remain nearly at rest in the center of mass after the collision, probably dispersing on a time scale ~ 10^{-22} sec. These Coulomb effects are thus a potentially powerful tool for investigating the dynamics of the nuclear charge distribution and the mechanisms of pion production in relativistic heavy-ion collisions.

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H(2s) Formation and the Lyman-α Polarization in 1–7-keV H^+-H Collisions

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A multistate molecular approach to the proton–hydrogen-atom collision is formulated. Spurious long-range couplings are avoided and Galilean invariance enforced through variationally determined momentum translation factors. Well-defined radial and rotational couplings are employed in the 1–7-keV energy range in a ten-state calculation. Good agreement with Bayfield is obtained for the 2s charge-exchange probability. Concerning polarization of Lyman-α radiation, comparison with Kauppila *et al.* is made.

The proton–hydrogen-atom collision has been well studied over a wide range of energy, angle, and final-state products. In this Letter we shall be concerned only with energies below 25 keV where a molecular or hybrid-molecular description would appear to be necessary.

Following the pioneering work of Mott,[1] Massey and Smith,[2] and Bates, Massey, and Stewart,[3] Bates and McCarroll[4] formulated the first satisfactory impact-parameter, perturbed–stationary-states (PSS) treatment, in that the inclusion of momentum translation factors avoided spurious long-range divergent couplings and enforced Galilean invariance. This treatment was first applied in the two-state approximation by Ferguson[5] and later in the three-state approximation and in the low-velocity limit by Bates and Williams[6] and McCarroll and Piacentini.[7] Later impact-parameter multistate PSS treatments[8-10] were unfortunately not Galilean invariant and did involve spurious long-range couplings.

Crothers and Hughes,[11] to be referred to as I, set out to improve the Bates-McCarroll theory by determining the momentum translation factors variationally, the exact molecular stationary states being already variational. In I an extremely accurate description of proton-hydrogen close-capture collision spectroscopy was given. In particular the locations of the turning points in the curve of capture probability against energy for large-angle scattering were found to be in excellent agreement with experiment[12] and to compare favorably with previous elaborate calculations.[13,14] More recently Crothers and Hughes,[15] to be referred to as II, have adopted the theory of I to provide a multistate molecular description which is both variational and Galilean invariant and which includes both rotational and radial physically meaningful couplings. The purpose of this Letter is to provide a timely preview of some of the results of II, which we compare and contrast with some experiments previously reported in this journal. In particular we concentrate attention on $2s$ charge exchange[16] and polarization.[17]

In the notation of I, we pose as *Ansatz* the wave function

$$\Psi(\vec{r}, t) = \textstyle\sum_q (c_q{}^+ \Phi_q{}^+ + c_q{}^- \Phi_q{}^-), \tag{1}$$

where

$$\Phi_q{}^\pm = \tfrac{1}{2}[(\chi_q{}^+ + \chi_q{}^-)\exp(-\tfrac{1}{2}ivzf) \pm (\chi_q{}^+ - \chi_q{}^-)\exp(+\tfrac{1}{2}ivzf)]\exp[-i\int_0^t(\epsilon_q{}^\pm(R) + \tfrac{1}{8}v^2f^2)dt'\}. \tag{2}$$

The "switching" function f is determined variationally and is illustrated by the solid line of Fig. 2 of I. In I we have already discussed its physical significance and have compared and contrasted our variational choice with a number of nonvariational choices, including the classical choice of Bates and McCarroll[4] (see Table I of I). The state amplitudes $c_q{}^\pm$ are likewise determined variationally so that substitution of Eq. (1) into Eq. (24) of I yields

$$iv\textstyle\sum_q S_{pq}{}^{\pm\pm}(dc_q{}^\pm/dz) = \sum_q F_{pq}{}^{\pm\pm} c_q{}^\pm, \tag{3}$$

where

$$S_{pq}{}^{\pm\pm} = \int \Phi_p{}^{\pm *}\Phi_q{}^\pm d^3r, \tag{4}$$

$$F_{pq}{}^{\pm\pm} = \int \Phi_p{}^{\pm *}(H_e - i\,d/dt_{\vec{r}})\Phi_q{}^\pm d^3r. \tag{5}$$

