vanish for large q, when a series expansion in q is no longer legitimate. We show in Fig. 3 how the ratio of positron and electron bremsstrahlung cross sections for Fe and Th vary in the high-frequency region of the spectrum. The results for Th are, of course, less accurate, but they show how the factor $e^{2\pi\alpha(1-\epsilon/q)}$ of the ratio keeps the cross sections significantly different much further back from the tip.

Predictions for the two limiting regions of the pair production spectrum require no further work. It has previously been shown[9] that the cross section for a pair production process in which the positron takes almost all the energy is identical to the cross section for the high-frequency region of the electron bremsstrahlung spectrum, under the usual assumption of a very high energy incident particle. Hence, all results for electron bremsstrahlung may be taken over without modifications, understanding q again as the momentum of the low-energy electron. In the same way, pair production in which the electron takes almost all the energy is identical with the high-frequency region of the positron bremsstrahlung spectrum, with q the momentum of the low-energy positron. Figure 3 may hence also be interpreted as the ratio of pair production cross sections for these two cases, production of low-energy positrons is suppressed.

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Excitation of Atomic Hydrogen by Fast Protons

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The excitation of the metastable state ($2S$) of atomic hydrogen by fast protons is discussed. The direct excitation cross section of $2S$ is calculated from a coupled set of equations ($1S$, $2S$, $2P$). The indirect population of the $2S$ state by excitation to higher states with subsequent cascade to the $2S$ state is described by Born approximation. The calculation is shown to apply to a fast crossed beam experiment.

I. INTRODUCTION

THE virtue of the proton-hydrogen scattering system is that it is the simplest of the atom-atom[1] type. It is worthwhile understanding this system as a prototype of a more general atom-atom collision thereby gaining some confidence in the theoretical methods which we would like to apply to these more complicated collisions.

It would appear that the general atom-atom scattering problem breaks into two natural subgroups. Firstly, at high energies (where the relative velocity of the atoms is larger than the circulating electron velocities) we have the problem of direct collisions (elastic and inelastic) and the problem of rearrangement collisions. The direct collisions are treated here neglecting rearrangement. The wave functions thus obtained can then be used to calculate the rearrangement collisions. The justification for this procedure is that rearrangement probabilities are small at high energies.[2]

Secondly, at low energies a molecular description is more appropriate and direct and rearrangement collisions can be treated on almost the same footing.[2] Only direct high-energy collisions will be treated here.

We have in mind the following experiment. A slow beam of ground-state atomic hydrogen is crossed with a high-energy proton beam. The slow hydrogen beam is then allowed to proceed sufficiently long for excited states to decay ($\sim 10^{-6}$ sec) leaving only the metastable $2S$ state. The beam then passes through a small electric field where the $2S$ state is quenched. The resultant Lyman α radiation is then detected. This then measures the $2S$ population due to the collisions and cascade from higher states.

In the next section we describe the population of the $2S$ level by a calculation by the method of coupled states ($1S$,$2S$,$2P$). This method yields a result in sharp disagreement with so-called distorted-wave methods[2,3] but in qualitative agreement with the second Born approximation.[4] The reasons for this are discussed. The method of closely coupled states is known to be an approximation to a more exact optical potential method.[5] The modifications introduced by this last method are also briefly discussed.

In the third section the population of the higher

[1] By atom-atom collision we mean here the collision between two heavy bodies. One or both may be ions.
[2] M. H. Mittleman, Phys. Rev. **122**, 499 (1961).
[3] D. R. Bates, Proc. Phys. Soc. (London) **73**, 227 (1959).
[4] A. E. Kingston, B. L. Moiseiwitsch, and B. G. Skinner, Proc. Roy. Soc. (London) **258**, 273 (1960). The second Born approximation is not calculated exactly here. Only the $1S$, $2S$, and $2P$ states are allowed of the infinite, set of intermediate states.
[5] M. H. Mittleman and R. Pu, Phys. Rev. **126**, 370 (1962).

(up to $n=6$) levels is calculated by Born approximation. The probabilities for the decay to the $2S$ level are then obtained from tables.[6] The resultant population of the $2S$ from higher levels is then given. This procedure can be justified as follows: Firstly, the Born approximation is probably fractionally better for the highly excited states than for the $2S$ excitation. Secondly, the cross section for excitation of the higher states is smaller than that for excitation of $2S$ so fractional errors are reduced, and finally the probability of decay to the $2S$ is small (a maximum of ~ 0.12) so that the fractional error in the total $2S$ population is still further reduced.

