Nonperturbative treatments of charge exchange at arbitrary energies: An alternative variational principle

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An alternative theory for charge exchange at arbitrary energies is introduced. The method is a Schwinger-type variational unification of the leading second-order Born perturbation approximations and the efficient L^2-expansion theories. This new variational principle is devised in accordance with the correct boundary conditions for three charged particles. The present theory exhibits a number of advantages over all the existing methods in regard to both the conceptual and computational points of view.

I. INTRODUCTION

The first convergent S-matrix time-dependent theory for Coulomb scattering was devised by Dollard[1] (for a review see Ref. 2). In this fundamental work of Dollard, the convergence of the theory emerged as a result of imposing the correct boundary conditions to the scattering wave functions in the initial and final states. His results relate to both potential scattering as well as multichannel collisions. At the same time, Cheshire[3] investigated the charge-exchange problem by paying particular attention to the correct boundary conditions (see also Ref. 4). The second-order continuum distorted-wave (CDW) approximation with correct boundary conditions was originally formulated and implemented by Cheshire[3] with respect to electron capture from atomic hydrogen by protons. Subsequently, Mapleton[5] studied the second-order Coulomb Born approximation in H^+-H charge exchange. He reported that this approximation is divergent if the correct boundary conditions are overlooked. Here, it is tempting to conclude that the H^+-H collision cannot seriously test the boundary-condition problem due to the absence of logarithmic Coulomb phase factors associated with the relative motion of heavy particles. However, such an argument, which has frequently been put forward in the literature, is misleading due the reduction of the boundary-condition problem to the sole distortion of the scattering wave functions. The correct boundary conditions imply that *both* the scattering wave functions and the perturbation potentials are consistent with each other in the entrance and exit channels. Thus, for H^+-H collisions, the first-order Brinkman-Kramers (BK1) approximation possesses the correct scattering wave functions but still violates the proper boundary conditions, because the perturbation potentials and the channel states are *not* the solutions of the same eigenvalue problem. This is precisely the reason for the failure of the BK1 approximation, which does not represent a consistent first-order perturbation theory and which significantly overestimates the experimental data in a systematic manner.

There has been considerable confusion in the literature about the role played by the first-order theories for charge exchange. The first Born approximation of Jackson and Schiff[6] (JS1), which has also been considered by Bates and Dalgarno,[7] is found to be in satisfactory agreement with the measurement for H^+-H charge exchange. However, applications of the JS1 method to other collisions, especially with highly asymmetrical nuclear charges, met with notable inadequacy, yielding cross sections which are larger than the experimental data by orders of magnitude.[8] This led researchers to discard altogether the first-order perturbation theories as inappropriate. Thus, according to the commonly held conception, charge exchange was thought for a long time to be a phenomenon which can be successfully treated by the perturbation interaction expansions only if the potentials at least to the second order are taken into account.

In a review paper, Belkić *et al.*[9] rigorously established several important results relating to charge exchange. By employing the well-known eikonal hypothesis which is appropriate for ion-atom scattering, they obtained an exact eikonal T matrix for electron capture in a general case of collisions with one-electron systems. Such a full T matrix was free from any divergencies. This is a direct result of imposing the correct boundary conditions to the scattering eigenvalue problems in the entrance and exit channel. The work of Belkić *et al.*[9] relies upon the formalism of Dollard.[1] In order to properly regularize the T matrix for Coulomb scattering, Dollard[1] modified the standard Møller scattering operators Ω^+ and Ω^- by inclusion of the appropriate logarithmic distortion factors. Such a modification in the operational form was difficult to implement in applications.[2] However, Belkić *et al.*[9] retained the usual Møller operators and introduced the Coulomb logarithmic phases into the scattering wave functions. In this way an exact, regular T matrix was obtained[9] which is manageable for calculations. In Ref. 9 it was conclusively proven that the internuclear potential does not contribute to an *exact* eikonal total cross section. This conclusion is of great importance in view of

the often repeated misconception concerning Wick's contention about the long-range Coulomb interaction between the nuclei. A large number of erroneous papers have been published due to lack of understanding of the role played by the internuclear potential and the correct boundary conditions. Such a situation was substantially changed by the appearance of Ref. 9 in which the issue of the nucleus-nucleus interaction was definitively settled in a satisfactory manner. Rather than giving a catalogue of existing theories together with a compilation and empirical evaluation of the available data base, as most of the review papers had done thus far, Belkić *et al.*[9] devised a different approach. They took upon themselves to (i) rigorously formulate the requirements from the first principles which a consistent theory must fulfill, (ii) determine the limitations and assess the domain of validity of virtually all the available high-energy theories for charge exchange, and (iii) perform the original exhaustive computations of the cross sections within a theory which best satisfies condition (i).

When dealing with point (i) above, Belkić *et al.*[9] found that the long-range Coulombic behavior of the interaction between the two charged atomic aggregates has been ignored in most studies. The usual scattering theory which employs plane waves for the relative motion of heavy particles can confidently be used in nuclear physics where the interactions are of short range. The situation is, however, quite different for atomic collisions, due to the peculiar long-range Coulomb potentials which are effective even at infinite distances. Hence, in solving task (i), Belkić *et al.*[9] concluded that whenever two charged atomic aggregates are present, the standard theory of scattering must be appropriately reformulated. This is most efficiently accomplished by replacing the plane waves by the Coulombic state for the relative motion of the heavy particles. This modification must be done in a consistent manner by requiring that perturbation potentials and the corresponding channel-scattering wave functions are the solutions to the same eigenvalue problem.[9]

Once the above consistency criterion has been established, the limitations and validity of the existing theories for charge exchange were examined in detail.[9] No theory was free from criticism but, nevertheless, the CDW approximation emerged as a model with the least number of shortcomings.[9] Choosing this approximation of Cheshire[3] in accordance with their task (iii), Belkić *et al.*[9] carried out comprehensive computations for more than 50 atomic collisions of charge exchange. They revealed that the CDW method is systematically in satisfactory agreement with the measurements at energies which are greater than 80 keV/amu. This conclusion has subsequently been found by others to hold for many more colliding systems.[10]

However, the CDW theory significantly overestimates experimental data at intermediate and lower energies. In this energy range, the usual close-coupling methods are customarily applied.[11] In particular, the three-center expansion technique appears to be quite reliable for certain cases.[12] However, widespread usage of these close-coupling theories is severely hampered by a large number of intermediate states which are required for many-electron atoms, multicharged ions, or even for hydrogenic systems at higher energies.

Hence, a new theory is sought, which could be applied to *any* colliding particles at *arbitrary* energies. We shall presently resort to nonperturbative methods and develop a Schwinger-type variational principle. (Atomic units will be used throughout unless stated otherwise.)

II. SCHWINGER-TYPE VARIATIONAL PRINCIPLE FOR THE TOTAL GREEN'S FUNCTION

Here, we shall consider a direct collision between two particles, which might be either structureless or composite. If the full Hamiltonian of the system is denoted by H, then the total Green's function reads as follows:

$$G(z)=(z-H)^{-1}, \quad z=E+i\epsilon \ (\epsilon\rightarrow 0+) , \tag{2.1}$$

where E is the positive energy of the two particles under study. Resolvent (2.1) is of primary importance, since it provides the entire physical information about the problem under investigation. In particular, eigenenergies and eigenfunctions can directly be extracted from the spectral representation of the Green's operator $G(z)$, without solving the Schrödinger equation.[13,14] Writing, as usual,

$$H=H_0+V , \tag{2.2}$$

where H_0 is the kinetic energy operator and V is the total interaction potential, we can introduce the transition T operator by

$$T=V+VGV . \tag{2.3}$$

Then the T matrix is given as an integral over the whole two-particle space by putting the T operator in between the initial and final unperturbed states of the system, i.e.,

$$T_{if}=\langle f|T|i\rangle=\langle f|V+VGV|i\rangle . \tag{2.4}$$

Since pair interactions are known in atomic physics, it follows from Eq. (2.4) that transition amplitude T_{if} and, consequently the related scattering S matrix, could, in principle, be obtained *exactly* if the total Green's operator G is available. Hence, obtaining the total Green's function is central to scattering theory. This is an extraordinarily difficult task and, therefore, resorting to approximate solutions is unavoidable. In fact, however, the essence of physics in most realistic applications lies in approximations and the main concern here is their consistent introduction. Unfortunately, quite frequently approximations have been proposed by selecting a few parameters, and subsequent good agreement with experiments was chosen as the only criterion for the validity of the theory. We shall presently devise a different approach to scattering problems and set up a framework for the theory in which *ab initio* computations are possible starting from *first principles.* This is very important for an intrinsic quality of the theory, which thus provides *absolute data* without any arbitrary parameter. Whenever possible these theoretical results should be compared with *absolute* measurements. In this way, reliable tests can be performed on both the *magnitude* and the *behav-*

ior of the obtained results as a function of scattering angles or impact energies.

