PHYSICAL REVIEW VOLUME 122, NUMBER 4 MAY 15, 1961

Application of the Impulse Approximation to the Scattering of Electrons by Atoms. I. Inelastic Scattering by Hydrogen Atoms*

R. Akerib
Convair, San Diego, California

AND

S. Borowitz
Physics Department, New York University, New York, New York

(Received November 17, 1960)

A calculation of the ionization cross section and the excitation cross section to the 2*S* and 2*P* states of hydrogen atoms by collision with electrons is carried through by the use of an impulse approximation. The results are then compared to the experimental data and to various other theoretical calculations. The cross sections obtained compare favorably with experiment. The calculations carried out by these methods are no more complicated than the usual approximation methods and are easily adaptable for use with more complicated atoms.

I. INTRODUCTION

Although the system consisting of a hydrogen atom and an electron is a relatively simple three-body system, and the forces between all particles are known, the theoretical analysis of the inelastic scattering of electrons by hydrogen atoms has not progressed very far in recent years. The methods which have been used have been the first Born approximation, the second Born approximation, the distorted-wave approximation, and variational methods. Of these methods, only the first can be readily generalized to more complicated systems. The Born approximation, which has a wider range of applicability, generally suffers from the defect that it tends to overestimate the cross section at lower energies sometimes by a factor of 2.

In recent years, experimental techniques for the measurement of the scattering cross section of electrons by atoms have improved considerably and the signal-to-noise ratio has increased sufficiently so that a separation of the various inelastic processes is now possible. With the accumulation of experimental information, it now becomes possible to check various approximation methods for the scattering of electrons by atoms.

We are presenting the first of a series of articles which will apply the impulse approximation to the problem at hand. This method had previously been formulated by Chew,[1] and applied by him to the analogous nuclear problem of the scattering of neutrons by deuterons. The basic idea of the impulse approximation is that one assumes that during the collision the interaction between the bound atomic particles is turned off; this implies that the incident particle spends a very short time in the field of the bound particles, and during this time the atomic configuration is frozen. This assumption is natural to make when the incident particle has a relatively high energy. A detailed analysis by Chew and Wick,[2] and by Chew and Goldberger,[3] shows that the impulse approximation is valid as long as $\tau|\epsilon|\ll\hbar$, where τ is the transit time of the incident electron and ϵ is the binding energy of the ground state of the atom. For our problem, namely, the ionization cross section and the excitation cross section of the 2*S* and 2*P* states of hydrogen by electron impact, this criterion implies that the energy of the incident electron should be approximately 150 ev. We have carried out the calculations in this approximation to much lower energies in hope that there would be some fairly good agreement with experiment. A fair agreement would then offer some encouragement to apply this method to the scattering of electrons by heavier atoms.

As it turns out, the approximation is fairly good at all energies and is no more complicated than the first Born approximation. We, therefore, think that we have still another approximation method which can be used for calculating the inelastic scattering of electrons by atoms.

In Sec. II we derive the various formulas necessary for our work. These formulas are then used in Sec. III and IV to compute the ionization and the excitation cross sections to the 2*S* and 2*P* states of hydrogen, respectively. A short discussion of some of the difficulties encountered is given in Sec. V.

II. THEORY

To study the problem of the scattering of an electron by a hydrogen atom, we must solve the following Schrödinger equation:

$$H\psi(\mathbf{r}_1,\mathbf{r}_2)=E\psi(\mathbf{r}_1,\mathbf{r}_2), \tag{1}$$

where

$$H=-\frac{\hbar^2}{2m}\Delta_1-\frac{\hbar^2}{2m}\Delta_2-\frac{e^2}{r_1}-\frac{e^2}{r_2}+\frac{e^2}{r_{12}}, \tag{2}$$

and

$$E=\frac{\hbar^2k_1^2}{2m}-|\epsilon|. \tag{3}$$

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* The research reported in this paper has been sponsored in part by the Geophysics Research Center, Air Research and Development Command, under contract, and in part by the Army Rocket and Guided Missile Agency under contract.

[1] G. F. Chew, Phys. Rev. **80**, 196 (1952).

[2] G. F. Chew and G. C. Wick, Phys. Rev. **85**, 636 (1952).

[3] G. F. Chew and M. L. Goldberger, Phys. Rev. **87**, 778 (1952).

In (2) and (3), Δ_1 and Δ_2 are the Laplacian operators in the space of electrons 1 and 2, respectively; $\mathbf{r}_1$ and $\mathbf{r}_2$ are, respectively, the position vectors of the incident and bound electrons referred to the proton (we assume that the mass of the proton is infinite); $\mathbf{k}_1$ is the propagation vector of the incident electron before collision and ϵ is the binding energy of the ground state of hydrogen; $\hbar$ is Planck's constant, e and m are the charge and mass of the electron, respectively, and $\mathbf{r}_{12}=\mathbf{r}_1-\mathbf{r}_2$.

Use of standard techniques converts the Schrödinger equation into an integral equation with the scattered part of the wave function given by

$$\psi_s(\mathbf{r}_1,\mathbf{r}_2)\underset{r_1\to\infty}{\sim}-\frac{m}{2\pi\hbar^2}\sum\nolimits_n\phi_n(\mathbf{r}_2)\frac{\exp[ik_nr_1]}{r_1}\times\int d\mathbf{r}_1'd\mathbf{r}_2'\phi_n^*(\mathbf{r}_2')\times\exp[-i\mathbf{k}_n\cdot\mathbf{r}_2']V\psi(\mathbf{r}_1',\mathbf{r}_2')\tag{4}$$

for direct scattering, and

$$\psi_s(\mathbf{r}_1,\mathbf{r}_2)\underset{r_2\to\infty}{\sim}-\frac{m}{2\pi\hbar^2}\sum\nolimits_n\phi_n(\mathbf{r}_1)\frac{\exp[ik_nr_2]}{r_2}\times\int d\mathbf{r}_1'd\mathbf{r}_2'\phi_n^*(\mathbf{r}_1')\times\exp[-i\mathbf{k}_n\cdot\mathbf{r}_2']U\psi(\mathbf{r}_1',\mathbf{r}_2')\tag{5}$$

for exchange scattering. Here, ϕ_n is the wave function of an electron in the field of a proton in the state n, $\mathbf{k}_n$ is the propagation vector of the scattered electron, $V=(e^2/r_{12})-(e^2/r_1)$ and $U=(e^2/r_{12})-(e^2/r_2)$.

