CROSS SECTIONS FOR EXCITATION OF THE 2^2S STATE
OF HYDROGEN BY ELECTRON IMPACT*

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Many attempts have been made to find simple approximations which yield accurate scattering cross sections for electron-atom collisions. The $1s$ - $2s$ transition in hydrogen is particularly interesting because it can be studied in the laboratory and because exact target wave functions are available for quantum mechanical calculations. We report several calculations of integral cross sections (Q) and differential cross sections (DCS) for this transition and compare them with each other, with other calculations, and with experiment.

The experimental numbers given in Table I are uncertain and were obtained by interpolation on large photographs of the published figures. The experimental data of Stebbings et al.¹ have been corrected, using the new value of the polarization² and using the cascade corrections of Morrison and Rudge.³ The cross sections of Hils et al.⁴ are given as they reported them (where they were corrected for cascade using semiempirical $1s$ - $3p$ cross sections). The LS-BTO data are from the experiments of

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Lichten and Schultz⁵ normalized to the correlation method calculations of Taylor and Burke at low energy.⁵

In perturbation theory the total scattering cross section can be expressed as the sum of the direct and exchange scattering cross sections and their interference. Since the interference term is generally important, the relative phase of the direct and exchange scattering amplitudes is important and deserves study. In the BO, BOMC, BBGM1, and E. I approximations the direct amplitude is calculated in Born approximation (B) and the exchange amplitude in Oppenheimer's approximation, in Oppenheimer's approximation without the core term,⁶ in the first order approximation of Bates,⁶ and in the first order exchange approximation,⁷ respectively. The exchange amplitudes often have the same sign in the BO and BBGM1 theories and opposite signs in the BO and BOMC theories. Figure 1 shows the effect of this on the DCS. The effect is less noticeable in the integral cross sections. There is no post-prior discrepancy in these theories or in the Born direct cross section.

In the O and BOR approximations the direct amplitude is calculated in the Born approximation and the exchange amplitude in the prior interaction forms of the Ochkur and Ochkur-Rudge approximations,^{8a, 6} respectively. The corresponding post interaction forms^{8b} are called OP and BORP. The post-prior discrepancy for the BOR and BORP approximations is removed if the ORB. I exchange amplitude⁶ is used with the Born direct amplitude (BORB. I approximation). The BOR, BORP, and BORB. I cross sections differ only in their interference term; of the three, the

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BORB. I predicts Q in best agreement with experiment (see Table I). They predict similar angular dependencies for the cross sections (see Figure 2). Rudge (R)^{8a} and Morrison and Rudge (MR)³ have used the Ochkur-Rudge exchange amplitude with different direct amplitudes. The BORB. I approximation is in better agreement with experiment for Q than are their calculations^{3, 8a} if we use the BTO normalization but not if we use the older experimental normalization (SFHB and HKK).

Vainshtein, Presnyakov and Sobelman (VPS)⁹ proposed a theory which accounts for the effect of electron-electron repulsion on the scattering wave function. Making several approximations, they derived a formula for the cross section which contains a real "effective charge". Cross sections in this approximation are included in Table I and Figure 1. The VPS theory leads to an Ochkur-like relation for exchange, i. e., the ratio of the exchange scattering amplitude to the direct one is independent of the structure of the target. We use this relation and the Born direct amplitude to predict an exchange amplitude which we call the transferred VPS amplitude (TVPS). We use this exchange amplitude with the Born direct amplitude to predict total cross sections (BTVPS approximation).

Surprisingly, considering the different derivations of the two theories, the O and BTVPS methods are very close approximations to each other for both Q and the DCS. Crothers and McCarroll (CM)¹⁰ proposed an alternative version of the VPS theory which requires less drastic simplifying approximations in the formulas but still uses a peaking approximation. Their theory, including a complex effective charge, gives a sharp peak in the $Q(E)$

curve near threshold and a broad secondary peak at higher energies. We note the qualitative similarity of this behavior to the $Q(E)$ curve in the OP approximation. The O, BORB. I, MR, VPS, BTVPS, and CM methods seem to predict Q in rough agreement with the various experimental results (see Table I) and may be useful simple theories.

