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CHARGE TRANSFER IN THE CLASSICAL BINARY ENCOUNTER APPROXIMATION

BY

J. D. GARCIA AND E. GERJUOY

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Charge Transfer in the Classical Binary Encounter Approximation

J. D. Garcia and E. Gerjuoy

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J. D. Garcia and E. Gerjuoy
Department of Physics
University of Pittsburgh
Pittsburgh, Pennsylvania 15213

Experimental determinations recently have been made[1] of the capture of electrons by protons into the 2s state from one-and-two electron systems for incident proton energies ranging from 40 - 200 keV. This note is intended to demonstrate that these measured values can be predicted as well by the classical binary encounter theory as by any existing quantum mechanical approximations.

We have calculated the cross sections for the reactions

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

$$H^+ + H_2 \rightarrow H(2s) + H_2^+ \tag{2}$$

$$H^+ + He \rightarrow H(2s) + He^+ \tag{3}$$

using the expression from the Gryzinski model[2] for classical binary encounter theory:

$$\sigma = \int_{\Delta E_L}^{\Delta E_u} \sigma_{\Delta E}(v_1, v_2)\, d\Delta E \quad ,$$

where $\sigma_{\Delta E}(v_1,v_2)$ is the cross section for energy exchange between an incident charged particle with velocity $\vec{v}_1$ and a bound atomic electron with velocity $\vec{v}_2$, averaged over all orientations of $\vec{v}_2$. The exact expression for $\sigma_{\Delta E}$ has been given by Gerjuoy,[3] and is easily integrated. For the

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integration limits we use the simple expressions given by Gryzinski[2]

$$\Delta E_L = 1/2\ m_e v_1^2 + U_A - U_B$$

$$\Delta E_u = 1/2\ m_e v_1^2 + U_A + U_B$$

where U_A is the binding energy of the electron in the target atom and U_B is the binding energy of the electron after capture. The resultant expression is to be multiplied by the number of equivalent electrons. It should also be averaged over the speed distribution of the target electron; we have used a delta function distribution only: $f(|\vec{v}_2|)$ proportional to $\delta(v_2 - \sqrt{\frac{2U_A}{m_e}})$. The primary assumptions of our model are then: (a) the interaction between the electron and the incident proton is the primary one in determining this cross section; (b) the incident proton's trajectory is essentially unaffected by the process; and (c) the magnitude of the energy transfer is the primary criterion for deciding whether or not capture occurs.

Of these assumptions, (c) is the weakest, since not all electrons whose energies after collision are in the correct energy range for capture will be captured; capture is not equally probable for all directions and magnitude of the electron momentum relative to the proton. Taking the electron momentum into account has been attempted.[4] The major effect is a more rapid decrease of the cross section at high energies, which in the present model is proportional to $\frac{1}{E^3}$. For the relatively low energies of these measurements, however the weaker assumption may suffice. Assumption (c) is not entirely independent of assumption (a), since classically the target atom-electron interaction provides the mechanism for binding the electron to the incident ion. In general, however, it appears to us that violation of assumption (a) would have important effects mainly at lower energies, presumably lower than those herein discussed.

Figure 1 shows the experimental results for reactions (1) and (2) given by Ryding, et.al. together with some theoretical curves (Figure 2 of Reference 1). No absolute determinations of the cross sections were made. The observed ratios for the two processes were converted to cross sections by normalizing to the theoretical Born approximation value[5] for reaction (1) at 100 keV, (including the proton-proton interaction matrix element). In other words, the circle at 100 keV was postulated to lie precisely on the dashed theoretical curve of Mapleton.[5] There appears to be no compelling evidence for this choice of normalization. In particular, we noticed in the process of comparing our calculations to experiment, that the energy dependence for reaction (2) was reasonably well given by our model. In Figure 2(a,b) we present the same data normalized to our theoretical value for reaction (2) at 50 keV (though most points would do, since the experimental values all lie near the theoretical values). Curves B and D in Figure 1, like the solid lines in Figure 2 involve no adjustable parameters.

Figure 2(c) shows the experimental cross sections for reaction (3), which were obtained by Ryding, et.al.[1] by normalizing their data for this reaction to the Born approximation[6] for reaction (3) at 160 keV. Also shown are some theoretical values.

Even without any change of normalization, the classical predictions agree with experiment remarkably well, appearing at least as consistent with the data as quantum approximations in the energy range of the measurements. The more rapid decrease with energy at larger energies is in part due to failure of assumption (c) as discussed above.

