## ASYMPTOTIC CROSS SECTION FOR ELECTRON CAPTURE BY FAST PROTONS

## MOLECULAR HYDROGEN AND HELIL'M

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Asymptotic expressions for the total and differential charge exchange cross sections for fast protons in molecular hydrogen and helium are found. The second Born approximation is employed for the amplitude of each of the processes considered. The formulas for the total capture cross sections are compared with the experimental data.

## 1. INTRODUCTION

Recent papers ${ }^{[1-5]}$ report the results of experimental investigations of the cross sections for the capture of an electron by a fast proton with energy higher than 1 MeV (lab) for a beam passing through hydrogen, helium, nitrogen, or argon targets ${ }^{[1-5]}$. In the present paper we calculate the asymptotic nonrelativistic quantum-mechanical amplitudes and cross sections for electron capture in the processes

$$
\begin{align*}
& p+\mathrm{H}_{2} \rightarrow \mathrm{H}+\mathrm{H}_{2}{ }^{+},  \tag{1}\\
& p+\mathrm{He} \rightarrow \mathrm{H}+\mathrm{He}^{+} \tag{2}
\end{align*}
$$

in the limit as $\mathrm{v}_{0} / \mathrm{v} \rightarrow 0$, where $\mathrm{v}_{0}$ is the "orbital" velocity of the captured electron and v is the relative velocity of the incident proton; the results of the calculation are also compared with the indicated experimental data.

There have been many theoretical studies ${ }^{[8-8]}$, within the framework of the first Born approximation, of the processes (1) and (2) in the limit in question. However, an earlier analysis of the charge-exchange reaction

$$
\begin{equation*}
p+\mathrm{H} \rightarrow \mathrm{H}+p \tag{3}
\end{equation*}
$$

as $\mathrm{v}_{0} / \mathrm{v} \rightarrow 0^{\left[9{ }^{1}\right.}$ has shown that the first Born approximation does not suffice for the amplitude, and it is necessary to take into account terms of second order in the interaction. Since this result is essentially due to kinematic factors, it is natural to expect the first approximation to be insufficient also in the more complicated cases of processes (1) and (2).

Indeed, as shown by our calculation, in the most important region of small scattering angles (forward scattering) it is necessary to take into account not only the first but also the second Born approximation. It is seen at the same time that the principal asymptotic amplitudes in first and second order decrease equally rapidly with increasing velocity, and their interference, just as in the case of the process (3), leads to the following consequences. First, the contribution of the sum of the terms of the first and second orders, which contain the interaction of the incoming proton with an He nucleus (or with $\mathrm{H}_{2}$ nuclei) turns out to be smaller by a factor $m_{p} / m_{e}$ than their individual contributions. At small scattering angles, as a result the first-order term containing the interaction of the incoming proton
with the captured electron, and the second-order term containing the interaction of the captured electron with the proton and with the He nucleus ( $\mathrm{H}_{2}$ nuclei for (1)), become the principal terms. Second, interference of these principal terms causes the total cross section $\mathbf{Q}$ for each of the processes (1), (2), and (3), at not too large v , takes on to the value $\mathrm{Q} \approx 0.3 \mathrm{Q}_{\mathrm{BK}}$, i.e., it becomes smaller by an approximate factor 3.3 than the Brinkman-Kramers cross section QBK obtained using only one first-order term, which contains the interaction of the incoming proton with a captured electron. The indicated interference phenomenon thus turns out to be common to the processes (1), (2), and (3).

Section 2 contains a definition of the symbols and the initial asymptotic expressions. Sections 3 and 4 give the results of a calculation of the asymptotic forms of the first and second order terms for (1) and (2) in parallel. We note that when the contributions from the different integration regions to the corresponding integrals are estimated, no model representations are used at all for the electron wave functions of He and $\mathrm{H}_{2}$, owing to the presence of the asymptotic expressions (18) and ( $18^{\prime}$ ) for the wave functions of the ground states in the momentum representation. A similar asymptotic form was used earlier for the helium wave function by Kabir and Salpeter ${ }^{[10]}$. As a result of the calculation, a linear relation is established in Sec. 5 between the asymptotic cross sections of the reactions (1) and (3), the proportionality coefficient being connected with the electron density at the nucleus in the ground state of $\mathrm{H}_{2}$.

## 2. INITIAL EQUATIONS

Let $r_{1}$ and $r_{2}$ be the laboratory coordinates of the electrons with masses $m_{1}=m_{2}=m_{e}$ and let $r_{3}$ and $r_{4}$ be the coordinates of protons with masses $m_{3}=m_{4}$ $=m_{p}$ in the $H_{2}$ molecule; $r_{5}$ is the coordinate of the incoming proton. In the expression for the total Hamiltonian of the $\mathrm{p}+\mathrm{H}_{2}$ system

$$
\begin{equation*}
\mathscr{H}=-\frac{\hbar^{2}}{2} \sum_{\alpha=1}^{s} \frac{1}{m_{\alpha}} \Delta_{\alpha}+\sum_{1<\alpha<\beta \leqslant 5} \nabla_{\alpha \beta}\left(\left|\mathbf{r}_{\alpha}-\mathbf{r}_{\beta}\right|\right), \tag{4}
\end{equation*}
$$

where $\tilde{\mathrm{V}}_{\alpha \beta}(\mathrm{r})=\mathrm{Z}_{\alpha} \mathrm{Z}_{\beta} \mathrm{e}^{2} / \mathrm{r}$ and $\mathrm{Z}_{\alpha} \mathrm{e}$ is the charge of the particle $\alpha$, we go over from $r_{\alpha}$ to the Jacobi coordinates

$$
\mathbf{R}_{\mathrm{cm}}=\sum_{\alpha=1}^{5} m_{\alpha} \mathbf{r}_{\alpha} / \sum_{\alpha=1}^{5} m_{\alpha}, \quad \rho=\mathbf{r}_{5}-\sum_{\alpha=1}^{4} m_{\alpha} \mathbf{r}_{\alpha} / \sum_{\alpha=1}^{4} m_{\alpha}
$$

$$
\begin{aligned}
& \mathbf{R}=\frac{m_{1} \mathbf{r}_{1}+m_{3} \mathbf{r}_{3}}{m_{1}+m_{3}}-\frac{m_{2} \mathbf{r}_{2}+m_{4} \mathbf{r}_{4}}{m_{2}+m_{4}}{ }_{2}^{2} \\
& \mathbf{r}_{13}=\mathbf{r}_{1}-\mathbf{r}_{3} \quad \mathbf{r}_{24}=\mathbf{r}_{2}-\mathbf{r}_{4}
\end{aligned}
$$

and in the center-of-mass system we omit the higher order terms in $m_{e} / m_{p}$. Then, using the Coulomb system of measurement units, we obtain

$$
\begin{equation*}
\mathscr{H}_{\mathrm{cm}}=-\frac{1}{2}\left[\frac{1}{m_{e}}\left(\Delta_{s_{1}}+\Delta_{s_{2}}\right)+\frac{1}{v_{p p}} \Delta_{R}+\frac{1}{\mu_{p}} \Delta_{\rho}+V\left(s_{1}, s_{2}, \rho, \mathbf{R}\right)\right], \tag{5}
\end{equation*}
$$

where

$$
\begin{aligned}
& V\left(\mathbf{s}_{1}, \mathbf{s}_{2}, \rho, \mathbf{R}\right)=\nabla_{p o}\left(\left|\mathbf{s}_{1}-\mathbf{R} / 2\right|\right)+\nabla_{p o}\left(\left|\mathbf{s}_{1}+\mathbf{R} / 2\right|\right) \\
& +\nabla_{p e}\left(\left|\mathbf{s}_{2}-\mathbf{R} / 2\right|\right)+\nabla_{p e}\left(\left|\mathbf{s}_{2}+\mathbf{R} / 2\right|\right)+\nabla_{c e}\left(\left|\mathbf{s}_{1}-\mathbf{s}_{2}\right|\right) \\
& +\nabla_{p p}(\mathbf{R})+\nabla_{p e}\left(\left|\rho-\mathbf{s}_{1}\right|\right)+\nabla_{p e}\left(\left|\rho-\mathbf{s}_{2}\right|\right) \\
& +\nabla_{p p}(|\rho-\mathbf{R} / 2|)+\nabla_{p p}(|\rho+\mathbf{R} / 2|) ; \\
& v_{p p}=1 / 2 m_{p}, \quad \mu_{p}=2 / 3 m_{p}, \quad \mathbf{s}_{1}=\mathbf{r}_{13}-\mathbf{R} / 2, \quad \mathbf{s}_{2}=\mathbf{r}_{24}+\mathbf{R} / 2 .
\end{aligned}
$$