Kang and Foland made a peaking approximation to evaluate the scattering amplitudes in the coulomb wave approximation.¹¹ This treatment gave an Ochkur-like relation for exchange. We use this relation with the B direct amplitude to obtain the "transferred" KF exchange amplitude (TKF) and the BTKF total scattering cross section. The TKF exchange DCS is more similar to the BO exchange DCS than are the other exchange cross sections which result from Ochkur-like relations (e. g., the O one). Since the BO exchange DCS is believed to have a more realistic shape for this transition than the O exchange DCS has,⁶ the TKF exchange DCS might also be more realistic than the O one. The BTKF cross sections are easier to calculate than BO cross sections and have a magnitude which agrees better with experiment than the BO does.

Table I also gives cross sections from the unitarized Born approximation (B. II),¹² from the simplified second Born approximation (B2),¹³ and from close coupling calculations (c. c.). Since only the first three partial waves have been calculated for the 1s-2s and 1s-2s-3s close coupling approximation including exchange,¹⁴ the cross sections from higher partial waves have been added from B. I calculations.¹² (B. I and B are two names for the same theory.)

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Figure Captions

Figure 1 Total DCS for 1s-2s excitation in H at $k^2 = 1.3 \text{ a}_0^{-2}$.

Figure 2 Total DCS for 1s-2s excitation in H at $k^2 = 1.3 \text{ a}_0^{-2}$.

The BORB. I is not shown because it is very similar to the BORP.

Table I. Integral total cross sections for 1s-2s transitions.

