Electron correlation and the cross sections for electron capture from He: The impulse approximation

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(Received 15 April 1976)

Electron-capture cross sections have been evaluated for high-velocity protons impinging on a ground-state helium target. The scattering matrix element was formulated within the quantum-mechanical impulse approximation and the resulting cross sections were examined as a function of various levels of sophistication for the description of the target atom. The helium wave functions used here were of a simple one-parameter (λ) variational form, a Hartree-Fock (HF) equivalent function and, finally, a configuration-interaction (CI) description. The projectile energy ranged from 25 keV to 3.5 MeV and, where possible, the cross sections were compared with experiment.

I. INTRODUCTION

We assess here the influence of electron correlation on the cross sections for the capture of an electron by a high-velocity proton in collision with a helium target atom when calculated, in this instance, by means of the impulse approximation. The quantum-mechanical impulse approximation[1-4] attempts to describe many-body scattering as a summation of two-body effects and, as is customary in the application of the method, contributions to the scattering matrix element T which arise from terms identifiable with multiple scattering effects are ignored. If the velocity of the projectile is large compared with that of the orbital electrons, then the "impulse hypothesis" can be invoked; this allows one to neglect terms in T which involve the binding potentials of the electrons within the target atom. The resulting expression for T has been shown to possess similarity with a second-order Born approximation.

The electron capture reaction

$$\text{H}^+ + \text{He}(1s^2) \rightarrow \text{H}(1s) + \text{He}^+(1s), \tag{1}$$
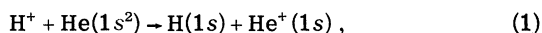
examined here, has also been studied in terms of the impulse approximation by Bransden and Cheshire.[5] For the spatial description of the ground state of He they used the simple one-parameter variational wave function $\Phi_\lambda(1, 2)$, with $\lambda = 1.6875$. The theoretical curve for the total cross section was found to lie below experiment and slowly diverged from it as the proton energy was increased, the latter feature being contrary to the expected behavior of the impulse approximation at high energies.

It was suggested[5,6] that these characteristics might arise from the use of the simple λ wave function and that an improved function with high momentum components should increase the theoretical cross sections at large energies. Hence

we have carried out calculations using the 35-term configuration-interaction (CI) wave function of Weiss[7] for He expressed in the form of a natural expansion.[8] The first term in the expansion represents a very close approximation to the Hartree-Fock (HF) wave function, and each additional natural configuration introduces electron correlation effects in the order of decreasing importance from an energy viewpoint. Thus following our previous cross-section studies[9] the 15 natural configurations which represent the total Weiss function were truncated to produce a renormalized wave function $\Phi_X(1, 2)$ containing only the first X configurations. Cross sections were evaluated for $X = 1(1)15$. For comparison, we have repeated the calculations of Bransden and Cheshire[5] and we have also extended their projectile energy range. Hence changes in the electron capture cross sections within the impulse approximation can be examined, firstly, as we approach the HF description of the target atom and, secondly, as we introduce correlation effects in a rational and systematic manner.

II. CALCULATIONS

The theory of the impulse approximation (IA) is well known (see McDowell and Coleman[10]); therefore we present only those equations which are essential for later discussion (Sec. III). Throughout this work we employ the notation of Bransden and Cheshire.[5] The capture cross section for reaction (1) is given in units of πa_0^2 by

$$Q_{if}(E) = \frac{1}{2\pi^2 c v_i^2} \left[\frac{\mu_f}{\mu_i} \right] \int_{\beta_{\min}^2}^{\beta_{\max}^2} |T_{if}|^2 \, d\beta^2, \tag{2}$$

where E is the energy of the high-velocity projectile, c is the mass ratio of a proton and a hydrogen atom, v_i is the relative velocity of the colliding systems with a reduced mass μ_i in the

initial state and μ_f in the final state and, here, T_{if} is the "post" form of the IA scattering matrix. The quantity β^2 is defined as the square of the change between the initial and final relative momenta and, since the total energy is conserved in the center-of-mass framework, we find that

$$\beta_{min} = (v_i^2 - \varepsilon)/2v_i \qquad (3)$$

and, in this calculation, β_{max} is effectively infinite. The energy defect ε equals $2[\epsilon(\mathrm{He}) - \epsilon(\mathrm{H}) - \epsilon(\mathrm{He}^+)]$, where $\epsilon(\mathrm{He})$, $\epsilon(\mathrm{H})$, and $\epsilon(\mathrm{He}^+)$ are the (negative) binding energies in atomic units[11] of the ground states of the He and H atoms and the He^+ ion.

