

## Excitation of Helium by Electrons and Protons

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The first part of this paper deals with generalized oscillator strengths  $f(K)$ . On the basis of previous work of Lassette, we obtain a suitable form for the power-series representations of the  $f(K)$  for transitions in which an electron jumps from a  $1s$  to an  $ns$ ,  $n\bar{p}$ , or  $nd$  orbital of an atom. We apply the method to give analytical representations of  $f(K)$  for the transitions  $1^1S \rightarrow 2^1P$  and  $1^1S \rightarrow 3^1P$  in helium. In the second part of this paper, we study the dependence of the "total" excitation cross sections  $\sigma_E$  on the velocity  $v$  of the incident electron or proton for various dipole-allowed and dipole-forbidden transitions. By expanding the theoretical  $\sigma_E$  (direct and interference) in a series in inverse powers of  $v^2$ , we find a qualitative interpretation of the variation with  $v$  of the experimental  $\sigma_E$  of Moustafa and de Heer (electrons) and of Van den Bos, Winter, and de Heer (protons) for the transitions  $1^1S \rightarrow n^1S$ ,  $n^1P$ , and  $n^1D$  in helium, with  $n=3, 4, 5$ , and  $6$ . From our analytical formula for  $f(K)$  in the transitions  $1^1S \rightarrow 2^1P$ ,  $3^1P$  in helium, we calculate the corresponding  $\sigma_E$ , and compare these values with some other theoretical and experimental ones. The influence of interference between direct and exchange scattering is taken into account by using the Ochkur approximation. It is shown that the Ochkur approximation can be obtained in a simple way from the Bethe and Mott formulas. In the final part of this paper we study the nature of  $f(K)$ , for complex  $K$ , for ionization of atoms, and find the positions of the singularities (poles).

### 1. INTRODUCTION

**T**HE generalized oscillator strength associated with a transition  $i \rightarrow f$  in an atom, as defined by Bethe,<sup>1</sup> is

$$f(K) = (E/R)(Ka_0)^{-2} \left| \sum_s (\psi_f | \exp(i\mathbf{K} \cdot \mathbf{r}_s) | \psi_i) \right|^2, \quad (1)$$

where  $E$  and  $R$  are the excitation energy and the rydberg energy,  $\psi_i$  and  $\psi_f$  are the initial- and final-state wave functions,  $\hbar\mathbf{K}$  is the momentum transfer, and  $a_0$  is the radius of the first Bohr orbit of hydrogen. The sum in Eq. (1) is over all atomic electrons, with coordinates  $\mathbf{r}_s$ .

According to the Bethe theory, the collision cross section for transfer of momentum  $Ka_0$  is

$$\sigma_{E,K} d(Ka_0)^2 = (4\pi a_0^2 R^2 / TE) f(K) [d(Ka_0)^2 / (Ka_0)^2], \quad (2)$$

where  $T = \frac{1}{2}mv^2$ ,  $m$  is the electron rest mass, and  $v$  the velocity of the incident electron. Equation (2) applies at great enough  $T$ .

By integrating Eq. (2) over  $K$ , we obtain the excitation cross section

$$\sigma_E = \frac{4\pi a_0^2 R^2}{TE} \int_{(Ka_0)_{\min}^2}^{(Ka_0)_{\max}^2} f(K) d(Ka_0)^2 / (Ka_0)^2, \quad (3)$$

where

$$(Ka_0)_{\min}^2 = (E^2 / 4TR) [1 + (E/2T) + O(E^2/T^2)]. \quad (4)$$

We may expand  $\exp(i\mathbf{K} \cdot \mathbf{r}_s)$  in Eq. (1) in a series of powers of  $i\mathbf{K} \cdot \mathbf{r}_s$ . It then follows that  $f(K)$  gets the form of an infinite series of even powers of  $Ka_0$ :

$$f(K) = \sum_{\nu=0}^{\infty} b_{\nu}(Ka_0)^{2\nu}.$$

The first few terms of this series may give a good repre-

sentation of the  $f(K)$  for small  $K$ , but not for large  $K$ . Since  $(Ka_0)_{\max}^2$  is proportional to  $T$  and is never small, we should not calculate  $\sigma_E$  with such series of  $f(K)$ .

Recently, Lassette<sup>2</sup> studied the nature of the function  $f(K)$  for complex values of  $K$ , for excitation to bound states, and came to the important conclusion that for finite values of  $K$ ,  $f(K)$  has singularities only for  $Ka_0 = \pm i\alpha$ , where  $\alpha = \alpha_i + \alpha_f$ ,  $\alpha_i = (-E_i/R)^{1/2} = (I/R)^{1/2}$ ,  $\alpha_f = (-E_f/R)^{1/2} = [(I-E)/R]^{1/2}$ . Here  $I$  is the ionization energy and  $E$ , as before, is the excitation energy. In order to obtain this result, one has to assume that the electrons in different shells of an atom (or molecule) are distinguishable so that in an excitation process we know the initial and final orbital of the electron which is excited. The  $E_i$  and  $E_f$  may then be considered to be the initial- and final-state energy eigenvalues of that electron. For bound initial and final states,  $E_i$  and  $E_f$  are negative and  $\alpha_i$ ,  $\alpha_f$ , and  $\alpha$  are real and positive.

On the basis of this conclusion, Lassette<sup>2</sup> introduced a power series representation of  $f(K)$  which contains terms like  $x/(1+x)$  with  $x = (Ka_0/\alpha)^2$ , so that  $f(K)$  has singularities for  $Ka_0 = \pm i\alpha$  ( $x = -1$ ), as should be the case. Furthermore, Lassette's power series converges for all physically attainable values of  $K$ , so that this series may be used to calculate the excitation cross section  $\sigma_E$ . Lassette<sup>2</sup> applied his method to find an analytic representation of the  $f(K)$  and to calculate the  $\sigma_E$  for the transition  $1^1S \rightarrow 2^1S$  in helium.

In this paper, we first study the nature of the  $f(K)$  for some transitions in atomic hydrogen. Since the exact atomic wave functions for all states in atomic hydrogen are known, the  $f(K)$  for any transition in H may be calculated exactly. The behavior of the  $f(K)$  found for atomic hydrogen provides a basis for the general trend of the  $f(K)$  for corresponding transitions in other atoms. This may be understood by the following. First,

<sup>1</sup> H. Bethe, Ann. Physik **5**, 325 (1930).

<sup>2</sup> E. N. Lassette, J. Chem. Phys. **43**, 4479 (1965).

Lassetre<sup>2</sup> found that the position and nature of the singularities of  $f(K)$  only depend on the behavior of  $\psi_i$  and  $\psi_f$  for very large  $r$  (distance from the nucleus). Second, the behavior of  $\psi_i$  and  $\psi_f$  is asymptotically similar for different atoms if the quantum numbers of initial and final states are the same. As we shall see for instance in Sec. 2, the  $f(K)$  for the transitions  $1s \rightarrow np$  in atomic hydrogen have sixth- and higher-order poles for  $Ka_0 = \pm i(\alpha_i + \alpha_f) = \pm i(1 + 1/n)$ . Consequently, the  $f(K)$  for the transitions  $1^1S \rightarrow n^1P$  in helium will also have sixth- and higher-order poles for  $Ka_0 = \pm i(\alpha_i + \alpha_f)$  with different  $\alpha_i$  and  $\alpha_f$ . In Secs. 2 and 8 we shall see, for the transitions  $1^1S \rightarrow 2^1P$ ,  $3^1P$ , and  $2^1S$  in He, that series expansions of  $f(K)$  similar to the ones found for the corresponding transitions in H, and a suitable choice of only one or two parameters, enable us to reproduce the experimental  $f(K)$  values within the experimental accuracy. The lowest-order pole of  $f(K)$  simultaneously determines how fast  $f(K)$  decreases for large  $K$ . We also study the nature of  $f(K)$  for ionization of atoms. In this case, however, we only give an analysis of the problem but no applications.

