AOV05090 *PG PLRAA,00APR3AW026002R024

[1] E. Karule, in *Proceedings of the Fourth International Conference on the Physics of Electronic and Atomic Collisions, Quebec, 1965*, edited by L. Kerwin and W. Fite (Science Bookcrafters, Hastings-on-Hudson, New York, 1965), p. 139; Tr. Inst. Fiz. Akad. Nauk Latv. SSR 3, 33 (1965).

[2] E. Karule and R. Peterkop, in *Proceedings of the Fourth International Conference on the Physics of Electronic and Atomic Collisions, Quebec, 1965*, edited by L. Kerwin and W. Fite (Science Bookcrafters, Hastings-on-Hudson, New York, 1965), p. 134.

[3] R. Marriott and M. Rotenberg, *Proceedings of the Fifth International Conference on the Physics of Electronic and Atomic Collisions* (Nauka Publishing House, Leningrad, U.S.S.R., 1967), p. 379.

[4] P. G. Burke and A. J. Taylor, J. Phys. B **2**, 869 (1969).

[5] J. Perel, P. Englander, and B. Bederson, Phys. Rev. **128**, 1148 (1962).

[6] B. Bederson and L. J. Kieffer, Rev. Mod. Phys. **43**, 601 (1971).

[7] A. Kasdan, T. Miller, and B. Bederson, Proceedings of the Third International Conference on Atomic Physics, Boulder, 1972 (unpublished). Authors are thankful to Professor Benjamin Bederson for pointing out this reference and for sending a copy of the same before publication.

[8] I. Z. Vinkalns, E. M. Karule, and V. D. Obedkov, Opt. Spectrosk. **17**, 197 (1964) [Opt. Spectrosc. **17**, 105 (1964)].

[9] A. Temkin, Phys. Rev. **107**, 1004 (1957).

[10] W. B. Garrett, Phys. Rev. **140**, A705 (1965).

[11] P. M. Stone, Phys. Rev. **141**, 137 (1966).

[12] N. Feautrier and V. K. Lan, C.R. Acad. Sci. B **267**, 124 (1968).

[13] V. K. Lan, J. Phys. B **4**, 658 (1971).

[14] B. T. Dai and A. D. Stauffer, Can. J. Phys. **49**, 1670 (1971).

[15] K. C. Mathur, A. N. Tripathi, and S. K. Joshi, J. Phys. B **4**, L39 (1971).

[16] R. J. Glauber, in *Lectures in Theoretical Physics*, edited by W. E. Brittin *et al.* (Interscience, New York, 1959), Vol. 1, p. 315.

[17] E. Clementi, Tables of Atomic Functions, IBM J. Res. Dev. **9**, 2 (1965).

[18] K. C. Mathur, A. N. Tripathi, and S. K. Joshi, Phys. Lett. A **38**, 159 (1972).

[19] B. C. Saha, Kalpana Sarkar, and A. S. Ghosh (unpublished).

[20] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), p. 582.

[21] B. T. Dai and A. D. Stauffer, Can. J. Phys. **49**, 2527 (1971).

[22] T. Tietz, Nuovo Cimento **36**, 1365 (1965).

[23] S. B. Gupta, Ph.D thesis (Calcutta University, 1967) (unpublished).

[24] J. C. Crown and A. Russek, Phys. Rev. 138, A669 (1965).

PHYSICAL REVIEW A VOLUME 8, NUMBER 1 JULY 1973

Charge Exchange: Theory and Application to Proton-Hydrogen-Atom Collisions*†

Yehuda B. Band

Department of Physics, University of Chicago, Chicago, Illinois 60637

(Received 5 July 1972; revised manuscript received 11 December 1972)

A theory of rearrangement collisions taking account of the nonorthogonality of initial and final states is presented. Detailed discussion of the range of validity of the theory is worked out. The method is applied to proton-hydrogen-atom charge exchange collisions. We find that at high energy the Jackson-Schiff results are obtained and that below 100 kev the cross section is raised significantly above the result of Jackson and Schiff. The new result is in better agreement with experimental results than the calculations based on the Jackson-Schiff formulation.

I. INTRODUCTION

I shall describe charge exchange collisions of the type $A+(B+e^-)\rightarrow(A+e^-)+B$, where A and B are cores which are difficult to excite. In the initial state ψ_i the electron is associated with core B and $(B+e^-)$ has a relative momentum $\vec{k}_i(\hbar=1)$ with respect to A. The final state that we shall consider is that of the electron associated with core A and $(A+e^-)$ having relative momentum $\vec{k}_f$ with respect to B.

There have been many different approaches to calculating charge exchange transition probabilities. In the energy range we are concerned with, relative velocities of 10^8 cm/sec or greater, there have been Born-approximation calculations carried out by Brinkman and Kramers,[1] by Saha and Basu,[2] and by Jackson and Schiff.[3] The last of these included the intercore potential and on the basis of their results, Jackson and Schiff claim that its neglect is not justified. Within the Born approximation no account has been taken of the nonorthogonality of initial and final states. Some attempts have been made at taking the nonorthogonality into account by Bassel and Gerjuoy[4] and by Grant and Shapiro[5] using a distorted-wave approximation. To first order the distorted-wave results tend asymptotically to the Brinkman–Kramers cross section. Cheshire[6] has also calculated the resonant charge exchange cross section using a distorted-wave approximation. McCarroll and Salin[7] obtain the same asymptotic result at large energies as Cheshire. Cheshire[8] has also calculated the charge exchange cross section into excited states using the results of Jackson and Schiff.[3] An impact-parameter formalism using straight-line trajectories (from which differential cross sections cannot be obtained) has been employed by McCarroll,[9] Mittleman,[10] and McElroy[11] to obtain the total charge exchange cross sections into a given final state.

The approach used here is a time-dependent quantum-mechanical formulation with a two-state approximation. Section II describes the kinematics of the problem. Section III presents the method and discusses the range of validity of the model. Section IV applies the method to proton–hydrogen-atom collisions and compares our results to experiments and previous calculations. Section V is a summary.

II. KINEMATICS

As Bohr[12] pointed out, charge exchange is a three-body problem whereas excitation is a two-body problem. Consequently, we must be careful in our consideration of the kinematics as well as the potentials between particles. Cores A and B have masses M_A, M_B and coordinates $\vec{R}_A$, $\vec{R}_B$ with respect to an inertial frame. The electron has mass m and position $\vec{r}$ (see Fig. 1). We define the vectors $\vec{R}$, $\vec{r}_A$, $\vec{r}_B$, and $\vec{R}_{\text{c.m.}}$:

$$\vec{R}=\vec{R}_B-\vec{R}_A, \tag{1}$$

$$\vec{r}_A=\vec{r}-\vec{R}_A, \tag{2}$$

$$\vec{r}_B=\vec{r}-\vec{R}_B, \tag{3}$$

$$\vec{R}_{\text{c.m.}}=(1/M_T)(M_A\vec{R}_A+M_B\vec{R}_B+m\text{r}), \tag{4}$$

where $M_T=M_A+M_B+m$.