Following closely the outline of the earlier analysis,[5] the evaluation of Q_{if} using $\Phi_X(1, 2)$ eventually involved numerical integration procedures. Unfortunately, because of the number and nature of the basis orbitals used here to describe the He atom, these procedures became extremely lengthy in execution; this was particularly noticeable at

large E because of the increased diffuseness of the integrands. Therefore, to extend the calculations to include capture into excited states was not feasible owing to the computation time becoming prohibitively large.

The Q_{if} values for reaction (1), namely, $Q(1s)$, were determined for $25 \leqslant E \leqslant 3500$ keV; this extends the upper limit of $E = 1000$ keV chosen by Bransden and Cheshire.[5] The results are given in Table I for $\Phi_\lambda(1, 2)$ and $\Phi_X(1, 2)$ for selected X values; the symmetry of the basis orbitals used to construct each additional natural configuration is quoted, for convenience, after each X value. For ease of discussion, Table I also contains the relative percentage change in $Q(1s)$, $\Delta(l \to m)$, when, for example, X is increased from l to m; $\Delta(l \to m)$ is defined as

$$[(Q_m - Q_l)/Q_l] \times 100\% .$$

TABLE I. Electron capture cross sections $Q(1s)$ for reaction (1), measured in units of πa_0^2, evaluated for various projectile energies E using the $(\Phi_\lambda, \epsilon_\lambda)$ and (Φ_X, ϵ_X) descriptions for $\mathrm{He}(1s^2)$, where $\lambda = 1.6875$ and $1 \leq X \leq 15$. The symmetry of the basis functions employed for each additional natural configuration is quoted after each X value. Also given are the relative percentage changes $\Delta(l \to m)$ in $Q(1s)$ when, for example, $X = l$ is changed to a better description $X = m$; $\Delta(l \to m)$ is defined as $[(Q_m - Q_l)/Q_l] \times 100\%$. The format $A - B$ means $A \times 10^{-B}$.