Chew[1] points out that it is simpler for our purposes to use the R matrix notation in expressing the various formulas that we need. We shall, in the following, follow the parallel derivation of Chew for the problem of the scattering of a neutron by a deuteron. We assume that $\psi(\mathbf{r}_1,\mathbf{r}_2)$ appearing under the integral sign in (4) and (5) can be expressed in the following approximate form:

$$\psi(\mathbf{r}_1,\mathbf{r}_2)\approx\psi_a(\mathbf{r}_1,\mathbf{r}_2)=\int d\mathbf{k}_2\,g_0(\mathbf{k}_2)\psi_{\mathbf{k}_1,\,\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2),\tag{6}$$

where the subscript a indicates that $\psi_a(\mathbf{r}_1,\mathbf{r}_2)$ is an approximation to the true wave function of the system, $g_0(\mathbf{k}_2)$ is the Fourier transform of the wave function for the ground state of the hydrogen atom, and $\psi_{\mathbf{k}_1,\,\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2)$ represents the wave function of an electron of momentum $\mathbf{p}_1=\hbar\mathbf{k}_1$ in the field of an electron of momentum $\mathbf{p}_2=\hbar\mathbf{k}_2$. Equation (6) is equivalent to considering the interaction of the incident electron with a free electron whose momentum distribution is given by the Fourier transform of the ground state wave function of hydrogen.

Substitution of (6) into (4) and (5) leads to the R matrices

$$(\mathbf{k}_n,n|R^{(d)}|\mathbf{k}_1,0)=-i\int d\mathbf{k}_2\,g_0(\mathbf{k}_2)\times\int\int d\mathbf{r}_1d\mathbf{r}_2\exp[-i\mathbf{k}_n\cdot\mathbf{r}_1]\phi_n^*(\mathbf{r}_2)V\times\psi_{\mathbf{k}_1,\,\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2)\tag{7}$$

for direct scattering and

$$(\mathbf{k}_n,n|R^{(e)}|\mathbf{k}_1,0)=-i\int d\mathbf{k}_2\,g_0(\mathbf{k}_2)\times\int\int d\mathbf{r}_1d\mathbf{r}_2\exp[-i\mathbf{k}_n\cdot\mathbf{r}_2]\phi_n^*(\mathbf{r}_1)U\times\psi_{\mathbf{k}_1,\,\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2)\tag{8}$$

for exchange scattering. If we define

$$f_n=(m/2\pi\hbar^2)(\mathbf{k}_n,n|R^{(d)}|\mathbf{k}_1,0)\tag{9a}$$

and

$$g_n=(m/2\pi\hbar^2)(\mathbf{k}_n,n|R^{(e)}|\mathbf{k}_1,0),\tag{9b}$$

then the cross section for excitation to the state n will be

$$\sigma_n=(k_n/k_1)\{\tfrac{1}{4}|f_n+g_n|^2+\tfrac{3}{4}|f_n-g_n|^2\}.\tag{10}$$

For ionization, we define

$$f(\mathbf{k}_1,\mathbf{k}_1',\mathbf{k}_2')=(\mathbf{k}_1',\mathbf{k}_2'|R^{(d)}|\mathbf{k}_1,0)\tag{11a}$$

and

$$g(\mathbf{k}_1,\mathbf{k}_1',\mathbf{k}_2')=(\mathbf{k}_1',\mathbf{k}_2'|R^{(e)}|\mathbf{k}_1,0).\tag{11b}$$

The cross section for ionization will then be

$$\sigma d\mathbf{k}_1'd\mathbf{k}_2'=(2\pi/\hbar v_1)\{\tfrac{1}{4}|f+g|^2+\tfrac{3}{4}|f-g|^2\}\times\delta(E_f-E_0)d\mathbf{k}_1'd\mathbf{k}_2'.\tag{12}$$

Here, $\mathbf{k}_1'$ and $\mathbf{k}_2'$ are, respectively, the propagation vectors of the incident and bound electrons after scattering and E_0 and E_f are the initial and final energies of the system before and after scattering.

We now note that $\psi_{\mathbf{k}_1,\,\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2)$ can be factored into the product of two functions, one representing the motion of center of mass of the two electrons, and the other the relative motion about the center of mass:

$$\psi_{\mathbf{k}_1,\,\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2)=(2\pi)^{-\frac{3}{2}}\exp\{\tfrac{1}{2}i(\mathbf{k}_1+\mathbf{k}_2)\cdot(\mathbf{r}_1+\mathbf{r}_2)\}\times\psi_{\frac{1}{2}(\mathbf{k}_1-\mathbf{k}_2)}(\mathbf{r}_1-\mathbf{r}_2).\tag{13}$$

