

## Electron Capture from Atomic Hydrogen by Protons

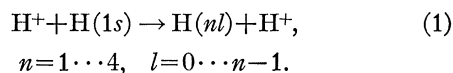
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In a paper by Bates and Dalgarno the BK (Brinkman-Kramers) cross sections together with the ground-state cross section of Jackson and Schiff were used to estimate the Born cross sections for capture into excited states of the hydrogen atom. In the present paper the Born cross sections are calculated numerically for capture into seven different final states. These results show that the estimates of Bates and Dalgarno are very good. In addition, the Born and BK cross sections for capture from  $\text{He}(1s^2)$  are compared with the corresponding quantities for capture from atomic hydrogen. The similarity of certain cross-section ratios for these two atoms suggests the possible use of these ratios to estimate the Born capture cross sections for other atoms from the BK cross sections for the corresponding atoms.

THE cross sections for the following processes have been calculated in the BK approximation by Bates and Dalgarno.<sup>1</sup>



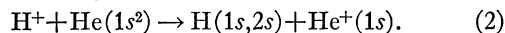
With these results and the Born cross section for capture into the  $1s$  state, they calculated the approximate Born cross sections for capture into excited states with the aid of one assumption; viz., they assumed the following equality of the cross-section ratios.

$$Q_B(nl)/Q_B(1s) = Q_{BK}(nl)/Q_{BK}(1s).$$

(The subscripts B and BK denote the Born and Brinkman-Kramers cross sections, respectively.) This assumption is supported by the calculations of Jackson and Schiff<sup>2</sup> who discuss the similarity of these ratios for  $nl=2s, 2p$ . In order to test this postulated equality of the ratios for a larger group of final states, the author has calculated the Born and BK cross sections to an accuracy of three significant figures for the following values of  $nl$ :

$$nl = 1s, 2s, 2p, 3s, 3p, 4s, 5s.$$

Another motivation for this calculation was to learn whether these cross-section ratios differed significantly from the corresponding ratios for electron capture from other atoms. In this connection, the Born cross sections are available for the helium capture problem,<sup>3</sup> and these cross sections have been supplemented<sup>4</sup> with the BK cross sections for the two processes of Eq. (2).



(Since the BK formulas listed by Bransden *et al.*<sup>4</sup> are approximations, these results were evaluated independently by the author.) A presentation of the numerical results is deferred until after a discussion of the

extension of the method of BD to more complicated atomic systems.

As was mentioned in I, the Born cross section may fail to converge to the correct cross section at high energies as well as at low energies, but it may provide a good estimate to the cross section over an intermediate energy range. Indeed, the results of I show that, for the case of helium, the agreement is quite good in the laboratory energy range from 40 keV to 1 MeV, the intermediate energy range. If, as suggested in I, the Born method is assumed to provide a good estimate to the capture cross section in this energy range, then a knowledge of the ratios

$$R_1(A) = Q_B(1s)/Q_{BK}(1s)$$

for several target atoms  $A$  can have practical value. (It is assumed that capture into the  $1s$  state of hydrogen dominates capture into all other states, and this is indeed the case for atomic hydrogen and helium). Whether or not the ratio  $R_1$  is of use depends upon its sensitivity to a change of target atom. If this variation is small, then the known ratio for one target atom could be used with some confidence to obtain an estimate of the Born cross section for another target atom. One simply calculates the BK cross section, and multiplies this result by the ratio  $R_1$  which has been calculated for a simpler atomic system at the same impact energy. These quantities are correlated at the same impact energy, the laboratory energy of the incident proton, since for a target atom initially at rest, this is the energy for which the velocity of relative translation is nearly the same for the separated aggregates of each system. At the present time,  $R_1$  is available only for atomic hydrogen and helium, and these ratios do not differ a great deal, as will be seen in the following paragraph. However, it is very speculative to predict how well these ratios would transform the BK cross sections into the Born cross sections for a system such as atomic oxygen. Nevertheless, when the enormous numerical task of computing Born cross sections for the above atomic system is considered—a distorted wave calculation would be more difficult<sup>5</sup>—such a crude estimation procedure becomes tolerable and, it is hoped, useful.