$(a_0k)^2$	Direct scattering only							Total scattering, including exchange and interference															"Experimental"						
	B ^a *	B.II ^b	MR ^c	B2 ^d	CM ^e	1s2s c.c. ^f	1s2s3s c.c. ^f	BO ^a *	BOMC ^a *	O ^a *	OP ^a *	BOR ^a *,†	BORP ^a *,†	BORB.I ^a *,†	R ^g †	MR ^c †	BBBGM1 ^a *	E1 ^h *	VPS ^a	BTVPs ^a *	BTKF ^a *	CM ^e	1s2s c.c. ⁱ	1s2s3s c.c. ⁱ	1s2s2p c.c. ^j	SFHB ⁱ	LS-BTO ⁱ	HKK ⁱ	
0.76	2.49 ⁻¹		1.12 ⁻¹					3.15	2.78	2.50 ⁻¹	1.41 ³	5.70 ⁻¹	2.95 ⁻¹	2.04 ⁻¹		1.28 ⁻¹	2.18		1.23 ⁻¹	2.50 ⁻¹	5.76 ⁻¹								
0.80	5.09 ⁻¹		2.38 ⁻¹		3.8 ⁻¹			5.77	5.33	5.17 ⁻¹	1.17 ²	1.12	6.00 ⁻¹	4.27 ⁻¹		2.73 ⁻¹	3.94		2.59 ⁻¹	5.20 ⁻¹	9.67 ⁻¹	5.1 ⁻¹					4.0 ⁻¹	5.7 ⁻¹	2.6 ⁻¹
1.00	7.80 ⁻¹	2.23 ⁻¹	4.21 ⁻¹		1.2 ⁻¹	1.62	1.37	5.18	5.63	7.85 ⁻¹	7.74	1.43	8.75 ⁻¹	6.91 ⁻¹	3.42 ⁻¹	4.65 ⁻¹	3.32	1.40	4.27 ⁻¹	7.96 ⁻¹	1.03	2.4 ⁻¹	1.04	8.11 ⁻¹	1.14	4.6 ⁻¹	7.5 ⁻¹	2.4 ⁻¹	
1.30	7.53 ⁻¹		4.68 ⁻¹		1.3 ⁻¹			2.55	3.07	7.18 ⁻¹	1.88	1.12	7.84 ⁻¹	6.73 ⁻¹		4.74 ⁻¹	1.57		4.28 ⁻¹	7.27 ⁻¹	8.21 ⁻¹	2.0 ⁻¹				3.3 ⁻¹	6.0 ⁻¹	1.7 ⁻¹	
1.44	7.16 ⁻¹	3.21 ⁻¹			1.4 ⁻¹	1.08	1.00	1.89	2.30	6.69 ⁻¹	1.29	9.87 ⁻¹	7.26 ⁻¹	6.38 ⁻¹			1.18		4.12 ⁻¹	6.76 ⁻¹	7.51 ⁻¹	2.0 ⁻¹	7.97 ⁻¹		8.28 ⁻¹	2.8 ⁻¹	5.5 ⁻¹	1.4 ⁻¹	
2.00	5.75 ⁻¹		4.21 ⁻¹		1.7 ⁻¹			8.09 ⁻¹	9.21 ⁻¹	5.15 ⁻¹	6.04 ⁻¹	6.59 ⁻¹	5.47 ⁻¹	5.09 ⁻¹		3.86 ⁻¹	5.88 ⁻¹		3.48 ⁻¹	5.19 ⁻¹	5.68 ⁻¹	1.9 ⁻¹				2.0 ⁻¹	4.6 ⁻¹	9.5 ⁻²	
2.25	5.25 ⁻¹	3.07 ⁻¹		2.56 ⁻¹	1.8 ⁻¹	6.75 ⁻¹	6.47 ⁻¹	6.39 ⁻¹	6.95 ⁻¹	4.68 ⁻¹	5.10 ⁻¹	5.74 ⁻¹	4.92 ⁻¹	4.65 ⁻¹	1.46 ⁻¹		4.99 ⁻¹	4.65 ⁻¹	3.25 ⁻¹	4.70 ⁻¹	5.13 ⁻¹	1.9 ⁻¹	5.28 ⁻¹	5.09 ⁻¹	5.04 ⁻¹	1.8 ⁻¹	4.3 ⁻¹	9.1 ⁻²	
4.00	3.20 ⁻¹	2.32 ⁻¹	2.73 ⁻¹		1.7 ⁻¹	3.68 ⁻¹	3.58 ⁻¹	3.01 ⁻¹	2.91 ⁻¹	2.89 ⁻¹	2.87 ⁻¹	3.12 ⁻¹	2.95 ⁻¹	2.90 ⁻¹	1.32 ⁻¹	2.48 ⁻¹	2.85 ⁻¹	2.84 ⁻¹	2.26 ⁻¹	2.90 ⁻¹	3.09 ⁻¹	1.7 ⁻¹			3.18 ⁻¹	1.8 ⁻¹		1.1 ⁻¹	
6.00	2.20 ⁻¹				1.4 ⁻¹			2.05 ⁻¹	2.00 ⁻¹	2.04 ⁻¹	2.02 ⁻¹	2.11 ⁻¹	2.06 ⁻¹	2.04 ⁻¹			2.01 ⁻¹		1.69 ⁻¹	2.04 ⁻¹	2.13 ⁻¹	1.4 ⁻¹				1.9 ⁻¹		9.6 ⁻²	
9.00	1.50 ⁻¹			1.39 ⁻¹	1.1 ⁻¹			1.41 ⁻¹	1.40 ⁻¹	1.41 ⁻¹	1.41 ⁻¹	1.44 ⁻¹	1.42 ⁻¹	1.42 ⁻¹	9.86 ⁻²		1.40 ⁻¹	1.40 ⁻¹	1.23 ⁻¹	1.41 ⁻¹	1.46 ⁻¹	1.1 ⁻¹				1.0 ⁻¹		8.8 ⁻²	
20.00	6.86 ⁻²		6.66 ⁻²		6.2 ⁻¹			6.67 ⁻²	6.66 ⁻²	6.68 ⁻²	6.68 ⁻²	6.70 ⁻²	6.69 ⁻²	6.69 ⁻²		6.47 ⁻²	6.66 ⁻²		6.20 ⁻²	6.68 ⁻²	6.75 ⁻²	6.2 ⁻¹				1.1 ⁻¹		8.6 ⁻²	

*Indicates the direct scattering is calculated in Born approximation (B).

†Indicates the exchange scattering is calculated in Ochkur-Rudge approximation (OR). ^aCalculated in present work. ^bRef. 12. ^cRef. 3. ^dRef. 13.^eRef. 10. ^fK. Smith, W. F. Miller, and A. J. P. Mumford, Proc. Phys. Soc., 76, 559 (1960). ^gRef. 8a. ^hRef. 7. ⁱSee text. ^jP. G. Burke, H. M. Schey, and K. Smith, Phys. Rev., 129, 1258 (1963).

The superscripts in the table indicate the power of ten by which the number is to be multiplied, if any.