We represent the total interaction $\hat{\mathbf{V}}$ in the form

$$
\hat{V}=\hat{V}_{I}+\hat{v_{I}}=\hat{V}_{F}+\hat{v}_{F}
$$

where

$$
\begin{aligned}
& \left\langle\boldsymbol{\rho}^{\prime} \mathbf{s}_{1} \mathbf{s}_{2}{ }^{\prime} \mathbf{R}^{\prime}\right| \hat{v}_{I}\left|\mathbf{\rho}_{\mathbf{1}} \mathbf{s}_{2} \mathbf{R}\right\rangle=\delta^{\mathbf{3}}\left(\boldsymbol{\rho}^{\prime}-\boldsymbol{\rho}\right) \delta^{\mathbf{3}}\left(\mathbf{s}_{1}{ }^{\prime}-\mathbf{s}_{1}\right) \delta^{\mathbf{3}}\left(\mathbf{s}_{2}-\mathbf{s}_{2}{ }^{\prime}\right) \\
& \times \boldsymbol{\delta}^{3}\left(\mathbf{R}-\mathbf{R}^{\prime}\right)\left[\nabla_{p e}\left(\left|\rho-\mathbf{s}_{1}\right|\right)+\tilde{\sigma}_{p c}\left(\left|\rho-\mathbf{s}_{2}\right|\right)\right. \\
& \left.+\nabla_{p p}(|\boldsymbol{\rho}-\mathbf{R} / 2|)+\nabla_{p p}(|\rho+\mathbf{R} / 2|)\right]
\end{aligned}
$$

is an interaction that vanishes when the subsystems are asymptotically separated in the initial channel and

$$
\begin{gathered}
\langle\ldots| \hat{V_{F}}|\ldots\rangle=\delta^{3}\left(\rho^{\prime}-\rho\right) \ldots \delta^{3}\left(\mathbf{R}-\mathbf{R}^{\prime}\right)\left[\nabla_{p p}(|\boldsymbol{\rho}-\mathbf{R} / 2|)\right. \\
+\widetilde{\nabla}_{p p}(|\boldsymbol{\rho}+\mathbf{R} / 2|)+\nabla_{p e}\left(\left|\boldsymbol{\rho}-\mathbf{s}_{2}\right|\right)+\widetilde{V}_{p e}\left(\left|\mathbf{s}_{1}-\mathbf{R} / 2\right|\right) \\
\left.+\widetilde{\nabla}_{p e}\left(\left|\mathbf{s}_{1}+\mathbf{R} / 2\right|\right)+\widetilde{\nabla}_{p e}\left(\left|\mathbf{s}_{1}-\mathbf{s}_{2}\right|\right)\right]
\end{gathered}
$$

is an interaction that vanishes in the final channel.
It should be noted that although (5) is indeed the principal asymptotic term of the expansion (4) in powers of $1 / \mathrm{m}_{\mathrm{p}}$, the possibility of using (5) to find the asymptotic solution as $1 / \mathrm{v} \rightarrow 0$ in a sufficiently wide range of scattering angle calls for a special analysis. We have in mind here the three-body problem. Thus, for the process (3) the solution obtained from the corresponding expansion of the exact Hamiltonian in powers of $1 / \mathrm{m}$ agrees, as $1 / \mathrm{v} \rightarrow 0$, with the solution expanded in $1 / m_{p}$ only in the region of small scattering angles $\theta \lesssim 1 / \mathrm{m}_{\mathrm{p}}^{3}$. At larger angles $\theta$ there is an appreciable discrepancy between these solutions. It is important to note, however, that in practice the entire contribution to the total cross section comes precisely from the indicated region of small scattering angles. We assume therefore that as $1 / v \rightarrow 0$ the asymptotic expression for the amplitude of the charge-exchange processes (1) and (2), obtained on the basis of the Hamiltonian (5), is valid in the region of the small scattering angles actually measured in the experiment.

The wave functions $|I\rangle$ and $\langle F|$ of the initial and final states are eigenfunctions of the simplified Hamiltonians $\mathrm{H}_{\mathrm{I}}=\mathrm{H}_{0}+\hat{\mathrm{V}}_{\mathrm{I}}$ and $\mathrm{H}_{\mathrm{F}}=\mathrm{H}_{0}+\hat{\mathrm{V}}_{\mathrm{F}}\left(\mathrm{H}_{0}\right.$ is the kinetic-energy operator in (5)):

$$
H_{\alpha}|\alpha\rangle=E_{\alpha}|\alpha\rangle \quad(\alpha=I, F),
$$

and have the following form in the coordinate representation

$$
\begin{gather*}
\left\langle\mathbf{R}_{\mathrm{s}_{1} \mathrm{~s}_{2} \rho|I\rangle=\frac{1}{(2 \pi)^{3 / 2}} \exp \left\{i \mathbf{k}_{i} \rho\right\} X_{n_{i}}(\mathbf{R}) \widetilde{\Psi}_{i}\left(\mathbf{s}_{1}, \mathbf{s}_{2}, \mathbf{R}\right),}\right. \\
\left\langle\mathbf{R s}_{\mathrm{s}_{1} \mathrm{~s}_{2} \rho|F\rangle}=\frac{1}{(2 \pi)^{3 / 2}} \exp \left\{\left[\mathbf{k}_{f} \frac{m_{\rho} \rho+\mathrm{s}_{1}}{m_{p}+1}\right\} \widetilde{\varphi}_{\widetilde{n}_{n}}\left(\rho-\mathrm{s}_{1}\right) X_{n_{f}}(\mathbf{R}) \widetilde{\Psi}_{f}^{(n)}\left(\mathbf{s}_{2}, \mathbf{R}\right) .\right.\right. \tag{6}
\end{gather*}
$$

The complete wave functions of $\mathrm{H}_{2}$ and $\mathrm{H}_{2}^{+}$have been written out here in the approximation of the theory of diatomic molecules, which makes it possible to sepa-
rate the electronic and nuclear motions. Here $\widetilde{\Psi}_{i}$ and $\widetilde{\Psi}_{f}^{(n)}$ are the electronic wave functions of the ${ }^{1} \Sigma_{2}^{+}$state of $\mathrm{H}_{2}$ and of the stationary state of $\mathrm{H}_{2}^{+}$, characterized by the required set of quantum numbers $\{n\} ; \chi n i(R)$ and $\chi_{n f}(R)$ are the corresponding nuclear functions. Finally, $\widetilde{\varphi} \widetilde{\mathrm{n}}\left(\rho-\mathrm{s}_{1}\right)$ is the wave function of the produced atomic hydrogen, characterized by the quantum numbers $\tilde{n}$. In (6), $k_{i}$ and $k_{f}$ are the momenta of the relative motion of the fragments in the initial and in the final states.

On the energy-conservation surface we have

$$
E=E_{I}=k_{i}^{2} / 2 \mu_{p}-E_{0 i}=E_{F}=k_{t}^{2} / 2 M_{t}-E_{n_{f}}-E_{\tilde{n}}-E_{\{n\}},
$$

where $E_{n f}$ and $E\{n\}$ are the energies of the nuclear and electronic motions in $\mathrm{H}_{2}^{+}$, respectively, $\mathrm{E}_{\widetilde{\mathrm{n}}}$ is the energy of the bound state of the H atom, and $\mathrm{M}_{\mathrm{f}}=1$ $+\mu \mathrm{p}$. Since both electrons are effectively different in the electronic ground state, the expression for the differential cross section of the reaction (1) is ${ }^{[6]}$

$$
\begin{equation*}
d Q_{\mathrm{H}_{2}}=2 d Q_{\mathrm{H}_{2}}^{(1)}, \tag{7}
\end{equation*}
$$

where $\mathrm{dQ}_{\mathrm{H}_{2}}^{(1)}$ is the cross section for the capture of a definite electron, in our case the first, from $\mathrm{H}_{2}$, followed by transition of $\mathrm{H}_{2}^{+}$to the n -th electronic state and of H to the $\tilde{\mathrm{n}}$-th state:

$$
\begin{equation*}
\left.\frac{d Q_{\mathrm{H}_{2}}^{(1)}}{d \Omega}=(2 \pi)^{4} \mu_{p}^{2} \oint_{n_{f}} \frac{k_{f}}{k_{i}}\left|\left\langle k_{f},\left\{n_{j} n\right\} ; \tilde{n}\right| \hat{T}_{f i}\right| I\right\rangle\left.\right|^{2} . \tag{8}
\end{equation*}
$$

The summation over $n_{f}$ is carried out here over all the nuclear-motion final states that are permitted by the conservation law, including a portion of the continuous spectrum belonging to the $n$-th electronic term of $\mathrm{H}_{2}^{+}$.