We thus use some analogies between the asymptotic behavior of hydrogenic wave functions and wave functions for complex atoms. However, it should be noted that our procedure is entirely different from the procedure in which hydrogenic wave functions with effective nuclear charges are used for complex atoms. The correct wave functions are proportional to  $\exp(-\alpha_f r/a_0)$  or  $\exp(-\alpha_i r/a_0)$ . Hydrogenic wave functions with effective nuclear charges  $Z_e$  are proportional to  $\exp(-Z_e r/na_0)$  and  $Z_e/n$  may be very different from  $\alpha_i$  or  $\alpha_f$ .

In this paper we further calculate cross sections  $\sigma_E$  from the obtained analytical expressions  $f(K)$  for the transitions  $1^1S \rightarrow 2^1P$ ,  $3^1P$  in He. We represent the  $\sigma_E$  analytically as series of powers in  $R/T$ . Such expansions, which are very suitable for large  $T$ , have been used before in the theory of stopping power.<sup>3</sup> Interference between direct and exchange scattering is approximately taken into account by using the Ochkur approximation.

Finally, we study the variation of experimental  $\sigma_E$  with  $T$ , for incident electrons and protons, for various transitions in helium. As far as possible, we give a theoretical interpretation of the difference in behavior of the  $\sigma_E$  for incident electrons and protons and for different sorts of transitions.

## 2. POWER-SERIES REPRESENTATIONS OF $f(K)$

### A. Atomic Hydrogen

On the basis of previous calculations of Massey and Mohr,<sup>4</sup> we found that for transitions in the series  $1s \rightarrow$

<sup>3</sup> L. M. Brown, Phys. Rev. **79**, 297 (1950); M. C. Walske, *ibid.* **88**, 1283 (1952); **101**, 940 (1956); U. Fano, Ann. Rev. Nucl. Sci. **13**, 1 (1963).

<sup>4</sup> H. S. W. Massey and C. B. O. Mohr, Proc. Roy. Soc. (London) **A132**, 605 (1931). (See also Ref. 11, p. 480.)

$ns$ ,  $1s \rightarrow np$ , and  $1s \rightarrow nd$  the following expansions may be given.

For  $1s \rightarrow ns$ :

$$f(K) = \frac{x}{(1+x)^6} \sum_{\nu=0}^{\infty} c_{\nu} \left( \frac{x}{1+x} \right)^{\nu} \quad (5)$$

with integer  $\nu$ . For instance, for the transition  $1s \rightarrow 2s$  one finds (Bates and Griffing,<sup>5</sup> Inokuti<sup>6</sup>)  $\alpha^2 = 9/4$ ,  $c_0 = 2^{13}/3^9$ , and  $c_{\nu} = 0$  for  $\nu \geq 1$ . For the transition,  $1s \rightarrow 3s$  is<sup>5,6</sup>  $\alpha^2 = 16/9$ ,  $c_0 = 3^3/2^9$ ,  $c_1 = c_2 = 3^3/2^7$ , and  $c_{\nu} = 0$  for  $\nu \geq 3$ .

For  $1s \rightarrow np$ :

$$f(K) = \frac{f(o)}{(1+x)^6} \left\{ 1 + \sum_{\nu=1}^{\infty} c_{\nu} \left( \frac{x}{1+x} \right)^{\nu} \right\}, \quad (6)$$

where  $f(o)$  is the optical oscillator strength. For the transition  $1s \rightarrow 2p$ , one finds<sup>5,6</sup>  $f(o) = 2^{13}/3^9$ ,  $\alpha^2 = 9/4$ , and  $c_{\nu} = 0$  for all  $\nu \geq 1$ . For  $1s \rightarrow 3p$ ,  $f(o) = 3^4/2^{10}$ ,  $\alpha^2 = 16/9$ ,  $c_1 = c_2 = 4$ , and  $c_{\nu} = 0$  for  $\nu \geq 3$ .

For  $1s \rightarrow nd$ :

$$f(K) = \frac{x}{(1+x)^8} \sum_{\nu=0}^{\infty} c_{\nu} \left( \frac{x}{1+x} \right)^{\nu}, \quad (7)$$

where for the transition  $1s \rightarrow 3d$ ,  $\alpha^2 = 16/9$ ,  $c_0 = 3^3/2^8$ , and  $c_{\nu} = 0$  for  $\nu \geq 1$ .

### B. Helium

On the basis of general considerations, Lassetre<sup>2</sup> found that the first term of the expansion of  $f(K)$  for the transition  $1^1S \rightarrow 2^1S$  is  $c_0 x/(1+x)^6$ , in agreement with Eq. (5), which is obtained in a different way. By only fitting this adjustable constant  $c_0$  to experiment, Lassetre obtained excellent agreement with his experimental  $f(K)$  values.

We will now use Eq. (6) to find analytical representations of  $f(K)$  for the transitions  $1^1S \rightarrow 2^1P$  and  $1^1S \rightarrow 3^1P$  in helium. The optical oscillator strengths have accurately been calculated by Schiff and Pekeris,<sup>7</sup> values of  $f(K)$  have been calculated and measured by Silverman and Lassetre<sup>8</sup> and measured by Lassetre, Krasnov, and Silverman.<sup>9</sup> The  $\alpha^2$  values can easily be calculated from the experimental  $E_i$  and  $E_f$  values (excitation and ionization energies). We found that the shape of the function  $f(K)$  according to Eq. (6) could be excellently fitted to experiment with only  $c_1$  unequal to zero for the transition  $1^1S \rightarrow 2^1P$  and with only  $c_1$  and  $c_2$  unequal to zero for the transition  $1^1S \rightarrow 3^1P$ . We thus found that a good representation of the  $f(K)$  is

<sup>5</sup> D. R. Bates and G. Griffing, Proc. Phys. Soc. (London) **66A**, 961 (1953).

<sup>6</sup> M. Inokuti (private communication).

<sup>7</sup> B. Schiff and C. L. Pekeris, Phys. Rev. **134**, A638 (1964).

<sup>8</sup> S. M. Silverman and E. N. Lassetre, J. Chem. Phys. **40**, 1265 (1964).