E (keV)	λ	$X = 1$ (s) [$\Delta(\lambda \to 1)$]	$X = 2$ (p) [$\Delta(1 \to 2)$]	$X = 3$ (s) [$\Delta(2 \to 3)$]	$X = 4$ (d) [$\Delta(3 \to 4)$]	$X = 5$ (p) [$\Delta(4 \to 5)$]	$X = 6$ (s) [$\Delta(5 \to 6)$]	$X = 15$ (s) [$\Delta(1 \to 15)$]	[$\Delta(\lambda \to 15)$]
25	3.952	3.693 [−6.6%]	3.569 [−3.4%]	3.352 [−6.1%]	3.350 [−0.1%]	3.339 [−0.3%]	3.333 [−0.2%]	3.375 [−8.6%]	[−14.6%]
50	1.168	1.112 [−4.8%]	1.100 [−1.1%]	1.051 [−4.5%]	1.053 [+0.2%]	1.052 [−0.1%]	1.051 [−0.1%]	1.066 [−4.1%]	[−8.7%]
100	2.088 −1	1.031 −1 [−2.7%]	2.042 −1 [+0.5%]	1.975 −1 [−3.3%]	1.983 −1 [+0.4%]	1.985 −1 [+0.1%]	1.985 −1 [+0.0%]	2.014 −1 [−0.8%]	[−3.5%]
150	5.931 −2	5.849 −2 [−1.4%]	5.928 −2 [+1.4%]	5.766 −2 [−2.7%]	5.797 −2 [+0.5%]	5.807 −2 [+0.2%]	5.812 −2 [+0.1%]	5.892 −2 [+0.7%]	[−0.7%]
200	2.174 −2	2.168 −2 [−0.3%]	2.203 −2 [+1.6%]	2.150 −2 [−2.4%]	2.163 −2 [+0.6%]	2.169 −2 [+0.3%]	2.172 −2 [+0.1%]	2.200 −2 [+1.5%]	[+1.2%]
400	1.374 −3	1.403 −3 [+2.1%]	1.431 −3 [+2.0%]	1.402 −3 [−2.0%]	1.412 −3 [+0.7%]	1.418 −3 [+0.4%]	1.422 −3 [+0.3%]	1.437 −3 [+2.4%]	[+4.6%]
600	2.262 −4	2.334 −4 [+3.2%]	2.376 −4 [+1.8%]	2.330 −4 [−1.9%]	2.346 −4 [+0.7%]	2.357 −4 [+0.5%]	2.364 −4 [+0.3%]	2.388 −4 [+2.3%]	[+5.6%]
800	5.876 −5	6.099 −5 [+3.8%]	6.199 −5 [+1.6%]	6.076 −5 [−2.0%]	6.112 −5 [+0.6%]	6.142 −5 [+0.5%]	6.162 −5 [+0.3%]	6.226 −5 [+2.1%]	[+6.0%]
1000	2.000 −5	2.082 −5 [+4.1%]	2.133 −5 [+1.5%]	2.070 −5 [−2.0%]	2.082 −5 [+0.6%]	2.091 −5 [+0.4%]	2.098 −5 [+0.3%]	2.122 −5 [+1.9%]	[+6.1%]
1500	2.656 −6	2.775 −6 [+4.5%]	2.807 −6 [+1.2%]	2.746 −6 [−2.2%]	2.759 −6 [+0.5%]	2.769 −6 [+0.4%]	2.777 −6 [+0.3%]	2.811 −6 [+1.3%]	[+5.5%]
2500	1.900 −7	1.995 −7 [+5.0%]	2.008 −7 [+0.7%]	1.961 −7 [−2.3%]	1.968 −7 [+0.4%]	1.973 −7 [+0.3%]	1.978 −7 [+0.3%]	1.999 −7 [+0.2%]	[+5.2%]
3500	3.187 −8	3.362 −8 [+5.5%]	3.375 −8 [+0.4%]	3.288 −8 [−2.6%]	3.298 −8 [+0.3%]	3.306 −8 [+0.2%]	3.314 −8 [+0.2%]	3.340 −8 [−0.7%]	[+4.8%]

III. DISCUSSION

For each choice of $\Phi(1, 2)$ we used the corresponding value for ϵ(He); consequently, an improvement in the description of He($1s^2$) had a twofold effect on $Q(1s)$. The nature of this dual dependence may be rationalized in the following way: Although the energy defect ϵ cannot be factorized from the resultant integrand for T_{if}, it always occurs in the form $v_i^2 - \epsilon = \delta$, say. The factor δ also occurs in β_{min}. At high impact energies the changes in δ due to improvements in ϵ(He), and hence ϵ, are minimal and therefore $Q(1s)$ is influenced only through changes in $\Phi(1, 2)$. For relatively low E, the capture cross sections reflect modifications in both the wave function and δ, the latter being most effective through its determination of β_{min}. Finally, pilot studies indicated that when ϵ(He) was held constant an improvement in $\Phi(1, 2)$ alone gave an *increase* in magnitude for $Q(1s)$ at each E used here.

Variations in $Q(1s)$ due to a systematic enhancement in the description of the target atom can be seen in Table I. Going from λ to the HF-equivalent description ($X = 1$) gives a reduction in $Q(1s)$ at low E but produces a slowly growing increase in its value as E becomes larger. Thus although the use of a HF wave function alone would, as discussed above, increase $Q(1s)$ for all E, the concomitant improvement in ϵ(He) causes an overall reduction in the cross section when $E \leq 200$ keV. Introduction of the leading electron correlation term, of essentially an angular nature based on p orbitals, results in a percentage change which is again negative at low E; $\Delta(1 \to 2)$ then becomes positive but drops away as we move to higher energies. When X is increased from 2 to 3 a purely radial correlation term is added to the description of He. The behavior of $\Delta(2 \to 3)$ is in marked contrast with that of $\Delta(1 \to 2)$, being negative at all impact energies, of relatively large magnitude at low E, and showing a slow *increase* in magnitude when $E > 1000$ keV. Although these initial angular and radial configurations recover about 48% and 37% of the total correlation energy, respectively, the radial term consistently gives the larger absolute shift in $Q(1s)$—particularly at the ends of our energy range. The addition of individual higher-order correlation terms $X \geq 4$ produces changes in the capture cross sections which, in general, are small and positive.