We calculate the asymptotic form of (8) as $1 / v \rightarrow 0$ by using the second Born approximation for the transition amplitude $\widetilde{\mathrm{T}}_{\mathrm{fi}}$

$$
\begin{gather*}
T_{f i} \approx T_{f i}^{1 I B}=\left\langle F \mid \hat{v}_{I}+\hat{v}_{F} G_{v} \hat{v}_{I} I I\right\rangle,  \tag{9}\\
G_{0}\left[E+i 0-H_{0}\right]^{-1} .
\end{gather*}
$$

Since the relative velocity of the nuclei in both $\mathrm{H}_{2}$ and $\mathrm{H}_{2}^{+}$is small in comparison with the velocity of the electron motion and in comparison with the velocity of the incoming proton, we can neglect in the operator $G_{0}$ the kinetic energy of the relative nuclear motion, i.e., we can assume that

$$
\begin{equation*}
H_{0} \approx-1 / 2\left(\Delta_{\mathrm{s} 1}+\Delta_{\mathrm{s} 2}+\mu_{p}^{-1} \Delta_{\rho}\right) \tag{10}
\end{equation*}
$$

Under this assumption, the operator (9) becomes diagonal in $\mathbf{R}$ :

$$
\begin{align*}
\langle\mathbf{R}| \hat{T} \hat{f i}_{H B}^{H B}\left|\mathbf{R}^{\prime}\right\rangle & =\delta^{3}\left(\mathbf{R}-\mathbf{R}^{\prime}\right)\left[\hat{v}_{I}(\mathbf{R})+\hat{v}_{F}(\mathbf{R}) \hat{G}_{o} \hat{v}_{I}(\mathbf{R})\right] \\
& \equiv \delta^{3}\left(\mathbf{R}-\mathbf{R}^{\prime}\right) \hat{\tau}_{f i}(\mathbf{R}) \tag{11}
\end{align*}
$$

(here $\widetilde{\mathrm{G}}_{0}$ is the resolvent of the operator (10)) and the expression for the matrix element takes the form

$$
\begin{gather*}
\left\langle\mathbf{k}_{f} ; n, n_{f} ; \tilde{n}\right| \hat{T}_{f i}^{\mathrm{II} B}\left|\mathbf{k}_{i} ;{ }^{1} \Sigma_{g}^{+}, n_{i}\right\rangle \\
=\int d^{3} \mathbf{R}_{\chi_{n_{f}}} \cdot(\mathbf{R}) \chi_{n_{i}}(\mathbf{R})\left\langle\mathbf{k}_{f} ; n ; \tilde{n}\right| \hat{\tau}_{f i}(\mathbf{R})\left|\mathbf{k}_{i} ;{ }^{1} \Sigma_{g}{ }^{+}\right\rangle . \tag{12}
\end{gather*}
$$

We substitute (12) in (8) and let the upper limit of summation with respect to $\mathrm{n}_{\mathrm{f}}$ tend to infinity at large E. Then, expanding the integrand asymptotically in powers of $1 / E$ and using the completeness condition of the functions $\chi_{n f}(R)$, we obtain for the principal asymptotic term of (8) the expression

$$
\begin{equation*}
\left.\frac{d Q_{\mathbf{H}_{2}}^{(1)}}{d \Omega}=(2 \pi)^{4} \mu_{p}^{2} \int d^{3} \mathbf{R}\left|\chi_{n_{i}}(\mathbf{R})\right|^{2} \right\rvert\,\left\langle\mathbf{k}_{f} ; n ; \tilde{n}\right| \hat{\tau}_{f f}(\mathbf{R})\left|\mathbf{k}_{i} ;{ }^{1} \Sigma_{g}{ }^{+}\right|^{2} \tag{13}
\end{equation*}
$$

which has an obvious physical meaning: $\mathrm{dQ}_{\mathrm{H}_{2}}^{(1)}$ is the cross section, averaged all the possible values of $R$, for the capture of an electron by an incident particle $\tilde{p}_{i}$ with mass $\mu_{p}$, charge +1 , and momentum $k_{i}$, the electrons being initially in a bound state in the field of two immobile Coulomb centers located at the point $\pm R / 2$. The particle $\tilde{p}_{i}$ possessing the indicated characteristics will henceforth be called a proton, in spite of the fact that its mass differs from $m_{p}$.

In the case of reaction (2), a transition from the exact Hamiltonian to the one expanded in powers of $1 / m_{p}$, analogous to the transition from (4) to (5), lead to the following picture. The particle $\widetilde{\mathrm{p}}_{\mathrm{i}}$ with mass $\mu_{\mathrm{p}}$ and charge +1 is incident on a Coulomb center with charge +2 , in the field of which two electrons are situated in a bound state, and the interaction causes a transition of one of the electrons into the bound state of the hydrogen atom. The expression for the cross section of such a process, at which $\mathrm{He}^{+}$turns out to be in a stationary state characterized by the set of quantum numbers $\{n\}$, is

$$
\begin{align*}
& d Q_{\mathrm{H}_{0}}=2 d Q_{\mathrm{H0}}^{(1)}, \\
& \frac{d Q_{\mathrm{H0}}^{(1)}}{d \Omega}=(2 \pi)^{4} \mu_{p}^{2}\left|\left\langle\mathbf{k}_{f} ; n ; \tilde{n} \hat{\tau}_{f i}^{(\mathrm{H0})} \mid \mathbf{k}_{i} ; 1 s^{2}\right\rangle\right|^{2}, \tag{14}
\end{align*}
$$

and since

$$
\hat{\tau}_{f i}^{\left(\mathrm{H}_{\mathrm{t}}\right)}=\hat{\tau}_{f i}^{\left(\mathrm{H}_{2}\right)}(0),
$$

it suffices to obtain the asymptotic form of the amplitude $\hat{\tau}_{\mathrm{fi}} \mathrm{H}_{2}(R)$. We shall henceforth denote the sets of quantum numbers specifying the initial and final states in (13) and (14) by $\{i\}$ and $\{f\}$, respectively, and the states themselves will be designated $|i\rangle$ and $\langle f|$.

## 3. FIRST-ORDER TERMS

We proceed to calculate the asymptotic behavior of the matrix elements $\langle\mathrm{f}| \hat{\tau}_{\mathrm{fi}}^{\left(\mathrm{H}_{2}\right)}(\mathrm{R})|\mathrm{i}\rangle$ as $1 / \mathrm{v} \rightarrow 0$. The first-order terms are

$$
\begin{equation*}
T^{\mathrm{I}}=\langle f| \hat{v}_{I}|i\rangle \tag{15}
\end{equation*}
$$

We consider first a matrix element containing the interaction $\hat{\mathrm{V}}_{\mathrm{pi}_{\mathrm{i}}}$ with the electron 1. A diagram of this matrix element is shown in Fig. 1a and corresponds to the integral

$$
\begin{equation*}
T_{B K}=g_{\mathrm{H}}\left(\Delta_{i}\right) \int d^{3} \mathbf{q}_{2} \Psi_{i}\left(\Delta_{f}, \mathbf{q}_{2}\right) \Psi_{f}\left(\mathbf{q}_{2}\right) . \tag{16}
\end{equation*}
$$

Here $\Delta_{i}=\mathbf{k}_{\mathbf{i}}-\mu \mathbf{p} \mathbf{k}_{\mathbf{f}} / \mathbf{M}_{\mathrm{f}}, \Delta_{\mathbf{f}}=\mathbf{k}_{\mathbf{f}}-\mathbf{k}_{\mathbf{i}}$ are the transferred momenta, with $\left\{\Delta_{\mathrm{i}}^{2}, \Delta_{\mathrm{f}}^{2}\right\} \geq \mathrm{v}^{2} / 4$, so that $\Delta_{\alpha}^{2}$ $\rightarrow \infty$ as $v \rightarrow \infty(\alpha=\mathrm{i}, \mathrm{f}) ; \Psi_{\mathrm{i}}$ and $\Psi_{\mathrm{f}}$ are the wave functions in the momentum representation:

$$
\begin{gathered}
\Psi_{i}\left(\mathbf{q}_{1}, \mathbf{q}_{2}\right)=\frac{1}{(2 \pi)^{3}} \iint d^{3} \mathbf{s}_{1} d^{3} \mathbf{s}_{2} \exp \left\{i\left[\mathbf{q}_{1} \mathbf{s}_{1}+\mathbf{q}_{2} \mathbf{s}_{2}\right]\right\} \tilde{\Psi}_{i}\left(\mathbf{s}_{1}, \mathbf{s}_{2}\right), \\
\left.\Psi_{/}(\mathbf{q})=\frac{1}{(2 \pi)^{3 / 2}} \int d^{3} \mathbf{s} \exp \{i \mathbf{q}\}\right\} \tilde{\Psi}_{f}(\mathbf{s}) \\
g_{\mathrm{H}}(\mathbf{q})=-\left(\frac{q^{2}}{2}+E_{\tilde{n}}\right) \varphi_{\mathrm{H}}(\mathbf{q}) \\
\varphi_{\mathrm{H}}(\mathbf{q})=\frac{1}{(2 \pi)^{3 / 2}} \int d^{3} \mathbf{s} \exp \{i \mathbf{q s}\} \tilde{\varphi}_{\mathrm{H}}(\mathbf{s})
\end{gathered}
$$

Since $\Delta_{\alpha}^{2} \rightarrow \infty$, to find the asymptotic form of (16)