II. METHOD OF COUPLED STATES

We are concerned here with relative energies of the order of keV. At these energies the proton wave packets can be made extremely small so that a classical description of the proton motion is sufficient. In addition, the cross section for appreciable proton deflection is small so that we may approximate the proton motion by a classical unaccelerated motion, the usual impact parameter method.[7] The Schrödinger equation for the electron can then be written

$$\left(i\frac{\partial}{\partial t}+\nabla^2+\frac{2}{|\mathbf{x}-\mathbf{R}/2|}+\frac{2}{|\mathbf{x}+\mathbf{R}/2|}\right)\psi(\mathbf{x},t)=0, \quad (1)$$

where

$$\mathbf{R}=\mathbf{b}+\mathbf{V}t. \quad (1a)$$

Here $\mathbf{b}$ is the impact parameter and $\mathbf{V}$ is the relative velocity of the two protons. Dimensionless quantities are used, distances being measured in Bohr radii and energies in rydbergs. The lab frame energy of the proton is given by $E=25\ \text{keV}\times(V/2)^2$. We chose an initial state with the electron centered on the proton at $-\mathbf{R}/2$.

$$\psi_i=\Phi_1(\mathbf{x}+\mathbf{R}/2)\exp[-i(\mathbf{V}\cdot\mathbf{x}/4)-i(W_1+V^2/16)t], \quad (2)$$

here Φ_1 is the ground state of the complete set of hydrogenic states, Φ_n, with eigenvalues W_n.

$$[\nabla^2+(2/x)+W_n]\Phi_n(\mathbf{x})=0 \quad (3)$$

We may expand the total wave function in terms of these states as

$$\psi(\mathbf{x},t)=\sum_n a_n(t)\Phi_n(\mathbf{x}+\mathbf{R}/2)\times\exp[-i(\mathbf{V}\cdot\mathbf{x}/4)-i(V^2/16+W_n)t]. \quad (4)$$

Substitution of (4) into (1) with some obvious manipulation yields the coupled set

$$\dot{a}_n=i\sum_m V_{nm}(t)a_m, \quad (5)$$

where

$$V_{nm}(t)=\int d^3x\,\Phi_n(\mathbf{x}+\mathbf{R}/2)\frac{2}{|\mathbf{x}-\mathbf{R}/2|}\times\Phi_m(\mathbf{x}+\mathbf{R}/2)e^{i(W_n-W_m)}. \quad (5a)$$

The initial condition can now be written

$$\lim_{t\to-\infty} a_n(t)=\delta_{n1}. \quad (6)$$

The infinite set of coupled equations (5) is of course intractable. We could arbitrarily cut off the sum in (4) at N and then determine the a_n variationally.[8] We would then arrive at Eqs. (5) with the sum truncated as in (4) at N. Another method for determining a_n is the so-called optical-potential method. We can arrive at a finite set of coupled equations for a_n except that now V_{nm} in (5) is replaced by an equivalent potential $\mathcal{V}_{nm}$ to be determined from an integral equation.[6]

$$\mathcal{V}_{nm}=V_{nm}+\sum_{j>N}\frac{1}{A_j}V_{nj}\mathcal{V}_{jm}. \quad (7)$$

Here A_j^{-1} is the propagator of the unperturbed electron. It should be pointed out that the infinite set of states has been removed from (5) at the expense of including it in (7). This is in principle exact. The difficulty arises from our inability to solve (7). We may attempt the solution by iteration. The leading term agrees with the previous method. We may attempt to obtain corrections from the next term

$$\mathcal{V}_{nm}^{(2)}=\sum_{j>N}\frac{1}{A_j}V_{nj}V_{jm}. \quad (8)$$

This sum has been investigated previously.[9] Its exact

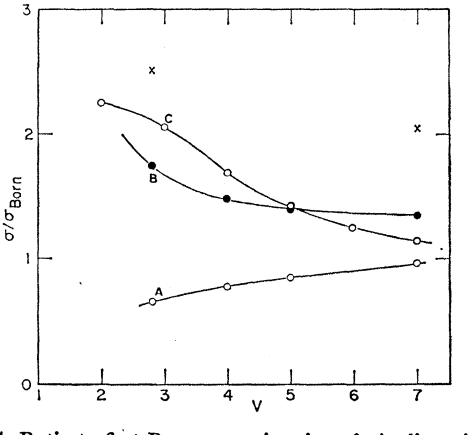

FIG. 1. Ratio to first Born approximation of: A, distortion approximation; B, second Born approximation; C, coupled states. The points x are optical-potential calculations.

[6] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Academic Press Inc., New York, 1957), p. 266.

[7] These approximations are discussed more fully in reference 2 where Eq. (1) is derived.

