Charge exchange between simple structured projectiles in high-energy collisions

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The continuum–intermediate-states approximation has been adapted for application to charge-exchange collisions between high-energy structured projectiles. A critical test of the scheme is provided by the reaction $H(1s)+H(1s)\rightarrow H^-(1s^2)+H^+$; the overall agreement with the limited experimental data is encouraging.

I. INTRODUCTION

Electron capture from small atomic targets by fast structureless projectiles such as protons and α particles can be described quite successfully by modifying the continuum-distorted-wave (CDW) method developed by Cheshire.[1] However, its application to charge exchange between structured systems is more difficult. Therefore, in a desire to examine such high-energy collisions between simple atoms, or ions, we suggest an adaptation of the method of continuum intermediate states (CIS). The CIS approach, devised by Belkić[2] for electron capture by a structureless projectile, is closely related to the CDW method but accounts for distortion effects in only one of the two channels. This feature not only produces considerable simplification from both the analytical and computational viewpoint, but also provides flexibility for generalization to electron capture by structured projectiles. In addition, the CIS method has the particular advantage of being more reliable than the CDW approximation for describing capture at large impact parameters (Shakeshaft,[3] Belkić[2]).

The reliability of the approximations involved in the proposed scheme is tested here by examining the reaction

$$H(1s)+H(1s)\rightarrow H^-(1s^2)+H^+ . \tag{1}$$

For this example, a comparison can be made with capture cross sections derived from the results of a CDW calculation for the reverse reaction; see Janev and Salin[4,5] and Moore and Banyard.[6] The former workers described the H^- target by a $1s1s'$ wave function, whereas, in an electron correlation study, the latter workers used the wave function of Weiss.[7] The only experimental results available for reaction (1) are those of McClure[8] and, unfortunately, these are restricted to impact energies $E \leq 63$ keV.

II. METHOD

The cross section $\sigma(nl)$ for the capture of electron 1, say, by a fast structured projectile system (Z_A, e_2) of energy E in collision with a target (Z_B, e_1) considered to be at rest, is written as

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

(in units of πa_0^2), where b is the impact parameter and (nl) is the capture state. Atomic units are used throughout unless stated otherwise. It follows from the definition of the prior form of the transition amplitude (see, for example, Cheshire[1] that, for this reaction, a_{if} can be expressed as

$$a_{if} = i\int_{-\infty}^{+\infty} dt \int d\vec{r}_1 d\vec{r}_2 \Psi_f^{-*}\left(\frac{Z_A}{s_1} - \frac{1}{s_{12}} + \frac{Z_B}{x_2} + \frac{(1-Z_A-Z_B)}{R} - U_i\right)\chi_i , \tag{3}$$

where χ_i is the initial distorted wave satisfying

$$\left(\tfrac{1}{2}\nabla_1^2 + \tfrac{1}{2}\nabla_2^2 + \frac{Z_B}{x_1} + \frac{Z_A}{s_2} - \frac{(Z_A-1)(Z_B-1)}{R} + i\frac{\partial}{\partial t} + U_i\right)\chi_i = 0. \tag{4}$$

The position vectors $\vec{s}_j, \vec{x}_j$, and $\vec{r}_j$ locate electron j relative to Z_A, Z_B, and the midpoint of R, respectively, where R is the internuclear separation. The final-state complete wave function Ψ_f^- is determined in the same manner as in the CDW method and therefore it incorporates the ground-state electronic wave function of the (Z_A, e_1, e_2) system and the distortion effects due to inclusion of continuum intermediate states which arise from the interaction of the active electron 1 with Z_B in the outward channel. In the CIS approximation, we choose the arbitrary distorting potential U_i such that χ_i involves only the eigenfunctions for (Z_A, e_2) and (Z_B, e_1) along with an appropriate phase function of the form defined by Belkić.[2] This requirement is satisfied by $U_i = -(Z_A-1)R^{-1}$ and, as a consequence, Eq. (3) becomes

$$a_{if} = i \int_{-\infty}^{+\infty} \left[\left\langle \Psi_f^- \left| \left(\frac{Z_A}{s_1} - \frac{1}{s_{12}} \right) \right| \chi_i \right\rangle + \left\langle \Psi_f^- \left| Z_B \left(\frac{1}{x_2} - \frac{1}{R} \right) \right| \chi_i \right\rangle \right] dt . \quad (5)$$

When the passive electron 2 remains tightly bound to Z_A throughout the whole interaction, then it is not unreasonable to suppose that the second matrix element provides a negligible contribution to a_{if}. Thus, in the calculation of $\sigma(nl)$, we consider only the first term in Eq. (5). The reliability of this approximation should increase when $Z_A >> Z_B$; such a relationship between the nuclear charges should also emphasize the importance of capture at large impact parameters and thus support our use of the CIS approach. Consequently, a very severe test of the present scheme is provided by applying it to the forward direction of reaction (1).