<sup>5</sup> R. H. Bassel and E. Gerjuoy, Phys. Rev. **117**, 749 (1960).

<sup>1</sup> D. R. Bates and A. Dalgarno, Proc. Phys. Soc. (London) **A66**, 972 (1953). This paper is denoted by BD.

<sup>2</sup> J. D. Jackson and H. Schiff, Phys. Rev. **89**, 359 (1953). This paper is denoted by JS.

<sup>3</sup> Robert A. Mapleton, Phys. Rev. **122**, 528 (1961). This paper is denoted by I.

<sup>4</sup> B. H. Bransden, A. Dalgarno, and N. M. King, Proc. Phys. Soc. (London) **A67**, 1075 (1954).

TABLE I. Cross sections and cross-section ratios.  $Q(nl)$  = cross section in units of  $\pi a_0^2 = 8.79 \times 10^{-17}$  cm<sup>2</sup> for capture into the state  $nl$ .  $E$  = center-of-mass energy in units of kev. (See text for explanation of other symbols.)

$nl \backslash E$		31.62	56.23	100	177.8	316.2	562.3	800	1000
1s	B	$2.84 \times 10^{-1}$	$5.00 \times 10^{-2}$	$6.01 \times 10^{-3}$	$5.04 \times 10^{-4}$	$3.15 \times 10^{-5}$	$1.58 \times 10^{-6}$		$6.77 \times 10^{-8}$
	BK	1.75	$2.63 \times 10^{-1}$	$2.64 \times 10^{-2}$	$1.84 \times 10^{-3}$	$9.62 \times 10^{-5}$	$4.14 \times 10^{-6}$		$1.57 \times 10^{-7}$
2s	B	$4.42 \times 10^{-2}$	$7.94 \times 10^{-3}$	$9.27 \times 10^{-4}$	$7.38 \times 10^{-5}$	$4.38 \times 10^{-6}$	$2.11 \times 10^{-7}$		$8.86 \times 10^{-9}$
	BK	$3.04 \times 10^{-1}$	$4.68 \times 10^{-2}$	$4.42 \times 10^{-3}$	$2.83 \times 10^{-4}$	$1.38 \times 10^{-5}$	$5.62 \times 10^{-7}$		$2.06 \times 10^{-8}$
2p	B	$5.03 \times 10^{-2}$	$5.93 \times 10^{-3}$	$4.08 \times 10^{-4}$	$1.83 \times 10^{-5}$	$6.02 \times 10^{-7}$	$1.60 \times 10^{-8}$		$3.72 \times 10^{-10}$
	BK	$3.45 \times 10^{-1}$	$3.28 \times 10^{-2}$	$1.80 \times 10^{-3}$	$6.58 \times 10^{-5}$	$1.81 \times 10^{-6}$	$4.16 \times 10^{-8}$		$8.59 \times 10^{-10}$
3s	B	$1.37 \times 10^{-2}$	$2.47 \times 10^{-3}$	$2.86 \times 10^{-4}$	$2.26 \times 10^{-5}$	$1.32 \times 10^{-6}$	$6.33 \times 10^{-8}$		$2.63 \times 10^{-9}$
	BK	$9.50 \times 10^{-2}$	$1.48 \times 10^{-2}$	$1.38 \times 10^{-3}$	$8.72 \times 10^{-5}$	$4.19 \times 10^{-6}$	$1.69 \times 10^{-7}$		$6.16 \times 10^{-9}$
3p	B	$1.67 \times 10^{-2}$	$2.07 \times 10^{-3}$	$1.45 \times 10^{-4}$	$6.52 \times 10^{-6}$	$2.14 \times 10^{-7}$	$5.68 \times 10^{-9}$		$1.31 \times 10^{-10}$
	BK	$1.20 \times 10^{-1}$	$1.19 \times 10^{-2}$	$6.57 \times 10^{-4}$	$2.38 \times 10^{-5}$	$6.48 \times 10^{-7}$	$1.48 \times 10^{-8}$		$3.09 \times 10^{-10}$
4s	B	$5.87 \times 10^{-3}$	$1.06 \times 10^{-3}$	$1.23 \times 10^{-4}$	$9.63 \times 10^{-6}$	$5.62 \times 10^{-7}$	$2.68 \times 10^{-8}$		$1.11 \times 10^{-9}$
	BK	$4.08 \times 10^{-2}$	$6.39 \times 10^{-3}$	$5.95 \times 10^{-4}$	$3.73 \times 10^{-5}$	$1.78 \times 10^{-6}$	$7.18 \times 10^{-8}$		$2.61 \times 10^{-9}$
5s	B	$3.03 \times 10^{-3}$	$5.46 \times 10^{-4}$	$6.32 \times 10^{-5}$	$4.95 \times 10^{-6}$	$2.89 \times 10^{-7}$	$1.38 \times 10^{-8}$		$5.71 \times 10^{-10}$
	BK	$2.11 \times 10^{-2}$	$3.30 \times 10^{-3}$	$3.07 \times 10^{-4}$	$1.92 \times 10^{-5}$	$9.16 \times 10^{-7}$	$3.68 \times 10^{-8}$		$1.34 \times 10^{-9}$
1s <sup>a</sup>	BK	8.04	2.74	$6.51 \times 10^{-1}$	$1.03 \times 10^{-1}$	$1.07 \times 10^{-2}$	$7.69 \times 10^{-4}$	$1.32 \times 10^{-4}$	
2s <sup>a</sup>	BK	$9.70 \times 10^{-1}$	$4.16 \times 10^{-1}$	$1.08 \times 10^{-1}$	$1.68 \times 10^{-1}$	$1.66 \times 10^{-3}$	$1.12 \times 10^{-4}$	$1.85 \times 10^{-5}$	
R <sub>1</sub>	H	0.162	0.190	0.228	0.274	0.327	0.382		0.431
	He	0.190	0.199	0.217	0.244	0.275	0.302	0.315	
R <sub>2</sub>	H	0.156	0.159	0.154	0.146	0.139	0.134		0.131
	He	0.086	0.107	0.125	0.134	0.137	0.135	0.133	
R <sub>3</sub>	H	0.174	0.178	0.167	0.154	0.143	0.136		0.131
	He	0.121	0.152	0.166	0.163	0.155	0.146	0.140	