Traditionally, the total Green's function G has been generated by the perturbation techniques, through an introduction of intermediate propagator G_x, such as

$$G=G_x+G_xV_xG\ , \tag{2.5a}$$

$$G=G_x+GV_xG_x\ , \tag{2.5b}$$

where

$$G_x(z)=(z-H+V_x)^{-1}\ . \tag{2.6}$$

Then, the well-known Born series for G is obtained by iterating Lippmann-Schwinger Eqs. (2.5a) and (2.5b). In practice, however, the third and higher orders in the Born series are unmanageable and this severely limits the perturbation theories. Hence, obtaining the full T matrix should proceed through introduction of nonperturbative methods. In order to achieve this goal, we shall presently investigate a variational principle for total Green's operator $G(z)$, which automatically will supply a variational estimate of the full T matrix. We first add and then subtract term GV_xG_x in the right-hand side of Eq. (2.5a), i.e.,

$$\begin{aligned} G&=G_x+G_xV_xG\ ,\\ &=G_x+(G_xV_xG+GV_xG_x)-GV_xG_x\ , \end{aligned} \tag{2.7}$$

and, subsequently, insert $G_x=G-G_xV_xG$ into the last term GV_xG_x of Eq. (2.7) to obtain

$$\begin{aligned} G&=G_x+(G_xV_xG+GV_xG_x)-GV_x(G-G_xV_xG)\ ,\\ &=G_x+(G_xV_xG+GV_xG_x)-G(V_x-V_xG_xV_x)G\ . \end{aligned} \tag{2.8}$$

Thus, by using Lippmann-Schwinger Eq. (2.5a) *twice* in the above derivation, we obtain the following identity for the exact total Green's operator G:

$$G=G_x+(G_xV_xG+GV_xG_x)-GDG\ , \tag{2.9}$$

where

$$D=V_x-V_xG_xV_x\ . \tag{2.10}$$

Further, replacing G by a trial estimate $\bar{G}$, i.e.,

$$\bar{G}=G_x+(G_xV_x\bar{G}+\bar{G}V_xG_x)-\bar{G}D\bar{G}\ , \tag{2.11}$$

and performing a small variation around $\bar{G}$ will imply

$$\begin{aligned} \delta\bar{G}&=G_xV_x(\delta\bar{G})-(\delta\bar{G})V_xG_x-(\delta\bar{G})[(V_x-V_xG_xV_x)\bar{G}]-[\bar{G}(V_x-V_xG_xV_x)](\delta\bar{G})\\ &=[G_x-\bar{G}(1-V_xG_x)]V_x(\delta\bar{G})+(\delta\bar{G})V_x[G_x-(1-G_xV_x)\bar{G}]\\ &=[G(1-V_xG_x)-\bar{G}(1-V_xG_x)]V_x(\delta\bar{G})+(\delta\bar{G})V_x[(1-G_xV_x)G-(1-G_xV_x)\bar{G}]\ , \end{aligned} \tag{2.12}$$

so that

$$\delta\bar{G}=(\Delta G)D(\delta\bar{G})+(\delta\bar{G})D(\Delta G)\ , \tag{2.13}$$

where $\Delta G=G-\bar{G}$. If trial operator $\bar{G}$ were exact, i.e.,

$$\bar{G}=G\ \ (\Delta G=0)\ , \tag{2.14a}$$

then the right-hand side of Eq. (2.13) would be identical to zero. Further, Eq. (2.14a) implies that the left-hand side of Eq. (2.13) also vanishes:

$$\delta\bar{G}=0\ . \tag{2.14b}$$

This is the condition for operator $\bar{G}$ to be a stationary functional. Hence we obtain bilinear form (2.11) of the variational principle for the total Green's function, since small variations of trial operator $\bar{G}$ around exact value G are found to vanish identically by virtue of (2.14b).

For practical purposes, however, it would be advantageous to derive an alternative form for Eq. (2.11), which will be independent of the norm of trial operators. This is accomplished by casting operator $\bar{G}$ into an arbitrary representation $\{|a\rangle,\langle b|\}$:

$$\begin{aligned} \langle b|\bar{G}|a\rangle&=\langle b|G_x|a\rangle+\langle b|G_xV_x|a'\rangle\\ &\quad+\langle b'|V_xG_x|a\rangle-\langle b'|D|a'\rangle\ , \end{aligned} \tag{2.15}$$

where $|a'\rangle=\bar{G}|a\rangle$ and $\langle b'|=\langle b|\bar{G}^{\dagger}$. Further, considering $|a'\rangle$ and $\langle b'|$ as trial functions, we shall expand them as follows:

$$|a'\rangle=\sum_i a_i|i\rangle,\ |b'\rangle=\sum_j b_j|j\rangle\ , \tag{2.16}$$

where $\{|i\rangle,\langle j|\}$ are linearly independent complete basis sets, and a_i and b_j are unknown expansion coefficients. Two sets $\{|i\rangle\}$ and $\{\langle j|\}$ do not need to be identical to each other. Inserting (2.16) into Eq. (2.15) and carrying out independent variations of a_i and b_j^*, we obtain

$$\begin{aligned} \langle b|\delta\bar{G}|a\rangle&=\sum_i(\delta a_i)[\langle b|G_xV_x|i\rangle-\sum_j b_j^*\langle j|D|i\rangle]\\ &\quad+\sum_j(\delta b_j^*)[\langle j|V_xG_x|a\rangle-\sum_i a_i\langle j|D|i\rangle]\ . \end{aligned} \tag{2.17}$$

For independent variations of coefficients a_i and b_j^*, stationary condition (2.14b) is satisfied provided that

$$\sum_j b_j^*\langle j|D|i\rangle=\langle b|G_xV_x|i\rangle\ , \tag{2.18}$$

$$\sum_i a_i\langle j|D|i\rangle=\langle j|V_xG_x|a\rangle\ , \tag{2.19}$$

or, in the matrix form

$$\underline{a}\,\underline{D}=\underline{A},\ \ \underline{b}^{\dagger}\underline{D}=\underline{B}\ , \tag{2.20}$$

where $A_j=\langle j|V_xG_x|a\rangle$ and $B_i=\langle b|G_xV_x|i\rangle$. We assume that inverse $\underline{D}^{-1}$ exists, i.e.,

$$\underline{D}^{-1}\underline{D}=\underline{1}\ , \tag{2.21}$$

so that

$$\underline{a}=\underline{A}\,\underline{D}^{-1},\quad \underline{b}^{\dagger}=\underline{B}\,\underline{D}^{-1}\ . \tag{2.22}$$

Substituting (2.22) into Eq. (2.15), we derive the following result:

$$\begin{aligned}\langle b|\overline{G}|a\rangle&=\langle b|G_x|a\rangle+\underline{b}^{\dagger}\underline{A}+\underline{a}\,\underline{B}-\underline{a}\,\underline{b}^{\dagger}\underline{D}\\&=\langle b|G_x|a\rangle+\underline{B}\,\underline{D}^{-1}\underline{A}\\&\quad+\underline{A}\,\underline{D}^{-1}\underline{B}-\underline{A}\,\underline{D}^{-1}\underline{B}\,\underline{D}^{-1}\underline{D}\ ,\end{aligned} \tag{2.23}$$

and, after canceling term $\underline{A}\,\underline{D}^{-1}\underline{B}$ by $-\underline{A}\,\underline{D}^{-1}\underline{B}\,\underline{D}^{-1}\underline{D}$ through the use of Eq. (2.21), we deduce

$$\begin{aligned}\langle b|\overline{G}|a\rangle&=\langle b|G_x|a\rangle\\&\quad+\sum_{i,j}\langle b|G_xV_x|i\rangle D_{ij}\langle j|V_xG_x|a\rangle\ ,\end{aligned} \tag{2.24}$$

where

$$(D^{-1})_{ji}=\langle j|D|i\rangle\ . \tag{2.25}$$

Finally, since basis sets $\{|a\rangle,\langle b|\}$ are arbitrary, we can write Eq. (2.24) in a more general form, which is independent of representations $\{|a\rangle\}$ and $\{\langle b|\}$, i.e.,

$$\overline{G}=G_x+\sum_{i,j}G_xV_x|i\rangle D_{ij}\langle j|V_xG_x\ . \tag{2.26}$$

It is immediately apparent that fractional form (2.26) of the variational principle for the total Green's function does not depend upon the norm of the basis set functions $|i\rangle$ and $\langle j|$. Bilinear form (2.11) has previously been reported by Newton,[15] whereas fractional version (2.26) was derived by Belkić and Taylor.[16(f)] Practical implementations of variational principle (2.26) were deferred until now since the so-called "boundary-condition problem" took a great deal of our attention.[17]

III. APPLICATION TO CHARGE EXCHANGE AT ARBITRARY ENERGIES

In this section we shall apply variational principle (2.26) to electron capture from hydrogenlike atomic systems $(Z_T,e)_i$ by completely stripped projectiles Z_P:

$$Z_P+(Z_T,e)_i\rightarrow(Z_P,e)_f+Z_T\ , \tag{3.1}$$

where Z_K is the nuclear charge of the Kth nucleus $(K=P,T)$ and j is the usual set of quantum numbers, i.e., $j=\{n^jl^jm^j\}$ $(j=f,i)$. Let $\mathbf{r}_K$ be the position vector of the electron e with respect to the Kth nucleus $(K=P,T)$ and, further, let $\mathbf{R}$ be the relative vector of Z_T toward Z_P. We also introduce relative vectors $\mathbf{r}_i$ and $\mathbf{r}_f$ by

$$\mathbf{r}_i=a_T\mathbf{r}_T-\mathbf{r}_P,\quad \mathbf{r}_f=a_P\mathbf{r}_P-\mathbf{r}_T,\quad \mathbf{R}=\mathbf{r}_T-\mathbf{r}_P\ , \tag{3.2}$$

where $a_K=m_Km/(m_K+m)$, $m=1$ is the electron mass and m_K is the mass of the Kth nucleus $(K=P,T)$. The total Hamiltonian of the three-particle system under study is given by

$$H=H_0+V\ , \tag{3.3}$$

where H_0 is the kinetic-energy operator and V is the full interaction potential,

$$H_0=-\frac{1}{2\mu_i}\nabla^2_{r_i}-\frac{1}{2a_T}\nabla^2_{r_T}\equiv K_i-\frac{1}{2a_T}\nabla^2_{r_T}\ , \tag{3.4}$$

$$=-\frac{1}{2\mu_f}\nabla^2_{r_f}-\frac{1}{2a_P}\nabla^2_{r_P}\equiv K_f-\frac{1}{2a_P}\nabla^2_{r_P}\ , \tag{3.5}$$

$$V=V_P(r_P)+V_T(r_T)+V_{PT}(R)\ ,$$

$$V_K(r)=-Z_K/r,\quad V_{PT}=Z_PZ_T/R\ , \tag{3.6}$$

$$\mu_i=m_P(m_T+m)/(m_P+m_T+m)\ ,$$

$$\mu_f=m_T(m_P+m)/(m_T+m_P+m)\ . \tag{3.7}$$

The entrance- and exit-channel scattering wave functions Φ_i^+ and Φ_f^- with the correct boundary conditions are respectively given by

$$\Phi_i^-=\varphi_i^T(\mathbf{r}_T)\exp[i\mathbf{k}_i\cdot\mathbf{r}_i+i\nu_i\ln(k_ir_i-\mathbf{k}_i\cdot\mathbf{r}_i)]\ , \tag{3.8a}$$