<sup>9</sup> E. N. Lassetre, M. E. Krasnov, and S. Silverman, J. Chem. Phys. **40**, 1242 (1964).

given by Eq. (6) with:

For  $1^1S \rightarrow 2^1P$ :

$$\alpha^2 = 3.391, c_1 = 0.86, c_\nu = 0 \text{ for } \nu \geq 2, \text{ and } f(o) = 0.27616.$$

For  $1^1S \rightarrow 3^1P$ :

$$\alpha^2 = 2.896, c_1 = 1.5, c_2 = 20, c_\nu = 0 \text{ for } \nu \geq 3, \text{ and } f(o) = 0.0734.$$

When, for the transition  $1^1S \rightarrow 2^1P$ , we use Eq. (6) with Lassettre's value of  $f(o)$  and with the values of  $\alpha^2$  and  $c_1$  given above, then we reproduce the theoretical  $f(K)$  of Silverman and Lassettre<sup>8</sup> within 1 to 2%. For the transition  $1^1S \rightarrow 3^1P$  we cannot very well give an error margin since the experimental values of  $f(K)$  are too much scattered.

### 3. THE CROSS SECTION $\sigma_E$ FOR INCIDENT ELECTRONS

#### A. Dipole-Allowed Transitions

For dipole-allowed transitions, we may rewrite Eq. (3) as

$$\sigma_E = (4\pi a_0^2 R^2 / TE) [\ln(4c_E T/R) - \phi(E, T)] f(o) \quad (8)$$

with

$$\ln c_E = \lim_{\epsilon \rightarrow 0} \left[ \int_{\epsilon}^{\infty} \frac{f(K)}{f(o)} \frac{d(Ka_0)^2}{(Ka_0)^2} + \ln \left( \frac{\epsilon R^2}{E^2} \right) \right] \quad (9)$$

and

$$\begin{aligned} \phi(E, T) = \ln \left[ \frac{4TR}{E^2} (Ka_0)_{\min}^2 \right] \\ + \int_0^{(Ka_0)_{\min}^2} \left[ \frac{f(K)}{f(o)} - 1 \right] \frac{d(Ka_0)^2}{(Ka_0)^2} \\ + \int_{(Ka_0)_{\max}^2}^{\infty} \frac{f(K)}{f(o)} \frac{d(Ka_0)^2}{(Ka_0)^2}. \quad (10) \end{aligned}$$

Equation (9) has been used before by Miller and Platzman<sup>10</sup> and by Inokuti.<sup>6</sup> The function  $\phi(E, T)$  may be expanded in a series of powers of  $R/T$ , where the first term is of the order  $R/T$  so that  $\phi(E, T)$  may be put equal to zero in the limit of large  $T$ .

Inserting Eq. (6) into Eqs. (9) and (10) results in

$$\ln c_E = 2 \ln \left( \frac{\alpha R}{E} \right) - \frac{137}{60} + \frac{c_1}{6} + \frac{c_2}{42} + \frac{c_3}{168} + \frac{c_4}{504} + \dots \quad (11)$$

and

$$\phi(E, T) = E/2T + (c_1 - 6) E^2/4\alpha^2 RT + O(R^2/T^2). \quad (12)$$

With Eqs. (11) and (12) and the values of  $f(o)$ ,  $\alpha^2$ ,  $c_1$ , and  $c_2$  given in Sec. 2B, we find for the transition  $1^1S \rightarrow 2^1P$  ( $E = 21.22$  eV),  $\ln c_E = -1.81$  and  $\phi(E, T) =$

<sup>10</sup> W. F. Miller and R. L. Platzman, Proc. Phys. Soc. (London) **70**, 299 (1957).

$-0.144R/T + O(R^2/T^2)$ . For the transition  $1^1S \rightarrow 3^1P$  ( $E = 23.08$  eV), we find  $\ln c_E = -1.56$  and  $\phi(E, T) = -0.27R/T + O(R^2/T^2)$ . Thus Eq. (8) gives:

For  $1^1S \rightarrow 2^1P$ :

$$\sigma_E = (4\pi a_0^2 R/T) [0.177 \ln(T/R) - 0.075 + 0.0255(R/T) + O(R^2/T^2)]. \quad (13)$$

For  $1^1S \rightarrow 3^1P$ :

$$\sigma_E = (4\pi a_0^2 R/T) [0.0432 \ln(T/R) - 0.0075 + 0.0117(R/T) + O(R^2/T^2)]. \quad (14)$$

For  $T/R > 10$ , the contribution of the third term in Eqs. (13) and (14) is less than 1%. Further, interference between direct and exchange scattering will also give a term of the order  $(R/T)^2$  in  $\sigma_E$ . The interference term will diminish the cross sections and will therefore work in the opposite direction to the third term of Eqs. (13) and (14). In Sec. 5 we calculate the interference terms with the Ochkur approximation. The sum of the direct and interference  $\sigma_E$  are given by Eqs. (31) and (32) of Sec. 5.

Some cross sections calculated with Eqs. (13), (14), (31), and (32) are given in Table I for different energies  $E_{e1}$  of the incident electron. The relation between  $T$  and  $E_{e1}$  is  $T = E_{e1} [1 - 3E_{e1}/2mc^2 + O(E_{e1}^2/m^2c^4)]$ , where  $c$  is the velocity of light. In the table are also included some theoretical cross sections given by Mott and Massey<sup>11</sup> (these cross sections were calculated by Fox), some experimental cross sections of Moustafa and de Heer,<sup>12</sup> and theoretically calculated (including interference and exchange) cross sections of Ochkur and Brattsev.<sup>13</sup> No comparison has been made with the theoretical work of Altshuler<sup>14</sup> and experimental results of St. John *et al.*<sup>15</sup> (this is done in Ref. 12).

The agreement of the  $\sigma_E$  for the transition  $1^1S \rightarrow 2^1P$  is reasonable. The discrepancies between the  $\sigma_E$  for the transition  $1^1S \rightarrow 3^1P$  may be due to (i) errors in the  $c_0$  and  $c_1$  values used in the present calculation. Such errors may have been caused by uncertainties in the  $f(K)$  values of Silverman and Lassettre<sup>8,9</sup> as well as by our fitting procedure. However, since the major contribution to  $\ln c_E$  comes from small  $Ka_0$ , it is not very probable that our fitting procedure alone leads to large errors in  $\sigma_E$ ; (ii) inaccuracies in the wave functions used in the theoretical calculations of Refs. 11 and 13; (iii) errors in the experimental  $\sigma_E$ . According to Moustafa and de Heer,<sup>12</sup> these errors may be 10%.

<sup>11</sup> N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, London, 1965), 3rd ed., p. 498.

<sup>12</sup> H. R. Moustafa and F. J. de Heer, *Physica* (to be published).

<sup>13</sup> V. I. Ochkur and V. F. Brattsev, *Opt. i Spektroskopiya* **19**, 490 (1965) [English transl.: *Opt. Spectry.* (USSR) **19**, 274 (1965)].

<sup>14</sup> S. Altshuler, *Phys. Rev.* **87**, 992 (1952).

<sup>15</sup> R. M. St. John, C. J. Bronco, and R. G. Fowler, *J. Opt. Soc. Am.* **50**, 28 (1960); R. M. St. John and R. G. Fowler, *Phys. Rev.* **122**, 1813 (1961).

TABLE I. Theoretical and experimental excitation cross sections  $\sigma_E$  in units  $\pi a_0^2$ .