<sup>a</sup> See Eq. (2) of text.

The numerical results are tabulated as a function of the center-of-mass energy in Table I. [ $E$  = tabulated energy,  $E'$  = impact energy,  $E'(H) = 2E$ ,  $E'(He) = 1.25E$ .] For  $s$ -state capture from atomic hydrogen, the  $n^{-3}$  law of JS is obeyed very well over the entire energy range. In addition, the two ratios

$$R_2(H) = Q_B(2s)/Q_B(1s), \quad R_3(H) = Q_{BK}(2s)/Q_{BK}(1s)$$

agree rather well, the disagreement becoming negligible as the energy increases. These results show that the estimates of BD are excellent except at very low impact energies. Also included in the table are the BK cross sections for the processes of Eq. (2). The agreement between the two most important ratios,  $R_1(H)$  and  $R_1(He)$ , is not as good as desired; however, either one can be used to obtain a fair estimate of the Born cross section,  $Q_B(1s)$ , for the other atom at the same impact energy. In the Appendix, the high-energy limit of  $R_1(He)$  is calculated with the same helium wave function that is used in I. This limit is 0.535, in contrast to the corresponding value of 0.661 for atomic hydrogen as given in JS. It is not known how sensitive  $R_1(He)$  is to the choice of the helium wave function; in this connection the author is currently calculating the prior, post, and BK ground-state cross sections using the six-parameter wave function of Hylleras. The results of this investigation will be reported in future work.

