Electron Capture from He$(1s^2)$ by Protons. II

ROBERT A. MAPLETON
Air Force Cambridge Research Laboratories, Laurence G. Hanscom Field, Bedford, Massachusetts
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The Born prior and post cross sections are calculated for the process, $H^+ + He(1s^2) \rightarrow H(1s) + He^+(1s)$, using the six-parameter helium wave function of Hylleras. The prior-post discrepancy (i.f.d.) is usually less than 1% in the energy range of this investigation, 40 keV to 1 MeV. Thus, the wave function is apparently adequate for this type of scattering calculation. These new cross sections are compared with the corresponding old cross sections calculated with the wave function, $\exp[-Z(x_1+x_2)]$, $(Z=1.6875)$; the new average cross sections, average of prior and post, are usually less than the old average values. The BK (Brinkman-Kramers) cross sections are also calculated. Although the new BK values are usually less than the old values, the new BK cross section at 10 MeV exceeds the old value by 47%.

IN a previous paper by this author, the calculations of the Born prior and post cross sections for electron capture from helium by protons were presented.[1] The simple helium wave function, $\exp[-Z(x_1+x_3)]$ $(Z=1.6875)$, was used in that calculation. The dominant process of I has been recalculated using the six-parameter helium wave function of Hylleras,[2] and the results of these calculations form the central topic of this paper. The process and the helium wave function are

$$H^+ + He(1s^2) \rightarrow H(1s) + He^+(1s);$$

$$\psi(\mathbf{x}_1,\mathbf{x}_3) = N[1+c_1|\mathbf{x}_1-\mathbf{x}_3| + c_2({}_1x-x_3)^2 + c_3(x_1+x_3) + c_4(x_1+x_3)^2 + c_5|\mathbf{x}_1-\mathbf{x}_3|^2] \times \exp[-Z(x_1+x_3)]; \quad (1)$$

$$Z=1.818,\quad c_1=0.353,\quad c_2=0.128,\quad c_3=-0.101,\quad c_4=0.033,\quad c_5=-0.032,\quad N=4.34198/\pi.$$

The BK (Brinkman-Kramers) cross sections have been calculated for this same process in order to determine the sensitivity of the ratio, $R=Q_B/Q_{BK}$, to the choice of the helium wave function.[3] The interaction terms given by Eq. (1a) of I are reproduced in Eq. (2) for convenient reference.

$$V_i = V_{pn} + V_{p1} + V_{p2} = 2|\mathbf{x}_3-\mathbf{x}_2|^{-1} - |\mathbf{x}_3-\mathbf{x}_2-\mathbf{x}_1|^{-1} - |\mathbf{x}_2|^{-1};$$
$$V_f = V_{pn} + V_{21} + V_{2n} + V_{p1} = 2|\mathbf{x}_3-\mathbf{x}_2|^{-1} + |\mathbf{x}_3-\mathbf{x}_1|^{-1} - 2|\mathbf{x}_3|^{-1} - |\mathbf{x}_3-\mathbf{x}_2-\mathbf{x}_1|^{-1}. \quad (2)$$

[With reference to Eq. (2), Born prior and post cross sections signify the cross sections obtained using the Born approximation with the interactions V_i and V_f, respectively, whereas the BK approximation refers to the cross sections obtained using the Born approximation with the interaction, V_{p2}.[4]] Although it would be desirable to recalculate all the processes of I with the improved helium wave function, such an extensive calculation does not appear necessary in order to obtain fairly reliable estimates of the total Born cross sections. Thus, as will be shown later, the ratios, R, are not very sensitive to the helium wave function used; therefore, it seems very unlikely that the cross-section ratios of the omitted processes of I to the dominant process of Eq. (1) would likewise be very sensitive to the helium wave function. Consequently, if this assumption is accepted, then the ratios of I together with the cross sections of this paper will provide a fairly accurate estimate of the total Born cross sections.

The reduction of the integrals which is treated in I and elsewhere[5] is mentioned only briefly here. In order to simplify the integral of the term, $c_1|\mathbf{x}_1-\mathbf{x}_3|V_{pn}$, the approximation, $\mathbf{A}_1=0$, is used; otherwise, a triple Feynman integral would have to be evaluated numerically.[5] The integral of the term, $c_1|\mathbf{x}_1-\mathbf{x}_3|V_{p1}$, reduces to a very long double integral.[5] Although the preceding approximation permits considerable simplification of this integral,[3] it was decided not to approximate this integral in the interest of achieving the best possible numerical accuracy. The results of the calculations, labeled II, are presented in Table I.

For convenient reference, some of the results of I and other results[3] are reproduced in the table. Attention is first directed to the new Born prior and post cross sections, Q(II). The i.f.d. (prior-post discrepancy[1]) seldom exceeds 1% and is usually less than this amount. These new cross sections are rather close to the old post cross sections, Q_f(I); moreover, as suggested in I, these new values tend to be less than the corresponding old values (especially the prior values) with a few exceptions. Not only is the i.f.d. of the cross section small, but the i.f.d. of the angular distribution—not shown—is likewise small. Only in the neighborhood of the angle where the amplitude changes sign does the i.f.d. become relatively large; this increase in magnitude could be caused by a loss in significant figures since the Feynman integrals are calculated only to an accuracy of five significant figures. However, the increase in the i.f.d. in

[1] R. A. Mapleton, Phys. Rev. **122**, 528 (1961). This reference is denoted by I.
[2] L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1935), p. 224; H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Academic Press Inc., New York, 1957), p. 151.
[3] R. A. Mapleton, Phys. Rev. **126**, 1477 (1962).
[4] D. R. Bates and R. McCarroll, Suppl. Phil. Mag. **11**, 39 (1962).
[5] R. A. Mapleton, Phys. Rev. **117**, 479 (1960).