$E_{e1}$ in eV	Eq. (13)	Eq. (31)	$\sigma_E(1^1S \rightarrow 2^1P)$			$\sigma_E(1^1S \rightarrow 3^1P)$					
			O & B <sup>a</sup>	M & M <sup>b</sup>	ZOC	Eq. (14)	Eq. (32)	M & M	Mo & H <sup>c</sup>	O & B	ZOC <sup>d</sup>
200	0.109	0.106	0.099	0.111	-0.007	0.0297	0.0287	0.0275	0.0240	0.025	0.0004
400	0.0712	0.0706	0.066	0.072	-0.0035	0.0189	0.0186	0.0180	0.0159	0.017	0.0002
1000	0.0372	0.0371			-0.0014	0.0097	0.00966		0.00835		0.00008
2000	0.0220	0.0220			-0.0007	0.00565	0.00564		0.00491		0.00004

<sup>a</sup> Ochkur and Brattsev (Ref. 13).

<sup>b</sup> Mott and Massey (values calculated by Fox) (Ref. 11).

<sup>c</sup> Moustafa and de Heer (Ref. 12).

<sup>d</sup> Zeroth-order correction, giving the values which should be added to the cross sections calculated with Eqs. (13) and (14) in order to get the cross sections corresponding to  $c_1=0(1^1S \rightarrow 2^1P)$  and  $c_1=c_2=4(1^1S \rightarrow 3^1P)$ .

However, Moustafa and de Heer find that a plot of their experimental  $\sigma_E T/R$  against  $\ln(T/R)$  gives a straight line, as should be the case for large  $T$  [see Eq. (14)]. From the slope of this straight line, they obtain an  $f(o)$  value of 0.073 which excellently agrees with the theoretical  $f(o)$  value 0.0734. This suggests that the  $\sigma_E$  of Moustafa and de Heer are reasonably accurate.

From the  $\sigma_E$  values obtained via Eqs. (13), (14), (31), and (32), it follows that interference may give a 2% reduction of the  $\sigma_E$  for  $E_{e1}=200$  eV. Since this effect of 2% is very small, we cannot give much weight to it. Higher-order terms in  $\sigma_E$  (see Sec. 8) and failure of the Ochkur approximation may easily compensate the 2% reduction of the  $\sigma_E$  for  $E_{e1}=200$  eV.

### B. Dipole-Forbidden Transitions

For dipole-forbidden transitions we may rewrite Eq. (3) as

$$\sigma_E = (4\pi a_0^2 R^2 / TE) [C - \eta(E, T)] \quad (15)$$

with

$$C = \int_0^\infty f(K) \frac{d(Ka_0)^2}{(Ka_0)^2} \quad (16)$$

and

$$\eta(E, T) = \int_0^{(Ka_0)_{\min}^2} f(K) \frac{d(Ka_0)^2}{(Ka_0)^2} + \int_{(Ka_0)_{\max}^2}^\infty f(K) \frac{d(Ka_0)^2}{(Ka_0)^2}. \quad (17)$$

According to Eq. (5) we find

$$C = \sum_{\mu=0}^\infty \sum_{\nu=\mu}^\infty \frac{(-1)^\mu}{5+\mu} \binom{\nu}{\mu} c_\nu \quad (18)$$

and according to Eq. (7)

$$C = \sum_{\mu=0}^\infty \sum_{\nu=\mu}^\infty \frac{(-1)^\mu}{7+\mu} \binom{\nu}{\mu} c_\nu. \quad (19)$$

For large  $T$ , it is again very suitable to expand  $\sigma_E$  in a series of powers of  $R/T$ , and because  $f(K)$  decreases very rapidly for large  $K$ , we may neglect the second term of Eq. (17) with respect to the first term. For very

small  $Ka_0$  ( $x$ ) we rewrite Eqs. (5) and (7) as

$$f(K) = c_0 x + O(x^2), \quad (20)$$

so that Eq. (17) becomes [see Eq. (4)]

$$\eta(E, T) = c_0 E^2 / 4\alpha^2 TR + O(R^2/T^2). \quad (21)$$

The parameter  $c_0$  in Eqs. (5), (7), (18), (19), (20), and (21) is directly proportional to the square of the matrix element  $\sum_s (\psi_f | (\hat{K} \cdot \mathbf{r}_s)^2 | \psi_i)$ , where  $\hat{K}$  is the unit vector in the direction of  $\mathbf{K}$ . From the structure of Eq. (17),  $\eta(E, T)$  is always positive, and from the fact that interference also diminishes the cross sections for small  $T$ , it follows that plotting  $\sigma_E T/R$  against  $\ln T/R$  or against  $T/R$  would give a straight line with a zero slope for large  $T$  and deviations towards lower  $\sigma_E T/R$  values for small  $T$ . This is in accord with experimental observations by Moustafa and de Heer<sup>12</sup> (see Sec. 4 for a further discussion).

### 4. THE DIFFERENCE BETWEEN EXCITATION BY PROTONS AND BY ELECTRONS

It is interesting to consider how great the difference is between excitation by protons and excitation by electrons.

When  $T = \frac{1}{2}mv^2$ , where  $m$  is the electron rest mass and  $v$  the velocity of the proton, then all formulas of Secs. 1 and 2 remain applicable when  $v$  is much larger than the orbital velocity of the atomic electrons, except Eq. (4), which must be replaced by

$$(Ka_0)_{\min}^2 = E^2 / 4TR [1 + (mE/2MT) + O(E^2/T^2)]. \quad (22)$$

Here  $M$  is the mass of the proton.

#### A. Dipole-Allowed Transitions

Equations (8), (9), (10), and (11) of Sec. 3A also remain applicable, but the first term of Eq. (10) becomes negligible compared with the second term. The third term of Eq. (10) only gives terms of the order  $(R/T)^6$  and higher orders and is negligible for incident electrons and protons. The term  $E/2T$  in Eq. (12) must be replaced by  $mE/2MT$ . The coefficients 0.0255 and 0.0117 of the third term of Eqs. (13) and (14) must be replaced by 0.164 and 0.0484. Since there is no interference between direct and exchange scattering, as in the case of incident electrons, we find, according to

Eqs. (13) and (14) with the new coefficients given above, that for protons the plot of  $\sigma_E T/R$  against  $\ln T/R$  gives a straight line for large  $T/R (> 10)$  with a deviation towards higher  $\sigma_E T/R$  values for small  $T/R$ . This behavior is also found from the experimental  $\sigma_E$  of Van den Bos, Winter, and de Heer<sup>16</sup> (see also Sec. 8).

### B. Dipole-Forbidden Transitions

All equations of Sec. 3B remain unchanged in the case of incident protons. This has some interesting consequences. From measurements of Van den Bos, Winter, and de Heer<sup>16</sup> for incident protons it follows that plotting the experimental  $\sigma_E T/R$  against  $\ln T/R$  for the transitions  $1^1S \rightarrow 3^1S$ ,  $4^1S$ ,  $5^1S$ ,  $6^1S$ ,  $3^1D$ ,  $4^1D$ ,  $5^1D$ , and  $6^1D$  in helium gives a straight line with a zero slope for large  $T$ , while deviations towards lower  $\sigma_E T/R$  values [in agreement with the fact that  $\eta(E, T)$  is positive] start to become important for  $T/R \approx 3$ . From measurements of Moustafa and de Heer<sup>12</sup> for incident electrons for the same transitions in helium, an entirely different behavior is found. For the transitions  $1^1S \rightarrow n^1S$ , they find that deviations from the straight line towards lower  $\sigma_E T/R$  become important already for  $T/R \approx 110$  and for the transitions  $1^1S \rightarrow n^1D$  for  $T/R \approx 6$ . Since the term of the order  $R/T$  in  $\eta(E, T)$  is essentially the same for incident electrons and protons and since for incident protons the function  $\eta(E, T)$  is negligible for  $T/R > 4$  (see above), we cannot ascribe the difference in behavior for protons and electrons to the function  $\eta(E, T)$ . We will show in the next paragraph that interference between direct and exchange scattering may qualitatively explain a part of the difference in behavior for incident protons and electrons.