$$\equiv\Phi_i\exp[i\nu_i\ln(k_ir_i-\mathbf{k}_i\cdot\mathbf{r}_i)]\equiv\Phi_iF_i^+\ , \tag{3.8b}$$

$$\Phi_f^-=\varphi_f^P(\mathbf{r}_P)\exp[-i\mathbf{k}_f\cdot\mathbf{r}_f-i\nu_f\ln(k_fr_f-\mathbf{k}_f\cdot\mathbf{r}_f)]\ , \tag{3.9a}$$

$$\equiv\Phi_f\exp[-i\nu_f\ln(k_fr_f-\mathbf{k}_f\cdot\mathbf{r}_f)]\equiv\Phi_fF_f^-\ , \tag{3.9b}$$

where $\varphi_j^K(\mathbf{r}_K)$ describes the bound state of hydrogenic system $(Z_K,e)_j$ $(K=P,T;\ j=f,i)$, $\mathbf{k}_i$ and $\mathbf{k}_f$ are the initial and final wave vectors, respectively,

$$\nu_i=Z_P(Z_T-1)/v_i,\quad \mathbf{v}_i=\mathbf{k}_i/\mu_i\ , \tag{3.10a}$$

$$\nu_f=Z_T(Z_P-1)/v_f,\quad \mathbf{v}_f=\mathbf{k}_f/\mu_f\ . \tag{3.10b}$$

Total Hamiltonian H can be split into the following two symmetric forms:

$$H=H_0+V_i\ , \tag{3.11a}$$

$$=H_0+V_f\ , \tag{3.11b}$$

where V_i and V_f are the perturbation potentials in the entrance and exit channels,

$$V_i=V_P(r_P)+V_{\rm PT}(R)\ , \tag{3.12a}$$

$$V_f=V_T(r_T)+V_{\rm PT}(R)\ . \tag{3.12b}$$

We now resort to the well-known eikonal hypothesis, which assumes that k_i acquires large values. For heavy-particle collisions, we have that $\mu_i\gg m$ and, hence, k_i is large even at very small incident velocities v_i (of the order of 0.01 a.u.). Due to their large mass, heavy projectiles are only slightly deflected from the initial direction and the scattering is predominantly taking place in a narrow forward cone. This implies that $\hat{\mathbf{k}}_i\approx\hat{\mathbf{k}}_f$, but *not* $\mathbf{k}_i=\mathbf{k}_f$, however. Such an eikonal hypothesis permits the follow-

ing linearization of the kinetic energy operators for relative motion of heavy particles:[18]

$$K_i \equiv -\frac{1}{2\mu_i}\nabla^2_{r_i} \cong \frac{k_i^2}{2\mu_i} - \mathbf{v}_i\cdot(\mathbf{k}_i + i\nabla_{r_i}) \equiv K_{ie} \ , \tag{3.13a}$$

$$K_f \equiv -\frac{1}{2\mu_f}\nabla^2_{r_f} \cong \frac{k_f^2}{2\mu_f} - \mathbf{v}_f\cdot(\mathbf{k}_f - i\nabla_{r_f}) \equiv K_{fe} \ . \tag{3.13b}$$

Unperturbed asymptotic channel states Φ_i and Φ_f are the solutions of the following equations:

$$(E-H_i)\Phi_i = 0, \quad E = \frac{k_i^2}{2\mu_i} + E_i^T, \quad H_i = H_0 + V_T(r_T) \ , \tag{3.14a}$$

$$(E-H_f)\Phi_f = 0, \quad E = \frac{k_f^2}{2\mu_f} + E_f^P, \quad H_f = H_0 + V_P(r_P) \ , \tag{3.14b}$$

where E_j^K is the electronic binding energy of hydrogenlike atom $(Z_K, e)_j$:

$$E_j^K = -\tfrac{1}{2}(b_j^K)^2, \quad b_j^K = Z_K/n^j \quad (K = P,T; \quad j = f,i) \ . \tag{3.15}$$

Total exact Green's function G^+ is defined by

$$G^+ = (E - H + i\epsilon)^{-1} \ , \tag{3.16}$$

with the appropriate incoming boundary condition $(\epsilon \to 0+)$. This operator can be simplified by virtue of Eqs. (3.13a) and (3.13b) as follows:

$$G^+ \cong G_e^+ = (E_i^T - \mathbf{v}_i\cdot[\mathbf{k}_i + i\nabla_{r_i}] + \tfrac{1}{2}\nabla^2_{r_T} - V + i\epsilon)^{-1} \ , \tag{3.17a}$$

$$= (E_f^P - \mathbf{v}_f\cdot[\mathbf{k}_f - i\nabla_{r_f}] + \tfrac{1}{2}\nabla^2_{r_P} - V + i\epsilon)^{-1} \ , \tag{3.17b}$$

where the limits $\mu_i \gg m$ and $\mu_f \gg m$ are understood. Furthermore, within the same eikonal hypothesis, it is immediately seen that distorted waves F_i^+ and F_f^- satisfy the *linear* differential equations such as

$$(i\mathbf{v}_i\cdot\nabla_{r_i} - V_{ia})F_i^+ = 0 \ , \tag{3.18a}$$

$$(i\mathbf{v}_f\cdot\nabla_{r_f} - V_{fa})F_f^- = 0 \ , \tag{3.18b}$$

where V_{ia} and V_{fa} are the *asymptotic* values of perturbations V_i and V_f with the scattering particles being infinitely separated from each other in the entrance and exit channels,

$$V_{ia} = Z_P(Z_T - 1)/R, \quad V_i \xrightarrow[R\to\infty]{} V_{ia} \ , \tag{3.19a}$$

$$V_{fa} = Z_T(Z_P - 1)/R, \quad V_f \xrightarrow[R\to\infty]{} V_{fa} \ . \tag{3.19b}$$

Exact, full transition amplitudes T_{if}^- and T_{if}^+ with the *correct boundary conditions* for reaction (3.1) are introduced by

$$T_{if}^- = \langle \Psi_f^- | V_i' | \Phi_i^+ \rangle \ , \tag{3.20a}$$

$$T_{if}^+ = \langle \Phi_f^- | V_f' | \Psi_i^+ \rangle \ , \tag{3.20b}$$

where

$$\Psi_i^+ = (1 + G^+ V_i')\Phi_i^+ \ , \tag{3.21a}$$

$$\Psi_f^- = (1 + V_f' G^-)\Phi_f^- \ , \tag{3.21b}$$

and $V_{i,f}'$ are new perturbations

$$V_i' = V_i - V_{ia} = V_P(r_P) - V_P(R) \ , \tag{3.22a}$$

$$V_f' = V_f - V_{fa} = V_T(r_T) - V_T(R) \ . \tag{3.22b}$$

An explicit *eikonal* hypothesis should further consistently be invoked into the total Green's function via Eqs. (3.17a) and (3.17b) so that

$$T_{if}^- \cong T_{if}^{-(e)} \equiv \langle \Psi_f^{-(e)} | V_i' | \Phi_i^+ \rangle \ , \tag{3.23a}$$

$$T_{if}^+ \cong T_{if}^{+(e)} \equiv \langle \Phi_f^- | V_f' | \Psi_i^{+(e)} \rangle \ , \tag{3.23b}$$

where

$$\Psi_i^{+(e)} = (1 + G_e^+ V_i')\Phi_i^+ \ , \tag{3.24a}$$

$$\Psi_f^{-(e)} = (1 + V_f' G_e^-)\Phi_f^- \ , \tag{3.24b}$$

with G_e^+ given by Eqs. (3.17a) and (3.17b).

The "prior" and "post" T matrices T_{if}^- and T_{if}^+ as well as their respective exact eikonal simplifications $T_{if}^{-(e)}$ and $T_{if}^{+(e)}$ are defined in Eqs. (3.20a), (3.20b), (3.23a) and (3.23b) on the *energy shell* at which the total energy E is conserved, i.e., $E_i^T + k_i^2/(2\mu_i) = E_f^P + k_f^2/(2\mu_f)$ (see Eqs. (3.14a) and (3.14b). This fact together with the knowledge of the exact wave functions $\varphi_i^T(\mathbf{r}_T)$ and $\varphi_f^P(\mathbf{r}_P)$ for hydrogenlike atomic systems, imply that $T_{if}^- \equiv T_{if}^+$ and $T_{if}^{-(e)} \equiv T_{if}^{+(e)}$, i.e., there is no so-called "post-prior" discrepancy. Hence, for convenience, we shall hereafter employ only the post form $T_{if}^{+(e)}$ of the T matrix.

Modified perturbations V_i' and V_f' are of short range as $R \to \infty$, which can be easily seen by developing $V_K(r_K)$ into the Taylor expansions. By so doing, the lowest order in these expansions for $V_K(r_K)$ is found to coincide with $V_K(R)$, which then cancels term $-V_K(R)$ in Eqs. (3.22a) and (3.22b), i.e.,

$$V_K(r_K) - V_K(R) \cong \left[V_K(R) + \frac{\hat{\mathbf{R}}\cdot\mathbf{r}_K}{R^2} + \cdots \right] - V_K(R) = \frac{\hat{\mathbf{R}}\cdot\mathbf{r}_K}{R^2} + \cdots$$

$$(K = P,T; \quad j = f,i \quad R \to \infty; \quad \mu_{i,f} \gg 1) \ . \tag{3.25}$$

