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Rearrangement Collisions at Very High Energies*†

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The energy dependence of the charge-exchange cross section in proton–hydrogen-atom collisions at very high energies, within the framework of the Schrödinger equation, has long been a subject of controversy. We attempt to determine the energy dependence of the forward-scattering cross section at very high energies in an arbitrary rearrangement collision involving two heavy particles of masses M_a and M_b and a light particle of mass m, with m initially bound to M_a and finally bound to M_b. In the limits m/M_a, $m/M_b \to 0$ the scattering is entirely in the forward direction and the cross section σ for forward capture is given exactly by the impact-parameter treatment. A Born-type expansion is developed in the impact-parameter treatment for the forward-capture amplitude A. Thus, A is written as a sum of a finite number of Born terms plus a remainder R. The Schwarz inequality can be used to bound R since there are no non-normalizable plane-wave functions—the motion of M_a and M_b is treated classically. We can thereby show that for a certain class of nonsingular interactions the *second* Born term provides the dominant contribution to σ at high energies, whether or not the Born series converges. (This may be the first example for which it has been shown that the second Born term dominates.) This result makes plausible the dominance of the second Born term in p-H forward charge exchange.

I. INTRODUCTION

Within the framework of the Schrödinger equation, the determination of the energy dependence of the ground state to ground-state charge-transfer cross section in proton–hydrogen-atom collisions, as the relative kinetic energy E goes to infinity, is a vintage problem which continues to attract interest.[1] Capture into the backward direction is thought to dominate[2] for E sufficiently large, the main contribution coming from the first Born approximation[3] and being proportional to $(m_e/M_p)^2 E^{-3}$, with m_e and M_p the electron and proton masses, respectively. However, back scattering is unobservably small due to the $(m_e/M_p)^2$ factor, and we will concern ourselves with the result obtained by first letting $m_e/M_p \to 0$ and *then* considering arbitrarily large E. Capture into the forward direction then dominates, and it is the energy dependence of the forward-capture cross section which is of greatest interest and which is the subject of this paper.

The first quantum-mechanical calculation of the proton-hydrogen charge-transfer cross section was performed in 1930 by Brinkmann and Kramers.[4] Neglecting the proton-proton interaction and using the first Born approximation, they found that the forward-capture cross section behaved as C/E^6 for sufficiently high energy. (The rapid decrease with E is a consequence of the difficulty of having the electron undergo the necessary great change in its velocity.) The $1/E^6$ dependence disagreed with the $1/E^{11/2}$ dependence obtained earlier by Thomas[5] in a classical calculation, and was viewed with consternation by Bohr[6] and others. Much later, still using the first Born approximation, Jackson and Schiff[7] showed that the inclusion of the proton-proton interaction did not affect the energy dependence of forward capture; its only effect was to reduce the constant C. In 1955, however, Drisko[8] investigated the *second* Born term, and obtained, in agreement with the classical energy dependence, a limiting behavior $C'/E^{11/2}$ for forward capture. Drisko's result was a very strong indication that forward capture did not converge to the result obtained in the first Born approximation.

Dettmann and Leibfried[3] recently investigated each term in the Born series for a three-body rearrangement collision involving arbitrary masses m, M_a, and M_b, and a wide range of potentials, including Coulomb potentials. (It must be possible to express the Fourier transform of the potential as a power series in $1/k$ for large k.) For ground-state to ground-state capture, with m initially bound to M_a and finally to M_b, we introduce the notation σ_N^W for the cross section obtained by truncating the Born series after a large but finite number N of terms. (The superscript W indicates that the cross section is calculated in the correct wave treatment rather than the approximate impact-parameter treatment to be discussed later.) Dettmann and Leibfried proved that for any $N \geqslant 2$, the dominant contribution at high energies to σ_N^W comes from the first Born term if M_a equals M_b, and the second Born term if M_a differs from M_b. They also showed that the main contributions at high energies from the first and second Born terms come from the scattering of M_a and M_b into "critical" angles, angles which have a simple classical interpretation.[9] When M_a equals M_b equals M, say, as in proton-hydrogen charge transfer, there is a critical angle of 180° (in the center-of-mass frame) and back scattering then provides the main contribution at high energies from the first Born term. However, if the captured particle is light, critical back scattering is unobservably small and vanishes in the limit $m/M \to 0$.[10] In fact, when m/M_a and m/M_b are small there is always a small critical angle, of the order of $(\sqrt{\tfrac{3}{2}})[(m/M_a)+(m/M_b)]$ in the center-of-mass frame, which at high energies gives rise to a forward-capture peak in the *second* Born term, and in the limits m/M_a, $m/M_b \to 0$ forward capture dominates over critical scattering into other directions. In other words, after the limits m/M_a, $m/M_b \to 0$ are taken, the high-energy dependence of σ_N^W originates in the second Born term through forward capture, whether or not M_a equals M_b.

The proof that a given Born term determines the high-energy dependence of σ_N^W does not prove that this term determines the high-energy dependence of the actual cross section since the Born series may not converge for rearrangement collisions or even for direct collisions. The Born series for the Green's function diverges in the three-body problem, for rearrangement and direct collisions,[11] and therefore the Born series for the scattering amplitude may well diverge also in some cases.

The essence of the present approach is to avoid convergence questions. In the limits m/M_a, $m/M_b \to 0$ the scattering is entirely in the forward direction,[12] as suggested above. Now the impact parameter method treats forward scattering and in the limits m/M_a, $m/M_b \to 0$ the wave and impact parameter treatments yield identical cross sections.[12,13] But one can easily bound the cross section σ obtained in the impact-parameter treatment[14]; the heavy particles M_a and M_b are treated classically and there are no associated non-normalizable plane-wave functions. The light particle m is described by a normalizable wave function and is subject to a time-dependent potential, and matrix elements involving the unknown but normalizable wave function can be bounded by using the Schwarz inequality.

