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Continuum-distorted-wave calculations for rearrangement cross sections and their sensitivity to improvements in the target wave function: Proton-helium collisions

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The continuum-distorted-wave (CDW) approximation has been used to calculate the electron-capture cross sections $Q(nl)$ when a fast proton collides with a helium target atom. The range of the projectile energy is from 25 keV to 3 MeV and the electron-capture states considered are $nl = 1s$, $2s$, and $2p$. Of specific interest here is the sensitivity of these cross sections with respect to a systematic improvement in the description of the target ground-state wave function, both up to and beyond the Hartree-Fock level. Large changes were found to occur in the magnitude of each $Q(nl)$ as we progress from a simple one-parameter wave function for He up to a configuration-interaction description: The latter wave function accounted for about 99% of the electron correlation energy. Values of the total capture cross section were determined and compared with experiment over the available energy range of 100–2990 keV. The correlated results were, overall, in good agreement with experiment—especially in the high-energy region.

I. INTRODUCTION

The continuum-distorted-wave (CDW) method developed by Cheshire[1] for studying high-energy rearrangement collisions has received renewed application in recent years. Of particular interest here is the work of Salin.[2] He evaluated cross sections for electron capture into various excited states when fast protons collide with helium and, by describing the target atom by a simple one-parameter wave function $(1s)^2$ and then by a $(1s1s')$ function, his results changed by roughly 20% for projectile energies in excess of 1 MeV. Such differences in cross section at high energies due to this simple variation in the $He(^1S)$ wave function warrants further investigation. Therefore, for protons impinging on helium atoms, we examine in detail the sensitivity of the electron capture cross sections derived from the CDW method with respect to a systematic improvement in the description of the target wave function.

II. WAVE FUNCTIONS AND RESULTS

The rearrangement collisions considered here by the CDW method are

$$H^+ + He(1s^2) \rightarrow H(nl) + He^+(1s)\,, \tag{1}$$

where $nl \equiv 1s$, $2s$, and $2p$. The target electrons are regarded as distinguishable and, consequently, the single-electron-capture cross sections are twice the cross sections evaluated for the capture of the "active" electron, say, particle 1. For $\Phi(1,2)$, the ground-state wave function for He, we used various renormalized truncations of the natural expansion (Banyard and Baker[3]) derived from the 35-term configuration-interaction (CI) wave function of Weiss.[4] The leading term, $X = 1$, in such an expansion represents a good approximation to the Hartree-Fock (HF) wave function, and therefore truncations which include, in order, the first $X = 2, 3, 4, \ldots$ natural configurations introduce electron correlation into $\Phi_X(1,2)$ and its corresponding energy $\epsilon_X(\mathrm{He})$ in a well-defined manner. The complete Weiss wave function is attained when $X = 15$ and corresponds to $\epsilon(\mathrm{He}) = -2.90320$ a.u.[5]; this accounts for about 99% of the correlation energy. Cross sections were also evaluated using the simple one-parameter description $\Phi_\lambda(1,2)$, where $\lambda = 1.6875$, and comparisons were made with the $X = 1$ (~HF) results.

For a chosen projectile energy E, the capture cross section $Q(nl)$ is obtained from

$$Q(nl) = 2\int_0^\infty b\,|\,a_{nl}(b)\,|^2\,db\,, \tag{2}$$

(in units of πa_0^2) where $a_{nl}(b)$ is the prior form of the CDW transition amplitude[1,2] evaluated for reaction (1) and b is the impact parameter. The "nonactive" or "passive" electron (2) occurs in $a(nl)$ only in an overlap integral between its initial and final state; see, for example, the discussion by Belkić and Janev.[6] Therefore, for reaction (1), the influence of electron correlation on the capture cross sections derived from the present form of the CDW method will arise, in a direct manner, only from the *radial* correlation terms contained within $\Phi(1,2)$. We defined the polar axis z and the x axis of our coordinate framework to be in the directions of the projectile velocity and the impact parameter, respectively; thus it follows that $Q(2p_y) = 0$, and hence $Q(2p)$ is the sum of $Q(2p_z)$ and $Q(2p_x)$. Values of $Q(nl)$ for selected $\Phi(1,2)$ and its

TABLE I. Electron-capture cross sections $Q(nl)$, in units of πa_0^2, for reaction (1) when the target electrons are described, in turn, by a one-parameter variational wave function ($\lambda = 1.6875$) and the first X terms of a natural expansion of the Weiss 35-term CI function ($X = 15$ equals the total wave function). The symmetry of the basis functions used for each additional natural configuration is quoted after each X value. In brackets we give the percentage change $\Delta(i \to k)$ in $Q(nl)$ when the description for He is changed from $\Phi_i(1,2)$ to an energetically better function $\Phi_k(1,2)$; $\Delta(i \to k)$ is defined as $[Q_k - Q_i)/Q_i] \times 100\%$.