Equally important is the fact that new perturbations V_i' and V_f' do not contain internuclear potential $V_{\rm PT}(R)$, in contrast to the initial expressions (3.12a) and (3.12b) for V_i and V_f. However, there are three remaining terms in $T_{if}^{+(e)}$ which include the contributions from $V_{\rm PT}(R)$, and these are Φ_i^+, Φ_f^-, and G_e^+. This is an apparent drawback of our formalism, since in the eikonal limit, an exact T matrix should supply the total cross section which is independent of $V_{\rm PT}(R)$ according to Wick's contention. That this is indeed true will be immediately clear by using

the following identity:

$$G_e^+ V_i' \Phi_i^+ = F_i^+ G_e^{+'} V_i' \Phi_i \ , \tag{3.26}$$

where

$$G_e^{+'} = [E_i^T - \mathbf{v}_i \cdot (\mathbf{k}_i + i\nabla_{r_i}) + \tfrac{1}{2}\nabla_{r_T}^2 - V' + i\epsilon]^{-1} \tag{3.27}$$

and

$$V' = V - V_{ia} = V_i' + V_T(r_T) \ . \tag{3.28}$$

Since V_i' is a multiplicative operator and F_i^+ satisfies Eq. (3.18a), identity (3.26) can readily be proven if we multiply both sides of (3.26) by $1/G_e^{+'}$ and utilize the linearity of $G_e^{+'}$ with respect to ∇_{r_i}. Inserting identity (3.26) into Eq. (3.23b) we obtain

$$T_{if}^{+(e)} = \langle \Phi_f F | V_i' + V_f' G_e^{+'} V_i' | \Phi_i \rangle \ , \tag{3.29}$$

where

$$F = (F_i^+)^* F_f^- \ . \tag{3.30}$$

Finally, setting $\mathbf{R} = \boldsymbol{\rho} + \mathbf{Z} = (\rho\cos\varphi_\rho, \rho\sin\varphi_\rho, Z)$, where $\boldsymbol{\rho}\cdot\mathbf{Z} = 0$, we deduce in the eikonal limit

$$F = (\mu\rho v)^{+2i\nu_f} \exp[i\xi \ln(k_i r_i - \mathbf{k}_i \cdot \mathbf{r}_i)] \ , \tag{3.31a}$$

$$= (\mu\rho v)^{+2i\nu_i} \exp[-i\xi \ln(k_f r_f - \mathbf{k}_f \cdot \mathbf{r}_f)] \ , \tag{3.31b}$$

with

$$\mathbf{v}_f \cong \mathbf{v}_i \equiv \mathbf{v}, \ \mu = m_P m_T/(m_P + m_T)$$

and

$$\xi = (Z_T - Z_P)/v \ . \tag{3.32}$$

Thus we can rewrite Eq. (3.29) as follows:

$$T_{if}^{+(e)} = \langle \Phi_f \rho^{-2i\nu_f} e^{-i\delta_i} | V_i' + V_f' G_e^{+'} V_i' | \Phi_i \rangle \ , \tag{3.33a}$$

$$= \langle \Phi_f \rho^{-2i\nu_i} e^{+i\delta_f} | V_i' + V_f' G_e^{+'} V_i' | \Phi_i \rangle \ , \tag{3.33b}$$

where $\delta_{i,f} = \xi \ln(vR \mp \mathbf{v}\cdot\mathbf{R})$. Here, we ignore all the constant phase factors which do not contribute to either the differential $d\sigma_{if}^{+(e)}/d\Omega$ or total $\sigma_{if}^{+(e)}$ cross sections,

$$\frac{d\sigma_{if}^{+(e)}}{d\Omega} = \left| \frac{\mu}{2\pi} T_{if}^{+(e)} \right|^2 \text{(in } a_0^2\text{/sr atom)} \ , \tag{3.34a}$$

$$\sigma_{if}^{+(e)} = \int d\Omega \left[\frac{d\sigma_{if}^{+(e)}}{d\Omega} \right] \text{ (in units of } a_0^2) \ . \tag{3.34b}$$

Here Ω is the solid angle around $\mathbf{k}_i$,

$$\Omega = (\theta, \varphi), \quad \theta = \cos^{-1}(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f) \ , \tag{3.35a}$$

$$d\Omega = \sin\theta d\theta d\varphi, \quad \varphi \in [0, 2\pi], \quad \theta \in [0, \pi] \ , \tag{3.35b}$$

with θ being the scattering angle.

There are several important properties of the present Eq. (3.33), such as (i) Expression (3.33) for $T_{if}^{+(e)}$ represents an *exact eikonal T* matrix for a general three-body charge-exchange problem (3.1), (ii) Modified perturbations V_i' and V_f' are short range at infinite separations between the two aggregates, and (iii) The entire dependence of $T_{if}^{+(e)}$ upon internuclear potential $V_{\rm PT}(R)$ is contained in phase factor $\rho^{-2i\nu_i}$ or $\rho^{-2i\nu_f}$. In particular, employing feature (iii), it can be easily shown that the total cross section is independent of $V_{\rm PT}(R)$, i.e.,

$$\sigma_{if}^{+(e)} = \int d\boldsymbol{\eta} \left| \frac{R_{if}^{+(e)}}{2\pi v} \right|^2$$

$$= \int_0^{2\mu v} d\eta\eta \int_0^{2\pi} d\varphi_\eta \left| \frac{R_{if}^{+(e)}}{2\pi v} \right|^2 \text{ (in units of } a_0^2) \ , \tag{3.36}$$

where $\boldsymbol{\eta}$ is the transverse momentum transfer $\boldsymbol{\eta} = (\eta\cos\varphi_\eta, \eta\sin\varphi_\eta, 0)$ and

$$R_{if}^{+(e)} = \langle \Phi_f e^{-i\delta_i} | V_i' + V_f' G_e^{+'} V_i' | \Phi_i \rangle \ , \tag{3.37a}$$

$$= \langle \Phi_f e^{+i\delta_f} | V_i' + V_f' G_e^{+'} V_i' | \Phi_i \rangle \ . \tag{3.37b}$$

Hence our basic matrix element $R_{if}^{+(e)}$ is entirely independent of the internuclear potential and, moreover, contains only *one* logarithmic Coulomb phase factor $\exp(i\delta_i)$ or $\exp(-i\delta_f)$. Even this remaining phase disappears for a general homonuclear (symmetric) collision (3.1) with specification $Z_P = Z_T$. We see that in this latter case ($Z_P = Z_T$), preserving the correct boundary conditions requires only trivial modification of the standard scattering theory, such as appropriate substitution of $V_{\rm PT}(R)$ by $-V_T(R)$ in V_f as well as by $-V_P(R)$ in V_i and G_e^+.

Exact expression (3.37) for $R_{if}^{+(e)}$ is free from the Coulombic divergencies which would arise if the correct boundary conditions were overlooked [see Refs. 19(a)-19(l)]. Hence, our matrix element $R_{if}^{+(e)}$ represents a natural starting point for developing approximate schemes, resorting to either perturbative or nonperturbative treatments. Perturbation methods based upon Eq. (3.37) have been previously studied by Belkić,[20] who expanded $G_e^{+'}$ in terms of the free three-particle Green's function G_{0e}^+ and performed *exact* numerical computation within the second-order Born approximation (see Sec. V). We shall presently develop nonperturbative methods starting from variational principle (2.26) for the total Green's operator. In particular, we choose

$$V_x = V' \ , \tag{3.38}$$

which implies

$$G_x^+ \equiv (E - H_0 - V' + V_x + i\epsilon)^{-1} = G_{0e}^+ \tag{3.39}$$

where G_{0e}^+ is the free-particle Green's function

$$G_{0e}^+ = (E_i^T - \mathbf{v}\cdot[\mathbf{k}_i + i\nabla_{r_i}] + \tfrac{1}{2}\nabla_{r_T}^2 + i\epsilon)^{-1} \ , \tag{3.40a}$$

$$= (E_f^P - \mathbf{v}\cdot[\mathbf{k}_f - i\nabla_{r_f}] + \tfrac{1}{2}\nabla_{r_P}^2 + i\epsilon)^{-1} \ . \tag{3.40b}$$

Hence the present variational estimate $\bar{G}_e^{+'}$ of exact eikonal Green's operator $G_e^{+'}$ is introduced by

$$\bar{G}_e^{+'} = G_{0e}^+ + \sum_{\lambda,\nu} G_{0e}^+ V' | \Phi_\lambda \rangle D_{\lambda\nu} \langle \Phi_\nu | V' G_{0e}^+ \ , \tag{3.41}$$

where

$$(D^{-1})_{\nu\lambda}=\langle\Phi_\nu|D|\Phi_\lambda\rangle\equiv\langle\Phi_\nu|V'-V'G_{0e}^{+}V'|\Phi_\lambda\rangle\ , \tag{3.42}$$

and

$$\Phi_\lambda=S_\lambda^T(\mathbf{r}_T)\exp(i\mathbf{k}_i\cdot\mathbf{r}_i)\ , \tag{3.43a}$$

$$\Phi_\nu=S_\nu^P(\mathbf{r}_P)\exp(-i\mathbf{k}_f\cdot\mathbf{r}_f)\ . \tag{3.43b}$$

Here $S_\gamma^K(\mathbf{r}_K)$ is a Coulombic-Sturmian wave function of Rotenberg:[21]

$$(-\tfrac{1}{2}\nabla_{r_K}^2-E_K)S_\gamma^K(\mathbf{r}_K)=\frac{Z_K a_{n^\gamma l^\gamma}^K}{r_K}S_\gamma^K(\mathbf{r}_K)\ , \tag{3.44}$$

where E_K is an arbitrary, but fixed negative energy parameter and coupling strength $Z_K a_{n^\gamma l^\gamma}^K$ represents an eigenvalue, such as

$$a_{n^\gamma l^\gamma}^K=(n^\gamma/Z_K)(-2E_K)^{1/2}\quad(K=P,T;\quad\gamma=\nu,\lambda) \tag{3.45}$$

and γ is the usual triplet of hydrogenic quantum numbers, i.e., $\gamma=\{n^\gamma l^\gamma m^\gamma\}$ $(\gamma=\nu,\lambda)$. In fact, there is a great similarity between the hydrogenlike and Sturmian wave functions, which can best be seen from the following simple scaling in the coordinate representation:[22]

$$S_{n^{j_l}j_m{}^j}^K(\mathbf{r}_K)=(a_{n^{j_l}j}^K)^{3/2}\varphi_{n^{j_l}j_m{}^j}^K(a_{n^{j_l}j}^K\mathbf{r}_K)\ . \tag{3.46}$$

Clearly, both wave functions in Eq. (3.46) relate to the same potential $V_K(r_K)$, but they nevertheless differ significantly in their respective spectrums. Specifically, although entirely *discrete,* spectrum $\{S_{n^\gamma l^\gamma m^\gamma}^K(\mathbf{r}_K)\}$ of Sturmian wave functions is known to be *complete.* In contrast, the set of the hydrogenlike bound-state wave functions $\{\varphi_{n^\gamma l^\gamma m^\gamma}^K(\mathbf{r}_K)\}$ can only be complete by inclusion of the corresponding *continuum* Coulomb waves. For this reason, the Sturmian expansion functions are much more convenient in practical computations than the hydrogenic basis set.