It might be noted that the bound on σ obtained in the impact-parameter method is a particular example of the existence of bounds[15] (indeed, of variational bounds[14]) on transition amplitudes in time-dependent problems. The essential point[14] is that the only unknown in a transition-amplitude matrix element is the unitary time-translation operator, and this operator can be eliminated by the use of the Schwarz inequality. The impact-parameter approximation reduces the original scattering problem to that of the determination of a transition amplitude.

Returning to the problem at hand, a Born-type expansion is developed in the impact-parameter method for the forward-capture amplitude A. Thus A is written as the sum S_N of a finite number N of Born terms plus a remainder R_N. The Born terms are, of course, given explicitly, and their velocity dependences can often be extracted even when the velocity-independent coefficients cannot be obtained. Let the contribution to σ from the dominant Born term be D/v^q, with q known; D may or may not be known. One then obtains a bound on the contribution to σ directly from R_N and from the cross term involving R_N and S_N, of the form D'/v^p with p known; D' may or may not be known. If $p > q$ it follows that the cross section behaves as $1/v^q$ whether or not the Born series diverges.

We have successfully applied the above approach only to a certain class of nonsingular potentials, and found that the second Born term dominates at high energies. To our knowledge this is the first example of a reasonably rigorous proof of the dominance of the second Born term in any scattering process for which the first Born term does not vanish by some selection rule, and it makes even more plausible the dominance of the second Born term in p-H forward charge exchange. The result is physically reasonable when one considers that classically forward capture is pictured as a two-step process[16]: m is first scattered by the incident particle towards the target particle, from which it is scattered a second time to emerge with the same velocity as the almost undeflected incident particle.[5]

In Sec. II we discuss the impact-parameter method for an arbitrary rearrangement collision involving two heavy particles M_a and M_b and a light particle m. We discuss the existence of the transition amplitude A and then upper and lower bounds on A are derived. Various expansions of A are considered; for most expansions the bounds are very poor. In Sec. III for interactions which are nonsingular and which fall off sufficiently rapidly with increasing distance, a particular expansion provides the high-energy dependence of the ground state to ground-state forward-capture cross section and shows it to originate in the second Born term.

II. IMPACT-PARAMETER METHOD

A. Preliminaries

In the eikonal or impact-parameter method the light particle of mass m is treated quantum mechanically but the heavy particles of masses M_a and M_b are treated classically and it is further assumed that they move with constant velocity. Thus, M_a and M_b become moving centers of force which subject m to a time-dependent potential. The state vector $|\Psi(t)\rangle$ of m at any time t is determined by

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle \tag{2.1}$$

and appropriate boundary conditions.

We work in the laboratory system with M_a initially and therefore permanently at rest. Let the vectors $\vec{r}$ and $\vec{R}(t)$ locate m and M_b with respect to M_a, the origin of coordinates. The interaction operator V_a between m and M_a is time independent but the interaction operators $V_b(t)$ and $V_{ab}(t)$ between m and M_b and between M_a and M_b depend on the time through

$$\vec{R}(t) = \vec{\rho} + \vec{v}t\,, \tag{2.2}$$

where $\vec{\rho}$ is the impact parameter and $\vec{v}$ is the (constant) velocity of M_b. The Hamiltonian $H(t)$ has the form

$$H(t) = H_0 + V_a + V_b(t) + V_{ab}(t)\,, \tag{2.3}$$

where

$$H_0 = -(\hbar^2/2m)\nabla_{\vec{r}}^{\,2} \tag{2.4}$$

is the kinetic energy operator of m. Note that the interaction between M_a and M_b is included in the Hamiltonian; a discussion of this point will be given later. All interactions are assumed to be Hermitian and local. In coordinate space we have, with $r = |\vec{r}|$ and $R(t) = |\vec{R}(t)|$,

$$\langle\vec{r}\,|V_a|\vec{s}\rangle = V_a(r)\delta(\vec{r}-\vec{s})\,, \tag{2.5a}$$

$$\langle\vec{r}\,|V_b(t)|\vec{s}\rangle = V_b(|\vec{r}-\vec{R}(t)|)\delta(\vec{r}-\vec{s})\,, \tag{2.5b}$$

$$\langle\vec{r}\,|V_{ab}(t)|\vec{s}\rangle = V_{ab}(R(t))\delta(\vec{r}-\vec{s})\,. \tag{2.5c}$$

Note that we use the same symbol for the interaction operators as we do for their coordinate representations, although of course the arguments differ. No confusion should arise in distinguishing between operators and their coordinate representations.

With the state vector of m specified at some time t_0, the formal solution of Eq. (2.1) is

$$|\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle\,. \tag{2.6}$$

The unitary time-translation operator $U(t,t_0)$ governs the time development of the state vector and satisfies

$$\left(H(t) - i\hbar\frac{\partial}{\partial t}\right)U(t,t_0) = 0\,, \tag{2.7}$$

with the boundary condition

$$U(t_0,t_0) = 1\,. \tag{2.8}$$

The definition of the transition amplitude depends on the existence of unperturbed ingoing and outgoing states. For later use we first define operators H_a, $H_b(t)$, $V_a'(t)$, $V_b'(t)$, and $V(t)$:

$$H_a \equiv H_0 + V_a\,, \tag{2.9a}$$

$$H_b(t) \equiv H_0 + V_b(t)\,, \tag{2.9b}$$

$$V_a'(t) \equiv H(t) - H_a = V_b(t) + V_{ab}(t)\,, \tag{2.9c}$$

$$V_b'(t) \equiv H(t) - H_b(t) = V_a + V_{ab}(t)\,, \tag{2.9d}$$

$$V(t) \equiv H(t) - H_0 = V_a + V_b(t) + V_{ab}(t)\,. \tag{2.9e}$$

We shall also need the unitary time-translation operators $U_a(t,t_0)$ and $U_b(t,t_0)$ defined by

$$\left(H_a - i\hbar\frac{\partial}{\partial t}\right)U_a(t,t_0) = 0\,,\quad U_a(t_0,t_0) = 1\,; \tag{2.10a}$$

and

$$\left(H_b(t) - i\hbar\frac{\partial}{\partial t}\right)U_b(t,t_0) = 0\,,\quad U_b(t_0,t_0) = 1\,. \tag{2.10b}$$

It is simple to write formal solutions for U_a and U_b. We have

$$U_a(t,t_0)=e^{-i(t-t_0)H_a/\hbar}\ , \tag{2.11a}$$

since H_a is time independent, but

$$U_b(t,t_0)=\mathcal{T}\exp[-i\int_{t_0}^{t}H_b(t')\,dt'/\hbar]\,, \tag{2.11b}$$

where $\mathcal{T}$ is Dyson's time-ordering operator.