	$Q(1s)$					$Q(2s)$			$Q(2p)$		
E (keV)	λ	$X=1(s)$ [$\Delta(\lambda \to 1)$]	$X=3(s)$	$X=6(s)$	$X=15(s)$ [$\Delta(1 \to 15)$]	λ	$X=1(s)$ [$\Delta(\lambda \to 1)$]	$X=15(s)$ [$\Delta(1 \to 15)$]	λ	$X=1(s)$ [$\Delta(\lambda \to 1)$]	$X=15(s)$ [$\Delta(1 \to 15)$]
25	7.552^{0} [a]	7.254^{0} [−3.9%]	6.578^{0}	6.498^{0}	6.472^{0} [−10.8%]	5.583^{-1}	5.118^{-1} [−8.3%]	4.351^{-1} [−15.0%]	9.546^{-1}	8.112^{-1} [−15.0%]	7.860^{-1} [−3.1%]
50	1.806^{0}	1.711^{0} [−5.3%]	1.627^{0}	1.617^{0}	1.614^{0} [−5.7%]	2.132^{-1}	2.026^{-1} [−5.0%]	1.862^{-1} [−8.1%]	1.495^{-1}	1.499^{-1} [+0.3%]	1.451^{-1} [−3.2%]
100	2.958^{-1}	2.701^{-1} [−8.7%]	2.617^{-1}	2.610^{-1}	2.608^{-1} [−3.4%]	4.228^{-2}	3.907^{-2} [−7.6%]	3.746^{-2} [−4.1%]	1.940^{-2}	1.956^{-2} [+0.8%]	1.864^{-2} [−4.7%]
200	3.055^{-2}	2.733^{-2} [−10.5%]	2.643^{-2}	2.640^{-2}	2.639^{-2} [−3.4%]	4.519^{-3}	4.052^{-3} [−10.3%]	3.913^{-3} [−3.4%]	1.486^{-3}	1.547^{-3} [+4.1%]	1.459^{-3} [−5.7%]
400	1.936^{-3}	1.807^{-3} [−6.7%]	1.727^{-3}	1.726^{-3}	1.726^{-3} [−4.5%]	2.776^{-4}	2.576^{-4} [−7.2%]	2.463^{-4} [−4.4%]	6.405^{-5}	7.571^{-5} [+18.2%]	7.078^{-5} [−6.5%]
600	3.131^{-4}	3.104^{-4} [−0.9%]	2.944^{-4}	2.945^{-4}	2.945^{-4} [−5.1%]	4.374^{-5}	4.309^{-5} [−1.5%]	4.090^{-5} [−5.1%]	8.225^{-6}	1.082^{-5} [+31.6%]	1.012^{-5} [−6.5%]
800	7.935^{-5}	8.306^{-5} [+4.7%]	7.847^{-5}	7.854^{-5}	7.854^{-5} [−5.4%]	1.089^{-5}	1.134^{-5} [+4.1%]	1.072^{-5} [−5.5%]	1.791^{-6}	2.547^{-6} [+42.2%]	2.393^{-6} [−6.0%]
1000	2.630^{-5}	2.882^{-5} [+9.6%]	2.718^{-5}	2.722^{-5}	2.722^{-5} [−5.6%]	3.566^{-6}	3.889^{-6} [+9.1%]	3.673^{-6} [−5.6%]	5.340^{-7}	8.048^{-7} [+50.7%]	7.597^{-7} [−5.6%]
1500	3.284^{-6}	3.920^{-6} [+19.4%]	3.692^{-6}	3.701^{-6}	3.700^{-6} [−5.6%]	4.368^{-7}	5.196^{-7} [+19.0%]	4.906^{-7} [−5.6%]	5.685^{-8}	9.414^{-8} [+65.6%]	8.984^{-8} [−4.6%]
2000	7.152^{-7}	9.052^{-7} [+26.6%]	8.535^{-7}	8.561^{-7}	8.559^{-7} [−5.4%]	9.414^{-8}	1.188^{-7} [+26.2%]	1.123^{-7} [−5.5%]	1.140^{-8}	1.996^{-8} [+75.1%]	1.920^{-8} [−3.8%]
2500	2.145^{-7}	2.833^{-7} [+32.1%]	2.675^{-7}	2.684^{-7}	2.683^{-7} [−5.3%]	2.804^{-8}	3.695^{-8} [+31.8%]	3.500^{-8} [−5.3%]	3.264^{-9}	5.929^{-9} [+81.6%]	5.741^{-9} [−3.2%]
3000	7.922^{-8}	1.081^{-7} [+36.5%]	1.022^{-7}	1.026^{-7}	1.025^{-7} [−5.2%]	1.031^{-8}	1.404^{-8} [+36.2%]	1.332^{-8} [−5.2%]	1.175^{-9}	2.189^{-9} [+86.3%]	2.130^{-9} [−2.7%]