There can be no doubt that the process occurring is one in which the quantum theory is needed for a proper description. It may be, however, that the quantum mechanical approximations extant in effect are "semi-classical", and that in fact the process is sufficiently structureless in this energy range to require little more than computing the phase space available. Evaluation of the available phase space appears to be done adequately by the classical theory, even under the restrictive assumptions used. In other words, it is possible that with proper account of the Coulomb nature of the problem, the kinematics dominate the behavior of the cross section. The dynamics, or actual structure of the transition amplitude specific to this problem, would then not be important at these energies. Evidence supporting these statements is available in terms of the success of the classical model in predicting excitation and ionization cross sections.[2,8,9]

The above discussion hinges in part on the fact that the measurements were relative measurements. It appears to us that absolute measurements of these cross sections to resolve the question of normalization are necessary and desirable.

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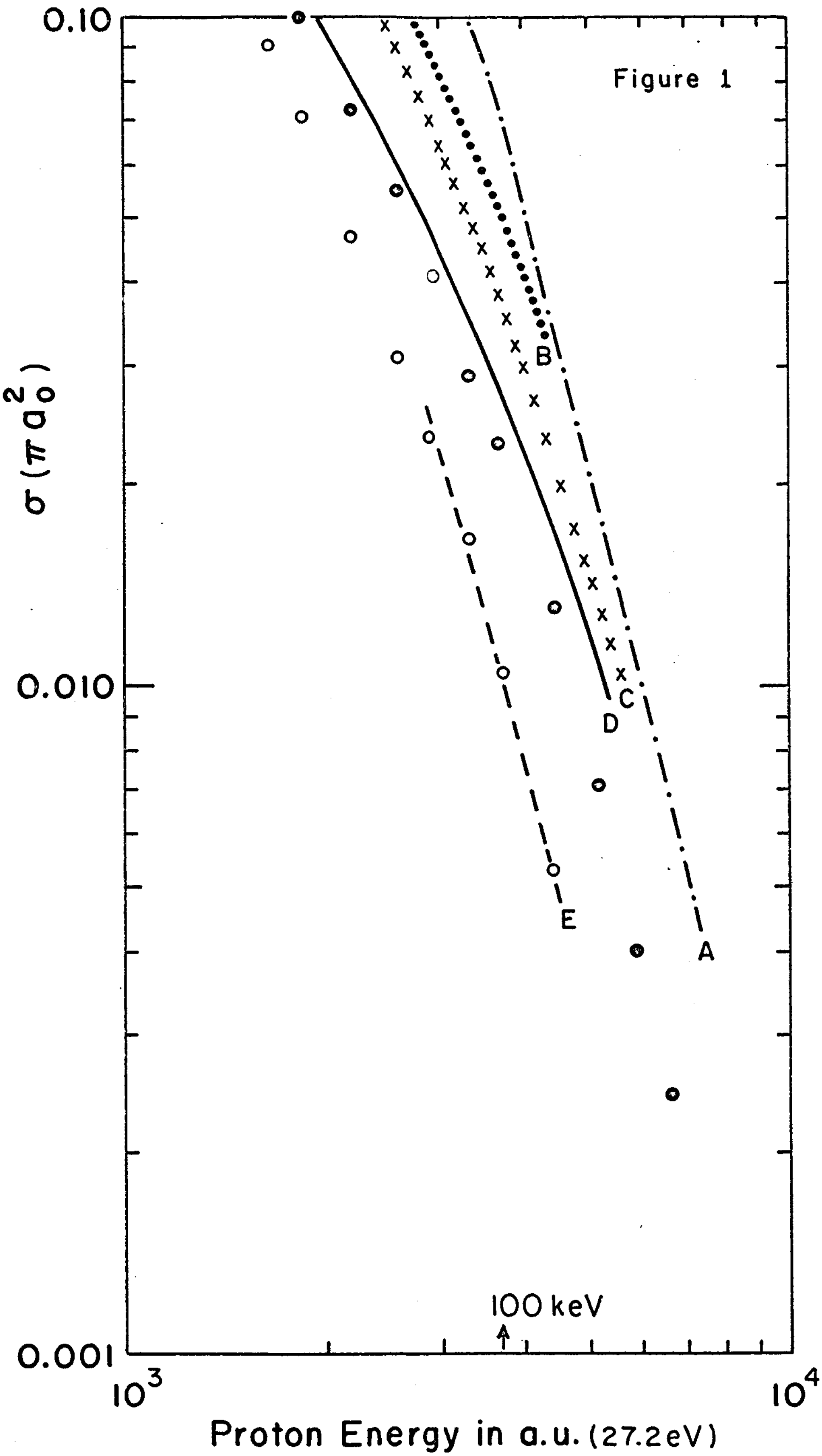

Figure 1. Charge capture by protons into a 2s state. o, experimental p + H; •, experimental p + H_2; A-·-, Brinkman-Kramers theory for p + H (Ref. 5); B····, present results for p + H_2; C+++, McElroy 2-state approximation for p + H (Ref. 7); D——, present results for p + H; E--- Born approximation for p + H (Ref. 5). See text for normalization of experimental values.