Now if at large negative times m is bound to M_a the unperturbed ingoing state $|\Psi_a(t)\rangle$ is defined by

$$|\Psi_a(t)\rangle\equiv\lim_{t_0\to-\infty}U_a(t,t_0)|\Psi(t_0)\rangle\ , \tag{2.12}$$

provided the limit exists. Thus, $|\Psi_a(t)\rangle$ represents the unperturbed propagation in time of the bound system $(m+M_a)$ and therefore

$$\langle\vec{r}|\Psi_a(t)\rangle=\Phi_a(\vec{r})e^{-iE_at/\hbar}\ , \tag{2.13}$$

where $\Phi_a(\vec{r})$ is the initial stationary bound-state wave function of m and E_a is the corresponding bound-state energy. In Appendix A we prove that the limit in (2.12) will exist if

$$\lim_{t\to-\infty}t\,\|\,V_a'(t)|\Phi_a\rangle\,\|=0\,, \tag{2.14}$$

where the norm $\|\,|\Phi\rangle\,\|$ of the vector $|\Phi\rangle$ is defined by

$$\|\,|\Phi\rangle\,\|=\langle\Phi|\Phi\rangle^{1/2}=(\int|\langle\vec{r}|\Phi\rangle|^2d\vec{r})^{1/2}\,. \tag{2.15}$$

Going into the coordinate representation and noting that the presence of $\Phi_a(\vec{r})$ restricts the range of r, Eq. (2.14) leads to the requirement

$$\lim_{R\to\infty}R(V_b(R)+V_{ab}(R))=0\,; \tag{2.16}$$

thus, if the interactions satisfy (2.14) or, equivalently, (2.16), the unperturbed ingoing state exists.

Similarly, if at large positive times m is bound to M_b, the unperturbed outgoing state $|\Psi_b(t)\rangle$ is defined by

$$|\Psi_b(t)\rangle\equiv\lim_{t_0\to\infty}U_b(t,t_0)|\Psi(t_0)\rangle\ , \tag{2.17}$$

provided the limit exists, and

$$\langle\vec{r}|\Psi_b(t)\rangle=\Phi_b(\vec{r}-\vec{R}(t))e^{im\vec{v}\cdot\vec{r}/\hbar}e^{-i(E_b+mv^2/2)t/\hbar}, \tag{2.18}$$

where Φ_b is the final stationary bound-state wave function of m and E_b is the corresponding bound-state energy. Note that through the translational motion of M_b, m acquires the additional energy $\frac{1}{2}mv^2$ and the additional momentum $m\vec{v}$. The unperturbed outgoing state exists if

$$\lim_{t\to\infty}t\,\|\,V_b'(t)|\Phi_b(t)\rangle\,\|=0\,, \tag{2.19}$$

which amounts to the requirement

$$\lim_{R\to\infty}R(V_a(R)+V_{ab}(R))=0\,. \tag{2.20}$$

Note that the difference in form between (2.13) and (2.18) plays no significant role in the conditions for the existence of the unperturbed ingoing and outgoing states: Eqs. (2.16) and (2.20) differ only in the interchange of a and b.

With the boundary condition that m is initially bound to M_a, the amplitude for forward capture is

$$A=\lim_{T_1\to\infty}\langle\Psi_b(T_1)|\Psi(T_1)\rangle \tag{2.21}$$

or, using (2.6) and recognizing that (2.12) implies that $\Psi(T_0)$ approaches $\Psi_a(T_0)$ for T_0 in the remote past,

$$A=\lim_{\substack{T_1\to\infty\\T_0\to-\infty}}\langle\Psi_b(T_1)|U(T_1,T_0)|\Psi_a(T_0)\rangle\ , \tag{2.22}$$

where the unperturbed ingoing and outgoing states are defined by (2.13) and (2.18). The cross section for forward capture is

$$\sigma=\int_0^\infty|A|^2 2\pi\rho\,d\rho\,. \tag{2.23}$$

We suppress the ρ and v dependence of A and the v dependence of σ.

We note that if we add a term $f(t)1$ to the Hamiltonian (2.3), where $f(t)$ is a real function rather than an operator and 1 is the unit operator in coordinate space, then

$$|\Psi(t)\rangle\to\exp[-i\int^t f(t')\,dt'/\hbar]|\Psi(t)\rangle\ ; \tag{2.24}$$

by (2.21) A is merely altered by a phase factor so that σ is unchanged. If we choose $f(t)$ to be $-V_{ab}(R(t))$ then $V_{ab}(t)$ disappears from $H(t)$ showing that, as is well known, this interaction cannot affect the cross section for forward capture in the impact-parameter treatment. Moreover, if the conditions (2.14) and (2.19) do not hold, we can, since $\Phi_a(\vec{r})$ and $\Phi_b(\vec{r}-\vec{R}(t))$ restrict the range of r and $|\vec{r}-\vec{R}(t)|$, respectively, always choose $f(t)$ so that with the modified forms of $V_a'(t)$ and V_b' these conditions do hold, and hence we can always define unperturbed ingoing and outgoing states. This is just a reflection of the fact that the perturbing potential, whatever its form is, provided it vanishes asympotically, has a vanishingly small probability for inducing transitions at long range. In this paper we always work specifically with the Hamiltonian given by (2.3), and with interactions which satisfy conditions (2.14) and (2.19). This is because although σ is unaffected by the addition of a term $f(t)1$ to the Hamiltonian, any trial (e.g., Born) estimate of σ, calculated with some trial U, will in general be affected by this term. Later we wish to develop a Born series in the impact-parameter treatment which in the limits m/M_a, $m/M_b \to 0$ corresponds term by term to the Born series obtained in the wave treatment, and this is possible only if the Hamiltonian includes those, and only those, interactions which occur in the real three-body problem. In particular, the Hamiltonian must include $V_{ab}(t)$.