## 5. THE OCHKUR APPROXIMATION

On the basis of the Born-Oppenheimer approximation, Ochkur<sup>17</sup> expanded the exchange amplitude of the Born-Oppenheimer approximation into powers of  $(R/T)^{1/2}$  and took into account only the first term of the expansion. Thus we may expect that Ochkur's method gives good results for large  $T$ . The Ochkur approximation is easy to apply and gives reasonable total cross sections for a given excitation, even for small  $T$ .

We will derive the Ochkur approximation in a simple way from the Bethe formulas [Eqs. (1) and (2) of this paper] and Mott's formula for scattering of electrons by free electrons at rest. Ochkur<sup>17</sup> already mentioned the analogy between his and Mott's formula. Therefore, we rewrite Eqs. (1) and (2) as

$$\sigma_{E,K} d(Ka_0)^2 = (4\pi a_0^2 R/T) [1/(Ka_0)^4] P(K, E) d(Ka_0)^2, \quad (23)$$

<sup>16</sup> J. Van den Bos, G. Winter, and F. J. de Heer, *Physica* (to be published).

<sup>17</sup> V. I. Ochkur, *Zh. Eksperim. i Teor. Fiz.* **45**, 734 (1964) [English transl.: *Soviet Phys.—JETP* **18**, 503 (1964)].

where

$$P(K, E) = \left| \sum_s (\psi_f | \exp(i\mathbf{K} \cdot \mathbf{r}_s) | \psi_i) \right|^2. \quad (24)$$

The Rutherford formula for scattering of electrons by free electrons at rest is

$$\sigma_K d(Ka_0)^2 = (4\pi a_0^2 R/T) [1/(Ka_0)^4] d(Ka_0)^2. \quad (25)$$

Equation (25) is also equal to Eq. (31) of Vriens<sup>18</sup> for scattering of electrons by free electrons moving in arbitrary directions. This confirms the interpretation of Fano (Ref. 3, p. 8) that  $\sigma_{E,K}$  is equal to  $P(K, E)$  times the cross section that one particular atomic electron receives a momentum  $Ka_0$ .

When we include exchange and interference in our treatment and when the velocity of the incident electron is much larger than the orbital velocities of the atomic electrons, then the cross section for one particular atomic electron to receive a momentum  $Ka_0$  is no longer given by the Rutherford formula but by the Mott formula.<sup>19</sup> Therefore,  $\sigma_{E,K}$  will better be given by  $P(K, E)$  times the Mott formula, which for  $T \gg E$  gives

$$\sigma_{E,K} d(Ka_0)^2 = \frac{4\pi a_0^2 R}{T} \left[ \frac{1}{(Ka_0)^4} + \frac{R^2}{T^2} - \frac{R}{(Ka_0)^2 T} \right] \times P(K, E) d(Ka_0)^2, \quad (26)$$

where the first term is the direct-scattering term, the second the exchange term, and the third the interference term. Thus Eq. (26) is an approximation in that in the exchange and interference terms the binding and orbital velocity of the atomic electrons are disregarded with respect to the velocity of the incident electron.

Before applying Eq. (26), we first need to consider the symmetry properties of the total wave functions. In the following, we will separately consider excitation of atomic hydrogen and excitation of helium.

### A. Excitation of Atomic Hydrogen

When  $f$  and  $g$  are the direct and exchange scattering amplitudes, the cross section  $\sigma_{E,K}$  is proportional to  $\frac{1}{4} |f+g|^2 + \frac{3}{4} |f-g|^2$ . With different  $f$  and  $g$ , this relation also holds for scattering of electrons by free electrons (not necessarily at rest) since the presence of the nucleus does not affect the symmetry properties of the wave functions. Equation (26) should therefore be applicable for excitation of atomic hydrogen. The Ochkur approximation also leads to Eq. (26) in this case.

In the preceding paragraphs, we confined ourselves to the terms of the order  $(R/T) \ln(T/R)$ ,  $R/T$ , and  $R^2/T^2$  in  $\sigma_E$ . Therefore, we will neglect the second term of Eq. (26).

We define the function

$$\mu(i \rightarrow f) = -\sigma_{E, \text{interference}} / \sigma_{E, \text{direct}}. \quad (27)$$

<sup>18</sup> L. Vriens, *Proc. Phys. Soc. (London)* **89**, 13 (1966).

<sup>19</sup> N. F. Mott, *Proc. Roy. Soc. (London)* **A126**, 259 (1930).

This function is a direct measure of the relative importance of interference between direct and exchange scattering. From Eqs. (1), (3), (5), (6), (7), (8), (9), (11), (15), (16), (24), and (26) and from the coefficients  $\alpha^2$ ,  $c_0$  and  $c_1$  given in Sec. 2A, it follows that

$$\mu(1s \rightarrow 2s) = 9R/16T + O(R^2/T^2),$$

$$\mu(1s \rightarrow 2p) = (9R/20T) \ln(4c_B T/R) + O(R^2/T^2),$$

where, according to Inokuti,<sup>20</sup>  $c_B = 0.4980579$ . Further,

$$\mu(1s \rightarrow 3s) = 244R/351T + O(R^2/T^2),$$

$$\mu(1s \rightarrow 3d) = 8R/27T + O(R^2/T^2).$$

Thus for large  $T/R$ ,

$$\mu(1s \rightarrow 2s)/\mu(1s \rightarrow 2p) \approx (5/4) \ln(4c_B T/R)$$

and

$$\mu(1s \rightarrow 3s)/\mu(1s \rightarrow 3d) \approx 2.35.$$

A direct consequence of the structure of Eq. (26) and of the nature of the functions  $f(K)$  is that  $\mu(i \rightarrow f)$  becomes larger when the major contribution to the direct term of  $\sigma_E$  comes from larger  $K$ . Consequently, for large  $T$ , interference will be more important for dipole-forbidden than for dipole-allowed transitions; this has already been noted by Ochkur.<sup>17</sup> Extensive calculations of Inokuti<sup>21</sup> concerning the nature of  $f(K)$  show that the major contribution to the direct term of  $\sigma_E$  comes from larger  $K$  for  $1s \rightarrow ns$  than for  $1s \rightarrow nd$  transitions. We may expect, therefore, that interference is more important for  $1s \rightarrow ns$  than for  $1s \rightarrow nd$  transitions. These conclusions agree with the few values of  $\mu$  calculated above and enable us (see below) to give a qualitative interpretation of the behavior of experimental excitation cross sections in He. Concerning the relative importance of interference for large  $T$ , one must be aware that the validity of our conclusions depends on the validity of the Ochkur approximation for large  $T$  for the total cross sections.