For this initial calculation, the interelectronic interaction was approximated by the average electrostatic potential due to the passive electron being described by a $1s$ hydrogen atom orbital. Thus, in Eq. (5),

$$\left(\frac{Z_A}{s_1} - \frac{1}{s_{12}} \right) \to e^{-2s_1} \left(1 + \frac{1}{s_1} \right), \quad (6)$$

when $Z_A = 1$. $H^-(1s^2)$ was described, firstly, by the Hartree-Fock (HF) fitted function of Curl and Coulson[9] and, secondly, by a "fixed-core" representation of the form $1s1s'$ in which the exponent of the valence-electron orbital is chosen to be $(2\epsilon)^{1/2}$, where ϵ is the experimental value of the single-ionization energy, and the fixed core is a $1s$ hydrogen orbital. The latter description of H^- has the advantage of having one electron loosely bound whilst the other electron remains comparatively tightly bound. Such a wave function, albeit empirical, could be particularly appropriate at the intermediate energies represented by experiment[8] since contributions to $\sigma(1s)$ from relatively large values of the impact parameter may then be significant. Finally, we used the configuration-interaction (CI) wave function of Weiss.[7] This function not only allowed for the high degree of electron correlation in H^-, and satisfied the energy variation principle, but it also enabled us to make numerical comparisons with the CDW results[6] at large E values. The energy decrement $\Delta\epsilon$ used in conjunction with the HF and CI wave functions was derived in each case from the corresponding theoretical energies, whereas, for the fixed-core description of H^-, we used the experimental value.

III. RESULTS AND DISCUSSION

Although the CIS method, like the CDW approach, is essentially a high-energy approximation, the comparison of our theoretical capture cross sections with experiment is limited to the data of McClure[8] (see Fig. 1). Also shown in Fig. 1 are the "post" and "prior" theoretical curves of Mapleton[10] used by McClure[8] for comparison with experiment. Mapleton[10] employed a Born approximation to describe reaction (1) with the ground state of H^- being represented by the correlated wave function of Chandrasekhar.[11] In Table I we compare the CIS-based results, using the HF and CI wave functions, with the CDW cross sections[6] for projectile energies E up to 1 MeV. The difference between the HF and CI values measures the influence of electron correlation within the current formulations of the CIS and CDW methods.

Figure 1 shows that the three CIS-based curves represent a considerable improvement on the Mapleton cross sections when compared with experiment, although at low energies the peak values are still too large. It is to be noted that, as observed for the CDW results,[4-6] each theoretical curve appears to fall off too rapidly as E increases in value. Additional experimental cross sections at higher energies would provide a most useful check with theory.

Of the curves presented in Fig. 1, that derived from the HF wave function is perhaps the best—this is somewhat surprising and may, as discussed

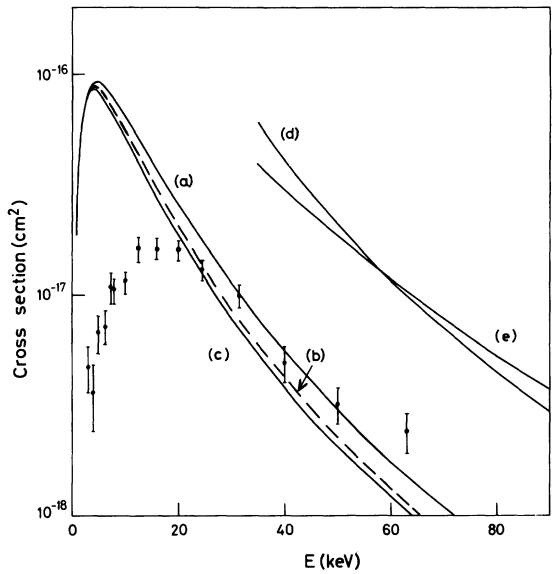

FIG. 1. Electron-capture cross sections $\sigma(1s)$ for $H(1s) + H(1s) \to H^-(1s^2) + H^+$. The CIS results are shown in curves (a), (b), and (c) and are derived, respectively, from the use of the Hartree-Fock (HF) function, the "fixed-core" model, and the configuration-interaction (CI) description for $H^-(1s^2)$. Curves (d) and (e) are the "prior" and "post" results of Mapleton (Ref. 10) calculated using a Born approximation. The experimental points are those of McClure (Ref. 8).