It will be convenient to define vectors $\vec{R}'_A$ and $\vec{R}'_B$ as

$$\vec{R}'_A=\vec{R}_A-\frac{m\vec{r}+M_B\vec{R}_B}{M_B+m}, \tag{5}$$

$$\vec{R}'_B=\vec{R}_B-\frac{m\vec{r}+M_A\vec{R}_A}{M_A+m}. \tag{6}$$

These are the relative coordinates between A and $(B+e)$, and B and $(A+e)$, respectively.

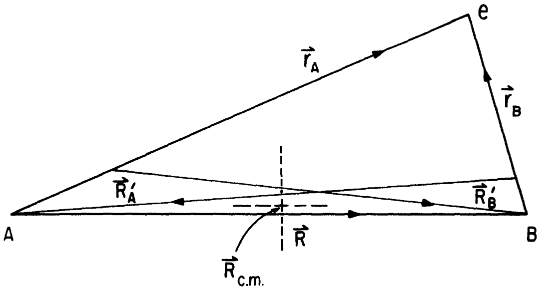

FIG. 1. Coordinate system.

The initial state consists of core A with momentum $\vec{k}_A$ and $(B+e)$ with momentum $\vec{k}_B$ in our inertial frame. In the c.m. frame, initially A and $(B+e)$ have relative momentum $\vec{k}_i$. The internal energy of $(B+e)$ in the initial state is β. The momentum and energy of the c.m. are constants of motion and are trivial to handle. The final state that we consider is $(A+e)$ and B with relative momentum $\vec{k}_f$ in the c.m. frame and $(A+e)$ has internal energy α.

The kinetic energy of the system is given by

$$T=\tfrac{1}{2}M_A\vec{V}_A^2+\tfrac{1}{2}M_B\vec{V}_B^2+\tfrac{1}{2}m\vec{v}^2. \tag{7}$$

It will be useful to find expressions for T in terms of two different sets of variables, $\{\vec{P}_{R'_A},\vec{P}_B\}$, where $\vec{P}_{R'_A}$ is the momentum of A with respect to $(B+e)$ and $\vec{P}_B$ is the momentum of e with respect to B, and $\{\vec{P}_{R'_B},\vec{P}_A\}$, where $\vec{P}_{R'_B}$ is the momentum of B with respect to $(A+e)$ and $\vec{P}_A$ is the momentum of e with respect to A. In order to express T in terms of $\{\vec{P}_{R'_A},\vec{P}_B\}$ we obtain the expressions of $\vec{V}_B$, $\vec{V}_A$, and $\vec{v}$ in terms of $\vec{V}'_A$ and $\vec{v}_B$ by using Eqs. (1)–(5) after they have been differentiated with respect to time. We find

$$\vec{V}_A=\frac{M_B+m}{M_T}\vec{V}'_A, \tag{8}$$

$$\vec{V}_B=-\frac{M_A}{M_T}\vec{V}'_A-\frac{m}{M_B+m}\vec{v}_B, \tag{9}$$

$$\vec{v}=\vec{V}_B+\vec{v}_B. \tag{10}$$

We conclude

$$T=\frac{1}{2}\frac{M_A(M_B+m)}{M_T}\vec{V}_A'^2+\tfrac{1}{2}m\vec{v}_B^2, \tag{11}$$

where we have dropped the c.m. kinetic energy. Similarly, in terms of $\vec{V}'_B$ and $\vec{v}_A$ we find

$$T=\frac{1}{2}\frac{M_B(M_A+m)}{M_T}\vec{V}_B'^2+\tfrac{1}{2}m\vec{v}_A^2. \tag{12}$$

We now define the eigenfunctions $\varphi_i(\vec{r}_B)$ and $\varphi_f(\vec{r}_A)$ which satisfy the equations

$$\begin{aligned}\left(-\frac{1}{2m}\nabla_{r_B}^2+V^B(\vec{r}_B)\right)\varphi_i(\vec{r}_B)&=\beta\,\varphi_i(\vec{r}_B),\\ \left(-\frac{1}{2m}\nabla_{r_A}^2+V^A(\vec{r}_A)\right)\varphi_f(\vec{r}_A)&=\alpha\,\varphi_f(\vec{r}_A),\end{aligned} \tag{13}$$

where $V^A(\vec{r}_A)$ and $V^B(\vec{r}_B)$ are potential energies of the electron in core A and B, respectively.

III. METHOD

When the Hamiltonian is expressed in terms of $\{\vec{P}_{R'_A},\vec{P}_B\}$ or $\{\vec{P}_{R'_B},\vec{P}_A\}$ and we quantize the theory and make the operator replacements

$$\frac{1}{i}\vec{\nabla}_{R'_A}\longleftrightarrow\vec{P}_{R'_A}\quad\text{and}\quad\frac{1}{i}\vec{\nabla}_{r_B}\longleftrightarrow\vec{P}_{r_B}$$

or

$$\frac{1}{i}\vec{\nabla}_{R'_B} \longleftrightarrow \vec{P}_{R'_B} \text{ and } \frac{1}{i}\vec{\nabla}_{r_A} \longleftrightarrow \vec{P}_{r_A},$$

we obtain the expression

$$\mathcal{H} = -\frac{1}{2\mu_i}\nabla^2_{R'_A} - \frac{1}{2m}\nabla^2_{r_B} + V^A(\vec{r}_A) + V^B(\vec{r}_B) + V^{AB}(\vec{R}) \tag{14}$$

or

$$\mathcal{H} = -\frac{1}{2\mu_f}\nabla^2_{R'_B} - \frac{1}{2m}\nabla^2_{r_A} + V^A(\vec{r}_A) + V^B(\vec{r}_B) + V^{AB}(\vec{R}), \tag{15}$$

where

$$\mu_i = \frac{M_A(M_B+m)}{M_T}, \quad \mu_f = \frac{M_B(M_A+m)}{M_T}$$

for the Hamiltonian operator depending upon which set of independent variables we choose.

So far we have not made any approximations. The Hamiltonian operator expressions are exact. Expanding the wave function in a complete set of basis functions which satisfy the initial conditions that at $t = -\infty$, we have the state

$$\psi(t=-\infty) = \varphi_i(\vec{r}_B)\, e^{-i\vec{k}_i \cdot \vec{R}'_A} e^{-i(\beta + k_i^2/2\mu_i)t}$$

will give the exact answer. We shall make a two-state approximation which consists of ignoring all states except the initial state and the particular final state of interest. A discussion of when such an approximation is justified will be given in what follows. We should actually consider a two-state wave function of the form given in the Appendix. However, as is shown in the Appendix the result is not changed by our approximation. We take our *Ansatz* wave function of the form

$$\psi(\vec{R}, \vec{r}, t) = b_i(t)\, \varphi_i(\vec{r}_B)\, e^{-i\vec{k}_i \cdot \vec{R}'_A} e^{-i(\beta + k_i^2/2\mu_i)t} + a_i(t)\, \varphi_f(\vec{r}_A)\, e^{i\vec{k}_f \cdot \vec{R}'_B} e^{-i(\alpha + k_f^2/2\mu_f)t}, \tag{16}$$

where $\vec{R}'_A$ and $\vec{R}'_B$ are given in Eqs. (5) and (6), respectively, and $a_f(t)$ and $b_f(t)$ are coefficients.