B. Upper and Lower Bounds on A

Following the procedure of Ref. 14 we introduce the integral equation

$$U(T_1, T_0) = \overline{U}(T_0, T_1)^\dagger - (i/\hbar)\int_{T_0}^{T_1} dt_2[\mathcal{H}(t_2)\overline{U}(t_2,T_1)]^\dagger U(t_2,T_0) \tag{2.25}$$

for $U(T_1,T_0)$, and the adjoint integral equation

$$U(t_2,T_0) = \hat{U}(t_2,T_0) - (i/\hbar)\int_{T_0}^{t_2} dt_1\, U(t_2,t_1)\mathcal{H}(t_1)\hat{U}(t_1,T_0) \tag{2.26}$$

for $U(t_2,T_0)$. Here

$$\mathcal{H}(t) \equiv H(t) - i\hbar\frac{\partial}{\partial t} \tag{2.27}$$

and $\overline{U}$ and $\hat{U}$ are any two trial operators, not necessarily unitary, which satisfy the conditions

$$\overline{U}(t,t) = 1, \quad \hat{U}(t,t) = 1\,. \tag{2.28}$$

If we use (2.26) in the right-hand side of (2.25) and use the resulting expression for $U(T_1,T_0)$ in (2.22), we obtain

$$A = A_0 + A_1 + R_1\,, \tag{2.29}$$

where, in the limits $T_0 \to -\infty$ and $T_1 \to \infty$,

$$A_0 = \langle \Psi_b(T_1)|\,\overline{U}(T_0,T_1)^\dagger\,|\Psi_a(T_0)\rangle\,, \tag{2.30}$$

$$A_1 = -(i/\hbar)\int_{T_0}^{T_1} dt\,\langle \Psi_b(T_1)|\{\mathcal{H}(t)\overline{U}(t,T_1)\}^\dagger \times\hat{U}(t,T_0)|\Psi_a(T_0)\rangle\,, \tag{2.31}$$

$$R_1 = (-i/\hbar)^2\int_{T_0}^{T_1} dt_2\int_{T_0}^{t_2} dt_1\,\langle \Psi_b(T_1)|\{\mathcal{H}(t_2)\overline{U}(t_2,T_1)\}^\dagger \times U(t_2,t_1)'\mathcal{H}(t_1)\hat{U}(t_1,T_0)|\Psi_a(T_0)\rangle\,. \tag{2.32}$$

We can use the Schwarz inequality to eliminate U from (2.32) since U is unitary. We then obtain a bound on the remainder R_1 of the form

$$|R_1| \le R_1^{Bd} \equiv \lim_{\substack{T_1\to\infty\\ T_0\to-\infty}} (1/\hbar)^2\int_{T_0}^{T_1} dt_2\int_{T_0}^{t_2} dt_1 \times\|\mathcal{H}(t_2)\overline{U}(t_2,T_1)|\Psi_b(T_1)\rangle\| \times\|\mathcal{H}(t_1)\hat{U}(t_1,T_0)|\Psi_a(T_0)\rangle\|\,. \tag{2.33}$$

We therefore have the upper and lower bounds

$$|A_0 + A_1| - R_1^{Bd} \le |A| \le |A_0 + A_1| + R_1^{Bd} \tag{2.34}$$

on A.[14]

C. Examples

If we choose

$$\hat{U}(t_1,t_0) \equiv \exp\{-i\int_{t_0}^{t_1}[H_a + V_{ab}(t)]dt/\hbar\} = U_a(t_1,t_0)\exp[-i\int_{t_0}^{t_1}V_{ab}(t)dt/\hbar] \tag{2.35}$$

and

$$\overline{U}(t_1,t_0) \equiv \mathcal{T}\exp\{-i\int_{t_0}^{t_1}[H_b(t) + V_{ab}(t)]dt/\hbar\} = U_b(t_1,t_0)\exp[-i\int_{t_0}^{t_1}V_{ab}(t)dt/\hbar]\,, \tag{2.36}$$

we obtain

$$A_0 = \alpha \lim_{T_0\to-\infty}\langle\Psi_b(T_0)|\Psi_a(T_0)\rangle = 0\,, \tag{2.37}$$

since Ψ_a and Ψ_b do not overlap in the remote past; we also have

$$A_1 = (-i\alpha/\hbar)\int_{-\infty}^{\infty} dt\langle\Psi_b(t)|V_a|\Psi_a(t)\rangle \tag{2.38}$$

and

$$|R_1| \le R_1^{Bd} = (1/\hbar)^2\int_{-\infty}^{\infty} dt_2\,\|V_a|\Psi_b(t_2)\rangle\| \times\int_{-\infty}^{t_2} dt_1\,\|V_b(t_1)|\Psi_a(t_1)\rangle\|\,. \tag{2.39}$$

The coefficient α appearing in (2.37) and (2.38) is simply a phase factor defined as

$$\alpha = \exp[-i\int_{-\infty}^{\infty}V_{ab}(t)dt/\hbar]\,. \tag{2.40}$$

A_1 is just the Brinkmann-Kramers-type amplitude which, in the case of proton-hydrogen ground state to ground-state charge transfer, leads to a cross section which behaves as v^{-12} at very high energies, as noted earlier. Note that even if α, and therefore A_1, does not exist, the relevant quantity, i.e., $|A_1|$, does exist. We can easily determine the velocity dependence of R_1^{Bd} [for Eqs. (2.5), (2.13), and (2.18)],

$$\|V_b(t)|\Psi_a(t)\rangle\| = (\int d\vec{r}\,|V_b(|\vec{r} - \vec{\rho} - \vec{v}t|)\Phi_a(\vec{r})|^2)^{1/2} \tag{2.41}$$

and

$$\|V_a|\Psi_b(t)\rangle\| = (\int d\vec{r}\,|V_a(r)\Phi_b(\vec{r} - \vec{\rho} - \vec{v}t)|^2)^{1/2}\,. \tag{2.42}$$