In order to show other similarities between the two capture problems, the ratios

$$R_2(He) = Q_B(2s)/Q_B(1s), \quad R_3(He) = Q_{BK}(2s)/Q_{BK}(1s)$$

are also included in the table. The two ratios  $R_3(A)$  agree more closely, for the same impact energies, than the ratios  $R_2(A)$ . This is not surprising, since the BK cross sections are very similar to one another in their energy dependence, whereas the Born cross sections can be expressed in terms of the corresponding BK quantity by multiplication with an energy-dependent factor which depends upon the target atom and the final  $s$  state of the hydrogen atom. (Only capture into  $s$  states is being considered.) Since these factors approach constants at high energies, this description of the cross-section energy dependence, and hence, of the ratios,  $R_2$  and  $R_3$ , is in clear accord with the numerical results of the table. [One example of an energy-dependent factor is found in Eq. (17) of JS.] The foregoing explanation likewise applies to the approximate  $n^{-3}$  law which is satisfied by the hydrogen and helium capture problems.

It is this host of similarities among the ratios for these two atoms that suggests the possible use of these ratios to estimate the Born cross section for capture from an atom such as oxygen, a capture process of considerable interest in certain areas of upper atmospheric research.

## APPENDIX

The calculation of the high-energy limit (non-relativistic) of the ratio,  $R_1(\text{He})$ , is presented in this appendix. The point of departure of the calculation is the prior Born amplitude given by Eq. (1a) of I, which is written for convenient reference.

$$g = \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 V_i \exp[-\alpha x_1 - x_2 - Zx_3 + i(\mathbf{A}_1 \cdot \mathbf{x}_1 + \mathbf{A}_2 \cdot \mathbf{x}_2 - \mathbf{A}_3 \cdot \mathbf{x}_3)],$$

$$V_i = 2|\mathbf{x}_2 - \mathbf{x}_3|^{-1} - |\mathbf{x}_1 - (\mathbf{x}_2 - \mathbf{x}_3)|^{-1} - |\mathbf{x}_2|^{-1},$$

$$Z = 1.6875, \quad \alpha = 2 + Z.$$

The common factor is omitted, and other common factors which will emerge during the course of the calculation likewise will be omitted, since they are not needed. The quantity  $\mathbf{A}_1$  is set equal to zero, for reasons given in I, and the integration over  $\mathbf{x}_1$  is performed, all of which reduces  $g$  to<sup>4</sup>

$$g = \int d\mathbf{x}_2 d\mathbf{x}_3 (|\mathbf{x}_2 - \mathbf{x}_3|^{-1} + [|\mathbf{x}_2 - \mathbf{x}_3|^{-1} + \frac{1}{2}\alpha] \times \exp[-\alpha|\mathbf{x}_2 - \mathbf{x}_3|] - |\mathbf{x}_2|^{-1}) \times \exp[-x_2 - Zx_3 + i(\mathbf{A}_2 \cdot \mathbf{x}_2 - \mathbf{A}_3 \cdot \mathbf{x}_3)].$$

The remaining integrations can be effected using standard methods,<sup>5</sup> so with the omission of these details, the amplitude may be represented by

$$g = V_1 + V_2 - V_{p2},$$

$$V_1 = \int_0^1 dx x(1-x) \left( \frac{\partial}{\partial U} + \frac{\partial}{\partial V} \right)^2 U^{-1} V^{-\frac{1}{2}},$$

$$V_2 = \left[ 1 - \frac{\alpha}{2} \frac{\partial}{\partial \alpha} \right] \int_0^1 dx x(1-x) \left( \frac{\partial}{\partial U} + \frac{\partial}{\partial V} \right) \times [(\alpha^2 + U)V^{-\frac{1}{2}} - 2\alpha][(\alpha^2 - U)^2 + 4\alpha^2 Q^2]^{-1},$$

$$V_{p2} = (Z^2 + A_3^2)^{-2} (1 + A_2^2)^{-1},$$

$$U = (1 + A_2^2)(1 - x) + (Z^2 + A_3^2)x, \quad R = |\mathbf{A}_2 - \mathbf{A}_3|^2,$$

$$V = 1 + (Z^2 - 1)x + x(1 - x)R, \quad Q^2 = |(1 - x)\mathbf{A}_2 + x\mathbf{A}_3|^2.$$