We now substitute the wave function into the Schrödinger equation to obtain

$$\begin{aligned} i\dot{b}_i(t)\, \varphi_i(\vec{r}_B)\, e^{-i\vec{k}_i \cdot \vec{R}'_A} e^{-iut} + i\dot{a}_f(t)\, \varphi_f(\vec{r}_A)\, e^{i\vec{k}_f \cdot \vec{R}'_B} e^{-i\nu t} &= [V^A(\vec{r}_A) + V^{AB}(\vec{R})]\, b_i(t)\, \varphi_i(\vec{r}_B)\, e^{-i\vec{k}_i \cdot \vec{R}'_A} e^{-iut} \\ &\quad + [V^B(\vec{r}_B) + V^{AB}(\vec{R})]\, a_f(t)\, \varphi_f(r_A)\, e^{i\vec{k}_f \cdot \vec{R}'_B} e^{-i\nu t}, \end{aligned} \tag{17}$$

where we have let

$$u = \beta + k_i^2/2\mu_i, \quad \nu = \alpha + k_f^2/2\mu_f.$$

We used the expression in Eq. (15) for the Hamiltonian when we operated on the term with coefficient $b_i(t)$ and Eq. (16) on the $a_f(t)$ term.

Now in the limit as $|R| \to \infty$, when $t \to \pm\infty$ we find that $\dot{a}(\pm\infty) = 0$; this is due to our choice of exponential t dependence and

$$\lim_{|R|\to\infty} V^{AB}(R) = 0, \quad \lim_{|R|\to\infty} V^A(r_A)\, \varphi_i(r_B) = 0,$$

$$\lim_{|R|\to\infty} V^B(r_B)\, \varphi_f(r_A) = 0.$$

The wave function in Eq. (16) is constructed so that the electron is carried with the moving cores A and B at infinite nuclear separation so that the difficulty pointed by Thorson[13] does not arise.

Before we continue with the method to obtain our results, we know enough about the model to discuss in what situations it may be applied. We are concerned with collisions of atoms, one of which $(B+e)$ has an electron that is more loosely bound than any of the rest (if there is more than one) so that, except for the "active" electron, the atom may be considered as a core. Examples are hydrogen and sodium atoms. Atom A must also be a core with respect to state $\varphi_f(\vec{r}_A)$.

We are interested in finding the charge exchange probability $|a_f(\infty)|^2$ in a particular state $\varphi_f(\vec{r}_A)$. To do so by this method, the probability of finding different excited states $\varphi_j(\vec{r}_B)$, excited core states [when more than one electron in $(B+e)$] and different states $\varphi_l(\vec{r}_A)$, must be small compared to the probability of elastic scattering. Also, no other channels besides the elastic one should couple strongly with $\varphi_f(\vec{r}_A)$. If these conditions are not met, then our two-state approximation is not valid.

Criteria governing the collision energy must also be met if we wish to use this model. The relative momentum of A and $(B+e)$, and $(A+e)$ and B should remain more or less constant for trajectories which contribute heavily to the charge exchange cross section.[14] That is, we require

$$k_i > \{\mu_i[V^A(\vec{r}_A) + V^{AB}(\vec{R})]\}^{1/2},$$

$$k_f > \{\mu_f[V^B(\vec{r}_B) + V^{AB}(\vec{R})]\}^{1/2}$$

for trajectories which contribute to charge exchange.[15] In what follows we shall substitute $|\psi_f\rangle$ and $|\psi_i\rangle$ for projections onto charge transfer and elastic channels of $|\psi^{(+)}\rangle$. This is justified when $ka > 1$ and $M\langle V\rangle a/k < 1$, that is, when the criteria for the validity of the Born approximation are satisfied. These conditions are satisfied in the collisions of light atoms A and B when the relative kinetic energy > 10 keV.

If the relative kinetic energy is above this limit and the other conditions are met, we expect that the method will work.

Taking the inner product (integral over $\vec{r}_A$ and $\vec{r}_B$) of $\varphi_i(\vec{r}_B)e^{-i\vec{k}_i\cdot\vec{R}'_A}$ with $\varphi_i(\vec{r}_B)e^{-i\vec{k}'_i\cdot\vec{R}'_A}$ we obtain

$$\iint \varphi_i^*(r_B)e^{i\vec{k}'_i\cdot\vec{R}'_A}\varphi_i(r_B)e^{-i\vec{k}_i\cdot\vec{R}'_A}d^3r_A d^3r_B$$
$$=\int |\varphi_i(\vec{r}_B)|^2\exp\left(-i(\vec{k}_i-\vec{k}'_i)\cdot\frac{M_B}{M_B+m}\vec{r}_B\right)d^3r_B$$
$$\times\int e^{i(\vec{k}_i-\vec{k}'_i)\cdot\vec{r}_A}d^3r_A=(2\pi)^3\,\delta^3(\vec{k}_i-\vec{k}'_i).$$

The integral over $\vec{r}_B$ is always finite. We have chosen to normalize in an infinite volume which is why we obtained the Dirac δ function rather than the Kronecker δ. The δ function is handled by taking a narrow wave packet about $\vec{k}'_i$ in the usual fashion.

We multiply Eq. (17) by $\varphi_i^*(r_B)e^{+i\vec{k}'_i\cdot\vec{R}'_A}e^{iut}$ and integrate over $\vec{r}_A$ and $\vec{r}_B$ (which is equivalent to integrating over r_B and R'_A) to deduce

$$i[\dot{b}_i(t)+\dot{a}_f(t)S_{if}e^{i(u-\nu)t}]=b_i(t)h^A_{ii}+a_f(t)h^B_{if}e^{i(u-\nu)t}. \tag{18}$$