Substitution of (13) into (7) and (8) and replacement of the hydrogen wave function $\phi_n(\mathbf{r})$ by its Fourier transform, we are led to the general expression

$$(\mathbf{k}_n,n|R|\mathbf{k}_1,0)=\int\int d\mathbf{k}_2d\mathbf{k}_2''g_n^*(\mathbf{k}_2'')\times(\mathbf{k}_n,\mathbf{k}_2''|R|\mathbf{k}_1,\mathbf{k}_2)g_0(\mathbf{k}_2)\tag{14}$$

where the R matrix under the integral sign is given by

$$(\mathbf{k}_n,\mathbf{k}_2''|R^{(d)}|\mathbf{k}_1,\mathbf{k}_2)$$
$$=-\frac{i}{(2\pi)^3}\int\int d\mathbf{r}_1 d\mathbf{r}_2 \exp[-i(\mathbf{k}_n\cdot\mathbf{r}_1+\mathbf{k}_2''\cdot\mathbf{r}_2)]$$
$$\times\exp[\tfrac{1}{2}i(\mathbf{k}_1+\mathbf{k}_2)\cdot(\mathbf{r}_1+\mathbf{r}_2)]V\psi_{\frac{1}{2}(\mathbf{k}_1-\mathbf{k}_2)}(\mathbf{r}_1-\mathbf{r}_2) \quad (15)$$

for direct scattering and

$$(\mathbf{k}_n,\mathbf{k}_2''|R^{(e)}|\mathbf{k}_1,\mathbf{k}_2)$$
$$=-\frac{i}{(2\pi)^3}\int\int d\mathbf{r}_1 d\mathbf{r}_2 \exp[-i(\mathbf{k}_n\cdot\mathbf{r}_2+\mathbf{k}_2''\cdot\mathbf{r}_1)]$$
$$\times\exp[\tfrac{1}{2}i(\mathbf{k}_1+\mathbf{k}_2)\cdot(\mathbf{r}_1+\mathbf{r}_2)]U\psi_{\frac{1}{2}(\mathbf{k}_1-\mathbf{k}_2)}(\mathbf{r}_1-\mathbf{r}_2) \quad (16)$$

for exchange scattering. We will now proceed to compute (15) and (16). We will confine our remarks to the R matrix for direct scattering and give the results for exchange since the same treatment is applicable. We substitute for the potential V the expression $(e^2/r_{12})-(e^2/r_1)$ into (15) and carry out the transformation

$$\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2,$$
$$\boldsymbol{\varrho}=\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2).$$

These steps lead to

$$(\mathbf{k}_n,\mathbf{k}_2''|R^{(d)}|\mathbf{k}_1,\mathbf{k}_2)=-[ie^2/(2\pi)^3]\{I_1-I_2\} \quad (17)$$

where

$$I_1=\int\int\frac{d\mathbf{r}d\boldsymbol{\varrho}}{r}\exp[-i(\mathbf{k}_n+\mathbf{k}_2''-\mathbf{k}_1-\mathbf{k}_2)\cdot\boldsymbol{\varrho}]$$
$$\times\exp[-i\mathbf{k}'\cdot\mathbf{r}]\psi_{\mathbf{k}}(\mathbf{r}) \quad (18a)$$

and

$$I_2=\int\int\frac{d\mathbf{r}d\boldsymbol{\varrho}}{|\boldsymbol{\varrho}+\frac{1}{2}\mathbf{r}|}\exp[-i(\mathbf{k}_n+\mathbf{k}_2''-\mathbf{k}_1-\mathbf{k}_2)\cdot\boldsymbol{\varrho}]$$
$$\times\exp[-i\mathbf{k}'\cdot\mathbf{r}]\psi_{\mathbf{k}}(\mathbf{r}) \quad (18b)$$

with

$$\mathbf{k}=\tfrac{1}{2}(\mathbf{k}_1-\mathbf{k}_2) \quad\text{and}\quad \mathbf{k}'=\tfrac{1}{2}(\mathbf{k}_n-\mathbf{k}_2''). \quad (19)$$

Now $\psi_{\mathbf{k}}(\mathbf{r})$ represents the motion of a charged particle in a Coulomb field and is given by[4]

$$\psi_{\mathbf{k}}(\mathbf{r})=N(k)e^{i\mathbf{k}\cdot\mathbf{r}}F[(-i/2a_0k);1;ikr-i\mathbf{k}\cdot\mathbf{r}], \quad (20a)$$

where F is the confluent hypergeometric function of its argument and

$$N(k)=(m/\hbar k)^{\frac{1}{2}}\Gamma[1+(i/2a_0k)]e^{-\pi/4a_0k}. \quad (20b)$$

Here, $\Gamma[1+(i/2a_0k)]$ is the gamma function of its argument. When $\psi_{\mathbf{k}}(\mathbf{r})$ is substituted into (18a), we obtain

$$I_1=(2\pi)^3N(k)\delta(\mathbf{k}_n+\mathbf{k}_2''-k_1-k_2)$$
$$\times\int\frac{d\mathbf{r}}{r}\exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]$$
$$\times F((-i/2a_0k);1;ikr-i\mathbf{k}\cdot\mathbf{r}). \quad (21)$$

The $\mathbf{r}$ integral has been carried through by various authors,[5] and leads to

$$\int\frac{d\mathbf{r}}{r}\exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]F[(-i/2a_0k);1;ikr-i\mathbf{k}\cdot\mathbf{r}]$$
$$=\frac{4\pi}{(\mathbf{k}-\mathbf{k}')^2}N(k)\left\{\frac{(\mathbf{k}-\mathbf{k}')^2-2\mathbf{k}\cdot(\mathbf{k}-\mathbf{k}')}{(\mathbf{k}-\mathbf{k}')^2}\right\}^{i/2a_0k}. \quad (22)$$

Now, let us consider I_2. This represents the contribution, to the inelastic process, of the wave that has been scattered from the proton. Thus, I_2 represents a multiple scattering effect that is of a higher order and should be negligible compared to I_1. To show this, we carry out the integrals represented in I_2. We let $\mathbf{r}=\mathbf{r}$ and $\boldsymbol{\varrho}'=\boldsymbol{\varrho}+\frac{1}{2}\mathbf{r}$ in (18b) which separates the $\mathbf{r}$ and $\boldsymbol{\varrho}$ integrals and leads to

$$I_2=\frac{\pi^2}{64a_0}N(k)\frac{(\mathbf{k}-\mathbf{k}')^4}{[\mathbf{k}\cdot(\mathbf{k}-\mathbf{k}')]^4(\mathbf{k}-\mathbf{k}')^2}$$
$$\times\left\{1-\frac{2\mathbf{k}\cdot(\mathbf{k}-\mathbf{k}')}{(\mathbf{k}-\mathbf{k}')^2}\right\}^{-1+(i/2a_0k)}.$$