Inserting $\bar{G}_e^{+\prime}$ from (3.41) into Eq. (3.37a) in place of $G_e^{+\prime}$, we obtain the present variational estimate $\bar{R}_{if}^{+(e)}$ of our exact eikonal matrix element $R_{if}^{+(e)}$:

$$\bar{R}_{if}^{+(e)}=\langle\Phi_f e^{-i\delta_i}|V_i'+V_f'\bar{G}_e^{+\prime}V_i'|\Phi_i\rangle\ , \tag{3.47a}$$

$$=R_{if}^{+(\mathrm{CB2})}+\sum_{\lambda,\nu}A_{\lambda f}D_{\lambda\nu}B_{i\nu}\equiv R_{if}^{+(\mathrm{CB2})}+S_{if}^{+(e)}\ , \tag{3.47b}$$

where

$$R_{if}^{+(\mathrm{CB2})}=\langle\Phi_f e^{-i\delta_i}|V_i'+V_f'G_{0e}^{+}V_i'|\Phi_i\rangle\ , \tag{3.48a}$$

$$A_{\lambda f}=\langle\Phi_f e^{-i\delta_i}|V_f'G_{0e}^{+}V'|\Phi_\lambda\rangle\ , \tag{3.48b}$$

$$B_{i\lambda}=\langle\Phi_\nu|V'G_{0e}^{+}V_i'|\Phi_i\rangle\ . \tag{3.48c}$$

The *second Born* approximation with the *correct* boundary conditions (CB2) has previously been introduced by Belkić[20] precisely in the form of Eq. (3.48a) for general reaction (3.1). In Ref. 20, *exact* numerical computations within the CB2 approximation has been carried out for H^+-H charge exchange and we shall discuss these results in Sec. V. General homonuclear (symmetric) collisions with $Z_P=Z_T$ are the subject of thorough investigation in Sec. IV.

IV. EXACT CALCULATIONS OF THE VARIATIONAL T MATRIX FOR SYMMETRIC-CHARGE-CHANGING COLLISIONS

Here we consider the symmetric version of reaction (3.1) in which case

$$Z_P=Z_T\ , \tag{4.1}$$

$$\xi=0\ . \tag{4.2}$$

In the present derivation, we shall keep notation Z_P and Z_T for the charge of the impact and target nucleus, respectively, as if they were different. For our variational principle with the correct boundary conditions, however, identity (4.1) will be understood throughout. The only place at which identity (4.1) will explicitly be used is the definition of parameter ξ [see Eqs. (3.32) and (4.2)]. In this way, it will be possible to use the same algorithm for computations of variational T matrices *with* and *without* the correct boundary conditions. A variational principle of the Schwinger-type can also be obtained starting from the standard, full T matrix *without* preserving the proper boundary conditions. This can be accomplished for general reaction (3.1) by considering ξ as a parameter which is independent of Z_K $(K=P,T)$, then setting $\xi=0$ in either the homonuclear $(Z_P=Z_T)$ or heteronuclear $(Z_P\neq Z_T)$ case, and using variational principle (3.47a), (3.47b) with the formal substitutions of $V_{i,f}'$ and V' by $V_{i,f}$ and V, respectively. In this case, the factored high-energy leading term in Eq. (3.47b) would be the second-order Jackson-Schiff (JS2) approximation.[23] The difference between the results obtained by means of the first-order Born approximations CB1 and JS1 *with* and *without* the correct boundary conditions, respectively, has previously been found to be extremely significant.[17,24] It would be interesting to see whether this conclusion can be extended to the computations performed within the variational principles for the full T matrices.

The calculation of all the matrix elements will be carried out in a rigorous manner, thus yielding exact results. This is to be contrasted to the standard peaking approximation of unknown validity, which has customarily been employed in various second Born-type approximations such as the impulse or strong-potential Born (SPB) theories.[19,25]

We shall be working in the momentum space for which we need to introduce the Fourier transform of the type

$$f(\mathbf{q})=(2\pi)^{-3}\int d\mathbf{r}e^{i\mathbf{q}\cdot\mathbf{r}}f(\mathbf{r})\ , \tag{4.3}$$

and the complete set of plane waves,

$$|\mathbf{k}\,\mathbf{K}\rangle=(2\pi)^{-3}|\exp(i\mathbf{k}\cdot\mathbf{r}_T+i\mathbf{K}\cdot\mathbf{r}_P)\rangle\ , \tag{4.4a}$$

$$\langle\mathbf{k}'\,\mathbf{K}'|\mathbf{k}\,\mathbf{K}\rangle=\delta(\mathbf{k}-\mathbf{k}')\delta(\mathbf{K}-\mathbf{K}')\ . \tag{4.4b}$$

Then, we obtain

$$T_{if}^{+(\mathrm{CB2})}=T_{if}^{+(\mathrm{CB1})}+Q_{if}^{+}\ , \tag{4.5}$$

where

$$T_{if}^{+(\mathrm{CB1})}=\langle\Phi_f|V_i'|\Phi_i\rangle\ , \tag{4.6a}$$

$$=(2\pi)^6\{-\tfrac{1}{2}\rho_{\beta,i}[\tilde{\varphi}_f^{\,P}(-\boldsymbol{\alpha})]^*\tilde{\varphi}_i^{\,T}(\boldsymbol{\beta}) + \int d\mathbf{p}[\tilde{\varphi}_f^{\,P}(\mathbf{p}-\boldsymbol{\alpha})]^*\tilde{W}_P(-\mathbf{p})\tilde{\varphi}_i^{\,T}(\mathbf{p}+\boldsymbol{\beta})\}\ , \tag{4.6b}$$

$$Q_{if}^{+}=\langle\Phi_f|V_f'G_{0e}^{+}V_i'|\Phi_i\rangle\ , \tag{4.7}$$

$$\begin{aligned}Q_{if}^{+}=(2\pi)^6\Big[&\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{\varphi}_f^{\,P}(\mathbf{p}+\mathbf{q}-\boldsymbol{\alpha})]^*\tilde{W}_T(-\mathbf{q})E_{pq}^{-1}\tilde{V}_P(\mathbf{p})\tilde{\varphi}_i^{\,T}(\mathbf{q}+\boldsymbol{\beta})\\ &+\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{\varphi}_f^{\,P}(\mathbf{p}+\mathbf{q}-\boldsymbol{\alpha})]^*\tilde{W}_T(-\mathbf{q})E_{pq}^{-1}\tilde{W}_P(-\mathbf{p})\tilde{\varphi}_i^{\,T}(\mathbf{p}+\mathbf{q}+\boldsymbol{\beta})\\ &+\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{\varphi}_f^{\,P}(\mathbf{p}-\boldsymbol{\alpha})]^*\tilde{V}_T(-\mathbf{q})E_{pq}^{-1}\tilde{V}_P(\mathbf{p})\tilde{\varphi}_i^{\,T}(\mathbf{q}+\boldsymbol{\beta})\\ &+\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{\varphi}_f^{\,P}(\mathbf{p}-\boldsymbol{\alpha})]^*\tilde{V}_T(-\mathbf{q})E_{pq}^{-1}\tilde{W}_P(-\mathbf{p})\tilde{\varphi}_i^{\,T}(\mathbf{p}+\mathbf{q}+\boldsymbol{\beta})\Big]\ ,\end{aligned} \tag{4.8}$$

with

$$W_K(R)=-V_K(R),\quad K=P,T \tag{4.9}$$

$$E_{pq}=E_i^T+\mathbf{p}\cdot\mathbf{v}/2-|\mathbf{p}+\mathbf{q}+\boldsymbol{\beta}|^2/2+i\epsilon\ , \tag{4.10}$$

$$\boldsymbol{\alpha}=\boldsymbol{\eta}+\alpha_z\hat{\mathbf{v}},\quad \alpha_z=-v/2+\Delta E/v\ , \tag{4.11}$$

$$\boldsymbol{\beta}=-\boldsymbol{\eta}+\beta_z\hat{\mathbf{v}},\quad \beta_z=-v/2-\Delta E/v\ , \tag{4.12}$$

$$\rho_{\beta,i}=\beta^2+(b_i^T)^2,\quad \Delta E=E_i^T-E_f^P,\quad \beta=|\boldsymbol{\beta}|\ . \tag{4.13}$$