However, since at this stage of development we are primarily concerned with the 1–7-keV range we are content to retain just sufficient terms to give the coefficients in the coupled equations (3) correct to the second power. Then isolating the derivatives by rearrangement we obtain

$$iv\frac{dc_p{}^\pm}{dz} = \sum_q \{F_{pq}{}^{\pm\pm} - \sum_{r\neq p,q} S_{pr}{}^{\pm\pm} F_{rq}{}^{\pm\pm}\} c_q{}^\pm, \tag{6}$$

where

$$S_{pq}{}^{\pm\pm} \approx \pm\tfrac{1}{2}\exp\{-i\int_0^z[\epsilon_p{}^\pm(R) - \epsilon_q{}^\pm(R)]dz'/v\}[ivf(\mathcal{J}_{pq}{}^{-+} + \mathcal{J}_{pq}{}^{+-}) + \tfrac{1}{2}v^2f^2(\mathcal{Q}_{pq}{}^{--} - \mathcal{Q}_{pq}{}^{++})], \tag{7}$$

$$\begin{aligned} F_{pq}{}^{\pm\pm} = {} & \tfrac{1}{2}\exp\{-i\int_0^z[\epsilon_p{}^\pm(R) - \epsilon_q{}^\pm(R)]dz'/v\}\{iv[f(\epsilon_q{}^\pm - \epsilon_p{}^\pm)\mathcal{J}_{pq}{}^{\pm\mp} - 2\mathcal{R}_{pq}{}^{\pm\pm}] \\ & + \tfrac{1}{4}v^2[f^2(\epsilon_q{}^\mp + \epsilon_p{}^\mp - 2\epsilon_q{}^\pm)\mathcal{Q}_{pq}{}^{\mp\mp} + f^2(\epsilon_q{}^\pm - \epsilon_p{}^\pm)\mathcal{Q}_{pq}{}^{\pm\pm} \pm 4f(\mathcal{S}_{pq}{}^{-+} - \mathcal{S}_{pq}{}^{+-}) - 4(df/dz)\mathcal{J}_{pq}{}^{\pm\mp}]\}, \end{aligned} \tag{8}$$

$$\mathcal{J}_{pq}{}^{\pm\mp} = \int \chi_p{}^{\pm *} z \chi_q{}^\mp d^3r, \tag{9}$$

$$\mathcal{Q}_{pq}{}^{\pm\pm} = \int \chi_p{}^{\pm *} z^2 \chi_q{}^\pm d^3r, \tag{10}$$

$$\mathcal{R}_{pq}{}^{\pm\pm} = \int \chi_p{}^{\pm *}(\partial\chi_q{}^\pm/\partial z_{\vec{r}})\, d^3r, \tag{11}$$

$$\mathcal{S}_{pq}{}^{\pm\mp} = \int \chi_p{}^{\pm *} z(\partial\chi_q{}^\mp/\partial z_{\vec{r}}) d^3r. \tag{12}$$

In actual practice we solve (9) in the form

$$dc_p{}^\pm/dz = -\textstyle\sum_q A_{pq}{}^{\pm\pm} c_q{}^\pm \exp\{-i\int_0^z[\epsilon_q{}^\pm(\mathcal{R}) - \epsilon_p{}^\pm(\mathcal{R})]dz'/v\}, \tag{13}$$

but with $A_{pq}{}^{\pm\pm}$ and $A_{qp}{}^{\pm\pm *}$ replaced by their arithmetic average, as has been justified by a variation-perturbation treatment.[18] The well-defined radial and rotational components of $\mathcal{R}_{pq}{}^{\pm\pm}$ [Eq. (11)] are illustrated in II for various selections of the ten states $\chi_0{}^+(1s\sigma_g)$, $\chi_0{}^-(2p\sigma_u)$, $\chi_1{}^+(3d\pi_g)$, $\psi_1{}^-(2p\pi_u)$, $\chi_2{}^+(2s\sigma_g)$, $\chi_2{}^-(3p\sigma_u)$, $\chi_3{}^+(3d\sigma_g)$, $\chi_3{}^-(4f\sigma_u)$, $\chi_4{}^+(4d\pi_g)$, and $\chi_4{}^-(3p\pi_g)$.