When (21) and (22) are combined and $\mathbf{k}$ and $\mathbf{k}'$ are replaced by their values as given in (19), we find that $I_2\sim 1/k_1^6$ and $I_1\sim 1/k_1^2$; thus, $I_2/I_1\sim 1/k_1^4$. It follows then that we can neglect the $1/r_1$ term in (15) and $1/r_2$ term in (16). This is to be expected, since if we consider I_1, the orthogonality of the initial and final states of hydrogen will give zero contribution in the Born approximation. By combining (14), (15), and the expression for I_1, we obtain

$$(\mathbf{k}_n,n|R^{(d)}|\mathbf{k}_1,0)$$
$$=-ie^2\int d\mathbf{k}_2 g_n^*(\mathbf{k}_1+\mathbf{k}_2-k_n)(\mathbf{k}'|r^{(d)}|\mathbf{k})g_0(\mathbf{k}_2), \quad (24)$$

for direct scattering. The $\mathbf{k}_2''$ integral has been carried through. Here,

$$(\mathbf{k}'|r^{(d)}|\mathbf{k})=\frac{4\pi}{(\mathbf{k}-\mathbf{k}')^2}N(k)$$
$$\times\left\{\frac{(\mathbf{k}-\mathbf{k}')^2-2\mathbf{k}\cdot(\mathbf{k}-\mathbf{k}')}{(\mathbf{k}-\mathbf{k}')^2}\right\}^{i/2a_0k}, \quad (25)$$

with

$$\mathbf{k}=\tfrac{1}{2}(\mathbf{k}_1-\mathbf{k}_2);\quad \mathbf{k}'=\tfrac{1}{2}(2\mathbf{k}_n-\mathbf{k}_1-\mathbf{k}_2). \quad (26)$$

The above treatment applied to exchange leads to

$$(\mathbf{k}_n,n|R^{(e)}|\mathbf{k}_1,0)$$
$$=-ie^2\int d\mathbf{k}_2 g_n^*(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_n)(\mathbf{k}'|r^{(e)}|\mathbf{k})g_0(\mathbf{k}_2), \quad (27)$$

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[4] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), 1st ed., Chap. V, p. 117.

[5] T. Pradhan, Phys. Rev. **105**, 1250 (1957). A. Nordsieck, *ibid.* **93**, 785 (1954).

where

$$(\mathbf{k}'|r^{(e)}|\mathbf{k})=\frac{4\pi}{(\mathbf{k}+\mathbf{k}')^2}N(k)\times\left\{\frac{(\mathbf{k}+\mathbf{k}')^2-2\mathbf{k}\cdot(\mathbf{k}+\mathbf{k}')}{(\mathbf{k}+\mathbf{k}')^2}\right\}^{i/2a_0k}, \quad (28)$$

with $\mathbf{k}$ and $\mathbf{k}'$ as given in (26).

III. IONIZATION CROSS SECTION

We are interested here in the case where the bound electron emerges in the continuum state after collision. We will assume it can be represented by a plane wave. If we let $\mathbf{k}_1'$ and $\mathbf{k}_2'$ be the propagation vectors of the incident and bound electrons, respectively, after collision, the R matrix for direct scattering becomes

$$(\mathbf{k}_1',\mathbf{k}_2'|R^{(d)}|\mathbf{k}_1,0)=-ie^2\int d\mathbf{k}_2 g_{\mathbf{k}_2'}^*(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_1')(\mathbf{k}'|r^{(d)}|\mathbf{k})g_0(\mathbf{k}_2). \quad (29)$$

Recalling that

$$\phi_0(\mathbf{r})=(\pi a_0^3)^{-\frac{1}{2}}e^{-r/a_0},$$

we can compute $g_0(\mathbf{k}_2)$; since we are assuming that the final state is a plane wave, $g_{\mathbf{k}_2'}$ will be a δ function and thus:

$$(\mathbf{k}_1',\mathbf{k}_2'|R^{(d)}|\mathbf{k}_1,0)=\frac{a_0^{\frac{3}{2}}e^2\sqrt{2}}{\pi}N(\tfrac{1}{2}|2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2'|)\frac{1}{(\mathbf{k}_1-\mathbf{k}_1')^2[1+a_0^2(\mathbf{k}_1'+\mathbf{k}_2'-\mathbf{k}_1)^2]^2}\times\left\{\frac{(\mathbf{k}_1-\mathbf{k}_1')\cdot(2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2')-(\mathbf{k}_1-\mathbf{k}_1')^2}{(\mathbf{k}_1-\mathbf{k}_1')^2}\right\}^{i/a_0|2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2'|}. \quad (30)$$

In a similar way, we obtain for exchange scattering:

$$(\mathbf{k}_1',\mathbf{k}_2'|R^{(e)}|\mathbf{k}_1,0)=\frac{a_0^{\frac{3}{2}}e^2\sqrt{2}}{\pi}N(\tfrac{1}{2}|2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2'|)\frac{1}{(\mathbf{k}_1-\mathbf{k}_2')^2[1+a_0^2(\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2')^2]^2}\times\left\{\frac{(\mathbf{k}_1-\mathbf{k}_2')\cdot(2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2')-(\mathbf{k}_1-\mathbf{k}_2')^2}{(\mathbf{k}_1-\mathbf{k}_2')^2}\right\}^{i/a_0|2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2'|}. \quad (31)$$