We multiply Eq. (17) similarly, by $\varphi_f^*(\vec{r}_A)e^{-i\vec{k}'_f\cdot\vec{R}'_B}\times e^{i\nu t}$ and integrate over $\vec{r}_A$ and $\vec{r}_B$ to deduce

$$i[\dot{a}_f(t)+\dot{b}_i(t)S_{fi}e^{-i(u-\nu)t}]=a_f(t)h^B_{ff}+b_i(t)h^A_{fi}e^{-i(u-\nu)t}, \tag{19}$$

where

$$S_{fi}=S^*_{if}=\frac{1}{(2\pi)^3}\int d^3r_A\,\varphi_f^*(\vec{r}_A)\exp\left\{-i\left[\vec{k}_f\left(1-\frac{m}{M_A+m}\right)-\vec{k}_i\right]\cdot\vec{r}_A\right\}$$
$$\times\int d^3r_B\,\varphi_i(\vec{r}_B)\exp\left\{i\left[\vec{k}_f-\vec{k}_i\left(1-\frac{m}{M_B+m}\right)\right]\cdot\vec{r}_B\right\}, \tag{20}$$

$$h^A_{ii}=\frac{1}{(2\pi)^3}\int d^3R\left[V^{AB}(\vec{R})+\int d^3r_B\,\varphi_i^*(\vec{r}_B)\varphi_i(\vec{r}_B)\,V^A(\vec{r}_B-\vec{R})\right], \tag{21}$$

$$h^B_{ff}=\frac{1}{(2\pi)^3}\int d^3R\left[V^{AB}(\vec{R})+\int d^3r_A\,\varphi_i^*(\vec{r}_A)\,\varphi_i(\vec{r}_A)\,V^B(\vec{r}_A-\vec{R})\right], \tag{22}$$

$$h^B_{if}=\frac{1}{(2\pi)^3}\int d^3r_A\int d^3r_B\,\varphi_i^*(\vec{r}_B)\exp\left\{-i\left[\vec{k}_f-\vec{k}_i\left(1-\frac{m}{M_B+m}\right)\right]\cdot\vec{r}_B\right\}\,[V^{AB}(\vec{r}_A-\vec{r}_B)+V^B(\vec{r}_B)]\varphi_f(\vec{r}_A)$$
$$\times\exp\left\{i\left[\vec{k}_f\left(1-\frac{m}{M_A+m}\right)-\vec{k}_i\right]\cdot\vec{r}_A\right\}, \tag{23}$$

and

$$h^A_{fi}=\frac{1}{(2\pi)^3}\int d^3r_A\int d^3r_B\,\varphi_f^*(\vec{r}_A)\exp\left\{-i\left[\vec{k}_f\left(1-\frac{m}{M_A+m}\right)-\vec{k}_i\right]\cdot\vec{r}_A[V^{AB}(\vec{r}_A-\vec{r}_B)+V^A(\vec{r}_A)]\varphi_i(\vec{r}_B)\right.$$
$$\left.\times\exp\left\{i\left[\vec{k}_f-\vec{k}_i\left(1-\frac{m}{M_B+m}\right)\right]\cdot\vec{r}_B\right\}\right.. \tag{24}$$

Rearranging Eqs. (18) and (19), we obtain

$$i(1-|S_{fi}|^2)\dot{b}_i(t)=(h^A_{ii}-S_{if}h^A_{fi})b_i(t)$$
$$+(h^B_{if}-S_{if}h^B_{ff})e^{i(u-\nu)t}a_f(t) \tag{25}$$

and

$$i(1-|S_{fi}|^2)\dot{a}_f(t)=(h^B_{ff}-S_{fi}h^B_{if})a_f(t)$$
$$+(h^A_{fi}-S_{fi}h^A_{ii})e^{-i(u-\nu)t}b_i(t). \tag{26}$$

The form of these equations is determined, not by the specific model but by the fact that we used a two-state *Ansatz* wave function, the two states not being orthogonal, and the time-dependent Schrödinger equation.[16] It is the form of the S and h's that is determined by the Hamiltonian and the expressions $\varphi_i(r_B)e^{-i\vec{k}_i\cdot\vec{R}_{A'}}$, $\varphi_f(r_A)e^{i\vec{k}_f\cdot\vec{R}_{B'}}$.

The initial conditions are

$$|b_i(t=-\infty)|=1,\quad |a_f(t=-\infty)|=0. \tag{27}$$

We shall solve Eqs. (25) and (26) for $|a_f(t)|$ in perturbation theory. The solution obtained will be identical to the solution of the problem based on a wave function allowing elastic and charge exchange scattering into any solid angle, as shown in the Appendix. Into the left-hand side of (26), we substitute the zero-order coefficients $a^0(t)=a(t=-\infty)=0$ and $b^0(t)=b(-\infty)=1$ and find, for large values of t, that

$$|a_{f,\Omega_f}(t)|^2=2\pi\left|\frac{h_{fi}-S_{fi}h_{ii}}{1-|S_{fi}|^2}\right|^2 t\,\delta(u-\nu)\ . \tag{28}$$

We can now compute the charge exchange (C. E.) differential cross section

$$\frac{d\sigma^{\text{C.E.}}}{\sigma\Omega}=2\pi\overline{\sum_{\{i\}\{f\}}}\left|\frac{h^A_{fi}-S_{fi}h^A_{ii}}{1-|S_{fi}|^2}\right|^2 k_f^2\frac{dk_f}{d\nu}\bigg/\frac{1}{(2\pi)^3}\frac{k_i}{\mu}$$
$$=(2\pi)^4\frac{k_f}{k_i}(\mu)^2\overline{\sum_{\{i\}\{f\}}}\left|\frac{h^A_{fi}-S_{fi}h^A_{ii}}{1-|S_{fi}|^2}\right|^2, \tag{29}$$

where the sum over final and average of initial states are taken. We should comment at this point that the relative velocity should be large enough to justify using the Born approximation. This point will be discussed again in Sec. IV when we discuss the comparisons with experimental results.

Our expression for the cross section has the feature that a shift in the definition of the zero of energy will not affect the result. This is not the case in the standard Born approximation for rearrangement collisions because of the nonorthogonality of initial and final states.[17] The Born term h^A_{fi} is corrected in our expression for this effect. We shall now apply (29) to a simple example to investigate the corrections to the Born term and to compare our expression to experiment.

IV. PROTON-HYDROGEN-ATOM COLLISIONS

Perhaps the simplest application of the theory just presented is to collisions involving proton and hydrogen atom. Since in this system there is but one electron, the full potentials of the nuclei are felt by the electron (no screening) and there are no correlation effects due to other electrons. The initial and final wave functions of the electron are hydrogenic orbitals which are easy to work with. The identity of protons may be ignored in the energy range we are concerned with and negligible error results. This is because the cross section for charge exchange is peaked in the forward direction; hence in practice the protons are distinguishable.[3]

A word of caution concerning application of the theory to systems like $H^+ + H_2$ or $H^+ + He$ is in order. There is no *a priori* reason to assume that the correlation effects of the electrons in such systems will not greatly affect the charge exchange cross sections. Also, excitation of the "second" electron may have a large effect on the charge exchange cross section. Extreme caution should be applied when considering such systems where correlation effects between electrons are important when considering charge exchange.