Here we present an acid test of our theory, made possible by the measurements of Bayfield,[16] namely the 2*s* charge-exchange probability. In Fig. 1 we compare our six-state results at 6 keV with Bayfield, the four omitted states being $3d\pi_g$, $2s\sigma_g$, $3d\sigma_g$, and $4d\pi_g$. In fact, our ten-state results are virtually identical since *gerade* coupling is unimportant in the relevant impact range. Moreover, allowance for Coulomb repulsion has negligible affect in this θE range. Our agreement with Bayfield is excellent.

The results of Gaussorgues *et al.*[19] in this instance are an average of values obtained from the three-state molecular approach of McCarroll and Piacentini[7] and the four-state LCAO treatment of Gaussorgues and Salin.[20] Both theories neglect translation factors and in the molecular calculation the amplitude associated with the 2*s* asymptotic state is chosen to be half that associated with the $2p\pi_u$ state. This is a very poor assumption and accordingly agreement with experiment is very poor. The five-state molecular theory of Chidichimo-Frank and Piacentini[8] gives the correct order of magnitude in comparison with Bayfield[16] and ourselves. However, even this should be considered fortuitous in our view, since the neglect by these authors of both translation factors and radial couplings is particularly unjustifiable at 6 keV. A similar assessment is appropriate to Fig. 5 of Schinke and Krüger.[9]

Unfortunately, apart from Bayfield's measurement, there have been no other differential measurements above 2 keV, where the full significance of our approach might be adequately assessed. We are fairly confident, however, that our approach, based on a molecular PSS treatment, the velocity perturbations of which are determined variationally, is valid well into the keV range, and so we shall now consider total cross sections, concentrating attention on direct 2*p* excitation which provides a further acid test of our theory through the polarization of the emitted Lyman-α radiation.

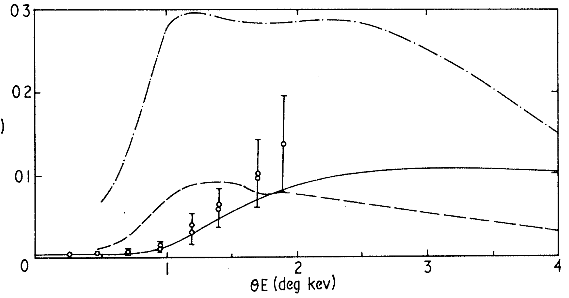

FIG. 1. Charge-exchange probability p_{2s}' of the 2*s* state of hydrogen plotted against the product of incident proton energy $E = 6$ (keV) and the laboratory scattering angle θ(deg). Solid line, this work; dash-dotted line, Gaussorgues *et al.* (Ref. 19); dashed line, Chidichimo-Frank and Piacentini (Ref. 8); circles, Bayfield (Ref. 16).