FIG. 1. Diagrams of the first-order terms that make the principal contribution to the asymptotic charge-exchange amplitude.
we use for the factors in (16) the following asymptotic expressions, which are obtained directly from the Schrödinger equation in the momentum representation ${ }^{[10]}$ for the ground state of the hydrogen molecule. As $q_{1} \rightarrow \infty$ we have

$$
\begin{align*}
\Psi_{i}\left(\mathbf{q}_{1}, \mathbf{q}_{2}\right) \rightarrow- & \frac{2(2 \pi)^{3 / 2}{ }^{2}}{q_{1}{ }^{2}} V_{p e}\left(q_{1}\right)\left[\exp \left\{\frac{i}{2} \mathbf{q}_{1} \mathbf{R}\right\} \bar{\Psi}_{i}\left(\frac{\mathbf{R}}{2}, \mathbf{q}_{2}\right)\right. \\
& \left.+\exp \left\{-\frac{i}{2} \mathbf{q}_{1} \mathbf{R}\right\} \bar{\Psi}_{i}\left(-\frac{\mathbf{R}}{2}, \mathbf{q}_{2}\right)\right], \tag{18}
\end{align*}
$$

where

$$
\begin{gathered}
\bar{\Psi}_{i}\left(\mathbf{s}_{1}, \mathbf{q}_{2}\right)=\frac{1}{(2 \pi)^{3 / 2}} \int d^{3} \mathbf{s}_{2} \exp \left\{i \mathbf{q}_{2} \mathbf{s}_{2}\right\} \tilde{\Psi}_{i}\left(\mathbf{s}_{1}, \mathbf{s}_{2}\right), \\
V_{p e}(q)=\frac{1}{(2 \pi)^{3 / 2}} \int \exp \{i q r\} \widetilde{\nabla}_{p e}(r) d^{3} \mathbf{r} .
\end{gathered}
$$

For atomic hydrogen we have

$$
\begin{equation*}
\varphi_{\mathrm{H}}(\mathbf{q}) \rightarrow-\frac{2(2 \pi)^{3 / 2} \widetilde{\varphi}_{\mathrm{H}}(0)}{q^{2}} V_{p c}(q), \quad q \rightarrow \infty . \tag{18'}
\end{equation*}
$$

Substituting these asymptotic expressions in (16), we obtain

$$
\begin{gather*}
T_{B K}=-\frac{2(2 \pi)^{3}}{\Delta_{f}^{2}} V_{p e}\left(\Delta_{i}\right) V_{p e}\left(\Delta_{f}\right)\left[\exp \left\{\frac{i}{2} \Delta_{f} \mathbf{R}\right\} \Gamma_{+}(0,0)\right. \\
\left.+\exp \left\{-\frac{i}{2} \Delta_{f} \mathbf{R}\right\} \Gamma_{-}(0,0)\right] \\
\Gamma_{ \pm}\left(t, t \mathbf{n}_{\Delta_{i}} \mathbf{R}\right)=\varphi_{H}\left(t \mathbf{n}_{\Delta_{t}}\right) \int d^{3} \mathbf{s}_{2} \tilde{\Psi}_{f}\left(\mathbf{s}_{2}\right) \tilde{\Psi}_{i}\left(t \mathbf{n}_{\Delta_{i}} \pm \frac{\mathbf{R}}{2}, s_{2}\right), \tag{19}
\end{gather*}
$$

where $n_{\Delta}=\Delta / \Delta$. The corresponding expression for (2) follows from (19) and (16) at $R=0$ when the hydrogen wave functions are replaced by the helium wave functions. Then

$$
\Gamma(t)=\tilde{\varphi}_{\mathrm{H}}\left(t \mathbf{n}_{\Delta_{j}}\right) \int d^{3} \mathbf{s}_{2} \tilde{\Psi}_{\mathrm{He}}+\left(\mathbf{s}_{2}\right) \tilde{\Psi}_{\mathrm{He}}\left(t \mathbf{n}_{\mathrm{s}_{i}} \mathbf{s}_{2}\right)
$$

We note that ( $16^{\prime}$ ) decreases like $1 / v^{6}$ as $v \rightarrow \infty$.
We consider further the first-order terms $\hat{\mathrm{V}}_{\mathrm{p}_{\mathrm{i}}}$, nuc $=\hat{\mathrm{V}}_{\mathrm{p}_{\mathrm{i}} \mathrm{p}_{3}}+\hat{\mathrm{V}}_{\mathrm{p}_{\mathrm{i}} \mathrm{p}_{4}}$ in (15), which contain the interactions of the incoming particle $\tilde{\mathrm{p}}_{\mathrm{i}}$ with the immobile Coulomb centers. This matrix element is shown graphically in Fig. 1b. The corresponding integral is

$$
\begin{align*}
& \boldsymbol{T}_{p_{i}, \text { nü }}=\iint d^{3} \mathbf{q}_{1} d^{3} \mathbf{q}_{2} \Psi_{i}\left(\mathbf{q}_{1}, \mathbf{q}_{2}\right) V_{p p}\left(\mathbf{q}_{1}+\Delta_{f}\right) \\
& \quad \times 2 \cos \frac{\left(\mathbf{q}_{1}+\Delta_{f}\right) \mathbf{R}}{2} \varphi_{\mathrm{H}}\left(\mathbf{q}_{1}-\mathbf{v}_{j}\right) \Psi_{f}\left(\mathbf{q}_{2}\right) . \tag{20}
\end{align*}
$$

We have introduced here the velocity vector $\mathrm{vf}_{\mathrm{f}}$ $=\mathrm{k}_{\mathrm{f}} / \mathrm{n}_{\mathrm{f}}$ of atomic hydrogen. In the integral with respect to $d^{3} q_{1}$, the most important regions, which make the principal contributions to the asymptotic expression, are the regions of localization of the wave functions $\Psi_{i}$ and $\varphi_{\mathrm{H}}$ in the momentum representation, i.e., the vicinities of the points $q_{1}=0$ (localization region of $\Psi_{i}$ ) and $\mathrm{q}_{1} \approx \mathrm{v}_{\mathrm{f}}$ (localization of $\varphi_{\mathrm{H}}$ ). These regions are well separated at large $v$, so that the contributions from them can be calculated separately. Expanding in the indicated vicinity the nonsingular parts of the inte-
grand and using the asymptotic expressions (18) and ( $18^{\prime}$ ), we obtain for the main contribution to (20)

$$
\begin{gather*}
T_{p_{i, \text { nuc }}=-\frac{2(2 \pi)^{3}}{v_{j}{ }^{2}} V_{p e}\left(v_{j}\right)\left\{V _ { p p } ( \Delta _ { f } ) \left[\exp \left\{-\frac{i}{2} \Delta_{i} \mathbf{R}\right\} \Gamma_{-}(0,0)\right.\right.}^{\left.\exp \left\{\frac{i}{2} \Delta_{j} \mathbf{R}\right\} \Gamma_{+}(0,0)\right]+\frac{4 V_{p p}\left(\Delta_{i}\right)}{(2 \pi)^{3}} \iiint d^{3} \mathbf{q}_{1} d^{3} \mathbf{q}_{1}{ }^{\prime} d^{3} \mathbf{q}_{2} \Psi_{i}\left(\mathbf{q}_{1}{ }^{\prime}, \mathbf{q}_{2}\right) \Psi_{f}\left(\mathbf{q}_{2}\right)} \\
\left.\times \cos \frac{\left(\mathbf{q}_{1}-\mathbf{q}_{1}{ }^{\prime}\right) \mathbf{R}}{2} \cos \frac{\left(\mathbf{q}_{1}-\Delta_{f}\right) \mathbf{R}}{2} \varphi_{\mathrm{H}}\left(\mathbf{q}_{1}-\mathbf{v}_{f}\right)\right\} .
\end{gather*}
$$

Each of the terms in this expression decreases like $1 / v^{6}$ as $1 / v \rightarrow 0$, just as the amplitude (16), and both matrix elements make comparable contributions to the asymptotic expression. The first-order term remaining in (15) and containing $\hat{\mathrm{V}}_{\mathrm{p}_{1} \mathrm{p}_{2}}$ (the interaction of $\widetilde{\mathrm{p}_{\mathrm{i}}}$ with electron 2) makes a smaller contribution than the terms considered above. Indeed, the integral corresponding to this matrix element is given by

$$
\begin{equation*}
T_{p_{i_{i} e_{2}}}=\int d^{3} \mathbf{q}_{1} d^{3} \mathbf{q}_{2} \Psi_{i}\left(\mathbf{q}_{1}, \mathbf{q}_{2}\right) V_{p e}\left(\mathbf{q}_{1}-\boldsymbol{\Delta}_{t}\right) \varphi_{\mathrm{H}}\left(\mathbf{q}_{1}-\mathbf{v}_{t}\right) \Psi_{t}\left(\mathbf{q}_{1}+\mathbf{q}_{2}-\boldsymbol{\Delta}_{t}\right) . \tag{22}
\end{equation*}
$$

The main contribution to the integral is made by the vicinities of the points $q_{1}=\Delta_{\mathrm{f}}$ and $\mathrm{q}_{2}=0$, which are the regions of localization of the wave function $\Psi_{f}$ and the wave function $\Psi_{i}\left(q_{1}, q_{2}\right)$ with respect to the argument $q_{2}$. In addition, the denominator of $V_{p e}$ also vanishes in these regions. At the same time we can use for $\Psi_{i}\left(q_{1}, q_{2}\right)$ with respect to the argument $q_{1}$ and for $\varphi_{\mathrm{H}}$ the asymptotic forms (18) and (18') in the vicinities of $q_{1} \approx \Delta_{f}$ and $q_{2} \approx 0$. Thus, we obtain the estimate

$$
\begin{equation*}
T_{p_{i} e_{2}} \approx \frac{\text { const }}{\Lambda_{t}^{2} v_{t}^{2}} V_{p e}\left(\Delta_{t}\right) V_{p e}\left(v_{t}\right), \tag{23}
\end{equation*}
$$

where const does not depend on $v$. This expression decreases like $1 / \mathrm{v}^{8}$, and is asymptotically small in comparison with the terms (16) and (21), so that the matrix element corresponding to the interaction $\mathrm{V}_{\mathrm{p}_{\mathrm{i}} \mathrm{e}_{2}}$ can be omitted in the calculation of the asymptotic form for large velocities ${ }^{1)}$. Thus, the asymptotic first-order matrix element (15) is given by a sum of the expressions (16') and (21).