TABLE I. A comparison of the electron-capture cross sections $\sigma(1s)$, measured in cms^2, for the reaction $H(1s) + H(1s) \rightarrow H^-(1s^2) + H^+$. The continuum–intermediate-states (CIS) results are calculated here for the forward reaction, whereas the continuum–distorted-wave (CDW) results are those of Moore and Banyard (Ref. 6) and were derived by them from the calculated results for the reverse reaction. For $H^-(1s^2)$, the Hartree-Fock (HF) function was that of Curl and Coulson (Ref. 9) and the configuration-interaction (CI) description was taken from Weiss (Ref. 7).

	CIS		CDW	
E (keV)	HF	CI	HF	CI
25	1.681×10^{-17}	1.173×10^{-17}	2.886×10^{-17}	2.067×10^{-17}
50	3.023×10^{-18}	2.067×10^{-18}	5.093×10^{-18}	3.526×10^{-18}
100	3.268×10^{-19}	2.268×10^{-19}	5.227×10^{-19}	3.600×10^{-19}
200	2.325×10^{-20}	1.650×10^{-20}	3.410×10^{-20}	2.379×10^{-20}
400	1.202×10^{-21}	8.696×10^{-22}	1.527×10^{-21}	1.087×10^{-21}
800	4.845×10^{-23}	3.636×10^{-23}	4.990×10^{-23}	3.618×10^{-23}
1000	1.688×10^{-23}	1.284×10^{-23}	1.570×10^{-23}	1.143×10^{-23}

below, arise from a cancellation of opposing effects. The more reasonable split-shell description of H^- embodied in the empirical fixed-core model and the Weiss wave function is seen to be reflected in the closeness of curves (b) and (c); both curves lie slightly below the experimental points when $E > 25$ keV. Our CIS-based approximation is only capable of responding to a split-shell or radial component of electron correlation and makes no allowance for the effects of angular correlation in H^-. Since the transition amplitude a_{if} is evaluated in terms of momentum space, it is possible that the opposing effects of angular and radial correlation—known to exist in momentum space[12]—may produce some cancellations. Thus, if the present method could be modified to allow for angular correlation, curve (c) might be raised. This is now under investigation.

For both descriptions of H^-, Table I indicates that for $E < 800$ keV, the CIS values are smaller than the corresponding cross sections derived from a CDW calculation for the reverse reaction. The relative merit of the two schemes is difficult to judge since, ideally, the comparisons with experiment should be made in the higher-energy region of Table I.

IV. SUMMARY

In view of the severity of the test of the present method, represented by its application to reaction (1), the comparison between theory and experiment was, overall, quite encouraging. The general procedure outlined above is now being examined in more detail and the method is also being applied to electron capture by fast Li ions impinging on H atoms. Such reactions have been the subject of a recent experimental investigation by Shah, Goffe, and Gilbody.[13] The preliminary comparisons are pleasing.

[1]I. M. Cheshire, Proc. Phys. Soc. London 84, 89 (1964).
[2]Dz. Belkić, J. Phys. B 10, 3491 (1977).
[3]R. Shakeshaft, J. Phys. B. 7, 1734 (1974).
[4]R. K. Janev and A. Salin, J. Phys. B 4, L127 (1971).
[5]R. K. Janev and A. Salin, Fizika 4, 165 (1972).
[6]J. C. Moore and K. E. Banyard, J. Phys. B 11, 1613 (1978).
[7]A. W. Weiss, Phys. Rev. 122, 1826 (1961).
[8]G. W. McClure, Phys. Rev. 166, 22 (1968).
[9]R. F. Curl and C. A. Coulson, Proc. Phys. Soc. London 85, 647 (1964); see also R. F. Curl and C. A. Coulson, J. Phys. B1, 325 (1978).
[10]R. A. Mapleton, Proc. Phys. Soc. London 85, 841 (1965).
[11]S. Chandrasekhar, Astrophys. J. 100, 176 (1944).
[12]K. E. Banyard and C. E. Reed, J. Phys. B 11, 2957 (1978).
[13]M. B. Shah, T. V. Goffe, and H. B. Gilbody, J. Phys. B 11, L233 (1978).