Hence $\vec{v}$, t_1, and t_2 appear only in the combinations $\vec{v}t_1$ and $\vec{v}t_2$ in the integrand in (2.39), and the v dependence can be extracted by changing the variables of integration to $u_1 = vt_1$ and $u_2 = vt_2$. Defining functions $f_1(u_1)$ and $f_2(u_2)$ by

$$f_1(u_1) = (\int d\vec{r}\,|V_b(|\vec{r} - \vec{\rho} - u_1\hat{z}|)\Phi_a(\vec{r})|^2)^{1/2} \tag{2.43}$$

and

$$f_2(u_2) = (\int d\vec{r}\,|V_a(r)\Phi_b(\vec{r} - \vec{\rho} - u_2\hat{z})|^2)^{1/2}\,, \tag{2.44}$$

where the unit vector $\hat{z}$ is simply $\vec{v}/v$, it follows that

$$R_1^{Bd} = F_1(\rho)/v^2 , \tag{2.45}$$

where the integral

$$F_1(\rho) = (1/\hbar)^2 \int_{-\infty}^{\infty} f_2(u_2)\, du_2 \int_{-\infty}^{u_2} f_1(u_1)\, du_1 \tag{2.46}$$

is independent of v. This result, if the integral (2.46) converges, is independent of the nature of the interactions and the initial and final states but it gives an extremely poor estimate of the velocity dependence of the remainder term R_1. The source of the trouble can be seen by comparing Eqs. (2.18) and (2.42). In applying the Schwarz inequality to the remainder we lose the translation factor $\exp(im\vec{v}\cdot\vec{r}/\hbar)$. This factor accounts for the change in momentum which m must undergo in being captured, and at high energies this change in momentum is very important in reducing the probability of capture.

We consider very briefly two further examples. The Jackson-Schiff approximation is obtained by choosing $\hat{U}$ equal to U_a and $\overline{U}$ equal to U_b, that is, we drop the term $V_{ab}(t)$ from (2.35) and (2.36). As before A_0 equals zero, but now we have

$$A_1 = (-i/\hbar)\int_{-\infty}^{\infty} dt \langle \Psi_b(t) | V_b'(t) | \Psi_a(t)\rangle , \tag{2.47}$$

which is the Jackson-Schiff term. However, R_1^{Bd} has the same velocity dependence as in the Brinkmann-Kramers approximation and again leads to an extremely poor result. A better bound on the remainder could probably be obtained by the use of the continuum distorted wave approximation of Cheshire.[17] In the continuum distorted wave approximation A_0 is zero and A_1 yields a cross section for forward capture in agreement with the second Born approximation at high energies. We have, however, been unable to determine the velocity dependence of R_1^{Bd} in this case. In any event, we can be fairly sure that although the bound may be improved it will still be far from reasonable since the same trouble occurs—the rapidly oscillating phase factor which accounts for the change in momentum of m disappears from the integrand of R_1 when we apply the Schwarz inequality. We note that this difficulty does not occur in direct collisions where the change in momentum of m is small.

III. BORN SERIES IN POWERS OF $V(t)$ FOR GROUND-STATE CAPTURE

In Sec. II we did not specify ϕ_a and ϕ_b. In this section we require that both ϕ_a and ϕ_b be ground states. The restriction to ground states is convenient because we will depend on the work of Dettmann and Liebfried[3] who themselves have only considered ground-state capture.

The Jackson-Schiff term (2.47) is the first term of the usual Born series and this series is obtained by expanding the Jackson-Schiff remainder [obtained from (2.32) by choosing $\hat{U}=U_a$ and $\overline{U}=U_b$],

$$R_1 = (-i/\hbar)^2 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{t_2} dt_1 \times \langle V_b'(t_2)\Psi_b(t_2) | U(t_2,t_1) | V_a'(t_1)\Psi_a(t_1)\rangle \tag{3.1}$$

in powers of

$$V(t) \equiv V_a + V_b(t) + V_{ab}(t) . \tag{3.2}$$

We use the integral equation [cf. Eq. (2.26)]

$$U(t_2,t_1) = U_0(t_2,t_1) - (i/\hbar)\int_{t_1}^{t_2} dt_3\, U(t_2,t_3)V(t_3)U_0(t_3,t_1) , \tag{3.3}$$

where

$$U_0(t_3,t_1) = \exp[-i(t_3-t_1)H_0/\hbar] . \tag{3.4}$$

We have, on iterating (3.3) $(N-2)$ times, inserting it in (3.1), and using (2.29),

$$A = A_1 + R_1 = \sum_{n=1}^{N} A_n + R_N , \tag{3.5}$$

where A_1 is given by (2.47), where A_n for $n \geq 2$ is given by

$$A_n = \left(\frac{-i}{\hbar}\right)^n \int_{D(t)} dt_n \cdots dt_1 \langle V_b'(t_n)\Psi_b(t_n) | U_0(t_n,t_{n-1}) \times \prod_{i=2}^{n-1} \{V(t_i)U_0(t_i,t_{i-1})\} | V_a'(t_1)\Psi_a(t_1)\rangle , \tag{3.6}$$

and where the remainder R_N differs from A_{N+1} only in the replacement of the single term $U_0(t_{N+1},t_N)$ by $U(t_{N+1},t_N)$ in the integrand of A_{N+1}. Here it is understood that

$$\prod_{i=m}^{n} \{a_i\} = \begin{cases} 1 & \text{if } n < m \\ a_n a_{n-1} \cdots a_m & \text{if } n \geq m \end{cases} \tag{3.7}$$

and that $D(t)$ is the infinite domain of integration with the variables of integration t_i ordered so that

$$\int_{D(t)} dt_n\, dt_{n-1} \cdots dt_1 \equiv \int_{-\infty}^{\infty} dt_n \int_{-\infty}^{t_n} dt_{n-1} \cdots \int_{-\infty}^{t_2} dt_1 . \tag{3.8}$$