## 4. SECOND-ORDER TERMS

Out of the twelve second-order terms

$$
\begin{equation*}
T^{\mathrm{II}}=\langle f| \hat{v}_{F} \vec{G}_{0} \hat{v}_{I}|i\rangle \tag{24}
\end{equation*}
$$

(in the case of the reaction (1) it is convenient to consider simultaneously the interactions $\hat{\mathrm{V}}_{\mathrm{p}_{\mathrm{i}} \mathrm{p}_{3}}+\hat{\mathrm{V}}_{\mathrm{p}_{\mathrm{i}} \mathrm{p}_{4}}$ $\equiv \hat{\mathrm{V}}_{\mathrm{p}_{\mathrm{i}}, \text { nuc }}$ and $\hat{\mathrm{V}}_{\mathrm{e}_{1} \mathrm{p}_{3}}+\hat{\mathrm{V}}_{\mathrm{e}_{1} \mathrm{p}_{4}} \equiv \mathrm{~V}_{\mathrm{e}_{1} \text { nuc }}$ of the exchanged electron with the two Coulomb centers) most terms are asymptotically small in comparison with the firstorder terms. Two terms that contain repeated interactions of the type indicated in Fig. 2a decrease like $\mathrm{v}^{-7} \ln \mathrm{v}$ as $\mathrm{v} \rightarrow \infty$ and are small in comparison with the corresponding first-order term (20) (Fig. 1b).

Further, all five second-order terms containing the interaction $\hat{\mathrm{V}}_{\mathrm{p}_{\mathrm{i}} \mathrm{e}_{2}}$ are small. We consider, e.g., the matrix element $\langle f| \hat{V}_{p_{i} e_{2}} \widetilde{G}_{o} \hat{V}_{p_{1} \text { nuc }}|i\rangle$ shown in Fig. 2b. Analysis of the integrand shows that at large $v$ the

[^0]principal contributions to the integrals with respect to $d^{3} q_{2}$ and $d^{3} q_{2}^{\prime}$ are made by the regions of localization of the wave functions in momentum space, viz., the vicinities of the points $q_{2}=0$ and $q_{2}^{\prime}=0$ at which the denominator of the potential $\mathrm{V}_{\text {pe }}$ also vanishes, and by the vicinities of the points $q_{1}=0$ and $q_{1}=v_{f}$ in the integral with respect to $\mathrm{d}^{3} \mathrm{q}_{1}$. The nonsingular functions are the potential $V_{p p}$, the wave function $\varphi_{\mathrm{H}}$, and the free Green's function. $\widetilde{G}_{0}$, in the system of regions $q_{2}$ $\approx 0, q_{2}^{\prime} \approx 0$, and $q_{1} \approx 0$ and respectively $V_{p p}$ and $\Psi_{i}$ with respect to the argument $q_{1}$, in the system of regions $q_{2}=0, q_{2}^{\prime} \approx 0$, and $q_{1} \approx v_{f}$. Expanding the nonsingular functions in the indicated regions and using (18) and (18'), we find that the principal contribution of the diagram of Fig. 2b is
\[

$$
\begin{gathered}
\langle f| \hat{V}_{p_{i} e_{2}} G_{0} \hat{V}_{p_{i}, \text { nuc }}|i\rangle \approx \frac{\text { const }_{1}}{v_{f}^{4}} V_{p p} \\
\left(\Delta_{f}\right) V_{p e}\left(v_{f}\right)+\text { const }_{2} \frac{\ln v}{v_{f}{ }^{3}} V_{p p}\left(\Delta_{i}\right) V_{p e}\left(v_{j}\right)
\end{gathered}
$$
\]

The leading term here is the second term (the contribution from the regions $q_{2} \approx 0, q_{2}^{\prime} \approx 0, q_{1} \approx v_{f}$, which decreases like $\mathrm{v}^{-7} \ln \mathrm{v}$ and becomes asymptotically small in comparison with the first-order terms.

Finally, among the remaining five second-order matrices we can neglect the contributions of the two terms containing the electron interaction $\hat{\mathrm{V}}_{\mathrm{e}_{1} \mathrm{e}_{2}}$. We consider, for example the diagram of Fig. 2c. The main contribution to the asymptotic form of the integral corresponding to this diagram is made by the regions $q_{p} \approx \mu p_{\mathrm{f}}, \mathrm{q}_{1} \approx 0, \mathrm{q}_{2} \approx \Delta_{\mathrm{f}}$, in which are localized the functions $\varphi_{\mathrm{H}}$ and $\Psi_{\mathrm{f}}$ as well as $\Psi_{\mathrm{i}}$ with respect to the variable $q_{1}$. In addition, the denominators of $V_{\text {ee }}$ and of the free Green's function $\widetilde{G}_{0}$ also vanish in them. The leading asymptotic form is then

$$
\begin{equation*}
\langle f| \hat{V}_{e_{1} e_{2}} G_{0} \hat{V}_{p_{i} e_{1}}|i\rangle \approx \mathrm{const} \frac{\ln v}{v} \frac{V_{p e}\left(\Delta_{i}\right) V_{p e}\left(\Delta_{f}\right)}{\Delta_{f}^{2}} \tag{26}
\end{equation*}
$$

and decreases like $\mathrm{v}^{-7} \ln \mathrm{v}$ as $\mathrm{v} \rightarrow \infty$.
It remains to consider only the three terms shown graphically in Fig. 3. The principal contributions to the integral corresponding to Fig. 3b are made by the localization regions of the wave functions $\Psi_{i}, \Psi_{\mathrm{f}}$, and $\varphi_{\mathrm{H}}$, the vicinities of the points $\mathrm{q}_{1}=0, \mathrm{q}_{2}=0, \mathrm{q}_{\mathrm{p}}=\mu \mathrm{p} \mathrm{v}_{\mathrm{f}}$. Expanding the potentials and the denominator of the Green's functions in the indicated vicinities, we obtain the following asymptotic expression for the diagram of Fig. 3b


FIG. 2. Diagrams of the second-order terms that are asymptotically small in comparison with the first-order terms.


FIG. 3. Diagrams of the second-order terms that make as important contributions to the asymptotic expression as the first-order terms shown in Fig. 1.

$$
\begin{align*}
& \left\langle f i V_{e, \text { nuc }} G_{:} \hat{\mathrm{r}}_{p, \text { nuc }} \mid i\right\rangle=\frac{8}{v_{t}^{2}} V_{p p}\left(\Delta_{i}\right) V_{e p}\left(v_{j}\right) \iiint d^{3} \mathbf{q}_{1} d^{3} \mathbf{q}_{2} d^{3} \mathbf{q} \Psi_{i}\left(\mathbf{q}_{1}, \mathbf{q}_{2}\right) \\
& \quad \times \Psi_{t}\left(\mathbf{q}_{2}\right) \cos \frac{\left(\mathbf{q}_{1}-\mathbf{q}-\mathbf{v}_{t}\right) \mathbf{R}}{2} \cos \frac{\left(\mathbf{q}+\Delta_{i}\right) \mathbf{R}}{2} \varphi_{\mathrm{H}}(\mathbf{q}), \tag{27}
\end{align*}
$$

where $q=q_{p}-\mu p_{\mathbf{f}}$. We have similarly for the asymptotic form of diagram 3c

$$
\begin{align*}
& \langle f| \hat{V}_{p_{i} \text { nuc }} G_{o} \hat{V}_{p_{i} e_{i}}|i\rangle=-\frac{2(2 \pi)^{3} M_{f} \mu_{p} V_{p e}\left(v_{f}\right) V_{p p}\left(\Delta_{f}\right)}{k_{f}^{2}-2 \mathbf{k}_{i_{j}}} \\
& \times\left[\exp \left\{\frac{i}{2} \Delta_{i} \mathbf{R}\right\} \Gamma_{+}(0,0)+\exp \left\{-\frac{i}{2} \Delta_{i} \mathbf{R}\right\} \Gamma_{-}(0,0)\right] . \tag{28}
\end{align*}
$$