The electron is initially on proton B in a 1s state. The potential energies are

$$V^B(r_B)=-1/r_B\ , \tag{30}$$

$$V^A(r_A)=-1/r_A, \tag{31}$$

$$V^{AB}(R)=1/R=1/|\vec{r}_A-\vec{r}_B|\ , \tag{32}$$

where $e=1$ and from now on atomic units are used throughout. The final state will have the electron in some state (nlm) about proton A where the quantization axis may be considered along $\vec{k}_i$. In the evaluation of cross section (29) the matrix elements h^A_{fi}, S_{fi}, and h^A_{ii} appear. To compute h^A_{fi} and S_{fi}, it is convenient, following Brinkman and Kramers, to use $\vec{r}_A$ and $\vec{r}_B$ as the independent coordinates in the evaluation of the integrals. When this is done we find,[3] from (20) and (24)

$$S_{fi}=\frac{1}{(2\pi)^3}\varphi_f^*(\vec{C})\varphi_i(\vec{B})\ , \tag{33}$$

$$h^A_{fi}=\frac{1}{(2\pi)^3}\left[-\left(\frac{C^2}{2}+|\alpha|\right)\varphi_f^*(\vec{C})\varphi_i(\vec{B})+\frac{1}{2\pi^2}\int\frac{d^3k}{k^2}\varphi_f^*(\vec{C}-\vec{k})\varphi_i(\vec{B}-\vec{k})\right], \tag{34}$$

where we have defined

$$\vec{B}=\vec{k}_f-\vec{k}_i\left(1-\frac{m}{M_B+m}\right), \tag{35}$$

$$\vec{C}=\vec{k}_f\left(1-\frac{m}{M_A+m}\right)-\vec{k}_i\ , \tag{36}$$

and the Fourier transform of the wave functions

$$\varphi(\vec{p})=\int e^{i\vec{p}\cdot\vec{r}}\varphi(\vec{r})d^3r\ . \tag{37}$$

For hydrogenic orbitals about a nucleus with charge Z,[18]

$$\varphi_{nlm}(\vec{p})=(2\pi)^{3/2}Y_{lm}(\Omega_p)F_{nl}(p)\ , \tag{38}$$

$$F_{nl}(p)=\left(\frac{2n(n-l-1)!}{\pi(n+l)!}\right)^{1/2}\frac{2^{2(l+1)}l\,!}{\gamma^{3/2}}\times\frac{(p/\gamma)^l}{[(p/\gamma)^2+1]^{l+2}}C^{l+1}_{n-l-1}\left(\frac{(p/\gamma)^2-1}{(p/\gamma)^2+1}\right)\ , \tag{39}$$

where $\gamma=Z/n$, $C^{l+1}_{n-l-1}(x)$ is the Gegenbauer function, and p is in atomic units.

The matrix element h^A_{ii} is easily evaluated if one uses the independent coordinates $\vec{R}$ and $\vec{r}_B$ in the integral. From (21) we see

$$h^A_{ii}=\frac{1}{(2\pi)^3}\int d^3R\left(\frac{1}{R}-\int d^3r_B\,|\varphi_i(r_B)|^2\frac{1}{|r_B+R|}\right)\ , \tag{40}$$

which for $(n,\ l=0)$ states is

$$h^{A}_{ii}=\frac{(n-1)!}{4\pi^2 n(n!)^3 z^3}\int_0^\infty dR\,R^2\int_{2\gamma R}^\infty dx\,xe^{-x}L^{(1)}_{n-1}(x)\left(\frac{x}{R}-2\gamma\right), \tag{41}$$

where $L^{(1)}_{n-1}(x)$ is an associated Laguerre function. We shall be concerned with the initial state, a 1S state, when dealing with $H^+ + H$, for which we obtain[19]

$$h_{ii}=1/4\pi^2 . \tag{42}$$

The matrix element which appears in the charge exchange cross section

$$M=\frac{M'}{1-|S_{fi}|^2}=\frac{h^A_{fi}-S_{fi}h^A_{ii}}{1-|S_{fi}|^2} \tag{43}$$

for transitions $1s\rightarrow nlm$, becomes with the aid of Eqs. (33), (34), and (42),

$$M=\left[-\frac{1}{2}\left(C^2+\frac{1}{n^2}+\frac{1}{2\pi^2}\right)F_{nl}(C)Y^*_{lm}(\Omega_C)F_{10}(B)\frac{1}{(4\pi)^{1/2}}+\frac{1}{2\pi^2}\int\frac{d^3k}{k^2}F_{nl}(|\vec{C}-\vec{k}|)Y^*_{lm}(\Omega_{\vec{C}-\vec{k}})\times F_{10}(|\vec{B}-\vec{k}|)\frac{1}{(4\pi)^{1/2}}\right]\Big/\left[1-\left(F_{nl}(C)Y^*_{lm}(\Omega_C)F_{10}(B)\frac{1}{(4\pi)^{1/2}}\right)^2\right] . \tag{44}$$

The "Born term" of the charge exchange matrix element, in the treatment by Jackson and Schiff,

$$M_{JS}=-\frac{1}{2}\left(C^2+\frac{1}{n^2}\right)F_{nl}(C)Y^*_{lm}(\Omega_C)F_{10}(B)\frac{1}{(4\pi)^{1/2}}+\frac{1}{2\pi^2}\int\frac{d^3k}{k^2}F_{nl}(|\vec{C}-\vec{k}|)Y^*_{lm}(\Omega_{\vec{C}-\vec{k}})\times F_{10}(|\vec{B}-\vec{k}|)\frac{1}{(4\pi)^{1/2}} , \tag{45}$$

is corrected by the term in the denominator of Eq. (44) which is $1-|S_{fi}|^2$ and by the term $h^A_{ii}S_{fi}$ in the numerator. We see that as long as C^2+1/n^2 is much larger than $1/2\pi^2$ and the two terms in M_{JS} do not cancel each other, then the $h^A_{ii}S_{fi}$ correction is unimportant. When $|S_{fi}|^2$ is small compared with 1 the denominator correction term is unimportant.

To find the charge exchange cross section to a given state (nlm) as a function of c.m. energy, $\frac{1}{2}E$, and scattering angle θ, we must express B^2 and C^2 in terms of these variables. This can be done by using Eqs. (35) and (36) and the conservation-of-energy relation $u=v$ so that k_f^2 is found in terms of α, β, and k_i^2. When this is done for equal-mass particles $M_A=M_B=M$ to lowest order in m/M we obtain for transitions into the ground state

$$B^2=C^2=E(1+\lambda),\quad (\vec{B}-\vec{C})^2=2E(1+\cos\theta)\simeq 4E, \tag{46}$$

where the last equality is made since the cross section will be extremely peaked, and

$$E=\left(\frac{m}{M+m}\right)^2 k_i^2 , \tag{47}$$

$$\lambda=4\left(\frac{M+m}{m}\right)^2\sin^2\tfrac{1}{2}\theta . \tag{48}$$

When E is measured in units of 100 keV then

$$E=\tfrac{1}{4}V^2 ,$$

where V is in atomic units.