The Born terms in the expansion (3.5) of A correspond to the Born terms in the expansion of the three-body scattering amplitude in the time-independent wave treatment, where the Green's function is there too expanded in powers of the sum of three interactions. In the limits m/M_a, $m/M_b \to 0$ the wave and impact-parameter treatments yield identical cross sections to all orders in the Born expansion.[18] Hence if σ_N denotes the cross section obtained from the first N Born terms in the impact-parameter treatment, i.e.,

$$\sigma_N = \int_0^{\infty} |S_N|^2 2\pi\rho\, d\rho , \quad S_N = \sum_{n=1}^{N} A_n , \tag{3.9}$$

then

$$\sigma_N = \lim_{\substack{m/M_a\to 0\\ m/M_b\to 0}} \sigma_N^W , \tag{3.10}$$

where σ_N^W was defined in the Introduction. Therefore, the energy dependence of σ_N at very high energies can be determined from the results of Dettmann and Liebfried.[3]

To bound the velocity dependence of R_N we apply the Schwarz inequality to eliminate U and obtain

$$|R_N| \le R_N^{Bd} = \left(\frac{1}{\hbar}\right)^{N+1} \int_{D(t)} dt_{N+1} \cdots dt_1 \times \| V_b'(t_{N+1}) | \Psi_b(t_{N+1})\rangle \| \times \left\| \prod_{i=2}^{N} \{V(t_i) U_0(t_i, t_{i-1})\} | V_a'(t_1) \Psi_a(t_1)\rangle \right\| . \tag{3.11}$$

Suppose that all interactions are nonsingular. Then $\|V(t)\|$ is finite for all t, where the norm $\|W\|$ of the operator W is defined by

$$\|W\| = \sup \frac{\| W|\phi\rangle \|}{\| |\phi\rangle \|} \tag{3.12}$$

for any choice of normalizable $|\phi\rangle$. Since

$$\|U_0(t_n, t_{n-1})\| = 1 \tag{3.13}$$

and since, by (3.12), $\| W|\phi\rangle \| \le \|W\| \times \| |\phi\rangle \|$, it then follows that

$$|R_N| \le R_N^{Bd} \le (1/\hbar)^{N+1} \int_{D(t)} dt_{N+1} \cdots dt_1 \times \| V_b'(t_{N+1}) | \Psi_b(t_{N+1})\rangle \| \times \prod_{i=2}^{N} \{\|V(t_i)\|\} \times \| V_a'(t_1) | \Psi_a(t_1)\rangle \| . \tag{3.14}$$

Now $\vec{v}$ and t_n, for all n, appear only in the combinations $\vec{v}t_n$ in the integrand of (3.14), and we can proceed as before, by changing the variables of integration to $u_n = vt_n$, to show that

$$|R_N| \le F_N(\rho)/v^{N+1} , \tag{3.15}$$

where

$$F_N(\rho) = \left(\frac{1}{\hbar}\right)^{N+1} \int_{D(u)} du_{N+1} \cdots du_1 \times g_2(u_{N+1}) \prod_{i=2}^{N} \{h(u_i)\} g_1(u_1) , \tag{3.16}$$

and where

$$g_1(u) = \{\int d\vec{r} \, |[V_b + V_{ab}]\Phi_a(\vec{r})|^2\}^{1/2} , \tag{3.17}$$

$$g_2(u) = \{\int d\vec{r} \, |[V_a + V_{ab}]\Phi_b(\vec{r} - \vec{\rho} - u\hat{z})|^2\}^{1/2} , \tag{3.18}$$

and where, ranging over all Φ normalized to unity,

$$h(u) = \sup\{\int d\vec{r} \, |[V_a + V_b + V_{ab}]\Phi(\vec{r})|^2\}^{1/2} ; \tag{3.19}$$

in Eqs. (3.17)–(3.19), we have $V_b = V_b(|\vec{r} - \vec{\rho} - u\hat{z}|)$, $V_{ab} = V_{ab}(|\vec{\rho} + u\hat{z}|)$, and $V_a = V_a(r)$. We have suppressed the ρ dependence of g_1, g_2, and h. The integral $F_N(\rho)$ is independent of ν. Whether or not it converges depends on how fast $g_1(u)$ and $g_2(u)$ fall off with increasing u since $h(u)$ contains a constant part with respect to u due to the term $V_a(r)$ which is independent of t. A sufficient condition for the integral to converge is that

$$\lim_{u\to\pm\infty} u^N g_1(u) = 0, \quad \lim_{u\to\pm\infty} u^N g_2(u) = 0 , \tag{3.20}$$

and this implies that as $R \to \infty$

$$R^N[V_a(R) + V_{ab}(R)] \to 0 , \qquad R^N[V_b(R) + V_{ab}(R)] \to 0 ,$$
$$R^N \frac{dV_a(R)}{dR} \to 0 , \qquad R^N \frac{dV_b(R)}{dR} \to 0 . \tag{3.21}$$

In the same way that we proved (3.15) we can show that $|A_n| \le O(1/v^n)$ and hence[19] that $|S_N| \le O(1/v)$. We then arrive at the result, which is proved in Appendix B,

$$|\sigma - \sigma_N| \le O(1/v^{N+2}) . \tag{3.22}$$

Now from the results of Dettmann and Liebfried[3] it follows that for nonsingular interactions having appropriate Fourier transforms

$$\sigma_N \sim O(1/v^{19}) , \quad N \ge 2 \tag{3.23}$$

and therefore by choosing N to be 18 we have that the high-energy dependence of σ is given by σ_{19} and hence by σ_2. Thus, the second Born term provides the dominant contribution to σ, provided (3.21) holds with N equal to 18. This is the main result of the paper.