[8] N. C. Sil, Proc. Roy. Soc. (London) **75**, 194 (1960).

[9] M. H. Mittleman, Ann. Phys. (New York) **14**, 94 (1961).

evaluation was not possible. However, its large distance (large $|R|$) behavior could be obtained. If for example we chose to keep the ground and first excited levels in our sum of (5), then it is known that the long-range potential on the electron is given incorrectly. The $2P$ state supplies only 0.65 of the correct polarizability.

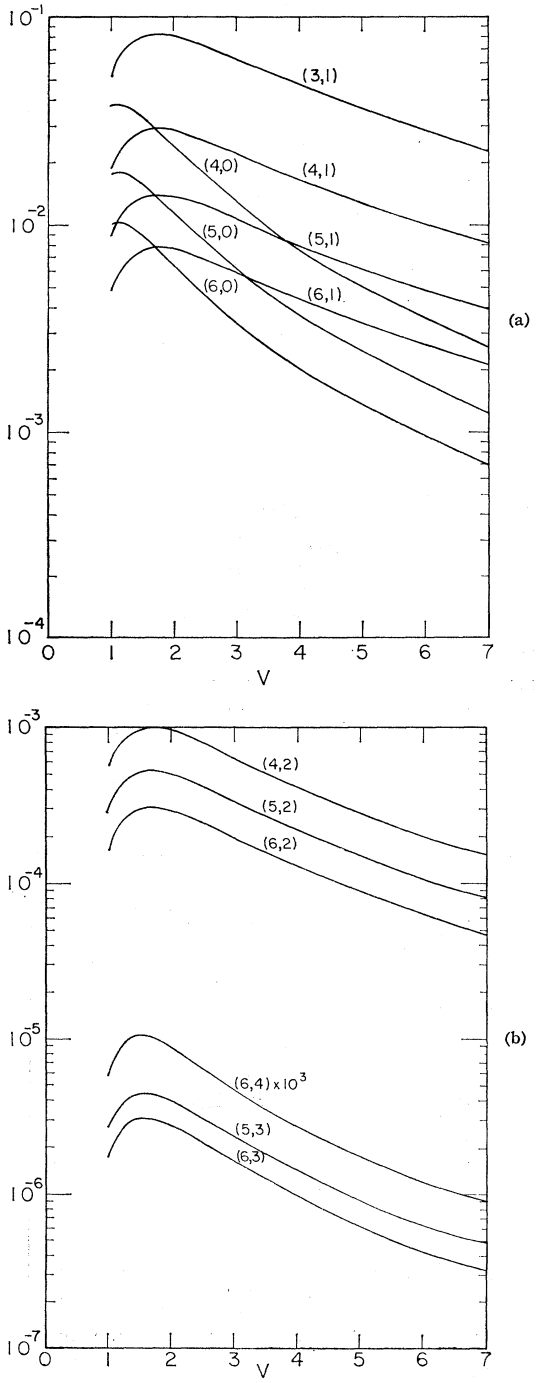

FIG. 2. (a) Born approximation cross section for the excitation of the level (n,l) in units of (πa^2). (b) Born approximation cross section for the excitation of the level (n,l) in units of (πa^2).

The situation is even worse for some of the off-diagonal elements of $\mathcal{U}_0 \cdot V_{1S,2S}$ has a long-range behavior which is essentially $e^{-3/2R}$. The correction $\mathcal{U}_{1S,2S}{}^{(2)}$ behaves like $1/R^4$. We emphasize again that the short-range behavior of $\mathcal{U}^{(2)}$ was not obtainable. The question of where the "long-range behavior" is indeed the true behavior of $\mathcal{U}^{(2)}$ could be answered at least qualitatively.[9] The result is that the distance at which the asymptotic behavior takes over increases with energy. Thus, at high energies we are only able to find the true long-range behavior where its effects are negligible.

We could also obtain an approximation to $\mathcal{U}^{(2)}$ for high energies.[9] The principal effect there is to give $\mathcal{U}$ an imaginary part representing excitation to all the states omitted from the sum in (5). We shall see in the next section that this is not a large effect so that its contribution was not included in (5). Finally we might point out that the optical-potential method for arriving at (5) is not variationally based. We may, therefore, use the wave function obtained from (5) to obtain a variational correction to the cross section due to the long-range or inelastic effects mentioned above.[5]