Let us compare the obtained asymptotic expressions (27) and (28) with the asymptotic first-order term of (21), which contains the interaction $\hat{\mathrm{V}}_{\text {pinuc }}$. We observe here that the second term of (21) is exactly cancelled by (27), and the algebraic sum of (21), (27), and (28) is equal to

$$
\begin{equation*}
T_{\mathrm{L}}(v)\left\{1-\frac{\mu_{\mathrm{p}}}{\mu_{\mathrm{p}}+1}\left[2 \frac{\mathbf{k}_{\mathrm{l}} \mathbf{k}_{f}}{k_{t}^{2}}-1\right]^{-1}\right\} \tag{29}
\end{equation*}
$$

where $T_{1}(v)$ is the first term of the (21). In the region of small scattering angles of interest to us, equation (29) is of the order of $T_{1}(v) / \mu \mathrm{p}$, and consequently the sum of (29) is smaller by a factor $\mu_{p}$ than each of the terms. Thus, as a result of the interference of the amplitudes corresponding to the indicated first- and second-order terms, their leading asymptotic forms cancel each other in part, as a result of which we have

$$
\langle f| \hat{V}_{p_{i} \text { nuc }}+\hat{V}_{\boldsymbol{V}_{i} \text { nuc }} G_{0} \hat{V}_{p_{\mathrm{i}} \text { nuc }}+\hat{V}_{p_{i} \text { nuc }} G_{i} \hat{V}_{i_{i}, \boldsymbol{e}}|i\rangle \approx\left(1 / \mu_{p}\right)\langle f| \hat{V}_{p_{i} \text { nuc }}|i\rangle .(30)
$$

Similarly, in case (2),
$\langle f| \hat{V}_{p_{i} \text { nuc }}+\hat{V}_{e, \text { nuc }} G_{0} \hat{V}_{p_{i} \text { nuc }}+\hat{V}_{p_{i} \text { nuc }} G_{0} \hat{V}_{e, p_{i}}|i\rangle \approx\left(1 / \mu_{p}\right)\langle f| \hat{V}_{p_{1} \text { nuc }}|i\rangle$.
Since the first-order terms shown in Fig. 1 make comparable contributions to (15) in the small-angle region, it follows that by virtue of ( 30 ) and ( $30^{\prime}$ ) the principal matrix element in this region is (16) (Fig. 1a).

Let us consider finally the matrix element $\langle f| \hat{\mathbf{V}}_{\mathrm{e}_{\perp} n u c} \widetilde{G}_{\mathbf{V}_{0}} \hat{\mathbf{V}}_{\mathrm{e}_{1} \mathrm{p}_{\mathrm{i}}}|\mathrm{i}\rangle$, shown in Fig. 3a. Expanding the nonsingular part of the integrand in the vicinities of the points $q_{1}=0, q_{2}=0, q_{p}=\mu_{p} \mathbf{v f}$, we obtain

$$
\begin{align*}
& \langle f| \hat{V}_{e, \text { nuc }} G_{0} \hat{V}_{e, p}|i\rangle=-2 V_{p e}\left(\Delta_{i}\right) V_{p e}\left(\Delta_{f}\right) \iiint d^{3} \mathbf{q}_{1} d^{3} \mathbf{q}_{2} d^{3} \mathbf{q} \Psi_{i}\left(\mathbf{q}_{1} \mathbf{q}_{2}\right) \\
& \times \Psi_{f}\left(\mathbf{q}_{2}\right) \varphi_{\mathrm{H}}(\mathbf{q}) \cos \frac{\left(\mathbf{q}_{1}+\Delta_{f}\right) \mathbf{R}}{2}\left[\frac{1}{2}\left(\Delta_{i}^{2}-v^{2}-i \varepsilon\right)+\mathbf{q}_{i} \Delta_{i}+\mathbf{q} \Delta_{f}\right]^{-1} \\
& =-\frac{(2 \pi)^{3} i}{v} V_{p e}\left(\Delta_{i}\right) V_{p e}\left(\Delta_{f}\right) \int_{j}^{\infty} d t \exp \left\{-\frac{i}{2} v t\left(\bar{\Delta}_{i}^{2}-1\right)\right\} \\
& \times\left[\exp \left\{\frac{i}{2} \Delta_{f} \mathbf{R}\right\} \Gamma_{+}\left(t, t \mathbf{n}_{\Delta_{i}} \mathbf{R}\right)+\exp \left\{-\frac{i}{2} \Delta_{f} \mathbf{R}\right\} \Gamma_{-}\left(t, t \mathbf{n}_{\Delta_{i}} \mathbf{R}\right)\right], \tag{31}
\end{align*}
$$

where $\widetilde{\Delta}_{i}^{2}=\Delta_{i}^{2} / v^{2}$. As $v \rightarrow \infty$, Eq. (31) decreases like $1 / v^{6}$ in the region $\left|\widetilde{\Delta}_{i}^{2}-1\right| \gg 1 / v$ and like $1 / v^{5}$ when $\left|\widetilde{\Delta}_{\mathrm{i}}^{2}-1\right| \lesssim 1 / \mathrm{v}$. Thus, the asymptotic sum of the firstand second-order terms coincides with the asymptotic sum of the diagrams shown in Figs. 1a and 3a at small scattering angles, and is given by the sum of the expressions (19) and (31):

$$
\begin{gather*}
\tau_{\tau_{i}}^{\left(\mathbf{H}_{2}\right)}(\mathbf{R})=\langle f| \hat{V}_{p_{i} e_{1}}+\hat{V}_{e_{i} \text { nuc }} G_{0} \hat{V}_{e_{1} p_{i}}|i\rangle \approx-\frac{2(2 \pi)^{3}}{v^{2}} V_{p e}\left(\Delta_{i}\right) V_{p e}\left(\Delta_{f}\right)^{\prime} \\
\times\left[\exp \left\{\frac{i}{2} \Delta_{f} \mathbf{R}\right\} T_{+}\left(\mathbf{R n}_{\Delta_{i}}, \Delta_{i}^{2}\right)+\exp \left\{-\frac{i}{2} \Delta_{f} \mathbf{R}\right\} T_{-}\left(\mathbf{R n}_{\Delta_{i}}, \Delta_{i}^{2}\right)\right] \\
T_{ \pm}\left(\mathbf{R n}_{\Delta}, \Delta^{2}\right)=\frac{\Gamma_{ \pm}(0,0)}{\Delta^{2}}+\frac{i v}{2} \int_{0}^{\infty} d t \cdot \exp \left[-\frac{i v t}{2}\left(\Delta^{2}-1\right)\right] \Gamma_{ \pm}\left(t, t n_{\Delta} \mathbf{R}\right) \tag{32}
\end{gather*}
$$

The corresponding expression for (2) takes the form $\tau_{i i}^{(\mathrm{H}+)}=\langle f| \hat{V}_{p_{i} e_{i}}+\hat{V}_{e ;}$ nuc $G_{0} \hat{V}_{e, p_{i}}|i\rangle \approx-\frac{4(2 \pi)^{3}}{v^{2}} V_{p e}\left(\Delta_{i}\right) V_{p c}\left(\Delta_{f}\right) T\left(\bar{\Delta}_{i}^{2}\right)$,

$$
\begin{equation*}
T\left(\bar{\Delta}^{2}\right)=\frac{\Gamma(0)}{\Delta^{2}}+\frac{i v}{2} \int_{0}^{\infty} d t \exp \left\{-\frac{i v}{2} t\left(\Delta^{2}-1\right)\right\} \Gamma(t) \tag{33}
\end{equation*}
$$

where $\Gamma(\mathrm{t})$ is defined in ( $19^{\prime}$ ).
The estimates of the contributions of the thirdorder terms of the Born series show that for processes (1) and (2) their contribution to the asymptotic amplitude $\mathrm{T}_{\mathrm{fi}}$ is smaller than that of the first- and secondorder terms. It is necessary to take into account two orders of perturbation theory because realization of the reactions in question calls for a change in the momenta of two particles, the incident proton (from $k_{i}$ to $\left(\mu_{\mathrm{p}} / \mathrm{M}_{\mathrm{f}}\right) \mathrm{k}_{\mathrm{f}}$ ) and the captured electron (from $\mathrm{g}_{0} \approx 1$ to $\mathrm{k}_{\mathrm{f}} / \mathrm{M}_{\mathrm{f}}$ ), something possible only as the result of at least two pair interactions. We note that to study the scattering at sufficiently large angles it is necessary to consider a perturbation-theory series based on the Hamiltonian (4). Account must be taken here of terms of still higher orders (in particular, for the reaction (2) the terms of the first three orders of the Born series make comparable contributions to the amplitude). The third-order terms become small only in the region of small scattering angles. Thus, the asymptotic amplitudes of reactions (1) and (2) are given respectively by expressions (32) and (33).