The scattering cross section is obtained by combining (30) and (31) with (12) which leads to

$$\sigma_{\text{ion}}d\mathbf{k}_1'd\mathbf{k}_2'=2^7\pi^2\frac{me^4}{\hbar^2a_0k_1}\frac{\exp[-\pi/a_0|2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2'|]}{\sinh[\pi/a_0|2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2'|]}\frac{\delta(E_1'+E_2'-E)}{(2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2')^2[1+a_0^2(\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2')^2]^4}\times\left\{\frac{1}{(\mathbf{k}_1-\mathbf{k}_1')^4}+\frac{1}{(\mathbf{k}_1-\mathbf{k}_2')^4}-\frac{1}{(\mathbf{k}_1-\mathbf{k}_1')^2(\mathbf{k}_1-\mathbf{k}_2')^2}\cos\vartheta\right\}d\mathbf{k}_1'd\mathbf{k}_2', \quad (32)$$

where

$$\vartheta=\frac{1}{|2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2'|}\frac{\{(2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2')\cdot(\mathbf{k}_1-\mathbf{k}_1')-(\mathbf{k}_1-\mathbf{k}_1')^2\}\{(2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2')\cdot(\mathbf{k}_1-\mathbf{k}_2')-(\mathbf{k}_1-\mathbf{k}_2')^2\}}{(\mathbf{k}_1-\mathbf{k}_1')^2(\mathbf{k}_1-\mathbf{k}_2')^2}. \quad (33)$$

The total cross section is obtained by integrating (32) over the entire space of $\mathbf{k}_1'$ and $\mathbf{k}_2'$. The limits on $\mathbf{k}_2'$ are set by the δ function. The limits on the magnitude of $\mathbf{k}_1$ are 0 and $(k_1^2-1)^{\frac{1}{2}}$ which correspond to the limiting cases where the emerging electron carries off all the excess energy and where the incident electron carries it off. However, as can be seen, the integrals cannot be carried through as they are, and certain transformations must be performed. We let $\mathbf{K}=2\mathbf{k}_1-\mathbf{k}_1'-\mathbf{k}_2'$ and $\mathbf{K}'=\mathbf{k}_2'-\mathbf{k}_1'$ which simplify the integrals. The angular integrations and the K' integral can then be carried through leaving us with one integral over K which must be computed numerically. Further, the transformation leads to the fact that, on the right-hand side of (32), the third term cancels the second. All this leads to

$$\sigma_t=\frac{2^8\pi^4}{k_1^2}\left\{-\frac{64}{15}\sigma_1+\frac{8}{5}\sigma_2+\frac{4}{15}\sigma_3+\frac{7}{3}\sigma_4+7\sigma_5-7\sigma_6\right\}, \quad (34)$$

where we have put $e=\hbar=m=1$ and σ_t is expressed in units of πa_0^2. Here,

$$\sigma_n=\int\frac{dK}{K^{2n-1}}\frac{e^{-\pi/K}}{\sinh(\pi/K)}\left\{\frac{[4k_1K-2k_1^2-K^2-2]^{\frac{1}{2}}}{[1+(k_1-K)^2]^{5-n}}-\frac{[4k_1K+2k_1^2+K^2+2]^{\frac{1}{2}}}{[1+(k_1+K)^2]^{5-n}}\right\}, \quad (35a)$$

with $n=1, \cdots 5$; and

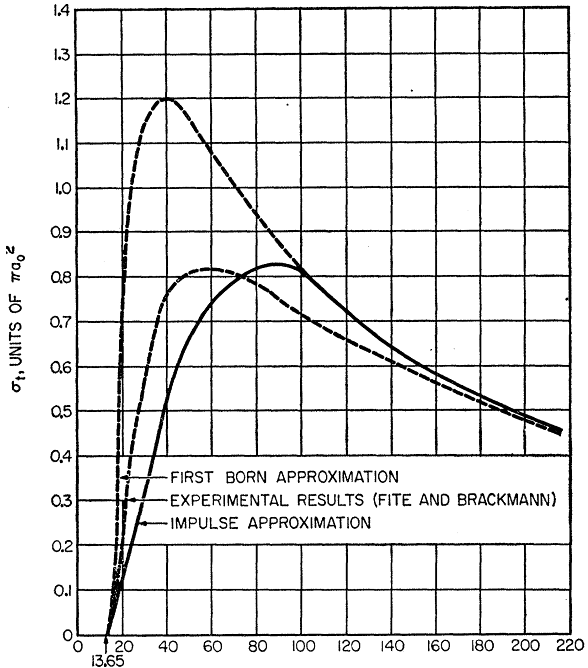

FIG. 1. Comparison of experimental and theoretical results: total ionization cross section for electron-hydrogen collisions.

$$\sigma_6=\int\frac{dK}{K^{10}}\frac{e^{-\pi/K}}{\sinh(\pi/K)}\left\{\tanh^{-1}\left[\frac{[4k_1K+2k_1^2+K^2+2]^{\frac{1}{2}}}{K(K^2+2k_1^2+2)}\right]\right.$$
$$\left.-\tanh^{-1}\left[\frac{[4k_1K-2k_1^2-K^2-2]^{\frac{1}{2}}}{K(K^2+2k_1^2+2)}\right]\right\},\quad(35\text{b})$$

where the limits of integration are $2k_1\pm(k_1^2-1)^{\frac{1}{2}}$. The numerical computation of (34) led to the curve given in Fig. 1. Two other curves are also given on this figure: the experimental result of Fite and Brackmann,[6] and the theoretical result obtained by them when they carried out the numerical integration of the Born approximation formula as given by Mott and Massey.[7] The Born approximation gives a maximum at a lower energy than the experimental and overestimates the cross section below 150 ev. Our result leads to a value for the cross section which is the same as the experimental although it is shifted to the higher energy. An examination of (35) shows that the cross section at high energies behaves as $1/k_1^{10}$. In fact, our approximation goes into the Born approximation at about 150 ev.