We have solved (5) in the approximation of keeping the $(1S)$, $(2S)$, $(2P_0)$, and $(2P_1)$ states[10] in (5). First, we use just V_{nm} for the potentials in (5). The ratio of the cross section[11] for $2S$ excitation from this calculation to the first Born approximation is shown in Fig. 1. The distortion approximation in which only $V_{1S,1S}$, $V_{2S,2S}$, and $V_{2S,1S}$ are kept, and the second Born approximation[4] are also shown in ratio to first Born approximation. Note that the second Born approximation is in qualitative agreement with our result while the distortion approximation goes in the wrong direction from the Born approximation. This may be understood qualitatively. The distortion approximation includes phase factors in the approximation to (4) which makes the overlap integral of the Born approximation oscillate more rapidly[2] thus reducing the result. The increase in the cross section, above the Born value in the other two curves, comes from the transition to the $2S$ state via the strongly coupled $2P$ state which is coupled to the ground state by an allowed transition. Explicit calculations show that at large impact parameters the amplitude for direct transition to the $2S$ state behaves like $e^{-(3/2)b}$ while the indirect transition through the $2P$ state behaves like $e^{-(3/2)b/V}$. The second may dominate at high velocities. Both the second Born approximation and our calculation contain this term.

We have also obtained solutions[12] to (5) when the long-range approximation for $\mathcal{U}^{(2)}$ was included. A

[10] The $2P$, $m=\pm 1$ states enter symmetrically so that only their sum need be kept.

[11] The cross section is obtained as

$$\sigma_n = \lim_{t\to\infty} 2\pi \int_0^\infty b\,db\,|a_n(t,b)|^2.$$

[12] These calculations were carried out with an IBM 650. Thanks are due to Tom Haritani for his invaluable assistance.

TABLE I. Probability of $2S$ population from state (nl).

n \ l	0	1	2	3	4	5
3	0	0.118	0			
4	0.0494	0.118	0.0302	0		
5	0.0654	0.119	0.040	0.011	0	
6	0.0690	0.120	0.046	0.016	0.005	0

reasonable cutoff was included for each term. These are shown as points in Fig. 1. They are not to be taken seriously. They certainly overestimate the magnitude of the effects they represent.

The corrections due to excitation of higher states which are neglected in (5) can be estimated by evaluating (8) in the high-energy limit.[9] The results of (5) can then be used to find the contribution of this high-energy limit. These give an estimated correction to curve C in Fig. 1 of no more than 10% in the direction of lowering the curve.

III. CONTRIBUTION FROM HIGHER STATES

The proton may excite higher states during the collision which may decay and populate the $2S$ state. We are therefore interested in the probability that a given state will decay to $2S$. This may be obtained from the tables[6] of transition probabilities between the various levels. We must simply add the probabilities of the various cascades. The results are given in Table I.

The cross section for excitation of these states has been calculated in the Born approximation. The result is

$$\sigma_{nlm}=\frac{16}{V^2}\int\frac{d^3k}{k^4}|\lambda_{nlm}(k)|^2\delta(k_z-W_n/V), \tag{9}$$

where

$$\lambda_{nlm}(k)=\int d^3y\,\Phi_{nlm}^*(y)\Phi_{1S}(y)e^{ik\cdot y}, \tag{9a}$$

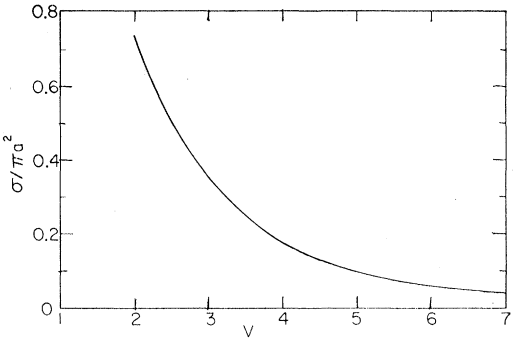

FIG. 3. $2S$ cross section in units of (πa^2).

and the excitation energy is $W_n=1-1/n^2$. The summation over the magnetic quantum number may easily be performed. The resultant cross sections are shown in Figs. 2(a) and (b).

The total $2S$ population is obtained by multiplying these curves by the appropriate number from the tables and summing. We then add the contribution from the direct excitation of $2S$ represented by curve C in Fig. 1. This contribution from excited states is small compared to the direct contribution; about 1% at $V=2$ and about 10% at $V=7$. The result is shown in Fig. 3.

The remarkable similarity of the curves for fixed l, could be used to extrapolate to higher n values. We could then sum over all n. This must be done with care. The lifetimes of the higher n states are longer. The number of such states which must be included depends on the experimental situation since only those states which can decay to $2S$ in the time between the excitation and the observation should be included. Strictly speaking, only those cascades which can end in the $2S$ in the available time should be included.