sum_{n=4}^{\infty} \frac{1}{n^3} = 1.08\sigma_{3s} \; . \tag{10}$$

This result is dependent on the Born approximation for validity and appears from our results to be an overestimate. We will write

$$\sum_{n=4}^{\infty} \sigma_{ns} = f\sigma_{3s} \; . \tag{11}$$

In general, $f$ is a function of energy, whose high-energy limit is 1.08. We can find $f$ at one specific energy, $k^2=1.00$, where no ionization is possible but all bound states can be excited. At this energy, we use our numerical results,

$$f = \frac{1}{\sigma_{3s}} \sum_{n=4}^{\infty} \sigma_{ns} = \frac{\sigma_t - \sigma_{123}}{\sigma_3} = 0.41 \; . \tag{12}$$

We conjecture that $f$ is a monotonic function of energy ranging between 0.41 and 1.08. If this is correct then $\sigma_I$ is bounded in the range between $\sigma_L$ and $\sigma_H$,

$$\sigma_L \le \sigma_I \le \sigma_H \; , \tag{13a}$$

with

$$\sigma_L = \sigma_t - \sigma_{123} - 1.08\sigma_{3s} \; , \tag{13b}$$

$$\sigma_H = \sigma_t - \sigma_{123} - 0.41\sigma_{3s} \; . \tag{13c}$$

We can interpolate $f$ roughly between these values using the following argument: The cross section for the excitation of the $n$th $s$ state from the $1s$ state can be expected to depend on the incident energy $E_i$, as

$$\sigma_n = \frac{a_n}{E_i} + \frac{b_n}{E_i^2} + \frac{c_n}{E_i^3} + \cdots \; . \tag{14}$$

The first term $a_n$ is correctly given by the Born approximation. So the correction to the Born value depends on $E$ as $1/E_i^2$ to leading order. It follows from this that the function $f$ departs from the Born value by terms of the same order in energy

$$f = f_B - \frac{C}{E_i^2} \; . \tag{15a}$$

We know that $f_B \approx 1.08$, and then using $f=0.41$ at $E_i=1$, we deduce

$$f = 1.08 - \frac{0.67}{E_i^2} \; . \tag{15b}$$

Although this estimate is quite rough because terms of order $1/E_i^2$ are not sufficient to give $f$ correctly near $E_i=1$, it is the best we can obtain from our data. We use Eq. (15b) to define an interpolated ionization cross section:

$$\sigma_I \approx \sigma_t - \sigma_{123} - f\sigma_{3s} \; . \tag{16}$$

We conclude this section with a remark about symmetrization. Equation (6) is an exact expression if the summation over $j$ includes all bound and continuum states. It is, however, not explicitly symmetric. Interchange of $r_1$ and $r_2$ takes one into a different region of configuration space (the upper triangle in Fig. 1), and the necessary symmetry can result only when all the (infinite number of) terms in the formal Eq. (6) are actually included.

One will, therefore, ask whether the results are improved by explicitly symmetrizing the practical form of Eq. (6) which contains only a finite number of terms. This is easily done by replacing $u_{kq}(r_1,r_2)$ by $u_{kq}(r_1,r_2)+u_{kq}(r_2,r_1)$, in (6) and making the corresponding replacement on the first term. However, the numerical results are distinctly inferior when this is done. The

TABLE I. Cross sections for elastic scattering, for excitation of the $2s$ and $3s$ states, and total cross section, all in units of $\pi a_0^2$. The last column $\sigma_I$ is the interpolated ionization cross section using Eq. (16).