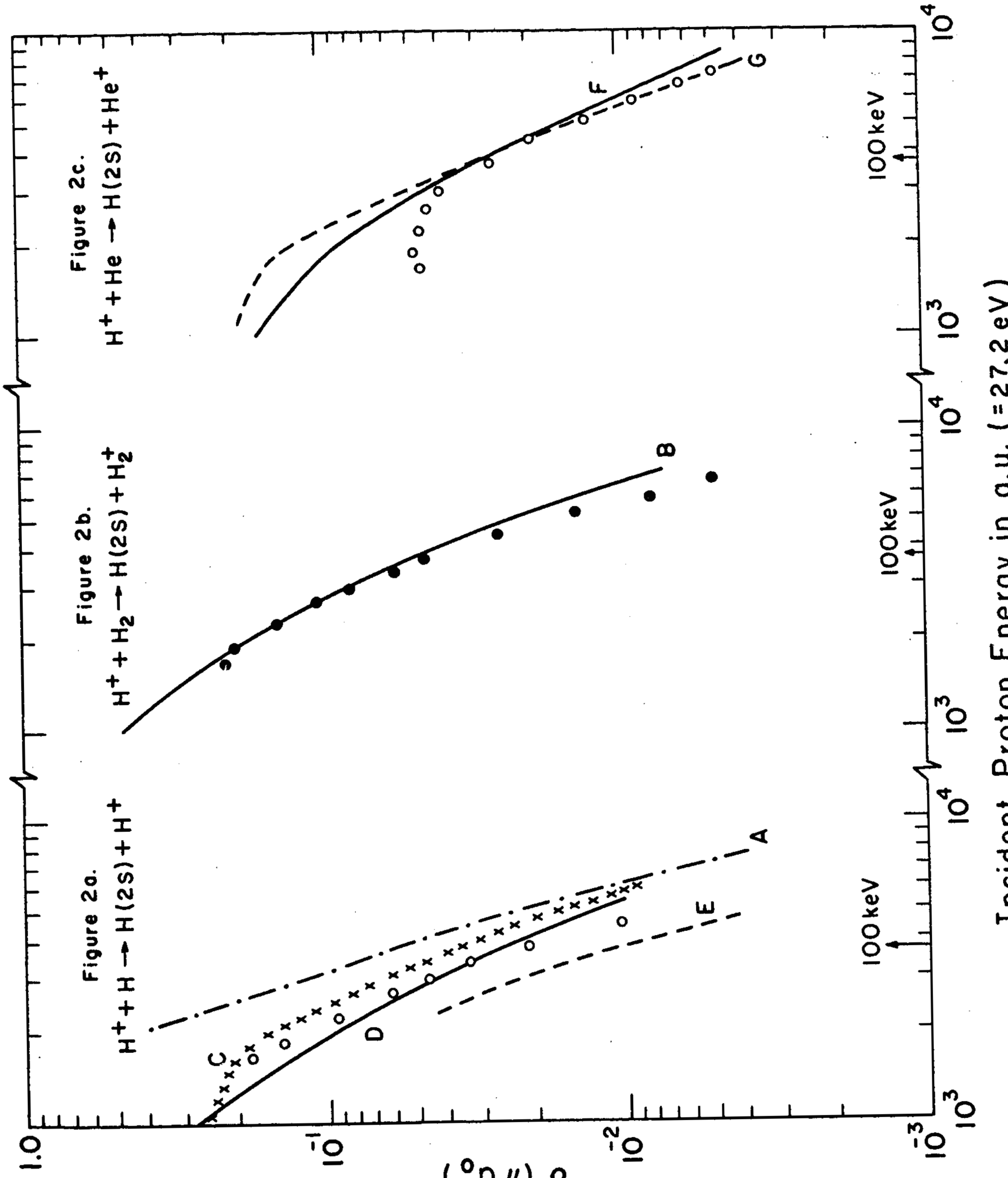

Figure 2. Charge capture by protons into a 2s state. (a) p + H; o, experiment (see text for normalization); curves A, C, D, E as in Figure 1: (b) p + H_2; ●, experiment (see text for normalization); curve B, present results: (c) p + He; o, experiment (see text for normalization); F——, present results; G----, Born approximation (Ref. 7).