The matrix element  $V_{p2}$  is proportional to the BK amplitude. In the high-energy limit, the preceding expression simplifies immensely. Attention is first directed to the evaluation of  $V_1$ . [In the subsequent calculations, the same symbol  $V_1$  ( $V_2$ ) will be used to represent the dominant part of  $V_1$  ( $V_2$ ).] If terms of the order of the ratio of the electron mass to the proton mass are neglected, then the following relations are valid at high energies.

$$A_3^2 = A_2^2 - \epsilon, \quad \mathbf{A}_2 \cdot \mathbf{A}_3 = A_2^2 - \epsilon/2, \\ Q^2 = A_2^2 - x\epsilon, \quad R = 4E, \quad A_2^2(m) = E.$$

In these relations,  $\epsilon$  denotes the change in internal energy, and  $A_2^2(m)$  represents the minimum value of  $A_2^2$ . The energy parameter  $E$  is the impact energy expressed in units of 100 kev. The angular dependence of  $R$  is omitted for the same reasons that are given by JS in the derivation of their Eq. (17). With this information, it can be shown that the dominant part of  $V_1$  originates from the term

$$V_1 = - \int_0^1 dx x(1-x) U^{-1} V^{-\frac{1}{2}},$$

and after integration of this expression and considerable simplification of the result, the leading terms of  $V_1$  can be shown to be given by

$$V_1 = \frac{1}{[4+R]^2} \left[ \frac{1}{1+A_2^2} + \frac{1}{Z(Z^2+A_3^2)} \right].$$

Although the integration was performed exactly in the derivation of this result, essentially the same result can be obtained by neglecting the  $x$  dependence in  $U$ . The effect of this approximation is to replace  $(Z^2 + A_3^2)$  by  $(1 + A_2^2)$  in the preceding result, and this is unimportant in the high-energy limit; moreover, this approximation greatly simplifies the calculation of  $V_2$  which is now sketched. In the expression that defines  $V_2$  the parametric differentiations are first performed; then the approximation for  $Q^2$  is used, and  $\alpha^2$  is neglected in comparison with  $U$ . With these tasks accomplished, it is not difficult to show that the dominant part of  $V_2$  originates from the term

$$V_2 = \frac{3}{4} \int_0^1 dx x(1-x) U^{-1} V^{-\frac{1}{2}},$$

and as before, one readily finds that the leading terms of  $V_2$  are given by

$$V_2 = \left( 1 + \frac{1}{Z} \right) \frac{1}{(1+A_2^2)(4+R)^2}.$$

Thus, apart from a factor, the expression written below represents the high-energy limit of  $g$ .

$$g = \frac{1}{(4+R)^2} \left[ \frac{1}{Z(Z^2+A_3^2)} + \frac{1}{(1+A_2^2)} + \left( 1 + \frac{1}{Z} \right) \frac{1}{(1+A_2^2)} \right] - \frac{1}{(1+A_2^2)(Z^2+A_3^2)^2}.$$

In order to obtain the cross section, the angular integration is replaced by integration over the momentum change variable  $A_2$  and the approximations

$$A_3^2 + Z^2 \approx 1 + A_2^2 \approx A_2^2, \quad 4 + R \approx R,$$

are used. It is now a simple task to obtain the following

high-energy relation between the two cross sections, in which relation  $K$  is an energy-independent factor.

$$Q_B(1s) = Q_{BK}(1s) [1 + 5/64(1 + 1/Z)^2 - 5/12(1 + 1/Z)] \\ = 0.535 Q_{BK}(1s), \quad Q_{BK} = KE^{-6}.$$