We have attempted, so far unsuccessfully, to generalize this result to singular interactions by expanding U in powers of $V_a'(t)$ rather than $V(t)$. Using the integral equation (2.26) with $\hat{U}$ equal to U_a we expand the remainder term (3.1) to obtain

$$A = \sum_{n=1}^{N} A_n + R_N , \tag{3.24}$$

where A_1 is the Jackson-Schiff term (2.47), but where now, for $n \ge 2$, A_n is given by

$$A_n = \left(\frac{-i}{\hbar}\right)^n \int_{D(t)} dt_n \cdots dt_1 \langle V_b'(t_n)\Psi_b(t_n) | U_a(t_n, t_{n-1}) \times \prod_{i=2}^{n-1} \{V_a'(t_i) U_a(t_i, t_{i-1})\} | V_a'(t_1)\Psi_a(t_1)\rangle . \tag{3.25}$$

The remainder R_N differs from A_{N+1} only in the replacement of the single term $U_a(t_{N+1}, t_N)$ by $U(t_{N+1}, t_N)$ in the integrand of A_{N+1}. Applying the Schwarz inequality to R_N and changing the variables of integration to $u_n = vt_n$ it follows that R_N is bounded by R_N^{Bd}, where

$$v^{N+1}R_N^{Bd} = \left(\frac{1}{\hbar}\right)^{N+1} \int_{D(u)} du_{N+1} \cdots du_1 \, g_2(u_{N+1}) \times \left\| \prod_{i=2}^{N} \{ V_a'(u_i/v) U_a(u_i/v, u_{i-1}/v) \} \times V_a'(u_i/v) | \Psi_a(u_i/v) \rangle \right\| , \quad (3.26)$$

where $g_2(u)$ is defined by Eq. (3.18). Suppose that $v^{N+1}R_N^{Bd}$ is continuous in v in the neighborhood of infinity, an assumption we have not attempted to justify since no conclusion can be reached with this approach yet anyway. Then in the limit $v \to \infty$ we can replace $U_a(u_i/v, u_{i-1}/v)$ by 1 in the integrand in (3.26) and therefore

$$\lim_{v\to\infty} v^{N+1}R_N^{Bd} = (1/\hbar)^{N+1} \int_{D(u)} du_{N+1} \cdots du_1 \, g_2(u_{N+1}) \, k, \quad (3.27)$$

where the function

$$k = k(u_N, u_{N-1}, \ldots, u_1) = \left\| \prod_{i=1}^{N} \left[V_a'\left(\frac{u_i}{v}\right) \right] \left| \Psi_a\left(\frac{u_1}{v}\right) \right\rangle \right\| \quad (3.28)$$

is independent of v, as can easily be checked.

Let us consider interactions not more singular than $1/r$ at the origin. Then $g_2(u)$ is defined for all u and $k(u_N, \cdots, u_1)$ is an analytic function except for possible singularities at points $u_i = u_j$, $i \neq j$. However, these singularities will be smoothed out by the integration over the u's and, for interactions not more singular than $1/r$ at the origin, the integral (3.27) will converge provided (3.21) holds with N equal to 1. Hence for p-H charge transfer

$$|R_N| \lesssim O(1/v^{N+1}) \quad (3.29)$$

and it can be shown that

$$|\sigma - \sigma_N| \lesssim O(1/v^{N+2}), \quad (3.30)$$

where R_N and σ_N are now defined with the series expansion (3.24).

The Born terms in (3.24) correspond to the Born terms in the time-independent wave treatment in which the Green's function is expanded in powers of the perturbation in the entrance channel. It can be shown that in the limits m/M_a, $m/M_b \to 0$ the two treatments yield identical cross sections to all orders in this Born-type expansion and hence σ_N can be determined from the wave treatment. Unfortunately only the first and second Born cross sections have, so far, been calculated in the wave treatment with this expansion,[20] it being very difficult to proceed to higher orders. Since for proton-hydrogen charge transfer $\sigma_2 \sim O(1/v^{11})$ we have been unable to draw any conclusions about the high-energy limit.

We remarked earlier that, whatever the nature of the interactions, the incident particle is not likely to induce transitions in the target when it is very far from the target. Hence we expect the capture cross section at very high energies to depend on the short-range rather than the long-range parts of the interactions, and if the interactions are singular at the origin these singularities will greatly influence the high-energy limit.[21] It would not, therefore, be wise to conclude immediately that the result we have obtained for a certain class of nonsingular interactions, namely, that in ground-state rearrangement the second Born term dominates at high energies in the forward direction, applies to singular interactions. Nevertheless, the result does make *plausible* the dominance of the second Born term when the interactions are singular as, for example, in p-H forward charge exchange.

Some of the techniques used in this paper can easily be applied to show that the first Born term dominates at high energies in direct inelastic collisions.

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APPENDIX A: EXISTENCE OF UNPERTURBED STATES

In this Appendix we prove that (2.14) is a sufficient condition for the unperturbed ingoing state to exist. A similar proof will establish that (2.19) is a sufficient condition for the unperturbed outgoing state to exist.

First we note that if $|\Psi_a(t)\rangle$ exists at one finite time it exists at all finite times. Thus, if we set t equal to zero in (2.12) and use (2.13) we are only required to prove that

$$|\Phi_a\rangle = \lim_{t_0\to-\infty} U_a(0,t_0) |\Psi(t_0)\rangle , \quad (A1)$$

subject to the boundary condition on Ψ that in the remote past m was bound to M_a in the state specified by Φ_a.

We begin the proof with the integral equation [cf. Eq. (2.26)]

$$U(0,t_0) = U_a(0,t_0) - (i/\hbar) \int_{t_0}^{0} dt \, U(0,t) V_a'(t) U_a(t,t_0) ; \quad (A2)$$

post multiplication of both sides of this equation by $U_a(t_0,0)|\Phi_a\rangle$ leads to the equation

$$U(0,t_0)U_a(t_0,0)|\Phi_a\rangle = |\Phi_a\rangle - (i/\hbar)\int_{t_0}^{0} dt\, U(0,t)V_a'(t)U_a(t,0)|\Phi_a\rangle \,. \tag{A3}$$

A sufficient condition for the last integral to converge as $t_0 \to -\infty$ is

$$\lim_{t\to-\infty} t\| U(0,t)V_a'(t)U_a(t,0)|\Phi_a\rangle \| = 0 \,. \tag{A4}$$

Since U is unitary and since U_a simply produces a phase factor, (A4) reduces to (2.14).