| $k^2$ | $\sigma_{1s}$ | $\sigma_{2s}$ | $\sigma_{3s}$ | $\sigma_t$ | $\sigma_I$ |
|---|---|---|---|---|---|
| 1.00 | 0.328 | 0.042 | 0.0069 | 0.379 | |
| 1.10 | 0.281 | 0.039 | 0.0081 | 0.356 | 0.0032 |
| 1.21 | 0.244 | 0.035 | 0.0084 | 0.300 | 0.0071 |
| 1.44 | 0.193 | 0.028 | 0.0071 | 0.249 | 0.0155 |
| 1.70 | 0.157 | 0.022 | 0.0056 | 0.209 | 0.0200 |
| 2.00 | 0.131 | 0.017 | 0.0047 | 0.178 | 0.0219 |
| 2.25 | 0.114 | 0.014 | 0.0036 | 0.158 | 0.0228 |
| 2.50 | 0.103 | 0.011 | 0.0029 | 0.142 | 0.0218 |
| 3.00 | 0.087 | 0.0077 | 0.0022 | 0.119 | 0.0201 |
| 4.00 | 0.065 | 0.0046 | 0.0013 | 0.087 | 0.0143 |

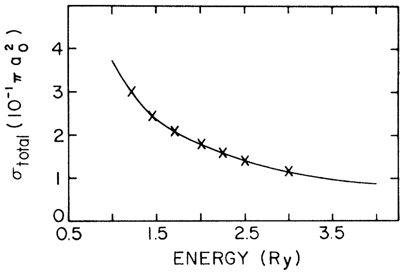

FIG. 2. Total cross section obtained from the numerical integration of the two-dimensional Schrödinger equation is shown as a solid line. The result obtained from a pseudostate expansion is shown as a set of crosses.

reason is that one has added to Eq. (6) functions which are not elementary solutions of Eq. (1); i.e., $u_{kq}(r_2,r_1)$ does not satisfy (1).

## III. RESULTS: COMPARISON WITH PSEUDOSTATE CALCULATIONS

The results of our calculations, based on solutions of the two-particle Schrödinger equation are given in Table I. We present there the cross sections for elastic scattering, for excitation of the $2s$ and $3s$ states, and the total cross section $\sigma_t$. These quantities are believed to be stable to about 0.001 with respect to variation of the calculational parameters (maximum radius, grid spacing, number of terms included).

The elastic and excitation cross sections for this model Hamiltonian have been compared with the results of our pseudostate calculations in Ref. 5. We report here similar comparisons for the total cross section (ionization is discussed subsequently). The comparison is made using the pseudostate results of Ref. 5 for $\mathrm{Im}(T_{11})$ as averaged over pseudothreshold structure. One comparison of this type with the seven-state basis is shown in Fig. 2. The agreement is excellent to graphical accuracy. Comparison of numerical values shows that in the range of incident energies from 1 to 3 Ry, the agreement between the values of $\mathrm{Im}(T_{11})$ obtained from the present numerical solutions and from the four pseudostate bases examined in Ref. 5 is within about 2% for each of the bases.

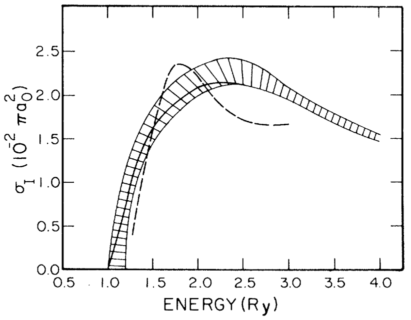

FIG. 3. Bounds on the ionization cross section $\sigma_L$ and $\sigma_H$ [defined by Eqs. (13b) and (13c)] are shown as functions of energy. The dashed line is a result obtained by the projection method applied to a pseudostate expansion according to Eq. (18). The solid line inside the shaded region is $\sigma_I$, obtained from Eq. (19), using Eq. (16) to estimate the higher bound-state contribution.

It is evident from the results presented in Table I that elastic scattering and excitation of the $2s$ and $3s$ states account for most of the total cross section. The quantities we believe bound the ionization $\sigma_L$ and $\sigma_H$ [see Eq. (13)] are much smaller, and are therefore not given as accurately as is $\sigma_t$. We show $\sigma_L$ and $\sigma_H$ in Fig. 3. The bounds are within about 5% of each other above $E_i = 3$ Ry. Our best estimate of the ionization cross section $\sigma_I$, obtained by using Eq. (16), is also shown. Numerical values for $\sigma_I$ are included in Table I.