Similarly, matrix elements $A_{\lambda f}$, $B_{i\nu}$, and $D_{\lambda\nu}$ of stationary part $S_{if}^{+(e)}$ are found to be

$$\begin{aligned}A_{\lambda f}=(2\pi)^6\Big[&\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{\varphi}_f^{\,P}(\mathbf{p}+\mathbf{q}-\boldsymbol{\alpha})]^*\tilde{W}_T(-\mathbf{q})E_{pq}^{-1}\tilde{V}_P(\mathbf{p})\tilde{S}_\lambda^{\,T}(\mathbf{q}+\boldsymbol{\beta})\\ &+\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{\varphi}_f^{\,P}(\mathbf{p}+\mathbf{q}-\boldsymbol{\alpha})]^*\tilde{W}_T(-\mathbf{q})E_{pq}^{-1}\tilde{W}_P(-\mathbf{p})\tilde{S}_\lambda^{\,T}(\mathbf{p}+\mathbf{q}+\boldsymbol{\beta})\\ &+\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{\varphi}_f^{\,P}(\mathbf{p}-\boldsymbol{\alpha})]^*\tilde{V}_T(-\mathbf{q})E_{pq}^{-1}\tilde{V}_P(\mathbf{p})\tilde{S}_\lambda^{\,T}(\mathbf{q}+\boldsymbol{\beta})\\ &+\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{\varphi}_f^{\,P}(\mathbf{p}-\boldsymbol{\alpha})]^*\tilde{V}_T(-\mathbf{q})E_{pq}^{-1}\tilde{W}_P(-\mathbf{p})\tilde{S}_\lambda^{\,T}(\mathbf{p}+\mathbf{q}+\boldsymbol{\beta})\\ &+\frac{l^\lambda+1}{n^\lambda}\int d\mathbf{q}[\tilde{\varphi}_f^{\,P}(\mathbf{q}-\boldsymbol{\alpha})]^*\tilde{W}_T(-\mathbf{q})+[\tilde{\varphi}_f^{\,P}(-\boldsymbol{\alpha})]^*\tilde{V}_T(-\mathbf{q})\frac{\rho_{\mathbf{q}+\boldsymbol{\beta},\lambda}}{\rho_{\mathbf{q}+\boldsymbol{\beta},i}}\tilde{S}_\lambda^{\,T}(\mathbf{q}+\boldsymbol{\beta})\Big]\ ,\end{aligned} \tag{4.14}$$

$$\begin{aligned}D_{\lambda\nu}=(2\pi)^6\Big[&-\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{S}_\nu^{\,P}(\mathbf{p}+\mathbf{q}-\boldsymbol{\alpha})]^*\tilde{W}_P(-\mathbf{q})E_{pq}^{-1}\tilde{V}_P(\mathbf{p})\tilde{S}_\lambda^{\,T}(\mathbf{q}+\boldsymbol{\beta})\\ &-\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{S}_\nu^{\,P}(\mathbf{p}+\mathbf{q}-\boldsymbol{\alpha})]^*\tilde{W}_P(-\mathbf{q})E_{pq}^{-1}\tilde{W}_P(-\mathbf{p})\tilde{S}_\lambda^{\,T}(\mathbf{p}+\mathbf{q}+\boldsymbol{\beta})\\ &-\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{S}_\nu^{\,P}(\mathbf{p}-\boldsymbol{\alpha})]^*\tilde{V}_T(-\mathbf{q})E_{pq}^{-1}\tilde{V}_P(\mathbf{p})\tilde{S}_\lambda^{\,T}(\mathbf{q}+\boldsymbol{\beta})\\ &-\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{S}_\nu^{\,P}(\mathbf{p}-\boldsymbol{\alpha})]^*\tilde{V}_T(-\mathbf{q})E_{pq}^{-1}\tilde{W}_P(-\mathbf{p})\tilde{S}_\lambda^{\,T}(\mathbf{p}+\mathbf{q}+\boldsymbol{\beta})\\ &+\frac{l^\lambda+1}{n^\lambda}\int d\mathbf{q}\{[\tilde{S}_\nu^{\,P}(\mathbf{q}-\boldsymbol{\alpha})]^*\tilde{W}_P(-\mathbf{q})+[\tilde{S}_\nu^{\,P}(-\boldsymbol{\alpha})]^*\tilde{V}_T(-\mathbf{q})\}\frac{\rho_{\mathbf{q}+\boldsymbol{\beta},\lambda}}{\rho_{\mathbf{q}+\boldsymbol{\beta},i}}\tilde{S}_\lambda^{\,T}(\mathbf{q}+\boldsymbol{\beta})\\ &+\frac{l^\nu+1}{n^\nu}\int d\mathbf{p}[\tilde{S}_\nu^{\,P}(\mathbf{p}-\boldsymbol{\alpha})]^*\frac{\rho_{\mathbf{p}-\boldsymbol{\alpha},\nu}}{\rho_{\mathbf{p}-\boldsymbol{\alpha},f}}[\tilde{S}_\lambda^{\,T}(\mathbf{p}+\boldsymbol{\beta})\tilde{W}_P(-\mathbf{p})+\tilde{S}_\lambda^{\,T}(\boldsymbol{\beta})\tilde{V}_P(\mathbf{p})]\\ &+\int d\mathbf{p}[\tilde{S}_\nu^{\,P}(\mathbf{p}-\boldsymbol{\alpha})]^*\tilde{W}_P(-\mathbf{p})\tilde{S}_\lambda^{\,T}(\mathbf{p}+\boldsymbol{\beta})\\ &-\left[\frac{l^\nu+1}{2n^\nu}\rho_{\alpha,\nu}+\frac{l^\lambda+1}{2n^\lambda}\rho_{\beta,\lambda}+\frac{(l^\nu+1)(l^\lambda+1)\rho_{\alpha,\nu}\rho_{\beta,\lambda}}{2n^\nu n^\lambda\rho_{\beta,i}}\right][\tilde{S}_\nu^{\,P}(-\boldsymbol{\alpha})]^*\tilde{S}_\lambda^{\,T}(\boldsymbol{\beta})\Big]\ ,\end{aligned} \tag{4.15}$$

$$B_{i\lambda}=(2\pi)^6\left[\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{S}^{P}_{\nu}(\mathbf{p}+\mathbf{q}-\boldsymbol{\alpha})]^*\tilde{W}_P(-\mathbf{q})E_{pq}^{-1}\tilde{V}_P(\mathbf{p})\tilde{\varphi}^{T}_{i}(\mathbf{q}+\boldsymbol{\beta})\right.$$
$$+\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{S}^{P}_{\nu}(\mathbf{p}+\mathbf{q}-\boldsymbol{\alpha})]^*\tilde{W}_P(-\mathbf{q})E_{pq}^{-1}\tilde{W}_P(-\mathbf{p})\tilde{\varphi}^{T}_{i}(\mathbf{p}+\mathbf{q}+\boldsymbol{\beta})$$
$$+\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{S}^{P}_{\nu}(\mathbf{p}-\boldsymbol{\alpha})]^*\tilde{V}_T(-\mathbf{q})E_{pq}^{-1}\tilde{V}_P(\mathbf{p})\tilde{\varphi}^{T}_{i}(\mathbf{q}+\boldsymbol{\beta})$$
$$+\int\int d\mathbf{p}\,d\mathbf{q}[\tilde{S}^{P}_{\nu}(\mathbf{p}-\boldsymbol{\alpha})]^*\tilde{V}_T(-\mathbf{q})E_{pq}^{-1}\tilde{W}_P(-\mathbf{p})\tilde{\varphi}^{T}_{i}(\mathbf{p}+\mathbf{q}+\boldsymbol{\beta})$$
$$\left.+\frac{l^{\nu}+1}{n^{\nu}}\int d\mathbf{p}[\tilde{S}^{P}_{\nu}(\mathbf{p}-\boldsymbol{\alpha})]^*\frac{\rho_{\mathbf{p}-\boldsymbol{\alpha},\nu}}{\rho_{\mathbf{p}-\boldsymbol{\alpha},f}}[\tilde{\varphi}^{T}_{i}(\mathbf{p}+\boldsymbol{\beta})\tilde{W}_P(-\mathbf{p})+\tilde{\varphi}^{T}_{i}(\boldsymbol{\beta})\tilde{V}_P(\mathbf{p})]\right], \tag{4.16}$$

where

$$\rho^{K}_{\tau,\gamma}=\tau^2+(b^{K}_{\gamma})^2,\quad b^{K}_{\gamma}=\frac{Z_K}{l^{\gamma}+1};\quad \gamma=\nu,\lambda\quad (K=P,T) \tag{4.17}$$

$$\rho^{K}_{\tau,j}=\tau^2+(b^{K}_{j})^2,\quad b^{K}_{j}=Z_K/n^{j};\quad j=f,i\quad (K=P,T)\,. \tag{4.18}$$

In these formulas, the following value of the Sturmian energy E_K was selected:

$$E_K=-(b^{K}_{\gamma})^2/2;\quad \gamma=\nu,\lambda\quad (K=P,T)\,. \tag{4.19}$$

This choice has the particular merit of making nodeless Sturmian wave functions ($n^{\gamma}=l^{\gamma}+1$) *identical* to the corresponding hydrogenlike wave functions ($1s,2p,3d,4f,5g,6h,\ldots$). The remaining Sturmian wave functions with $n^{\gamma}\neq l^{\gamma}+1$ represent certain pseudostates, which hopefully will mimic the hydrogenic continuum to a good approximation. Using the same Sturmian energy in computations of, for example, polarizability of atomic hydrogen, it can be verified that a Sturmian basis of *moderate size* provides excellent results in comparison with the exact values.[11(a)] This should be contrasted to the inability of even the *entire* set of hydrogenic bound states to provide satisfactory results without inclusion of the continuum.

For further analysis of matrix elements $A_{\lambda f}$, $B_{i\nu}$, and $D_{\lambda\nu}$ it will be useful to establish a relation between the momentum representations of Sturmian and bound-state hydrogenlike wave functions. Such a connection follows directly from Eqs. (3.46) and (4.3) in the form:[22]

$$\tilde{S}^{K}_{n^{\gamma}l^{\gamma}m^{\gamma}}(\mathbf{q})=(a^{K}_{n^{\gamma}l^{\gamma}})^{-3/2}\tilde{\varphi}^{K}_{n^{\gamma}l^{\gamma}m^{\gamma}}(\mathbf{q}/a^{K}_{n^{\gamma}l^{\gamma}})\,. \tag{4.20}$$

Also convenient is the relation between the momentum-space Sturmian wave functions and the Fourier transform of a Sturmian wave function weighted with the corresponding Coulomb potential, i.e.,

$$\tilde{\chi}^{K}_{\gamma}(\mathbf{q})=-\frac{l^{\gamma}+1}{2n^{\gamma}}\rho^{K}_{\mathbf{q},\gamma}S^{K}_{\gamma}(\mathbf{q});\quad \gamma=\nu,\lambda\quad (K=P,T)\,, \tag{4.21}$$

where $\rho^{K}_{\mathbf{q},\gamma}$ is given by Eq. (4.17) and

$$\chi^{K}_{\gamma}(\mathbf{r}_K)=V_K(r_K)S^{K}_{\gamma}(\mathbf{r}_K);\quad \gamma=\nu,\lambda\quad (K=P,T)\,. \tag{4.22}$$

It is straightforward to verify Eq. (4.21) by taking the Fourier transform of both sides of Sturmian eigenvalue problem (3.44) and employing Eqs. (3.45), (4.17), and (4.19). In deriving results (4.14), (4.15), and (4.16), we have already utilized Eq. (4.21).