The values obtained for $Q(1s)$ using the total Weiss wave function are listed under $X = 15$ in Table I, and the relative influence of all the correlation terms taken together is shown by $\Delta(1 \to 15)$. A significant reduction occurs for the cross sections at the lower end of the energy range followed by an increase which eventually falls away and, as we move to even higher impact energies, $Q(1s)$ is again reduced in value as a consequence of the overall effect of correlation. Of particular interest is the comparison between $\Delta(1 \to 15)$ and $\Delta(\lambda \to 1)$, especially at high energies, where these relative changes are seen to exhibit quite different trends. This gives rise to a total change $\Delta(\lambda \to 15)$ when E is large which, although positive, decreases in magnitude with increasing energy. For low E, the trends shown by $\Delta(\lambda \to 1)$ and $\Delta(1 \to 15)$ are now of a similar nature and produce a combined effect $\Delta(\lambda \to 15)$ which indicates a marked decrease in $Q(1s)$ as E becomes smaller.

To obtain some comparison with experiment a theoretical measure of the total capture cross section Q can be obtained by using the usual Oppenheimer[12] sum-rule relation $Q \simeq 1.202Q(1s)$. The results are given in Table II along with the experimental values obtained by Stier and Barnett[13] and Welsh et al.[14] Except at $E = 100$ keV, the comparison with experiment shows that the cross sections obtained from the improved descriptions of He are, as anticipated, superior to the λ-based results; the correlated values are seen to give, in general, the best agreement. However, at high impact energies the expected convergence between theory and experimental is not apparent.

IV. SUMMARY

The use of a CI wave function for He, which allowed for about 99% of the correlation energy, gave capture cross sections for reaction (1) within the impulse approximation which, relative to the λ-based results, were noticeably reduced at low E but became greater in value when $E \geq 200$ keV. The cross sections also showed an improvement when compared with experiment. We note that as E increased in value the major part of the improve-

TABLE II. Total electron capture cross sections $Q \simeq 1.202Q(1s)$ evaluated using, in turn, $(\Phi_\lambda, \epsilon_\lambda)$ and (Φ_X, ϵ_X) when $X = 1$ and 15 for He($1s^2$), compared with the experimental values. The units for Q are πa_0^2. A -B means $A \times 10^{-B}$.

E (keV)	λ	$X = 1$	$X = 15$	Experiment
100	2.510 −1	2.441 −1	2.421 −1	3.4 −1 [a]
440	1.093 −3	1.120 −3	1.146 −3	(1.8 ± 0.2) −3 [b]
654	1.825 −4	1.887 −4	1.930 −4	(3.3 ± 0.4) −4 [b]
851	5.255 −5	5.461 −5	5.570 −5	(9.4 ± 1.1) −5 [b]
1063	1.783 −5	1.857 −5	1.900 −5	(3.3 ± 0.4) −5 [b]
2450	2.540 −7	2.665 −7	2.672 −7	(3.6 ± 0.4) −7 [b]
2990	8.874 −8	9.337 −8	9.151 −8	(1.4 ± 0.1) −7 [b]

[a] Stier and Barnett, Ref. 13.
[b] Welsh et al., Ref. 14.

ment arose from the change in the wave function up to the HF level of description. At large E, however, the replacement of the λ wave function by the CI function caused a relative increase in Q which began to fall away in magnitude and was clearly not sufficient to produce the anticipated convergence with experiment. Thus this discrepancy must be attributable to the impulse approximation for T_{if} itself. From a theoretical viewpoint, the extended version of the impulse approximation is known to provide a better description for T_{if}, but the evaluation of the matrix element is extremely difficult and the overall procedure has yet to be shown tractable.

ACKNOWLEDGMENT

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