A final point of interest that emerges from this approximate calculation is the fact that the passive electron interaction  $V_{p1}$ , [see Eq. (1a) of I] does not contribute to the high-energy Born cross section. That is, the integration over  $\mathbf{x}_1$  provides a cancellation of one of the proton-nuclear terms,  $|\mathbf{x}_2 - \mathbf{x}_3|^{-1}$ ; however, the residual part of  $V_{p1}$ , the exponential term, supplies a high-energy term which replaces the original cancellation. This means that the effective interaction at high energies is

$$2|\mathbf{x}_2 - \mathbf{x}_3|^{-1} - |\mathbf{x}_2|^{-1}.$$

These mathematical details are consistent with the calculations of others.<sup>5</sup>

*Note added in proof.* This author is currently calculating BK cross sections for electron capture from O(<sup>3</sup>P) and N(<sup>4</sup>S) by protons. These results, together with the ratios of this paper, will be used to estimate the corresponding Born cross sections. This material will be included in a forthcoming publication.

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## Enhancement of Electron Density around Positive Point Charges in Metals and Lifetimes of Positrons

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By means of approximate self-consistent field calculations using a model of a finite metal with  $\sim 2000$  electrons, it is shown that over the range of densities appropriate to metals under normal conditions, the density at the position of a single positive charge varies by a factor of about 2, whereas the variation in the mean electron density ( $3/4\pi r_s^3$ ) is an order of magnitude greater. In a simple Hartree calculation of the type reported here, a bound state occurs when  $r_s > 4$  atomic units. Some brief remarks are made on the application of these results to the calculation of the lifetimes of positrons in various metals.

WE report in this note the results of some numerical calculations which we have carried out to estimate quantitatively the enhancement of the electron density around a single positive point charge in a metal. In earlier work we used both a finite metal model for finding electronic wave functions around a vacancy<sup>1</sup> and later we developed a density matrix approach based on low-order perturbation theory<sup>2</sup> which enabled us to pass to the limit of an infinite metal. Our earlier work<sup>1</sup> indicated that significant results could be obtained using as a model of a metal a finite spherical system containing 1734 particles in 867 doubly filled states and in such a model we have imposed approximate self-consistency in the Hartree sense when a single positive charge is placed at the origin. Mean interparticle spacings measured by  $r_s$  values<sup>3</sup> of 2, 2.66, 4, 5, and 6 have been considered and usually five or six iterations proved sufficient for achieving satisfactory self-consistency. In

each case we have taken the same number of particles and have obtained different  $r_s$  values by altering the size of the spherical system.

The main features of these results are then found to be as follows: First of all, as  $r_s$  is increased, we reach a point at which a bound state breaks off from the band. Our finite metal computations indicate that this is occurring when  $r_s > 4$ . The behavior of the electron density at the origin, denoted by  $\rho(0)$ , does not show any marked change due to the formation of a bound state, as may be seen from Table I below, which summarizes our results for a range of  $r_s$  values covering all metals under normal conditions.

It seemed useful to fit the numerical results given in the table by a simple analytical formula and we did this as follows. Two values of  $[\rho(0) - \rho_0]/\rho_0$  were obtained for each value of  $r_s$  corresponding to the upper and lower bounds of  $\rho(0)$  which differed by a few parts in a thousand. When polynomials with zero constant term were fitted to various groups of points, the quartic terms were found to be very small and random. It was found that a cubic could be constructed which lay within the bounds for each  $r_s$ . The formula which gave the best

<sup>1</sup> N. H. March and A. M. Murray, Proc. Roy. Soc. (London) **A256**, 400 (1960).

<sup>2</sup> N. H. March and A. M. Murray, Proc. Roy. Soc. (London) **A261**, 119 (1961).

<sup>3</sup> The mean electron density  $\rho_0 = 3/4\pi r_s^3$ . We use atomic units (au) throughout.