[a] The superscript denotes the power of ten by which each entry should be multiplied.

associated ϵ(He) are given in Table I for 25 keV $\leq E \leq 3$ MeV. Also quoted are some percentage changes in $Q(nl)$, $\Delta(i \to k)$, when, for example, X is increased from $i \to k$. The total capture cross section Q was obtained, following Salin,[2] from the "Oppenheimer n^{-3} rule"

$$Q = \sum_{nl} Q(nl) \simeq Q(1s) + 1.616\,[Q(2s) + Q(2p)]\,, \qquad (3)$$

and comparisons with experiment[7,8] are given in Table II.

III. DISCUSSION

As the ground-state wave function and energy for He are systematically improved, both the absolute and relative changes in each $Q(nl)$ can be seen by inspection of Table I. $\Delta(\lambda \to 1)$ measures the relative effect of improving $\Phi(1,2)$ from the simple one-parameter description up to the $X = 1$ (~HF) level, whereas $\Delta(1 \to 15)$ assesses the influence of correlation as we go beyond the independent-particle model and use, instead, the total wave function of Weiss. For each Δ quantity, a strong similarity is seen to exist between the corresponding values for $nl \equiv 1s$ and $2s$ and this becomes especially noticeable in the higher-energy range; the similarity does not extend to the $2p$ state. This may be rationalized as follows. At high projectile velocities, the major contributions to the cross sections arise at small values for the impact parameter, and therefore they will reflect the nature of the wave functions for the "active" electron, before and after capture, in regions close to both

TABLE II. A comparison with experiment of the total capture cross-sections Q, in units of πa_0^2, for the reaction $H^+ + He(1s^2) \rightarrow H + He^+(1s)$ evaluated using the continuum distorted wave approximation. The target electrons are described, in turn, by $(\Phi_\lambda, \epsilon_\lambda)$ and (Φ_X, ϵ_X) when $X = 1$, 3, and 15.

E (keV)	λ	$X=1$	$X=3$	$X=15$	Experiment
100	3.955^{-1} [a]	3.648^{-1}	3.527^{-1}	3.514^{-1}	3.4^{-1} [b]
440	1.637^{-3}	1.562^{-3}	1.489^{-3}	1.488^{-3}	$(1.8 \pm 0.2)^{-3}$ [c]
654	2.643^{-4}	2.868^{-4}	2.543^{-4}	2.545^{-4}	$(3.3 \pm 0.4)^{-4}$ [c]
851	7.367^{-5}	7.881^{-5}	7.438^{-5}	7.447^{-5}	$(9.4 \pm 1.1)^{-5}$ [c]
1063	2.418^{-5}	2.707^{-5}	2.552^{-5}	2.556^{-5}	$(3.3 \pm 0.4)^{-5}$ [c]
2450	2.959^{-7}	3.921^{-7}	3.705^{-7}	3.715^{-7}	$(3.6 \pm 0.4)^{-7}$ [c]
2990	9.959^{-8}	1.367^{-7}	1.295^{-7}	1.301^{-7}	$(1.4 \pm 0.1)^{-7}$ [c]

[a] The superscript denotes the power of ten by which the entry should be multiplied.
[b] Stier and Barnett (Ref. 7).
[c] Welsh *et al.* (Ref. 8).

the target nucleus and the projectile. While improvements in the inner regions of the target wave function will be common to all three cross sections, the 1*s* and 2*s* hydrogen orbitals possess quite different spatial characteristics from the 2*p* orbital at small electron-proton separations. At such small separations, the characteristics—but not the magnitude—of the 1*s* and 2*s* hydrogen orbitals are found to be very similar. Thus, for a fast proton this similarity will be reflected in the *percentage* changes observed for $Q(1s)$ and $Q(2s)$.