## 5. EXPRESSIONS FOR THE CROSS SECTIONS AND COMPARISON WITH EXPERIMENTAL DATA

To obtain asymptotic expressions for the total cross sections of the processes in question it is necessary to substitute (32) and (33) in (13) and (14), respectively, and integrate over the angle variables. Since the radial nuclear wave functions in (13) are localized in the vicinity $\Delta r \sim\left(1 / m_{p} \omega\right)^{1 / 2}$ near the point $R_{0}=1.4^{[11]}$, and the functions $\Gamma_{ \pm}$vary noticeably over the distances $\sim r_{0}=1$, it follows that $\Gamma_{ \pm}$can be expanded in the vicinity of $R_{0}$. In addition, owing to the presence of the rapidly oscillating factor $\exp \left(\mathrm{iR}_{0} \Delta_{\mathrm{f}} \cdot \mathrm{n}_{\mathrm{R}}\right)$, the contribution of the cross terms of the form $\exp \left(i \Delta_{f} \cdot R\right) T_{+} T_{-}^{*}$ to the integral over the angle variables in (13) is asymptotically small. Consequently, the asymptotic total cross section corresponding to (13) is of the form

$$
\begin{equation*}
Q_{\mathrm{H}_{2}}^{(1)}=4 \pi^{3} Q_{B K}^{(\mathrm{H})} \frac{5}{2^{10}} \int_{/ / 1}^{\infty} \frac{d \tau}{\tau^{4}} \int_{\subsetneq}^{\pi}\left|Y_{l_{i},-1}(\varphi, \theta)\right|^{2}\left|T_{+}\left(R_{0} \cos \theta, \tau\right)\right|^{2} \sin \theta d \theta, \tag{34}
\end{equation*}
$$

where $Q_{B K}^{(H)}=2^{18} \pi r_{0}^{2} / 5 v^{12}$ is the Brinkman-Kramers cross section for charge exchange on a hydrogen atom. Averaging (34) over the initial states, we obtain

$$
\begin{equation*}
\bar{Q}_{\mathrm{H}_{2}}^{(1)}=\pi^{2} Q_{B K}^{(\mathrm{H})} \int_{-1}^{ \pm 1} d z\left[0.296 \Gamma_{+}{ }^{2}(0,0)+\frac{5 \pi v}{2^{10}} \int_{0}^{\infty} d s \Gamma_{+}{ }^{2}\left(s, s R_{0} z\right)\right] . \tag{35}
\end{equation*}
$$

We have used here for the integral with respect to $d \tau$ in (34) the asymptotic expression

$$
\begin{gathered}
\lim _{N \rightarrow \infty} \int_{/ / 4}^{\infty} \frac{d \tau}{\tau^{4}}\left|\frac{f(0)}{\tau}+i N \int_{0}^{\infty} d t f(t) \exp \{-i N t(\tau-1)\}\right|^{2} \\
=\frac{2^{10}}{5}\left[0.296 f^{2}(0)+\frac{5 \pi}{2^{9}} N \int_{0}^{2} d t f^{2}(t)\right]
\end{gathered}
$$

The corresponding expression for (2) is

$$
\begin{equation*}
Q_{\mathrm{Ho}}^{(1)}=4 Q_{B K}^{(\mathrm{B})} \pi^{2}\left[0,296 \Gamma^{2}(0)+\frac{5 \pi v}{2^{10}} \int_{0}^{\infty} d s \Gamma^{2}(s)\right] . \tag{36}
\end{equation*}
$$

In the case when the final state of the target is not established in the experiment, it is necessary to sum (35) and (36) over the final states of the electron in $\mathrm{H}_{2}^{+}$ or in $\mathrm{He}^{+}$, including part of the continuous spectrum, and since the states with large electron energy make a small contribution, the summation can be extended over all the final states. Taking into account the completeness condition, and also Eqs. (7) and (14), we obtain for the total capture cross sections in a fixed final state of hydrogen

$$
\begin{gather*}
Q_{\mathrm{H}_{2}}=Q_{B K}^{(\mathrm{H})} \pi^{2} \cdot 4\left[0,296 \rho_{\mathrm{H}_{2}}\left(\frac{\mathbf{R}_{0}}{2}\right) \varphi_{\mathrm{H}}{ }^{2}(0)\right. \\
\left.+\frac{5 \pi v}{2^{11}} \int_{-1}^{+1} d\left(\mathbf{n}_{R^{\prime}} \mathbf{n}_{\Delta_{i}}\right) \int_{0}^{\infty} d \mathbf{s} \tilde{\varphi}_{\mathrm{H}}{ }^{2}(s) \rho_{\mathrm{H}_{2}}\left(s \mathbf{n}_{\Delta_{i}}+\frac{R_{0}}{2} \mathbf{n}_{R}\right)\right],  \tag{37}\\
Q_{\mathrm{He}}=8 Q_{B K}^{(\mathrm{H})} \pi^{2}\left[0,296 \rho_{\mathrm{He}}(0) \tilde{\varphi}_{\mathrm{H}}{ }^{2}(0)+\frac{5 \pi v}{2^{10}} \int_{0}^{\infty} d s \tilde{\varphi}_{\mathrm{H}}{ }^{2}(s) \rho_{\mathrm{He}}(s)\right], \tag{38}
\end{gather*}
$$

where

$$
\begin{gather*}
\rho_{\mathrm{H}_{2}}\left(\mathbf{s}_{1}\right)=\int d^{3} \mathbf{s}_{2}\left|\tilde{\Psi}_{\mathrm{H}_{2}}\left(\mathbf{s}_{1}, \mathbf{s}_{2}\right)\right|^{2}, \\
\rho_{\mathrm{He}_{\mathrm{e}}}\left(\mathbf{s}_{1}\right)=\int d^{3} \mathbf{s}_{2}\left|\tilde{\Psi}_{\mathrm{He}}\left(\mathbf{s}_{1}, \mathbf{s}_{2}\right)\right|^{2} \tag{39}
\end{gather*}
$$

are the corresponding electron densities. Summing finally over all the bound states of the hydrogen atom, we obtain an asymptotic expression for the total capture cross section

$$
\begin{align*}
& Q_{\mathrm{H}_{2}^{(t o t)}}^{(\text {(ot) }}=1,202 Q_{\mathrm{BK}}^{(\mathrm{H})}\left(0.296+\frac{5 \pi v}{2^{10}} J_{\mathrm{H}_{2}}\right),  \tag{40}\\
& Q_{\mathrm{He}}^{(\text {(ot) }}=1,202 Q_{\mathrm{BK}}^{(\mathrm{He})}\left(0.296+\frac{5 \pi v}{2^{20}} J_{\mathrm{He}}\right), \tag{41}
\end{align*}
$$

where

$$
\begin{gather*}
J_{\mathrm{H}_{2}}=\frac{1}{2.404} \int_{-1}^{ \pm 1} d z \int_{0}^{\infty} d t K(t) \frac{\rho_{\mathrm{H}_{2}}\left(\left(t^{2}+R_{0}{ }^{2} / 4+t z R_{0}\right)^{1 / 2}, z\right)}{\rho_{\mathrm{H}_{2}}\left(\mathbf{R}_{0} / 2\right)},  \tag{42}\\
J_{\mathrm{H} 0}=\frac{1}{1.202} \int_{0}^{\infty} d t K(t) \frac{\rho_{\mathrm{He}}(t)}{\rho_{\mathrm{He}}(0)}  \tag{43}\\
K(t)=\sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \frac{(2 l+1)}{R_{.0}{ }^{2}\left(\hat{)}()^{2}\right)} R_{\mathrm{R}_{1}{ }^{2}(t)} \tag{44}
\end{gather*}
$$

$\mathrm{R}_{\mathrm{n} l}(\mathrm{r})$ is the radial Coulomb function ${ }^{[11]} \cdot \mathrm{Q}_{\mathrm{BK}}^{\left(\mathrm{H}_{2}\right)}$ and $Q_{B K}^{(H e)}$ in (40) and (41) are the total cross sections for electron capture in the ls state of the hydrogen atom, calculated with allowance for only the first-order term $\hat{\mathbf{V}}_{\text {pie }_{1}}$ :

$$
\begin{equation*}
Q_{B K}^{\left(\mathrm{H}_{3}\right)}=4 Q_{B K}^{(\mathrm{H})} \rho_{\mathrm{H}_{2}}\left(\mathbf{R}_{0} / 2\right) \pi, \quad Q_{B K}^{(\mathrm{HO})}=8 Q_{B K}^{(\mathrm{H})} \rho_{\mathrm{Ho}}(0) \pi . \tag{45}
\end{equation*}
$$

The values of the electron densities that enter in (45) are known exactly near the nuclei:

$$
\rho_{\mathrm{H}_{2}}\left(\mathbf{R}_{0} / 2\right) \pi=0.723\left[{ }^{12}\right], \quad \rho_{\mathrm{He}}(0) \pi=5.688\left[{ }^{[3]}\right],
$$

so that

$$
\begin{equation*}
Q_{B K}^{(\mathrm{H})}=2.892 Q_{B K}^{(\mathrm{H})}, \quad Q_{B K}^{(\mathrm{HO})}=45.50 Q_{B K}^{(\mathrm{H})} . \tag{46}
\end{equation*}
$$