To examine the behavior at threshold, we go back to (32). Since we can write here $k_1^2=1+\epsilon(\epsilon\rightarrow 0)$, both $(k_1')^2$ and $(k_2')^2$ are small and

$$\sigma_t\approx\frac{2^6\pi^3}{k_1^3}\int\frac{d\mathbf{k}_1'}{(\mathbf{k}_1-\mathbf{k}_1')^4}[\epsilon-(k_1')^2].$$

When this integral is carried through, we obtain

$$\sigma_t\approx\text{const}\cdot\epsilon.$$

This is in agreement with Massey,[8] who points out that on the basis of the available evidence, the threshold law for ionization is $\sigma_t\propto\epsilon$ and in disagreement with Wannier,[9] who obtains $\sigma_t\propto\epsilon^{1.123}$.

IV. EXCITATION CROSS SECTIONS

Before we proceed to compute the excitation cross sections, one more approximation must be discussed. It is quite clear that, because of the complicated dependence of the R matrix on $\mathbf{k}_2$, it is not possible to carry out the $\mathbf{k}_2$ integral given in (24) and (27). We must attempt to take the r matrix out from under the integral sign at some suitable value of $\mathbf{k}_2$. To this end, we tabulate first the various Fourier transforms which arise in our calculations; namely,

$$g_0(\mathbf{k}_2)=\frac{\sqrt{2}}{\pi(1+k_2^2)^2},\qquad(36\text{a})$$

$$g_{200}(\mathbf{K})=-\frac{4}{\pi}\frac{-1+4K^2}{(1+4K^2)^3},\qquad(36\text{b})$$

and

$$g_{210}(\mathbf{K})=\frac{64}{i\pi}\frac{\mathbf{k}_1\cdot\mathbf{K}}{k_1(1+4K^2)^3},\qquad(36\text{c})$$

where $\mathbf{K}=\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_1'$. Now $g_0(\mathbf{k}_2)$ has a maximum at $k_2=0$ and falls off very rapidly as k_2 increases. We note that at high energies most of the scattering takes place in the forward direction and hence $\mathbf{k}_1-\mathbf{k}_1'\sim 0$. Thus, g_{200} and g_{210} will depend strongly on k_2. If we now examine the products $g_{100}g_{200}$ and $g_{100}g_{210}$, we see that the main contribution to the $\mathbf{k}_2$ integral will come from the region in which k_2 is small. An examination of the r matrix shows it to be a slowly varying function of k_2 over any given range of this variable. It has no singularities in the $\mathbf{k}_2$ plane and furthermore is bounded. The last point to be discussed occurs in (36c). In the numerator the term $\mathbf{k}_1\cdot\mathbf{K}$ occurs; (36c) can be rewritten in the form

$$f_{210}=\frac{g_{210}}{\cos\theta}=\frac{64}{i\pi}\frac{K}{(1+4K^2)^3}.$$

Thus, the only effect of the cosine is to change the scale of $g_{210}(\mathbf{K})$. In view of the previous discussion, we shall assume that we can take the r matrix out from under the integral sign at $k_2=0$ since it is around this region that the main contribution to the integral takes place. The above considerations apply to both direct and exchange scattering.

Once the procedure described is carried through, we

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[7] N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Oxford University Press, London, 1949), 2nd ed., Chap. XI, p. 235.

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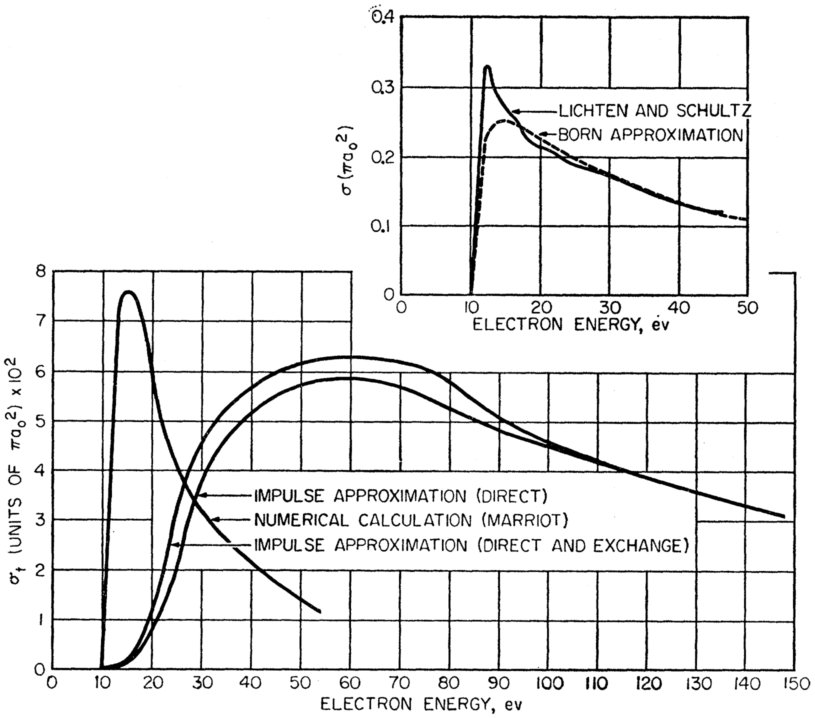

FIG. 2. Theoretical results: total cross section for $1S-2S$ transitions in electron-hydrogen collisions.

are left with the integral

$$I_{n0}=\int d\mathbf{k}_2 g_n^*(\mathbf{k}_1-\mathbf{k}_1'+\mathbf{k}_2')g_0(\mathbf{k}_2).$$

By substituting the Fourier integrals for g_0 and g_n, we obtain

$$I_{n0}=\int d\mathbf{r}\phi_n^*(\mathbf{r})e^{i(\mathbf{k}_1-\mathbf{k}_1)\cdot\mathbf{r}}\phi_0(\mathbf{r}). \tag{37}$$

We are now in a position to calculate the excitation cross sections.