The improvement in the target wave function up to the HF description reduces each $Q(nl)$ at low E but produces a large increase in value at high E and, for capture into the 2*p* states, the changes are quite dramatic. The most sensitive example was $Q(2p_x)$ where, at $E = 25$ and 3 MeV, $\Delta(\lambda \rightarrow 1)$ was -19% and $+92\%$, respectively. We also note that for each $Q(nl)$ an initial extension of the energy range should result in a continued increase for $\Delta(\lambda \rightarrow 1)$. Therefore, for reaction (1) a description of the target by at least an HF wave function is seen to be essential not only when $l = 0$ but is of even greater importance when considering electron capture into an excited state which possesses $l = 1$ angular characteristics.

An allowance for electron correlation reduces the value of every cross section, and for each $Q(nl)$ the major change occurs when $X = 1 \rightarrow 3$; see, for example, $Q(1s)$ in Table I. Except for $Q(1s)$ and $Q(2s)$ at low proton energies, the magnitude of $\Delta(1 \rightarrow 15)$ is seen to be generally small by comparison with $\Delta(\lambda \rightarrow 1)$. As we approach the upper limit for E, we observe that in contrast with the behavior of $\Delta(\lambda \rightarrow 1)$ the total effect of correlation shows a slow *decrease* in its relative importance. The *overall* change in cross section for each capture state due to the improvement in wave function from Φ_λ to the full CI function ranges from a reduction by 14% for $Q(1s)$, 22% for $Q(2s)$, and 18% for $Q(2p)$ at $E = 25$ keV up to an increase in value at $E = 3$ MeV of about 29% for $Q(1s)$ and $Q(2s)$ and 81% for $Q(2p)$.

At this stage it is of interest to compare the relative effects of the wave-function improvement within the CDW method with that for $Q(1s)$ in reaction (1) when determined by the impulse approximation (see Szuster and Banyard[9]). A striking difference occurs in the behavior of $\Delta(\lambda \rightarrow 1)$ which, in the present method, rises steeply with increasing E, whereas for the impulse approximation the rise is gradual and even at large E does not exceed 6%. Electron correlation also produced quite different trends since for most of our energy range the impulse approach showed an *increase* in $Q(1s)$ when $X = 1 \rightarrow 15$. However, we note that for both methods the initial introduction of radial correlation always reduces the capture cross section but, whereas in the impulse calculation this can be more than compensated for by an increase in value due to angular correlation, no such effect can occur in the present application of the CDW method.

Inspection of Table II indicates that when $\lambda \rightarrow X = 15$, the effect on Q varies from an 11% reduction at 100 keV to a 31% increase in value at 2990 keV. In particular, it is noted that the percentage increase will become larger as the energy range is extended. As occurred for each $Q(nl)$, the improvement in the wave function up to the HF approximation dominates the change in Q. When compared with experiment, the HF and fully correlated results are, overall, superior to the λ values. The agreement at high energies is particularly pleasing since the theoretical values are now within the limits of experimental error.

IV. CONCLUSIONS

For the CDW description of electron capture from He by fast protons, improvements in the target wave function up to and beyond the HF approximation can produce large changes in the cross sections $Q(nl)$ when $nl \equiv 1s$, $2s$, and $2p$. The most sensitive example was $Q(2p)$. Not only are such changes dominated by the HF contribution but relative to the λ-based cross sections, they also show every tendency to become larger when the projectile energy E is increased. Similar observations hold for Q—the total capture cross section. The HF and correlated values for Q were, overall, in reasonable accord with experiment throughout the available energy range. At large E these calculated values agree with experiment to within the observational error.

Finally, we recall that electron correlation has been introduced here only into the target wave function since the current application of the CDW method has, like previous applications, specifically removed direct interelectronic effects from the defining equations for the distortion functions. The consequence of this is being investigated. In addition, parallel calculations are now well advanced for reactions involving H^- where, energetically, correlation effects are of great importance.

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