Estimates of expressions (40) and (41) show that at moderately large $v$ the terms proportional to the velocity turn out to be actually corrections to the constant terms. We calculate the coefficient (42) and (43) with the aid of the very simple electron wave functions of the type

$$
\begin{gather*}
\widetilde{\Psi}_{\mathrm{H}_{2}\left(\mathbf{s}_{1} \mathbf{s}_{2}\right)=} \frac{1}{2\left[1+S\left(R_{0}\right)\right]}\left[\varphi\left(\left|\mathbf{s}_{1}-\frac{\mathbf{R}_{0}}{2}\right|\right)+\right. \\
\left.+\varphi\left(\left|\mathbf{s}_{1}+\frac{\mathbf{R}_{0}}{2}\right|\right)\right]\left[\varphi\left(\left|\mathbf{s}_{2}-\frac{\mathbf{R}_{0}}{2}\right|\right)+\varphi\left(\left\lvert\, \mathbf{s}_{2}+\frac{\mathbf{R}_{0}}{2} T\right.\right)\right], \\
\widetilde{\Psi}_{\mathrm{He}}\left(\mathbf{s}_{1} \mathbf{s}_{2}\right)=\varphi^{\prime}\left(s_{1}\right) \varphi^{\prime}\left(s_{2}\right), \tag{47}
\end{gather*}
$$

where

$$
\begin{gathered}
\varphi(s)=\left(Z^{3} / \pi\right)^{1 / 2} e^{-z_{s} s}, \quad \varphi^{\prime}(s)=\left(z^{\prime 3} / \pi\right)^{1 / 2} e^{-z^{\prime} s}, \\
S\left(R_{\mathrm{c}}\right)=\int d^{3} \mathbf{r} \varphi\left(\left|\mathbf{r}-\frac{\mathbf{R}_{0}}{2}\right|\right) \varphi\left(\left|\mathbf{r}+\frac{\mathbf{R}_{0}}{2}\right|\right), \\
Z=1.19, \quad z^{\prime}=1.7 .
\end{gathered}
$$

As shown in the Appendix, we have in this case $\mathrm{J}_{\mathrm{He}}$ $\approx 1 / 2\left(1+z^{\prime}\right)$, for process (2), so that

$$
\begin{equation*}
Q_{\mathrm{He}}^{\text {tot }} \approx 1.2\left(0.3+\frac{5 \pi v}{2^{11} \cdot 2,7}\right) Q_{B K}^{(\mathrm{HO})} . \tag{48}
\end{equation*}
$$

The corresponding expression for (1) is

$$
\begin{equation*}
Q_{\mathrm{H}_{2}}^{t t_{2} t} \approx 1.2\left(0.3+\frac{5 \pi v}{2^{12}}\right) Q_{B \mathrm{~K}}^{\left(\mathrm{H}_{2}\right)} . \tag{49}
\end{equation*}
$$

Recognizing that the cross section for the capture of an electron from the hydrogen atom is

$$
\begin{equation*}
Q_{\mathrm{H}}^{\text {tot }} \approx 1.2\left(0.3+\frac{5 \pi v}{2^{12}}\right) Q_{B K}^{(\mathrm{H})}, \tag{50}
\end{equation*}
$$

we see that there is a linear relation between the cross sections of the corresponding processes:

$$
\begin{equation*}
Q_{\mathrm{H}_{2}}^{\text {tot }}=4 \pi \rho_{\mathrm{H}_{2}}\left(\mathbf{R}_{0} / 2\right) Q_{\mathrm{H}}^{\text {bot }}, \tag{51}
\end{equation*}
$$

as previously obtained by Tuan and Gerjuoy ${ }^{[6]}$ within the framework of first-order theory.

The cross sections calculated from formulas (48) and (49) are compared in Fig. 4 with the experimental data $^{[1-5]}$ obtained for incident protons with energy above 1 MeV (in the lab). The lower series of the results corresponds to the process (1), and the upper to the process (2). As seen from the figure, there is satisfactory agreement between the experimental data


FIG. 4. Electron capture cross sections in processes (1) and (2) vs. the energy of the incident proton (in the laboratory system): $\mathrm{O}, \mathrm{O}-\mathrm{ex}-$ perimental data from $\left.\left[{ }^{1}\right], \diamond, \diamond-{ }^{2}\right], X-\left[{ }^{4}\right], \square,-\left[{ }^{5}\right]$. The theoretical plots 1 and 2 were calculated from formulas (49) and (48) for processes (1) and (2), respectively.
for (1) in the region $E<1.4 \mathrm{MeV}$. At larger values of $E$ there is a considerable discrepancy between data by different workers. The theoretical calculations for (1) agree well with the data of ${ }^{[1,2]}$ at $\mathrm{E} \gtrsim 2 \mathrm{MeV}$. For reaction (2), the scatter of the experimental points is much smaller, and at $\mathrm{E} \gtrsim 6 \mathrm{MeV}$ the points coincide with the theoretical values within the limits of experimental error. On the basis of the presented experimental data we can thus assume that the capture cross sections $Q_{H_{2}}^{\text {tot }} Q_{H e}^{\text {tot }}$ for $E \gtrsim 2 \mathrm{MeV}$ in the case of (1) and $\mathrm{E} \gtrsim 6 \mathrm{MeV}$ in the case of (2) reach their asymptotic values given by formulas (48) and (49). The reason why the asymptotic values of $Q_{H e}$ are reached at higher energies than those of $\mathrm{QH}_{2}$ is that the small parameter of the problem, namely the ratio of the "orbital" velocity of the exchanged electron to v , has a larger value in the case of capture from He than in capture from $\mathrm{H}_{2}$ at the same incident-proton energy. We note finally that if we neglect those terms of (35) and (36) which are proportional to the velocity and which make contributions of 20 and $15 \%$ at 6 MeV , respectively, then we can draw, with the same accuracy, the following conclusions, which do not depend on the employed many-electron wave functions of $\mathrm{H}_{2}$ and He .

First, only transitions to the final $\mathrm{n} \sigma_{\alpha}$ states ( $\alpha=\mathrm{g}, \mathrm{u}$ ) of $\mathrm{H}_{2}^{+}$and to (ns) states of $\mathrm{He}^{+}$are "allowed." The cross sections for capture with transition of $\mathrm{He}^{+}$to states with higher angular momenta and $\mathrm{H}_{2}^{+}$in states with larger projections of the angular momentum decrease much more rapidly as $\mathrm{v} \rightarrow \infty$. Second, the cross sections (48) and (49) decrease at equal rates as $\mathrm{v} \rightarrow \infty$, and consequently their ratio does not depend on the velocity of the incident proton.

## APPENDIX

If wave function (47) is used, the expression for the coefficient (43) takes the form

$$
\begin{equation*}
J_{\mathrm{He}}=\frac{1}{1,202} \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \frac{1}{n^{3}} J_{n l} \tag{A.1}
\end{equation*}
$$

where

$$
\begin{gather*}
J_{n l}=\frac{n^{3}(2 l+1)}{R_{18}{ }^{2}(0)} \int_{0}^{\infty} e^{-2 z^{\prime} t} R_{n l}{ }^{2}(t) d t \\
=\frac{(2 l+1)}{2} \frac{(n-l-1)!}{(n+l)!} \int_{0}^{\omega} d s \exp \left\{-s\left(1+n z^{\prime}\right)\right\} s^{2 l}\left[L_{n-l-1}^{(2 l+1)}(s)\right]^{2},  \tag{A.2}\\
L_{n}^{(m)}(s)=\frac{(m+n)!}{m!n!} F(-n, m+1 ; s), \tag{A.3}
\end{gather*}
$$

$F(\alpha, \beta ; s)$ is a confluent hypergeometric function. An integral of the type (A.2), in the form of a Laplace transform, has been calculated for a more general case in ${ }^{[14]}$. For the given values of the parameters we have

$$
\begin{align*}
J_{n l}= & \frac{1}{2\left(1+n z^{\prime}\right)^{2 l+1}} \sum_{v=0}^{n-l-1} \frac{(2 l+v)!}{(2 l)!v!}\left(1+\frac{1}{n z^{\prime}}\right)^{-v} \\
& \times F\left(-v,-v+1 ; 2 l+2 ; \frac{1}{n^{2} z^{\prime 2}}\right), \tag{A.4}
\end{align*}
$$

where $F(\alpha, \beta ; \gamma ; \mathrm{x})$ is a hypergeometric function that reduces in the present case to a polynomial of finite degree. Summing (A.4) over all $l$, we obtain

$$
\begin{equation*}
J_{n}=2\left(1+z^{\prime}\right) \sum_{l=0}^{n-1} J_{n l} . \tag{A.5}
\end{equation*}
$$

As a result of the calculation of the finite sums (A.4) and (A.5) we find that the coefficients $\mathrm{J}_{\mathrm{n}}$ are rather slowly varying functions of $n$. Thus, at $n=1,2$, and 3 they are equal to $1,1.12$, and 1.18 , respectively. Recognizing that (A.1) contains the rapidly decreasing factor $1 / \mathrm{n}^{3}$, we find, accurate to several tenths, that $\mathrm{J}_{\mathrm{He}}$ $\approx 1 / 2\left(1+z^{\prime}\right)$.

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[^0]:    ${ }^{1)}$ In their calculation of the asymptotic form of (22), Chatterjee and McDowell [ ${ }^{8}$ ] neglected the momentum transfer $\Delta_{e}=\mathrm{k}_{\mathrm{f}} / \mathrm{M}_{\mathrm{f}}=\mathrm{v}_{\mathrm{f}}$ of the electron $e_{1}$ in comparison with the Bohr value. However, since $\Delta_{\mathrm{e}} \gg 1$ when $\nu \gg 1$, the conclusion of $\left[{ }^{8}\right]$ that the matrix element (22) makes an important contribution is not justified.

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