TABLE I. Born cross sections, Q, in units of $\pi a_0^2 = 8.79\times10^{-17}$ cm^2 for capture into the state $He^+(1s)+H(1s)$. Q_{BK} are Brinkman-Kramers cross sections for the same process. I and II refer to old and new calculations, respectively; i = prior, f = post. E = incident energy of proton in keV—laboratory system.

	$E=$	39.53	70.29	125	222.3	300	395.3	600	702.9	1000	10 000
Q(I)	i	1.53	5.44×10^{-1}	1.41×10^{-1}	2.51×10^{-2}		2.94×10^{-3}		2.32×10^{-4}	4.16×10^{-5}	
	f	1.75	5.77×10^{-1}	1.34×10^{-1}	2.15×10^{-2}		2.41×10^{-3}		1.99×10^{-4}	3.86×10^{-5}	
Q(II)	i	1.72	5.73×10^{-1}	1.34×10^{-1}	2.13×10^{-2}	7.03×10^{-3}	2.34×10^{-3}	3.90×10^{-4}	1.90×10^{-4}	3.64×10^{-5}	
	f	1.75	5.75×10^{-1}	1.34×10^{-1}	2.13×10^{-2}	7.09×10^{-3}	2.36×10^{-3}	3.94×10^{-4}	1.92×10^{-4}	3.64×10^{-5}	
Q_{BK}(I)		8.04	2.74	6.51×10^{-1}	1.03×10^{-1}	3.33×10^{-2}	1.07×10^{-2}	1.64×10^{-3}	7.69×10^{-4}	1.32×10^{-4}	3.07×10^{-10}
Q_{BK}(II)		8.81	2.82	6.16×10^{-1}	9.02×10^{-2}	2.86×10^{-2}	9.20×10^{-3}	1.46×10^{-3}	7.00×10^{-4}	1.28×10^{-4}	4.50×10^{-10}

this part of the angular distribution is not inconsistent with the results of the table since this angular region contributes very little to the integrated cross section. The contribution to the amplitude by the unphysical interaction, V_{pn}, still has the relatively long angular tail as reported previously.[1,6] From the description of these results, it appears safe to conclude that the six-parameter helium wave function is adequate for this type of scattering calculation, and apparently Q(II) represents the actual Born cross sections for the process of Eq. (1) very well. Although Q(II) is smaller than Q(I) over most of the energy range of Table I, this situation probably is reversed at higher energies. Evidence for this view is given by the behavior of Q_{BK} at 10 MeV. At this value of E, Q_{BK}(II) exceeds Q_{BK}(I) by 47%, and thus it appears that Q(II) likewise would exceed Q(I) for values of E somewhat larger than 1 MeV. This conjecture is consistent with the judgement that the old helium wave function underestimates the high momentum-space components of the correct wave function[7]; one fact is evident: the BK results show that the six-parameter wave function does have the larger spread in momentum space. Another interesting comparison of Q(I) and Q(II) deserves mention. As discussed in I, the average value of Q_e(I) (average of prior and post values) at 1 MeV is less than the measured cross section. Now Q(II) is less than Q(I) (average values) and using the assumption that the cross section ratio, $R_e = Q_e/Q(1s;1s)$ (see I), is insensitive to the two helium wave functions, one can obtain a reliable estimate of the new average total Born cross section, $Q_e(\mathrm{II}) = Q(\mathrm{II})R_e(\mathrm{I})$. It is evident that Q_e(II) is less than Q_e(I), and this fact suggests that the Born approximation not only underestimates the cross section at 1 MeV, but also, at energies in excess of this value. This speculated behavior of the Born cross section is not obvious since Q_e(II) very likely exceeds Q_e(I) for energies slightly above 1 MeV. However, current research strongly suggests that the Born approximation is incorrect at sufficiently high energies although it may give rather accurate cross sections in the intermediate energy range.[4]

The new ratios, $R(\mathrm{II}) = Q_B(\mathrm{II})/Q_{BK}(\mathrm{II})$, are slightly smaller than the old ratios, R(I).[3] However, neither set of ratios differs appreciably from the corresponding ratios calculated for atomic hydrogen in this intermediate energy range from 40 keV to 1 MeV.[3] These new ratios are used in the estimation of the Born cross sections for electron capture from atomic nitrogen and atomic oxygen by protons, which results are presented in another publication.[8]

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[6] R. H. Bassel and E. Gerjuoy, Phys. Rev. **117**, 749 (1960).

[7] D. R. Bates, *Atomic and Molecular Processes* (Academic Press Inc., New York, 1962), p. 578.

[8] R. A. Mapleton, preceding paper [Phys. Rev. **130**, 1829 (1963)].