A. 1S→2S Transition

We recall that

$$\phi_0(\mathbf{r})=(\pi a_0^3)^{-\frac{1}{2}}e^{-r/a_0}$$

and

$$\phi_{200}(\mathbf{r})=(2^5\pi a_0^3)^{-\frac{1}{2}}(2-r/a_0)e^{-r/2a_0}.$$

Substitution of ϕ_0 and ϕ_{200} into (37) leads to

$$I_{200,100}=\frac{2^{13/2}(\mathbf{k}_1-\mathbf{k}_1')^2}{[9+4(\mathbf{k}_1-\mathbf{k}_1')^2]^3}. \tag{38}$$

By combining (38), (25), and (24), we obtain

$$(\mathbf{k}_1',200|R^{(d)}|\mathbf{k}_1,100)$$
$$=-\frac{2^{17/2}\pi e^2N(\frac{1}{2}k_1)}{[9+4a_0^2(\mathbf{k}_1-\mathbf{k}_1')^2]^3}\left\{\frac{\mathbf{k}_1\cdot(\mathbf{k}_1-\mathbf{k}_1')}{(\mathbf{k}-\mathbf{k}_1')^2}\right\}^{i/2a_0k_1'} \tag{39a}$$

for direct scattering and

$$(\mathbf{k}_1',200|R^{(e)}|\mathbf{k}_1,100)$$
$$=-\frac{2^{17/2}\pi e^2a_0^2N(\frac{1}{2}k_1)(\mathbf{k}_1-\mathbf{k}_1')^2\exp[-\pi/a_0k_1']}{(k_1')^2[9+4a_0^2(\mathbf{k}_1-\mathbf{k}_1')^2]^3}$$
$$\times\left\{\frac{\mathbf{k}_1'\cdot(\mathbf{k}_1-\mathbf{k}_1')}{(k_1')^2}\right\}^{i/2a_0k_1'} \tag{39b}$$

for exchange scattering. The scattering cross section is obtained by combining (39) and (10) which leads to

$$\sigma_{1S\to2S}=\frac{2^{17}\pi e^{-2\pi/k_1}}{k_1k_1'[\sinh(\pi/k_1')][9+4(\mathbf{k}_1-\mathbf{k}_1')]^6}$$
$$\times\left\{1+\frac{(\mathbf{k}_1-\mathbf{k}_1')^4}{(k_1')^4}\exp[-2\pi/k_1']\right.$$
$$+\frac{(\mathbf{k}_1-\mathbf{k}_1')^2\exp[-\pi/k_1']}{(k_1')^2}$$
$$\left.\times\cos\left[\frac{1}{k_1'}\ln\frac{(k_1')^2}{(\mathbf{k}_1-\mathbf{k}_1')^2}\right]\right\}. \tag{40}$$

Here we have put $e=\hbar=m=1$ and σ is expressed in units of πa_0^2. The total cross section will be obtained by integrating (40) over all scattering angles. Because of the interference term in (40), the integral involving this term was computed numerically. The total cross section led to the curve given in Fig. 2. We have also plotted on

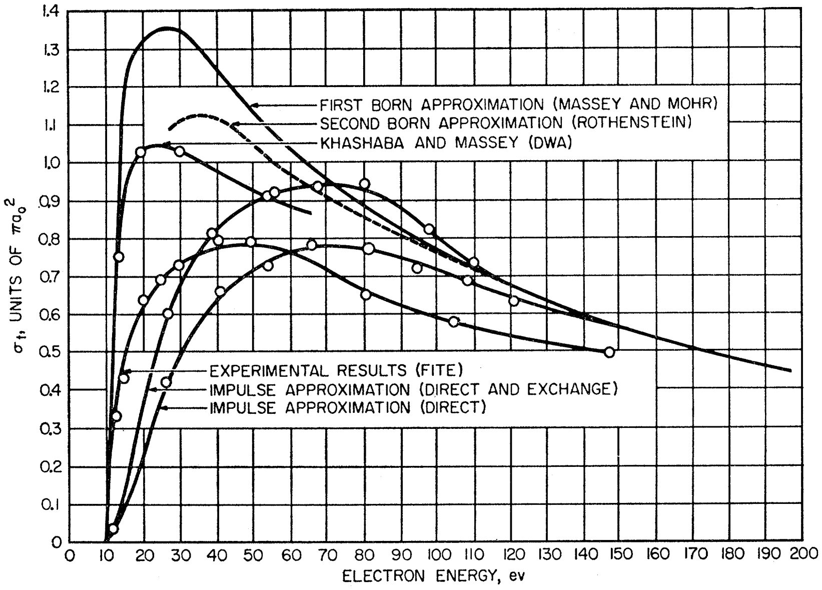

FIG. 3. Comparison of experimental and theoretical results: $1S-2P$ total cross section for electron-hydrogen collisions.

this figure the results of Marriott[10] and the Born approximation as given by Massey.[11] It is quite clear that we do not agree with Marriott's results and that the Born approximation is quite large. The experimental results of Lichten and Schultz[12] give a maximum of $0.35\pi a_0^2$ for the total cross section. This is higher than the maximum given by the Born approximation. Although our result is in disagreement with Lichten and Schultz, Fite and his co-workers[13] point out that their measurements indicate an agreement with our result[12a]: The maximum in our case is again shifted to the higher energies but the shape of the curve and the magnitude of the cross section agree quite well. We have also included in Fig. 2 the total direct cross section. Examination of this shows that exchange contributes about 20% of the scattering at 50 ev and a higher ratio as the energy decreases. As the energy of the incident electron increases, the exchange contribution approaches zero. We feel, however, that exchange can be neglected for heavier atoms in our approximation.