Since the momentum-space Sturmian wave functions are reduced to the scaled Fourier transforms of hydrogenlike wave functions by virtue of (4.20), inspection of Eqs. (4.5)–(4.16) will reveal that stationary part $S^{+(e)}_{if}$ requires the same type of three- and six-dimensional integrals in momentum space, as does $R^{+(\mathrm{CB2})}_{if}$. The three-dimensional integrals are the two-center Dalitz integrals which can be calculated either analytically or numerically in the form of parametric *one*-dimensional Feynmann quadratures. This has recently been shown by Belkić and Taylor[17(b),26] in both cases *with* and *without* the Coulombic phase distortions. The most difficult are the pure second Born-type six-dimensional integrals encountered in matrix elements Q^{+}_{if}, $A_{\lambda f}$, $B_{i\nu}$, and $D_{\lambda\nu}$ [see Eqs. (4.7), (4.14)–(4.16)]. These integrals have recently been reduced by Belkić[27] to only *two*-dimensional quadrature with smooth integrands for arbitrary pure three-body homonuclear charge exchange. Hence, in conclusion, we have shown that our variational principle (3.47) is very attractive from the computational point of view, since the T matrix for symmetric collisions requires, at most, two-dimensional integrals accompanied by a matrix inversion ($\underline{D}^{-1}$) at each incident energy and scattering angle.

V. NUMERICAL RESULTS OF THE CB2 APPROXIMATION FOR H^+-H CHARGE EXCHANGE AT INTERMEDIATE AND HIGH ENERGIES

A detailed account of the results obtained by the present variational principle is planned to be published separately in a forthcoming paper. The most critical is the intermediate and low-energy region at which stationary part $S^{+(e)}_{if}$ should compensate for deficiences of the first (CB1) and second (CB2) Born approximations. In fact, our experience shows that at low-incident energies as well as at the lower edge of intermediate energies, pure second Born-type matrix element $Q^{+}_{if}=\langle\Phi_f|V'_fG^{+}_{0e}V'_i|\Phi_i\rangle$ yields a negligible contribution to the transition amplitude $T^{+(\mathrm{CB2})}_{if}=T^{+(\mathrm{CB1})}_{if}+Q^{+}_{if}$ from Eq. (4.5). This becomes immediately clear by inspection of Figs. 1–3, which show the differential cross sections

for H^+-H charge exchange at 60, 125, and 5000 keV. Comparisons with the experimental data reveal that the first Born approximation (CB1) provides quite a satisfactory differential cross section $d\sigma_{if}^{+(\mathrm{CB1})}/d\Omega$ in the forward direction. Away from a narrow forward cone, theoretical data $d\sigma_{if}^{+(\mathrm{CB1})}/d\Omega$ decrease rapidly by orders of magnitude, which then yield adequate total cross sections despite the unphysical dip at intermediate scattering angles. Thus, at lower energies, a significant interplay will take place merely between the perturbation part $T_{if}^{+(\mathrm{CB1})}$ and stationary contribution $S_{if}^{+(e)}$ in the variational T matrix $\overline{T}_{if}^{+(e)}=T_{if}^{+(\mathrm{CB1})}+Q_{if}^{+}+S_{if}^{+(e)}$. Since the CB1 approximation gives an acceptable order of magnitude for the cross sections even at low energies, it is expected that the convergence over the basis states in $S_{if}^{+(e)}$

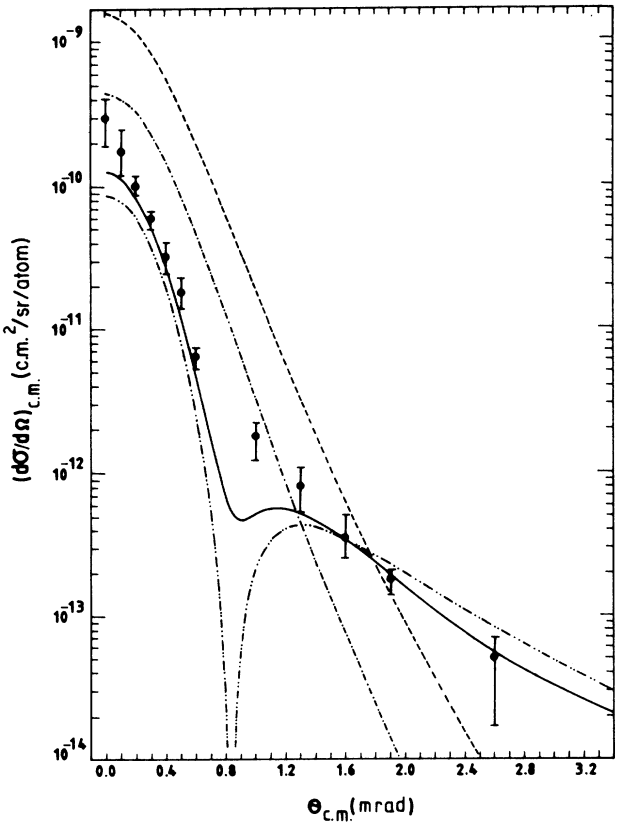

FIG. 1. Differential cross sections $(d\sigma/d\Omega)_\Sigma$ for charge exchange $H^+ + H(1s) \rightarrow H(\Sigma) + H^+$ as a function of scattering angle at 60-keV laboratory energy of the projectile. The theoretical curves are not folded over experimental resolution. Only the $1s \rightarrow 1s$ transition in atomic hydrogen is explicitly considered in the computations. The cross sections $(d\sigma/d\Omega)_\Sigma$ for capture into *any* state of H is estimated by using the simplest scaling formula, i.e., $(d\sigma/d\Omega)_\Sigma = 1.202(d\sigma_{1s,1s}/d\Omega)$. *Theory* (all the *exact* numerical computations obtained by Belkić, Ref. 20): ·-·-·, BK1, the first-order Brinkman-Kramers approximation, $T_{if}^{+(\mathrm{BK1})}=\langle\Phi_f|V_P(r_P)|\Phi_i\rangle$; — — — BK2, the second-order Brinkman-Kramers approximation proposed in Ref. 28, $T_{if}^{+(\mathrm{BK2})}=\langle\Phi_f|V_T(r_T)G_0^+V_P(r_P)|\Phi_i\rangle$; ·····, CB1 approximation, see the text, Eq.(4.6); and —— CB2 approximation, see text Eqs. (4.5)–(4.8). *Experiment*: Closed circles, Martin *et al.* (Ref. 29).

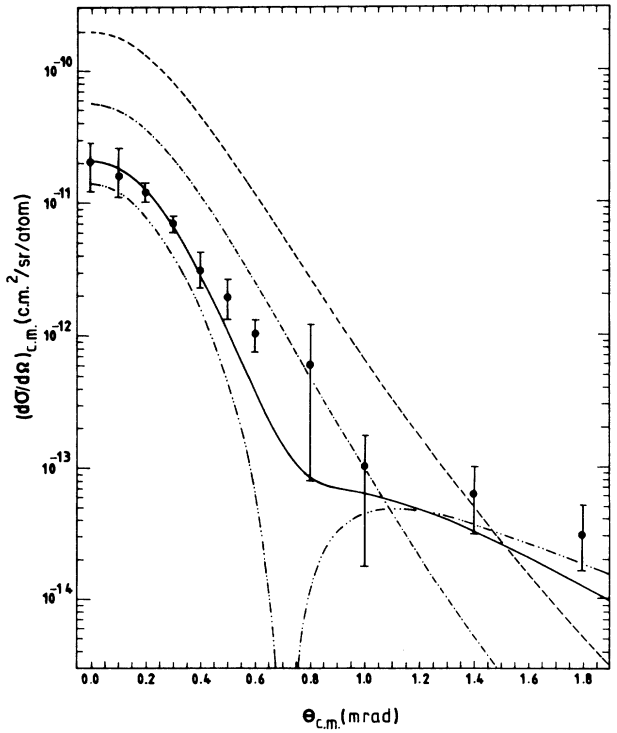

FIG. 2. Same as in Fig. 1, except for 125 keV.

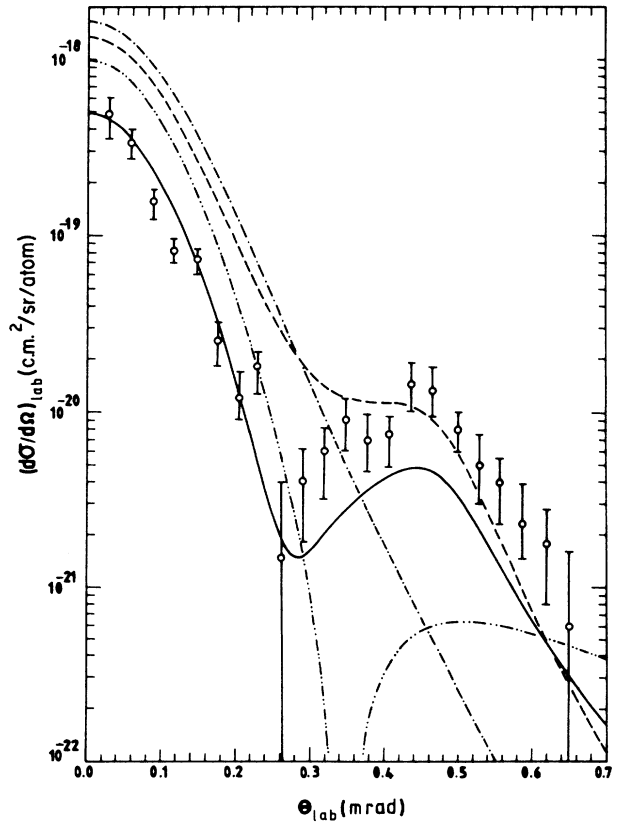

FIG. 3. Same as in Fig. 1, except for 5000 keV *and* the experimental data of Vogt *et al.* (Ref. 30) denoted by open circles.

can be achieved with low-rank matrices $\underline{A}$, $\underline{B}$ and $\underline{D}$.