The integral over $\vec{k}$ in Eq. (44) can be evaluated explicitly for transitions $(1S)\rightarrow(1S)$[3,4,20]

$$I'=\frac{1}{2\pi^2}\int\frac{d^3k}{k^2}\varphi^*_{1s}(|\vec{C}-\vec{k}|)\varphi_{1s}(|\vec{B}-\vec{k}|)=\frac{32}{\pi}\int\frac{d^3k}{k^2}\frac{1}{[(\vec{C}-\vec{k})^2+b^2]^2[(\vec{B}-\vec{k})^2+a^2]^2}=\frac{8}{\pi}\frac{1}{ab}\frac{\partial^2 L(-\vec{B},a;-\vec{C},b)}{\partial a\,\partial b}\bigg|_{a=1,b=1} , \tag{49}$$

where

$$L=\int\frac{d^3k}{k^2}\frac{1}{[(\vec{C}-\vec{k})^2+a^2][(\vec{B}-\vec{k})^2+b^2]}=\frac{2\pi^2}{(x-y^2)^{1/2}}\arctan\left(\frac{(x-y^2)^{1/2}}{y}\right) ,$$

$$x=[(\vec{B}-\vec{C})^2+(a+b)^2](B^2+a^2)(C^2+b^2), \tag{50}$$

$$y=b(B^2+a^2)+a(C^2+b^2).$$

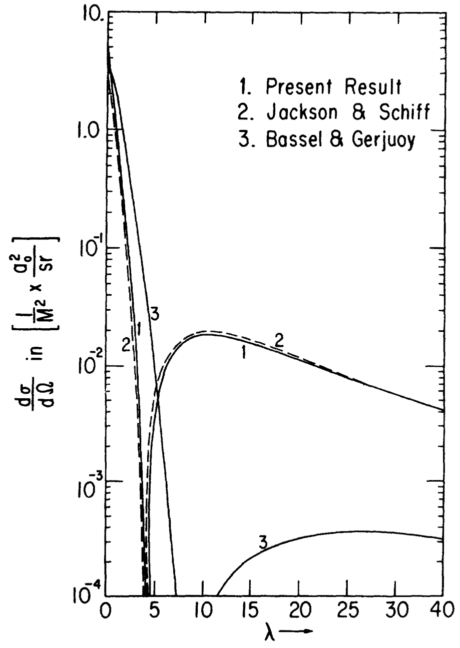

FIG. 2. Comparison of angular distributions at 25-keV proton energy.

With a little algebra we find

$$M_{1s\to 1s}=\frac{32\pi}{(2\pi)^3}\left(\left\{-\left[1+\frac{1}{2\pi^2[E(\lambda+1)+1]}\right]+\left(\frac{1}{2}+\frac{\lambda}{4}\right)\frac{\arctan E^{1/2}}{E^{1/2}}\right\}\frac{1}{[E(\lambda+1)+1]^3}+\frac{1}{8(E+1)^2[E(\lambda+1)+1]}-\frac{\lambda}{4(E+1)[E(\lambda+1)+1]^3}\right)\Big/\left[1-\left(\frac{8}{\pi^2[E(\lambda+1)+1]^4}\right)^2\right] \tag{51}$$

and therefore

$$\frac{d\sigma^{\text{C.E.}}}{d\Omega}=64\,M^2\left(\left\{-\left[1+\frac{1}{2\pi^2[E(\lambda+1)+1]}\right]+\left(\frac{1}{2}+\frac{\lambda}{4}\right)\frac{\arctan E^{1/2}}{E^{1/2}}\right\}\frac{1}{[E(\lambda+1)+]^3}+\frac{1}{8(E+1)^2[E(\lambda+1)+1]}-\frac{\lambda}{4(E+1)[E(\lambda+1)+1]^3}\right)^2\Big/\left(1-\frac{0.6570}{[E(\lambda+1)+1]^8}\right)^2 . \tag{52}$$

We can now see explicitly when the h_{ii}, S_{fi}, and $[1/(1-|S_{fi}|^2)]^2$ corrections will be important for the $1S\to 1S$ transition. We note that for forward scattering ($\lambda=0$), $h_{ii}^A S_{fi}$ will give a small contribution. At $E=0.25$ (proton lab energy of 25 keV) the differential cross section at $\lambda=0$ is increased by a factor of 1.52 over the Jackson–Schiff result. For comparison of results on the differential cross section at 25-keV proton energy with those of Jackson and Schiff and Bassel and Gerjuoy, see Fig. 2.

Before the arguments advanced in this paper it might have been concluded that the dip in Fig. 2 was due to the nonorthogonality of initial and final state. The argument is as follows: Since $|f\rangle$ is not orthogonal to $|i\rangle$ we can write

$$|f\rangle=|\perp\rangle\langle\perp|f\rangle+|i\rangle\langle i|f\rangle=|\perp\rangle S_{\perp f}+|i\rangle S_{if},$$

where $|\perp\rangle$ is perpendicular to $|i\rangle$. Therefore in the Jackson-Schiff Born approximation we could write

$$\begin{aligned}\langle f|V|i\rangle&=S_{f\perp}\langle\perp|V|i\rangle+S_{fi}\langle i|V|i\rangle\\&=S_{f\perp}\langle\perp|V|i\rangle+S_{fi}(1/4\pi^2)\,.\end{aligned}$$

Now at the angle at which the dip appears, perhaps the two terms cancel. Since the dip appears in our method as well, where we have

$$M=\frac{\langle f|V|i\rangle-S_{fi}\langle i|V|i\rangle}{1-|S_{fi}|^2}$$

we conclude that the nonorthogonality is not the cause for the dip.

To get the total $1S\to 1S$ cross section we integrate over all angles. Since the cross section is extremely peaked in the forward direction

$$\int|M|^2d\Omega\simeq\pi(m/M)^2\int_0^\infty|M|^2d\lambda. \tag{53}$$

If we were to neglect $h_{ii}^A S_{fi}$ and the denominator corrections, we would obtain the Jackson and Schiff cross section

$$\sigma_{1s\to 1s}^{\text{JS}}=\frac{2^6X}{5E(E+1)^5}(\pi a_0^2)\,, \tag{54}$$

where

$$X=\frac{1}{192}\left(127+\frac{14}{E}+\frac{2}{E^2}\right)-\frac{1}{96}\frac{\arctan E^{1/2}}{E^{1/8}}\left(83+\frac{15}{E}+\frac{2}{E^2}\right)+\frac{1}{96}\frac{\arctan E^{1/2}}{E^{1/2}}\left(31+\frac{8}{E}+\frac{1}{E^2}\right). \tag{55}$$

When the correction terms are taken into account we find the cross section substantially raised even for energies past 100 keV (see Fig. 3). At 25 keV our result is 28% larger than σ_{JS}. At an energy of 1 MeV our result is only 1% larger.