We would like to use the present results for ionization as a test of methods for the extraction of ionization cross sections from those for the excitation of pseudostates. It has been noted above that the pseudostate bases we have used give total cross sections within about 2% of the correct values. Roughly speaking, a 2% uncertainty in the total cross section implies for this model, about a 20% uncertainty in the ionization cross section, provided that the correct cross sections for the excitation of bound states were known. This is *not* the usual case, and instead, a projection technique has been employed.[10,11]

In the projection method, one determines the portion of a pseudostate wave function which pertains to the exact bound states. The cross section for ionization is approximated by the sum of the excitation cross sections multiplied by the probability that a particle in the pseudostate would be in the (exact) continuum. Let the pseudostates be denoted by $|\,p\,\rangle$ and the bound states by $|\,b\,\rangle$. Then

$$\sigma_I \approx \sum_p \left[ 1 - \sum_b |\langle b\,|p\rangle|^2 \right] \sigma_p \,. \tag{17}$$

The sum runs over open pseudostates whose excitation cross section is $\sigma_p$. It would be a better procedure to project transition amplitudes rather than cross sections. This approach remains to be explored. Another difficulty with this procedure is that the pseudostate cross sections have threshold structure, and therefore the approximate ionization cross section according to (17) will not be a smooth function of energy. It is therefore necessary to average the cross section for the excitation of each pseudostate over the threshold structure associated with higher pseudostates. We believe that the best results are obtained as follows. Replace Eq. (17) by

$$\sigma_I = \sigma_t - \sum_b{}' \sigma_b - \sum_{b,p} |\langle b\,|p\rangle|^2 \sigma_p \,. \tag{18}$$

Here $\sigma_b$ is the cross section for excitation of the bound state $|\,b\,\rangle$. The prime on the first sum in Eq. (18) is intended to denote that the sum includes only those bound states which are exactly represented in the pseudostate basis. Equation (18) is exactly equivalent to Eq. (17) if one uses in (17) the sum of cross sections as directly computed from the pseudostate expansion. We suggest, however, that it is better to use the optical theorem to relate $\sigma_t$

to the imaginary part of the $T_{11}$ matrix element, and then average this over resonances. So we have

$$\sigma_I = \frac{1}{k^2}\mathrm{Im}(T_{11}) - \sum_b{}' \sigma_b - \sum_{b,p} |\langle b\,|p\rangle|^2 \sigma_p \ . \tag{19}$$

Equation (19) would also be exactly equivalent to (17) except that we use smoothed quantities on the right side.

Equation (19) can yield quite reasonable results, as we see from Fig. 3. The ionization cross section for the present model as obtained from Eq. (19) using the seven-state basis described in Ref. 5 is shown there in comparison with the bounds $\sigma_L$ and $\sigma_H$. We see that $\sigma_I$ from (18) is not an unreasonable estimate, but is certainly too low at low energies, and probably somewhat too low at high energies. In other words, the projection technique tends to underestimate the ionization cross section. The results for $\sigma_I$ with the five-state bases discussed in Ref. 5 are generally similar. Best results for $\sigma_I$ with the five-state bases are obtained from the basis containing the longest range functions.

## IV. CONCLUSIONS

The total cross section has been obtained from the real part of the $S$-matrix element for elastic scattering for a model of electron-hydrogen scattering in which only the monopole component of the electron-electron interaction is retained, and only the ${}^1S$ state is considered. The calculation was performed by numerical integration of the two-body Schrödinger equation. Bounds are obtained for the ionization cross section under reasonable assumptions about the behavior of the excitation cross sections for high bound states.

The results obtained above are compared with those found from close-coupling calculations with a pseudostate basis. It is found that such calculations can give the total cross section with rather good accuracy. However, the projection method for determining ionization appears, in an example, to give an underestimate.

## ACKNOWLEDGMENT

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