B. $1S\rightarrow 2P$ Transition

In this case, the wave function for the final state of the atom is

$$\phi_{210}(\mathbf{r})=(2^5\pi a_0^3)^{-\frac{1}{2}}\frac{r}{a_0}e^{-r/2a_0}\cos\theta',$$

which leads to a value of $I_{210,100}$

$$I_{210,100}=\frac{3i2^{13/2}(k_1-k_1'\cos\theta)}{[9+4a_0^2(\mathbf{k}_1-\mathbf{k}_1')^2]^3}. \qquad (42)$$

The scattering cross section will then be:

$$\sigma_{1S\rightarrow 2P}=9\frac{2^{16}\pi e^{-2\pi/k_1}}{k_1k_1'\sinh(\pi/k_1')}\frac{(k_1-k_1'\cos\theta)^2}{(\mathbf{k}_1-\mathbf{k}_1')^4[9+4(\mathbf{k}_1-\mathbf{k}_1')^2]^6}$$
$$\times\left\{1+\frac{(\mathbf{k}_1-\mathbf{k}_1')^4}{(k_1')^4}\exp[-2\pi/k_1']+\frac{(\mathbf{k}_1-\mathbf{k}_1')^2}{(k_1')^2}\right.$$
$$\left.\times\exp[-\pi/k_1']\cos\left[\frac{1}{k_1'}\ln\frac{(k_1')^2}{(\mathbf{k}_1-\mathbf{k}_1')^2}\right]\right\}, \qquad (43)$$

where σ is again expressed in units of πa_0^2. The total cross section is obtained by integrating over all angles of scattering. The result is plotted in Fig. 3. Also given here are the first Born approximation,[11] the second Born approximation,[14] Fite's experimental results,[15] and the distorted wave approximation.[16] As can be seen, our result is better than the other approximations although it is again shifted to the higher energies.

In Tables I and II, we give some values for the differential cross section for excitation of the $2S$ and $2P$ states. We have included also the closest values computed by using the Born approximation (BA) for 100, 200, and 400 ev incident electron energy. Most of our values at high energy follow the same pattern as BA. However, at 100 ev our values are all lower. We have also included the values at 27 and 54 ev and no comparison exists for these values.

V. DISCUSSION

In addition to the basic assumptions of the impulse approximation two additional approximations have

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

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[12a] See Note added in proof.

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[15] W. L. Fite and R. T. Brackmann, Phys. Rev. **112**, 1151 (1958).

[16] S. Khashaba and H. S. W. Massey, Proc. Phys. Soc. (London) **71**, 574 (1958).

TABLE I. Differential cross section, $\sigma(\theta)$, for excitation of $2S$ state of hydrogen by electron impact. E_i, incident energy in ev; θ, scattering angle; $\sigma(\theta)$ in units of a_0^2; I.A., impulse approximation; B.A., Born approximation.

E_i	27	54	100	108	200	216	400	432
θ	I.A.	I.A.	B.A.	I.A.	B.A.	I.A.	B.A.	I.A.
0°	0.55	0.73	0.89	0.78	0.94	0.82	0.96	0.84
5°	0.51	0.62	0.77	0.75	0.70	0.75	0.55	···
10°	0.45	0.49	0.52	0.42	0.33	0.42	0.013	0.015
20°	0.30	0.29	0.133	0.194	0.031	0.028	0.0034	0.0045
30°	0.16	0.06	0.024	0.019	0.0024	0.0026	0.0312	0.0001
40°	0.058	···	0.0042	0.0023	0.00024	0.00024	0.0578	0.0578

TABLE II. Differential cross section for excitation of $2P$ state of hydrogen by electron impact. E_i, incident energy in ev; θ, scattering angle; $\sigma(\theta)$ in units of a_0^2; I.A., impulse approximation; B.A., Born approximation.

E_i	27	54	100	108	200	216	400	432
θ	I.A.	I.A.	B.A.	I.A.	B.A.	I.A.	B.A.	I.A.
0°	22.0	46.0	99.8	50.0	215.0	266.0	450.7	522.0
5°	21.0	36.0	23.7	18.0	13.3	10.0	5.43	5.0
10°	19.0	20.0	5.01	3.5	1.63	1.65	0.033	0.035
20°	10.0	6.0						
30°	0.13	0.1						
40°	0.05	0.01						

been made in the course of the calculation. One of these is a difficulty which will always arise when calculating the ionization cross section. The other occurs when one calculates an inelastic bound-bound transition.

In calculating the ionization cross section we have used plane waves for the final-state wave functions of the electron. This is a crude approximation but it would be difficult to know what the correct wave functions are. Coulombic wave functions have a logarithmic phase factor at infinity and apply only to the scattering by unshielded charges. In our case we have to describe the electron in the presence not only of a positive charge but other negative charges which provide some shielding. Consequently, a Coulombic wave function would not give the correct asymptotic behavior.

In calculating bound-bound transitions, in order to carry out the integrals, it is necessary to remove the r matrix from under the integral sign. In our application it was possible to do this because the product of the Fourier transforms of the bound-state wave functions peaked at some appropriate energy. The recipe that we have here does not necessarily apply for all bound-bound transitions. Each individual case must be examined separately to see what the appropriate value of the energy should be at which the r matrix is to be evaluated when removed from under the integral sign.

We have not made a detailed analysis of the nature of the fundamental impulse approximation and these additional approximations. We feel, however, that the results indicate that with labor no more complicated than that involved in the first Born approximation we have a supplementary approximation described here which is applicable to the calculation of inelastic scattering of electrons by atoms. If we were to generalize the results obtained for hydrogen, we could say that the true cross section for various processes lies somewhere in between the first Born approximation and the impulse approximation. We do not obtain the violent peaking at very low energies but rather our maximum cross section is approximately correct but occurs at an energy somewhat higher than the experimental results.

Note added in proof. W. Fite (private communication) has informed us that the experimental results for the $1S \rightarrow 2S$ transition should be raised by 50%.