### B. Excitation of Helium

When  $f$  and  $g$  are again the direct and exchange scattering amplitudes, the cross section  $\sigma_{E,K}$  for excitation of a singlet state is proportional to  $|f-g|^2$ . The relationship between  $f$  and  $g$  is different in H and He, and Eq. (2) of Ochkur and Brattsev<sup>13</sup> is incorrect on this point (at least for singlet excitation). For singlet excitation of He we find that Eq. (26) must be replaced by

$$\sigma_{E,K} d(Ka_0)^2 = \frac{4\pi a_0^2 R}{T} \left[ \frac{1}{(Ka_0)^2} + \frac{R^2}{4T^2} - \frac{R}{(Ka_0)^2 T} \right] \times P(K, E) d(Ka_0)^2. \quad (28)$$

<sup>20</sup> M. Inokuti, Argonne National Laboratory, Radiological Physics Division Report No. 6769, 1963 (unpublished).

<sup>21</sup> M. Inokuti, Argonne National Laboratory, Radiological Physics Division Report No. 7220, 1966 (unpublished).

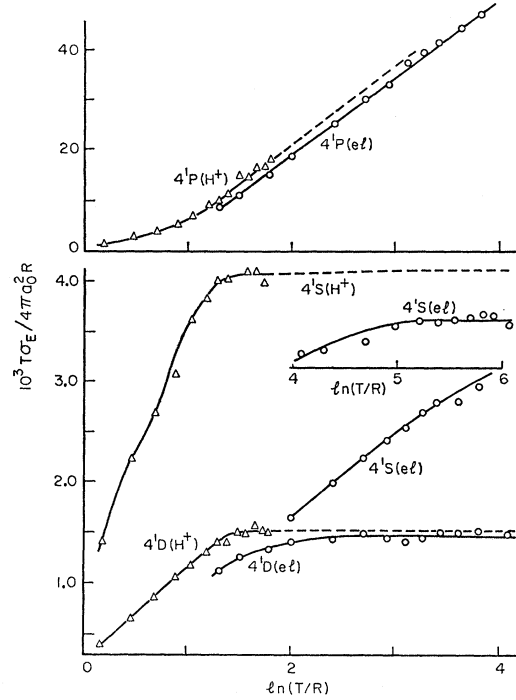


FIG. 1. Preliminary experimental (Refs. 12, 16) excitation cross sections times  $10^3 T/4\pi a_0^2 R$  plotted against  $\ln(T/R)$ . The dashed curves for incident protons are extrapolated (Ref. 16). The experimental curve for incident electrons for the transition  $1^1S \rightarrow 4^1S$  is given in two parts.

Using the same method as for atomic hydrogen and using the coefficients  $f(0)$ ,  $\alpha^2$ , and  $c_\nu$  of Sec. 2B, we find:

For  $1^1S \rightarrow 2^1P$ :

$$\sigma_{E, \text{interference}} = (4\pi a_0^2 R/T) [-0.138(R/T)], \quad (29)$$

For  $1^1S \rightarrow 3^1P$ :

$$\sigma_{E, \text{interference}} = (4\pi a_0^2 R/T) [-0.055(R/T)]. \quad (30)$$

By comparison with Eqs. (13) and (14), we see that interference corrections are much more important than the corrections of Sec. 3A. For the sum of the direct and interference terms, we get, according to Eqs. (13), (14), (29), and (30),

For  $1^1S \rightarrow 2^1P$ :

$$\sigma_E = (4\pi a_0^2 R/T) [0.177 \ln(T/R) - 0.075 - 0.112(R/T) + O(R^2/T^2)], \quad (31)$$

For  $1^1S \rightarrow 3^1P$ :

$$\sigma_E = (4\pi a_0^2 R/T) [0.0432 \ln(T/R) - 0.0075 - 0.043(R/T) + O(R^2/T^2)]. \quad (32)$$

Some cross sections calculated with Eqs. (31) and (32) have been listed in the table.

From the value  $\alpha^2 = 3.551$  for the transition  $1^1S \rightarrow 2^1S$  in helium and from the fact that  $c_\nu = 0$  for  $\nu \geq 1$  for that transition, it follows that

$$\mu(1^1S \rightarrow 2^1S) = \alpha^2 R/4T = 0.888R/T.$$

If we assume that the  $\mu(1^1S \rightarrow 3^1S)/\mu(1^1S \rightarrow 2^1S)$  in helium is approximately the same as the ratio  $\mu(1s \rightarrow 3s)/\mu(1s \rightarrow 2s) = 1.24$  for atomic hydrogen, then

$$\mu(1^1S \rightarrow 3^1S) \approx 1.10R/T$$

and interference gives a 5% reduction of  $\sigma_E$  for  $E_{e1} \approx 300$  eV. This does not quantitatively agree with the experimental result of Moustafa and de Heer<sup>12</sup> that deviations from the straight line in the plot of  $\sigma_E T/R$  against  $T/R$  become important for very large  $E_{e1}$  ( $\approx 1500$  eV) for transitions to  $n^1S$  states. For excitation of the  $2^1P$  and  $3^1P$  states we find from the small coefficients in Eqs. (29) and (30) that interference is not significant. This fact is consistent with Moustafa and de Heer's<sup>12</sup> result that the Bethe-Born approximation remains valid down to surprisingly low  $T$  for  $1^1S \rightarrow n^1P$  transitions. Moustafa and de Heer's<sup>12</sup> finding that the Bethe-Born approximation breaks down for higher  $T$  for  $n^1S$  than for  $n^1D$  excitation also agrees with our theoretical conclusions for  $ns$  and  $nd$  excitation in atomic hydrogen.

The behavior of the experimental  $\sigma_E$  for incident electrons<sup>12</sup> and protons<sup>16</sup> is illustrated in Fig. 1, which is reproduced here with the kind permission of de Heer.

## 6. EXCITATION AND IONIZATION BY ELECTRONS

For ionization of helium and other atoms, Schram *et al.*<sup>22</sup> found that in a plot of the ionization cross sections  $Q$  times  $T/R$  against  $\ln T/R$ , the deviations from the straight line towards lower  $Q T/R$  start to become important already for  $E_{e1} \approx 500$  eV. For excitation of helium to the  $3^1P$ ,  $4^1P$ , and  $5^1P$  states, Moustafa and de Heer<sup>12</sup> find that deviations from the straight line become important somewhere between 50 and 100 eV, in contrast with the 500 eV for ionization. This difference in behavior may be explained by the following:

(i) Interference will be most important when the velocities of the two outgoing electrons are comparable ( $E \approx \frac{1}{2}T$ ), and will become less and less important as  $E$  becomes smaller. Thus interference will give a more substantial reduction of the cross sections for ionization than for excitation.