To obtain our total cross section we choose a

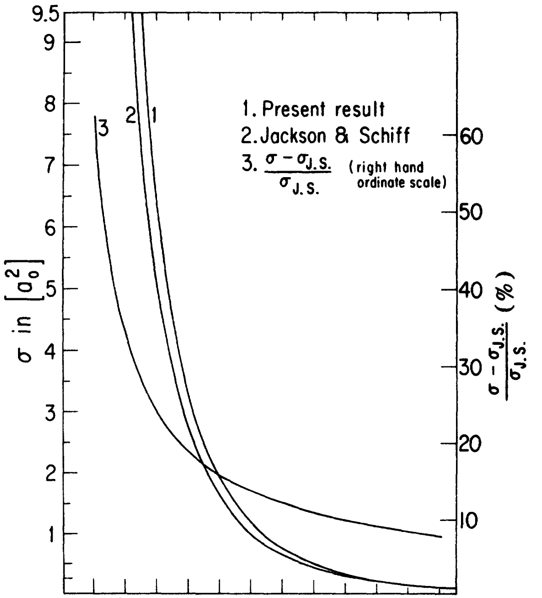

FIG. 3. Charge exchange cross section $1S\to 1S$ in (a_0^2). Right-hand ordinate is $(\sigma-\sigma_{\text{JS}})/\sigma_{\text{JS}}$ (%).

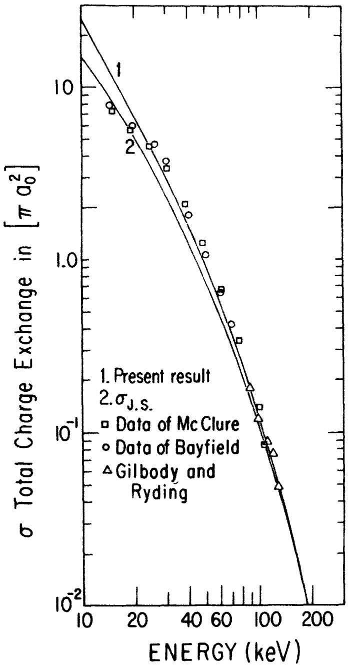

FIG. 4. Total charge exchange cross section (πa_0^2).

range of λ in which the correction terms are not negligible (i.e., $0<\lambda<20$ for 25 keV), and subtract our differential cross section from that of Jackson and Schiff in the range, integrate this difference over the range of λ and add this to σ_{JS}.

By multiplying our ground-state cross section σ_{1S-1S} by the ratio determined by Jackson and Schiff using scaling laws postulated in their paper, we would expect a reasonable estimate of the total charge exchange cross section. Figure 4 compares our calculation with that of Jackson and Schiff and the data of McClure,[21] Bayfield,[22] and Gilbody and Ryding.[23] Below 25 keV the data begin to drop below our calculation. This is owing to the breakdown of the Born approximation. Above 25 keV we can see that the correction terms to the Jackson-Schiff cross section help to bring about better agreement between theory and experiment. Between 25 and 90 keV our curve is lower than the data of McClure and Bayfield by about 15%. From 90 keV and above our curve lies on the data points of McClure and Gilbody and Ryding.

V. CONCLUSION

We have presented a method of calculation for cross sections of rearrangement collisions that includes the effects of the nonorthogonality of initial and final states; the nonorthogonality is due to the fact that the initial and final zero-order Hamiltonians are different. The method was applied to the charge transfer collision $P+H(1S)\rightarrow H(1S)+P$. In so doing we have justified Jackson and Schiff's calculation in the sense that the correction effects to the differential and total cross section, although significant on the scale of precision of experimental data, do not affect the magnitudes of shapes greatly. The cross section $1S\rightarrow 1S$ increased in this treatment by 28% at 25-keV proton energy and by 8% at 100 keV, above the Jackson-Schiff result. We estimate the energy range in which the method is expected to yield satisfactory results. Using the Jackson-Schiff scaling laws we find agreement of the theoretical and the experimentally determined total cross section.

Charge exchange scattering into higher states (nl, $l=0, 1, \ldots$) as well as perturbation effects of the proton on the ionization electrons that come off in the forward peak are now being studied.

ACKNOWLEDGMENTS

The author would like to express his gratitude to Professor R. Stephen Berry for his encouragement and interest and for reading the manuscript.

APPENDIX

I have been a bit cavalier in the *Ansatz* wave function (16). We should, until otherwise justified, consider a two-state wave function of the form

$$\Psi(Rrt)=e^{-iut}\varphi_i(\vec{r}_B)\int d\Omega_i b_{i,\Omega_i}(t)e^{-i\vec{k}_i\cdot\vec{R}'_A}+e^{-i\nu t}\varphi_f(\vec{r}_A)\int d\Omega_f a_{f,\Omega_f}(t)e^{i\vec{k}_f\cdot\vec{R}'_B}, \quad \text{(A1)}$$

where Ω_i and Ω_f are the directions in which $\vec{k}_i$ and $\vec{k}_f$ point. We impose initial conditions

$$b_{i,\Omega_i}(-\infty)=\delta(\Omega_i),\quad a_{f,\Omega_f}(-\infty)=0\,. \quad \text{(A2)}$$

Such a wave function allows elastic and inelastic scattering into the charge exchange channel in which we are interested, in all directions. After making arguments similar to those made in the text we obtain an equation of the form (17):

$$ie^{-iut}\varphi_i(\vec{r}_B)\int d\Omega'_i\dot{b}_{i,\Omega'_i}(t)e^{-i\vec{k}'_i\cdot\vec{R}'_A}+ie^{-i\nu t}\varphi_f(r_A)\int d\Omega'_f\dot{a}_{f,\Omega'_f}(t)e^{i\vec{k}'_f\cdot\vec{R}'_B}$$

$$=[V^A(\vec{r}_A)+V^{AB}(\vec{R})]e^{-iut}\varphi_i(\vec{r}_B)\int d\Omega'_i b_{i,\Omega'_i}(t)e^{-\vec{k}'_i\cdot\vec{R}'_A}+[V^B(\vec{r}_B)+V^{AB}(\vec{R})]e^{-i\nu t}\varphi_f(\vec{r}_A)\int d\Omega'_f a_{f,\Omega'_f}(t)e^{i\vec{k}'_f\cdot\vec{R}'_B}, \quad \text{(A3)}$$

where the prime on the momentum vector refers to the fact that its direction is in the solid angle $\Omega'_{i,f}$. By taking inner products with $e^{-i\vec{k}_i\cdot\vec{R}'_A}\varphi_i(\vec{r}_B)$ and $e^{-i\vec{k}_f\cdot\vec{R}'_B}\varphi_f(\vec{r}_A)$ we obtain