Assuming then that (2.14) is satisfied, the limit as $t_0 \to -\infty$ of the left-hand side of (A3) exists and can be used to specify the value of $\Psi(0)$, that is,

$$|\Psi(0)\rangle = \lim_{t_0\to-\infty} U(0,t_0)U_a(t_0,0)|\Phi_a\rangle \,. \tag{A5}$$

(This corresponds to the physical boundary condition that m is bound to M_a in the remote past.) Then, by definition, given any $\epsilon > 0$ there is some (large negative) T such that if $t_0 < T$,

$$\| U(0,t_0)U_a(t_0,0)|\Phi_a\rangle - |\Psi(0)\rangle \| < \epsilon \,. \tag{A6}$$

Since $\|\tilde{U}|\Phi\rangle\| = \| |\Phi\rangle \|$ for any unitary $\tilde{U}$, and since $U_a(0,t_0)U(t_0,0)$ is unitary, (A6) is equivalent to

$$\| |\Phi_a\rangle - U_a(0,t_0)|\Psi(t_0)\rangle \| < \epsilon \,, \tag{A7}$$

which implies (A1).

It is well known that when the Hamiltonian is time independent, $U(0,-\infty)$ is isometric. We should like to add that in the impact-parameter approximation it is sometimes possible to choose a representation in which $U(0,-\infty)$ is unitary.[22]

APPENDIX B

In this Appendix we prove Eq. (3.22). From Eqs. (2.23), (3.5), and (3.9) we have

$$\sigma - \sigma_N = \int_0^\infty [2\,\mathrm{Re}(S_N R_N) + |R_N|^2] 2\pi\rho\, d\rho \tag{B1}$$

and therefore

$$|\sigma - \sigma_N| \le (2\pi/v^{N+1}) \times \int_0^\infty \rho F_N(\rho)[2G_N(\rho) + F_N(\rho)/v^N]\, d\rho \,. \tag{B2}$$

using Eq. (3.15) in the second line. The ρ and v dependence of S_N has been suppressed. However, just as we obtained the bound (3.15) on R_N, we can show that

$$|S_N| \le G_N(\rho)/v \,, \tag{B3}$$

where $G_N(\rho)$ is some function which is independent of v. Hence

$$|\sigma - \sigma_N| \le (2\pi/v^{N+2}) \times \int_0^\infty \rho F_N(\rho)[2|S_N| + F_N(\rho)/v^{N+1}]\, d\rho \,. \tag{B4}$$

We have to show that the integral in Eq. (B4) is convergent. From Eqs. (3.17)–(3.19) *and* (3.21) we have, that for large ρ,

$$g_1(u) \le \frac{c_1}{(\rho^2 + u^2)^{(N/2)+\epsilon}} \,, \tag{B5}$$

$$g_2(u) \le \frac{c_2}{(\rho^2 + u^2)^{(N/2)+\delta}} \,, \tag{B6}$$

where ϵ and δ are positive, and

$$h(u) \le c_3 \,, \tag{B7}$$

where c_1, c_2, and c_3 are independent of u and ρ. Hence, by Eq. (3.16), for very large ρ, with $c_4 = c_1 c_2 (c_3)^{N-1}/(\hbar)^{N+1}$,

$$F_N(\rho) \le c_4 \int_{D(u)} du_{N+1} \cdots du_1 \times \frac{1}{(\rho^2 + u_{N+1}{}^2)^{(N/2)+\delta}} \frac{1}{(\rho^2 + u_1{}^2)^{(N/2)+\epsilon}} \tag{B8}$$

$$= \frac{c_4}{\rho^{N-1+2\epsilon+2\delta}} \int_{D(s)} ds_{N+1} \cdots ds_1 \times \frac{1}{(1 + s_{N+1}{}^2)^{(N/2)+\delta}} \frac{1}{(1 + s_1{}^2)^{(N/2)+\epsilon}} \,, \tag{B9}$$

where we have made the change of variables $s_n = u_n/\rho$. The integral in (B9) is convergent and is independent of ρ and v. Hence

$$F_N(\rho) \le O(1/\rho^{N-1+2\epsilon+2\delta}) \,. \tag{B10}$$

Similarly, we can show that

$$G_N(\rho) \le O(1/\rho^{N+2\epsilon+2\delta}) \tag{B11}$$

and therefore the integral in (B4) is certainly convergent if $N \ge 2$ and Eq. (3.22) then follows.

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Variational Formulation of the *R* Matrix Method for Multichannel Scattering*

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A variational treatment of the R matrix method for multichannel scattering is given, in which basis functions used for expanding the wave function within a boundary radius r_0 need not satisfy specific boundary conditions at r_0. As an illustration, a simple basis set of monomial functions (r^n, $n = 1,\dots,N$) is used in a two-channel-model problem with long-range potentials. Excellent results are obtained with ten such functions in each channel.

I. INTRODUCTION

Burke *et al.*[1] have recently formulated a computational procedure for electron-atom scattering problems, based on the R matrix theory of nuclear reactions.[2] In this formalism, the logarithmic derivative of the wave function at a boundary radius r_0 is determined by expanding the wave function within r_0 in terms of a basis set of functions. The reactance matrix K is then computed from knowledge of the numerical wave function for $r > r_0$, obtained by inward integration, starting from an asymptotic position. The boundary radius is chosen so that exchange can be neglected outside r_0, reducing the problem there to the solution of coupled ordinary differential equations. Matese and Henry[3] have proposed use of the variable-phase theory beyond r_0 to determine the K matrix.

In both of these approaches, the basis functions are constrained to have a fixed but arbitrary logarithmic derivative at r_0. Slow convergence with such a basis set has been observed in each of these two approaches.[3,4] A correction suggested by Buttle[5] has been used to approximate the effects of