(ii) For excitation, we distinguish between  $n^1S$ ,  $n^1P$ ,  $n^1D$ , and other states. For ionization we always take the sum, since we do not distinguish under usual experimental conditions between transitions with  $\Delta l = 0, 1, 2$ , and higher, where  $l$  is the azimuthal quantum number. Therefore, we should not compare the ionization cross sections with the cross sections for excitation to  $n^1P$  states, but with the sum of the cross sections for the excitation to  $n^1S$ ,  $n^1P$ ,  $n^1D$ , and following states. From the behavior of the  $\sigma_E T/R$  for dipole-forbidden

transitions (see Secs. 3B, 4B, and 5) it follows that in the plot of  $\sigma_E T/R$  against  $\ln T/R$ , deviations from the straight line start to become important at higher  $E_{e1}$  for  $\sigma_E(1^1S \rightarrow n^1S + n^1P + n^1D + \dots)$  than for  $\sigma_E(1^1S \rightarrow n^1P)$ .

(iii) The third term of Eq. (10) did not give a contribution to a term of the order  $R/T$  in  $\phi(E, T)$ , the first term gives  $E/2T + O(R^2/T^2)$ . For excitation of the  $2^1P$  and  $3^1P$  states in helium, we have found that  $f(K)$  decreases so rapidly when  $K$  becomes larger than zero, that the sum of the first two terms of  $\phi(E, T)$  is negative. For ionization,  $f(K)$  in general has a maximum for  $K > 0$ , and for large  $E$ ,  $f(K)$  has a maximum for  $(Ka_0)^2 \approx E/R$ . This behavior of  $f(K)$  for different  $E$  has been explained by Inokuti and Platzman.<sup>23</sup> The second term of Eq. (10) will thus become positive for larger  $E$  and will give an additional reduction of the (ionization) cross sections.

(iv) The energy transfers involved in ionization are substantially larger than the energy transfers needed for excitation of bound states. We may expect therefore that the Bethe-Born approximation breaks down at higher  $E_{e1}$  for ionization than for excitation.

## 7. POLES OF $f(K)$ FOR IONIZATION

In Sec. 2 we confined ourselves, just as Lassette<sup>2</sup> did before, to the excitation of bound states. We will now also consider ionization by electrons or protons.

For the excitation of bound states,  $E_f < 0$ , and  $\alpha_f = (-E_f/R)^{1/2}$  is real and positive. For ionization we have a different situation, since  $E_f > 0$ . However, it is still true that the position of the singularities (poles) of  $f(K)$  only depends on the behavior of  $\psi_i$  and  $\psi_f$  for very large  $r$ . This follows, just as for excitation to bound states,<sup>2</sup> from the structure of the matrix elements  $(\psi_f | \exp(i\mathbf{K} \cdot \mathbf{r}_s) | \psi_i)$  in Eq. (1). The integration over coordinate space may be divided into two parts, the first over the interior of a sphere with radius  $R_{sp}$ , with  $R_{sp}$  much larger than the atomic dimensions, and the second over the exterior of the sphere. The first part can never lead to poles for finite values of  $K$ , since we are integrating bounded functions over a finite region of coordinate space. Since the behavior of  $\psi_i$  and  $\psi_f$  for very large  $r$  is hydrogen-like and similar for all atoms, it will again (see Sec. 2) be sufficient<sup>24</sup> to study the behavior of  $f(K)$  for ionization of atomic hydrogen. For the generalized oscillator density associated with transitions to continuum states we now use the notation  $df(K)/d(E/R)$  instead of  $f(K)$ .

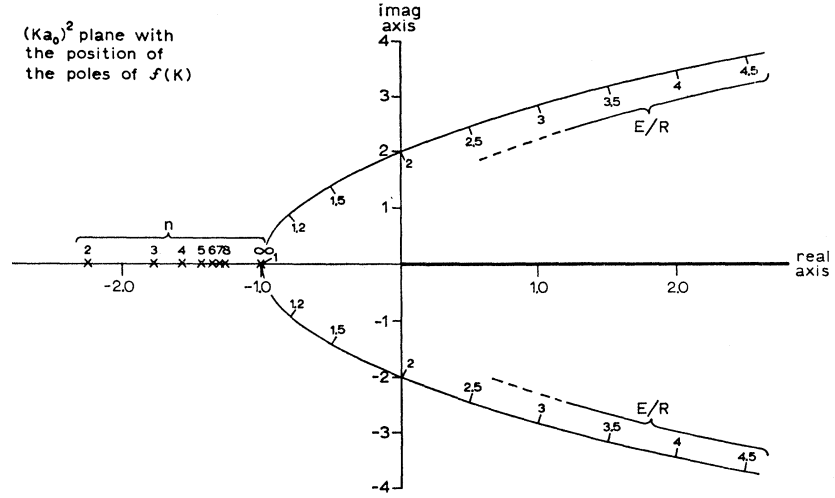
If we take the  $df(K)/d(E/R)$  calculated by Bethe<sup>1</sup>

<sup>23</sup> M. Inokuti and R. L. Platzman, *Abstracts of Papers, IVth International Conference on the Physics of Electronic and Atomic Collisions, Quebec, 1965* (Science Bookcrafters, Inc., New York, 1965), p. 408.

<sup>24</sup> We note that the behavior of the  $f(K)$  for ionization of complex atoms may for special energies become a little complicated because of things like auto-ionization. For instance (see below), for an auto-ionizing level between a lower ionization threshold indicated by suffix 1 and a higher-ionization threshold indicated by suffix 2,  $f(K)$  has poles for  $Ka_0 = \pm i(\alpha_{i1} \pm \alpha_{f1})$  and for  $Ka_0 = \pm i(\alpha_{i2} + \alpha_{f2})$ .

<sup>22</sup> B. L. Schram, F. J. de Heer, M. J. Van der Wiel, and J. Kistemaker, *Physica* **31**, 94 (1965); B. L. Schram, H. R. Moustafa, J. Schutten, and F. J. de Heer, *ibid.* **32**, 734 (1966); B. L. Schram, *ibid.* **32**, 197 (1966).

FIG. 2. Position of the poles of  $f(K)$  and  $df(K)/d(E/R)$  in the complex  $(Ka_0)^2$  plane for excitation and ionization of atomic hydrogen from the ground state. The only physically attainable values of  $(Ka_0)^2$  are real and positive. The  $n$  correspond to the principal quantum number of the excited states and the  $E/R$  to the (continuum) excitation energies.



for the ionization of atomic hydrogen from the ground state, and the  $df(K)/d(E/R)$  calculated by Burhop,<sup>25</sup> Mandl,<sup>26</sup> Walske,<sup>3</sup> and Khandelwal and Merzbacher<sup>27</sup>

for ionization of atomic hydrogen from the  $n=2$  and  $n=3$  states, it follows that in all these cases we may write

$$\frac{df(K)}{d(E/R)} = \{[(Ka_0)^2 + (\alpha_i + \alpha_f)^2][(Ka_0)^2 + (\alpha_i - \alpha_f)^2]\}^{-\nu} \xi(K, E) \quad (33)$$

with integer  $\nu \geq 3$  and with

$$\xi(K, E) = \frac{\exp[-(2/|\alpha_f|) \arctan(2\alpha_i |\alpha_f| / \{(Ka_0)^2 + \alpha_f^2 + \alpha_i^2\})]}{1 - \exp(-2\pi/|\alpha_f|)} \gamma(K, E), \quad (34)$$

where the  $\gamma(K, E)$  are simple analytic functions of  $K$  and  $E$  without any singularities for finite values of  $K$ .