$$i\dot{a}_{f,\Omega_f}(t)+ie^{-i(u-v)t}\int d\Omega_i'\,\dot{b}_{i,\Omega_i'}(t)S_{fi}(\Omega_f,\Omega_i')=\int d\Omega_f'\,a_{f,\Omega_f'}(t)h_{ff}^{B}(\Omega_f,\Omega_f')+e^{-i(u-v)t}\int d\Omega_i'\,b_{i,\Omega_i'}(t)\,h_{fi}(\Omega_f\Omega_i')\,, \tag{A4}$$

$$i\dot{b}_{i,\Omega_i}(t)+ie^{i(u-v)t}\int d\Omega_f'\,\dot{a}_{f,\Omega_f'}(t)S_{if}(\Omega_i\Omega_f')=\int d\Omega_i'\,b_{i,\Omega_i'}(t)h_{ii}(\Omega i,\Omega_i')+e^{i(u-v)t}\int d\Omega_f'\,a_{f,\Omega_f'}(t)h_{if}(\Omega_i,\Omega_f')\,, \tag{A5}$$

where

$$S_{fi}(\Omega_f,\Omega_i')=\frac{1}{(2\pi)^3}\int d^3r_A\,d^3r_B\,\varphi_f^{*}(\vec{r}_A)\,e^{-i\vec{k}_f\cdot\vec{R}_B'}\,\varphi_i(r_B)e^{-i\vec{k}_i'\cdot\vec{R}_A'}\,,$$

$$h_{ff}^{B}(\Omega_f,\Omega_f')=\frac{1}{(2\pi)^3}\int d^3r_A\,d^3r_B\,\varphi_f^{*}(r_A)e^{-i\vec{k}_f\cdot\vec{R}_B'}\,[V^B(\vec{r}_B)+V^{AB}(\vec{R})]\varphi_f(r_A)e^{i\vec{k}_f'\cdot\vec{R}_B'}\,, \tag{A6}$$

etc.

We solve Eqs. (A4) and (A5) thus: (i) Solve using perturbation theory taking $b_{i,\Omega_i}(t)=\delta(\Omega_i)$ and $a_{f,\Omega_f}(t)=0$ on the right-hand side of the equations; (ii) when solving for $a_{f,\Omega_f}(t)$, break the integrals on the left-hand side in the following way:

$$\int d\Omega_i'\,\dot{b}_{i,\Omega_f'}(t)\,S_{fi}(\Omega_f,\Omega_i')=\dot{b}^{(1)}_{i,\Omega_i'=0}(t)S_{fi}(\Omega_f,\Omega_i'=\hat{0})$$
$$+\int' d\Omega_i'\,\dot{b}_{i,\Omega_i'}(t)S_{fi}(\Omega_f,\Omega_i')\,,$$

where the prime on the integral sign means that $\Omega_i'=\hat{0}$ should not be included. Now neglect the primed integrals in solving for $a_{f,\Omega_f}(t)$.

This is a reasonable procedure: The $a_{f,\Omega_f}(t)$, and $b_{i,\Omega_i'}(t)$ $(\Omega_i'\neq 0)$ would be first order in the interaction, and they are multiplied by the small parameters $S_{if}(\Omega_i,\Omega_f)$ and $S_{fi}(\Omega_f,\Omega_i)$, respectively, so these terms should not be taken into account when computing $a_{f,\Omega_f}(t)$ to first order in perturbation theory. Using this procedure we obtain

$$i\dot{a}_{f,\Omega_f}(t)=\frac{h_{fi}^{A}-S_{fi}h_{ii}^{A}}{1-|S_{fi}|^2}e^{-i(u-v)t}\,,$$

where all symbols are defined in Eq. (28).

Without condition (ii), we would obtain

$$a_{f,\Omega_f}(t)$$
$$=-i\,\frac{h_{fi}^{A}(\Omega_f,\Omega_i=\hat{0})-\int d\Omega_i'\,S_{fi}(\Omega_f,\Omega_i')h_{ii}^{A}(\Omega_i',\Omega_i=\hat{0})}{1-\int d\Omega_i'\,S_{fi}(\Omega_f,\Omega_i')S_{if}(\Omega_i',\Omega_f)}\,,$$

which is more difficult to calculate.

---

[*] Submitted to the Department of Physics of the University of Chicago in partial fulfillment of the requirements for the degree of Ph. D.

[†] Work supported by the National Science Foundation under Grant No. GP26493, and The Advanced Research Projects Agency under Contract No. DAHC 15-67-C-0220.

[1] H. C. Brinkman and H. A. Kramers, Proc. Acad. Sci. Amsterdam **33**, 973 (1930).

[2] M. N. Saha and D. Basu, Indian J. Phys. **19**, 121 (1945).

[3] J. D. Jackson and H. Schiff, Phys. Rev. **89**, 359 (1953).

[4] R. H. Bassel and E. Gerjuoy, Phys. Rev. **117**, 749 (1960).

[5] J. Grant and J. Shapiro, Proc. Phys. Soc. Lond. **86**, 1007 (1965).

[6] J. M. Cheshire, Proc. Phys. Soc. Lond. **84**, 89 (1964).

[7] R. McCarroll and A. Salin, J. Phys. B **1**, 317 (1968).

[8] J. M. Cheshire, Proc. Phys. Soc. Lond. **82**, 113 (1963).

[9] R. McCarroll, Proc. R. Soc. **A264**, 547 (1961).

[10] M. H. Mittleman, Phys. Rev. **122**, 499 (1961).

[11] M. B. McElroy, Proc. R. Soc. **A272**, 542 (1963).

[12] N. Bohr, K. Dan. Vidensk. Selsk. Mat.-Fys. Medd. **18**, (8) (1948).

[13] W. R. Thorson, J. Chem. Phys. **42**, 3878 (1965).

[14] This is equivalent to the condition $\xi_2<1$ in L. Wilets and S. J. Wallace, Phys. Rev. **169**, 84 (1968).

[15] As we shall see, charge exchange is peaked in the forward direction.

[16] Bates gets the same form equations as (25) and (26) in D. R. Bates, Proc. R. Soc. **A247**, 294 (1958).

[17] B. H. Brandsden, *Atomic Collision Theory* (Benjamin, New York, 1970).

[18] B. Podolanski and L. Pauling, Phys. Rev. **34**, 109 (1929).

[19] It should be pointed out that if the potentials $V^{AB}(R)$ had been neglected, as was done in Ref. 1, h_{ii} would blow up. It is the delicate cancellation between the two terms in h_{ii} that keeps it finite.

[20] The scattering when A and B have charges Z_Ae, Z_Be then $I=(Z_AZ_B)^{5/2}(8/\pi)(1/ab)[\partial^2L(-B,a;-C,b)/\partial a\,\partial b]$, $a=Z_B$, $b=Z_A$.

[21] G. W. McClure, Phys. Rev. **148**, 47 (1966).

[22] J. E. Bayfield, Phys. Rev. **185**, 105 (1969).

[23] H. B. Gilbody and G. Ryding, Proc. R. Soc. **A291**, 438 (1966).