At energies below approximately 7 keV, the experimental data Morgan, Geddes, and Gilbody[21] exhibit a number of features which are consistent with a molecular description of the collision. In particular, they show that direct and exchange excitation are equally probable, which is consistent with our molecular model, since coupling between *gerade* states is very weak. Moreover, the experimental results show that the ratio of H(2*p*) to H(2*s*) production at low energies is much greater than unity. This is also consistent with the molecular model in which rotational coupling from the $2p\sigma_u$ to the $2p\pi_u$ channel [which dissociates to give H($2p_{\pm 1}$)] is the dominant inelastic component, while H(2*s*) production is enhanced mainly via $2p\sigma_u - 3p\sigma_u$ radial coupling which is of importance only in close encounters. However, as the energy increases from 1 to 7 keV, the probability of $2p_0$ production increases while that of $2p_{\pm 1}$ declines, and the probability of 2*s* production is increasingly reinforced by large-impact-parameter contributions. The former may be explained in terms of long-range rotational coupling between the $2p\pi_u$ and $4f\sigma_u$ states which cross near $16a_0$ as a result of the linear Stark effect. The latter, which results in a double-peaked structure, is due to long-range radial coupling between the $2p\sigma_u$, $3p\sigma_u$, and $4f\sigma_u$ states.

Although *gerade* coupling, especially the $1s\sigma_g$-$3d\sigma_g$ radial coupling, becomes significant for H(2*s*) production as the energy increases above 1 keV, it has little effect on the total 2*p* cross section below 7 keV, so that the six-state basis set ($1s\sigma_g$, $2p\sigma_u$, $2p\pi_u$, $3p\sigma_u$, $3p\pi_u$, $4f\sigma_u$) suffices. It is also important to note that translation factors have considerably more influence on total cross sections at large scattering angles. This is because the latter are governed primarily by nonadiabatic effects at small internuclear separations, where our switching function f is small. In II we present 2*s* and 2*p* direct and exchange total cross sections. Here we present in Fig. 2 our results for the polarization of the emitted Lyman-α radiation for direct excitation, given by[22]

$$\Pi = \frac{Q^d(2p_0) - Q^d(2p_{\pm 1})}{aQ^d(2p_0) + bQ^d(2p_{\pm 1})} \qquad (15)$$

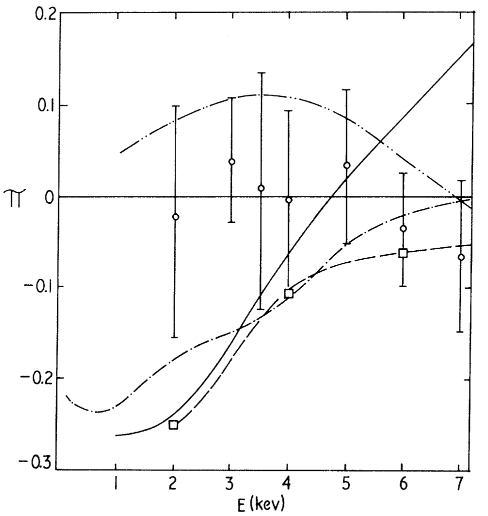

FIG. 2. The polarization Π of the Lyman-α radiation produced by direct excitation of hydrogen atoms by proton impact, against incident proton energy E (keV). Circles, Kauppila *et al.* (Ref. 17); solid line, this work (six states); dash-dotted line, Gaussorgues and Salin (Ref. 20); dashed line with squares, Rapp and Dinwiddie (Ref. 23); dash–double-dotted line, Gallaher and Wilets (Ref. 13).

in which $a = 2.375$ and $b = 3.749$. There is close accord with Rapp and Dinwiddie[23] at the lower energies but considerable disagreement with the experiment of Kauppila *et al.*[17] However, there is some doubt concerning the accuracy of the experimental values[20] and certainly a positive or nearly zero polarization value in the 1–3-keV range is at variance with the molecular model which predicts a value of -0.267 in the low-energy limit.

We conclude that the molecular PSS approach to low-energy homonuclear ion-atom collisions now appears to be a practical proposition and that valuable theoretical evidence may be adduced provided momentum translation factors are included in both rotational and radial couplings. We also conclude that it is necessary to determine specific momentum translation factors variationally as in I rather than merely to assume their existence.

In particular, our results for the 2*s* charge-exchange probability in proton–hydrogen-atom collisions over the 1–7-keV energy range are in excellent accord with experiment. In view of this and the discrepancy between theory and experiment for the polarization Π, a remeasurement of this quantity would appear desirable.

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