From Eq. (33) it follows that  $df(K)/d(E/R)$  has poles for  $Ka_0 = \pm i(\alpha_i \pm \alpha_f)$  instead of  $\pm i(\alpha_i + \alpha_f)$ , as was found for excitation to bound states. The position of the poles of  $f(K)$  and  $df(K)/d(E/R)$  for excitation and ionization of atomic hydrogen from the ground state is illustrated in Fig. 2. Similar figures can now be made for other initial states and for other atoms provided that the energy-eigenvalues are known from theory or experiment. Equation (33) gives us valuable information about the nature of  $df(K)/d(E/R)$  for complex atoms. When the ionization energy is  $I$ , the relations between the energy eigenvalues  $E_i$  and  $E_f$ , the excitation energy  $E$ , and  $I$  are:  $I = -E_i$  and  $E = I + E_f$ . For practical applications (not given here), Eq. (33) may more conveniently be rewritten as

$$\frac{df(K)}{d(E/R)} = \left\{ \left[ \frac{E}{R} - (Ka_0)^2 \right]^2 + 4 \left( \frac{I}{R} \right) (Ka_0)^2 \right\}^{-\nu} \xi(K, E). \quad (35)$$

## 8. DISCUSSION AND CONCLUSIONS

The basic subjects of this paper are (i) the nature and position of the poles of the functions  $f(K)$  and  $df(K)/d(E/R)$ , (ii) the power-series representations of  $f(K)$ , (iii) the expansion of  $\sigma_E$  in powers of  $R/T$ , and (iv) the derivation and application of the Ochkur approximation.

Power-series representations of  $f(K)$  such as given in Sec. 2 are of great practical importance since, when a transition  $f(K)$  is known for only a few  $K$  values, reasonable estimates of  $f(K)$  can be made for other  $K$  values and analytical expressions can be given for  $\sigma_E$ . Thus experimental differential and total cross sections can be correlated with each other in a simple way. Apart from the theoretical justification of the power-series expansions given by Lassetre,<sup>2</sup> some sort of justification is also given by the following:

In Secs. 3 and 5 we calculated  $\ln c_B$  and  $\sigma_E$  values for the transitions  $1^1S \rightarrow 2^1P$  and  $1^1S \rightarrow 3^1P$  in helium, using the analytical  $f(K)$  obtained in Sec. 2. Suppose we use the "zeroth-order" approximation of our method; i.e., for the transition  $1^1S \rightarrow 2^1P$  we take  $c_1 = 0$  instead of  $c_1 = 0.86$ , just as for the transition  $1s \rightarrow 2p$  in hydrogen; and for the transition  $1^1S \rightarrow 3^1P$  we take  $c_1 = c_2 = 4$  (instead of  $c_1 = 1.5$  and  $c_2 = 20$ ), just as for the transition  $1s \rightarrow 3p$  in hydrogen. Then the resulting differences in

<sup>25</sup> E. H. S. Burhop, Proc. Cambridge Phil. Soc. **36**, 43 (1940).

<sup>26</sup> F. Mandl, Report, Harwell, England, 1952 (unpublished).

<sup>27</sup> G. S. Khandelwal and E. Merzbacher, Phys. Rev. **151**, 12 (1966).



$\ln\sigma_E$  are 7.9% ( $1^1S \rightarrow 2^1P$ ) and 2.25% ( $1^1S \rightarrow 3^1P$ ), and the differences in the  $\sigma_E$  obtained are very small. This is illustrated in the table; if we add the values of the columns "ZOC" to the cross sections calculated with Eqs. (13) and (14), we get the "zeroth-order" cross sections. Further, in Sec. 2B we found already that Lassette's analytical  $f(K)$  for the transition  $1^1S \rightarrow 2^1S$  in helium did have the same "shape" as the function  $f(K)$  for the transition  $1s \rightarrow 2s$  in hydrogen. These results lead to the tentative conclusion that knowledge of the optical oscillator strength for a dipole-allowed transition and of the "quadrupole" matrix element for a dipole-forbidden transition in helium is sufficient for a quite accurate determination of the  $\sigma_E$  for large  $E_{e1}$ . Further research along these lines for other transitions (also to the continuum, see Sec. 7) and for other atoms would be of interest. The results of this paper also suggest that in choosing trial wave functions for complex atoms, it is quite important to give these trial wave functions the correct asymptotic behavior, since only in this way is a correct position of the poles of  $f(K)$  found. Research on this subject would also be of interest.

Expansions of  $\sigma_E$  (direct and interference) in powers of  $R/T$  such as given in Secs. 3, 4, and 5 are of importance when studying deviations from the asymptotic cross-section formulas. By considering the term of order  $(R/T)^2$  in  $\sigma_E$  for dipole-forbidden and dipole-allowed transitions in helium, we found a qualitative interpretation of the variation of experimental  $\sigma_E T/R$  with  $T$  for incident electrons and protons. One should clearly be aware, however, that expansions of  $\sigma_E$  in powers of  $R/T$  are only of value for sufficiently large  $T$ , for instance  $T/R > 10$ . For smaller  $T$ , too many terms have to be included in the expansions, and what is more important, the Bethe-Born and Ochkur approximations are no longer applicable for small  $T$ . Therefore, from expansions of  $\sigma_E$  in powers of  $R/T$  we can obtain information about the variation of  $\sigma_E$  with  $T$  for  $T/R > 10$ , but not for  $T/R < 10$ . Even for  $T/R > 10$  we cannot exclude the possibility that in some special cases the coefficient of the term of the order  $(R/T)^3$  in  $\sigma_E$  is much larger than the coefficient of the term of the order  $(R/T)^2$  in  $\sigma_E$ . Since for incident electrons only the first-order exchange and interference terms can properly be given, we cannot exactly derive the coefficient of the term of the order

$(R/T)^3$  in  $\sigma_E$ . For incident protons, more terms of the expansion may be given, as has been done, for instance, in the theory of stopping power.<sup>3</sup> We may further expect that the Ochkur approximation for incident electrons breaks down at higher  $T/R$  than the Bethe-Born approximation for incident protons. This may be made plausible by the fact that for given  $T$ ,  $E$ , and  $K$ , the distortion of the incident wave is much larger for incident electrons than for incident protons. Distortion can thus also be partly responsible for the difference in behavior of the  $\sigma_E$  for incident electrons and protons. Charge transfer and polarization may give further small differences.

That the Ochkur approximation can be obtained in this simple way from the Bethe and Mott formulas is interesting in that it gives us the simple pictorial representation of the collision process:  $\sigma_{E,K}$  is the cross section  $\sigma_K$ , for transfer of momentum  $K$  from the fast incident to one atomic electron, times the probability that such a momentum transfer leads to a certain final state (see also Fano, Ref. 3, p. 8).

*Note added in proof.* After the work described in this paper was finished, it was brought to the author's attention that the approximate relationship between exchange and direct scattering amplitudes derived by Ochkur<sup>17</sup> and usually referred to as "Ochkur approximation," was actually (except for some minor details) already found before by Bonham<sup>28</sup> [see Eqs. (1.18), (2.11), and (2.16) of Ref. 28].

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<sup>28</sup> R. A. Bonham, J. Chem. Phys. **36**, 3260 (1962).