On the other hand, as the incident energy is progressively augmented, the contribution from Q_{if}^{+} becomes increasingly more important as evidenced in Fig. 3. Computations show that both the real and imaginary parts of Q_{if}^{+} are of nearly equal importance at intermediate and higher energies (see Figs. 4–7). Finally, in the limit of very high impact energies, double scattering term Q_{if}^{+} dominates over the first-order contribution $T_{if}^{+(\mathrm{CB1})}$. Moreover, at these energies, the second Born (CB2) approximation yields the leading fraction of the total T matrix and, hence, here stationary part $S_{if}^{+(e)}$ is expected to be negligible.

VI. DISCUSSION AND CONCLUSION

In general, the methods currently used to deal with the problem of charge exchange may be classified into two distinct groups, i.e., perturbation theories and L^2-expansion techniques. In the former methods, each order of the perturbation potential series accounts for an

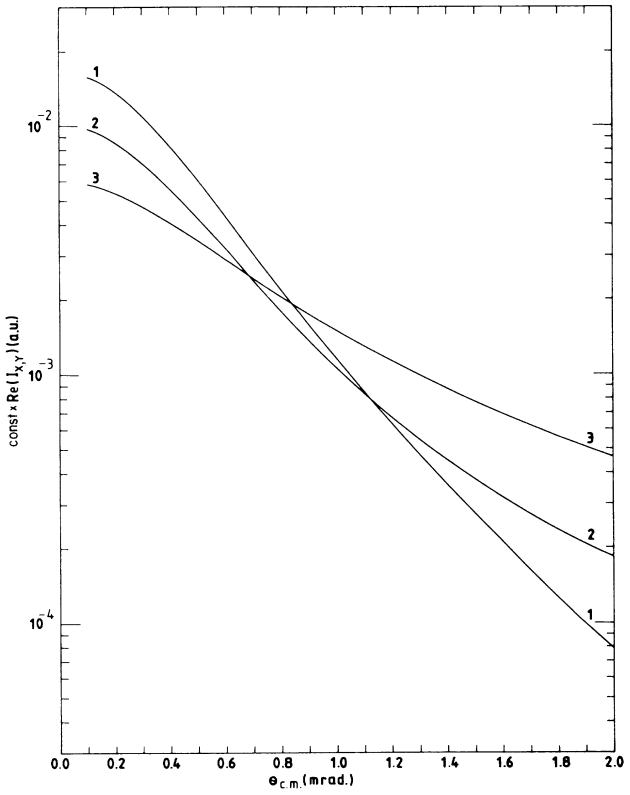

FIG. 4. Charge exchange in proton–atomic-hydrogen collisions, i.e., $H^+ + H(1s) \rightarrow H(1s) + H^+$ at 60-keV laboratory energy of the projectile. All the curves represent the real part of matrix element $\langle \Phi_f | XG_{0e}^{+} Y | \Phi_i \rangle = I_{X,Y}$ multiplied by a constant, const$=(-1)^n/(128\pi)$. Curve 1, $n=1$, $X=V_T(r_T)$, $Y=V_P(r_P)$; curve 2, $n=0$, $X=-V_T(R)$, $Y=V_P(r_P)$ [the same curve is obtained for $n=0$, $X=V_T(r_T)$ and $Y=-V_P(R)$]; curve 3, $n=1$, $X=-V_T(R)$, $Y=-V_P(R)$. These four matrix elements are computed *exactly* and they are all contained in the CB2 approximation [see Eqs. (4.5) and (4.7)] (a.u.=atomic units).

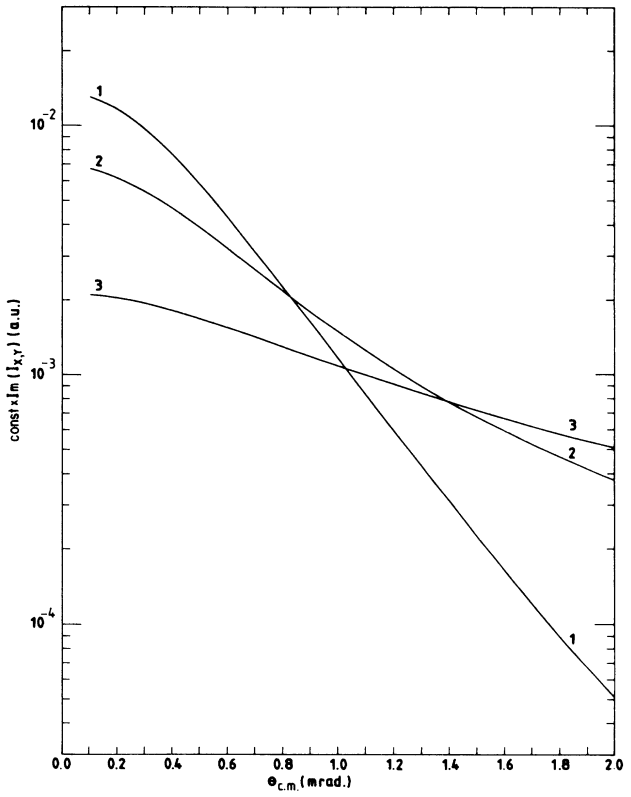

FIG. 5. Same as in Fig. 4, except for the imaginary part of $\langle \Phi_f | XG_{0e}^{+} Y | \Phi_i \rangle$.

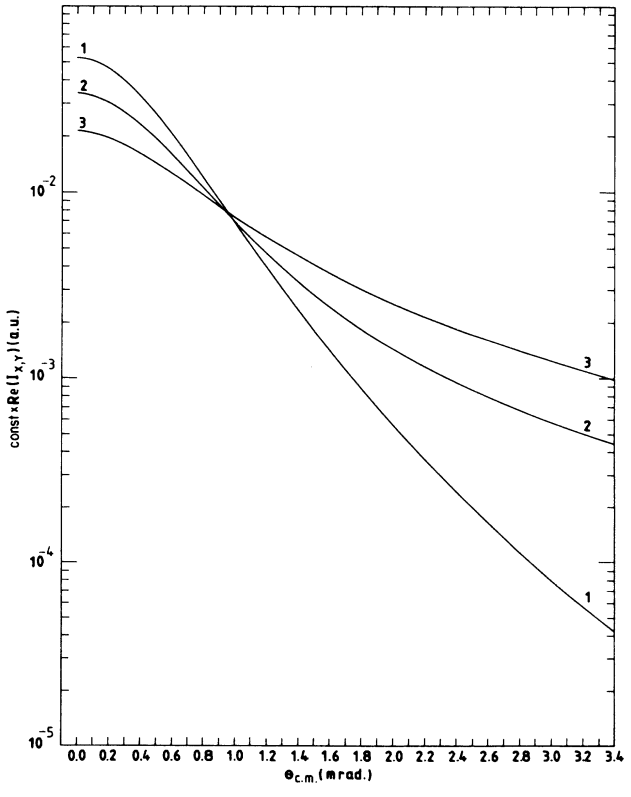

FIG. 6. Same as in Fig. 4, except for 125 keV.

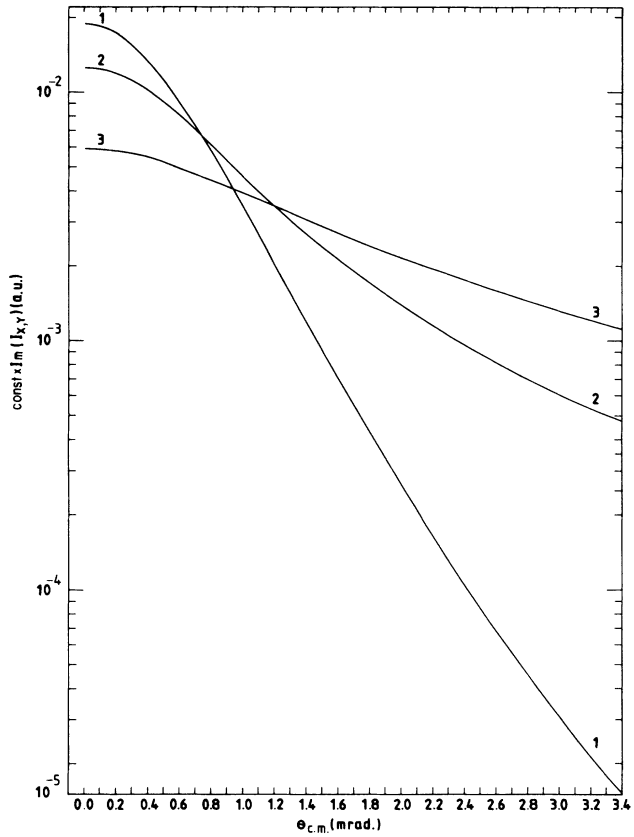

FIG. 7. Same as in Fig. 4, except for the imaginary part of matrix element $\langle \Phi_f | XG_{0e}^{+} Y | \Phi_i \rangle$ computed at 125 keV.

infinite number of intermediate transitions through the Green's functions. *Exact* computations, however, have thus far been carried out only up to the second order in the perturbation interactions, since the higher orders are practically unmanageable without resorting to peaking approximations of unknown validity. In contrast to this, the L^2-discretization methods (e.g., close-coupling techniques) take the perturbation potentials exactly into account and truncate the series of the total scattering wave functions developed in terms of certain expansion functions. Here only a limited number of intermediate channels can be accounted for, due to the complexity of the resulting system of coupled differential equations. This type of method is applicable, in practical terms, merely to lower energies, since at high energies all the channels are open and, hence, a large number of expansion functions is required. In fact, the high-energy behavior of the cross sections obtained by means of the close-coupling methods reduces to prediction of the first-order perturbation theories, irrespective of the basis-set size employed in the computations. The leading contribution at high energy is, however, determined by the second-order terms describing the Thomas double scattering.

Clearly, the most critical intermediate energy region of scattering is not well understood, within either of the aforementioned two groups of methods. They provide only partial answers, which could be considered satisfactory exclusively in their respective energy range of validity. Therefore, a new theory is sought which will potentially be applicable to all energies and, furthermore, will successfully encompass the best features of the leading second-order methods together with the efficient L^2-expansion techniques. Such a theory with the correct boundary conditions is proposed in the present paper through introduction of a Schwinger-type variational principle for the total Green's function and T matrix.

We first show that an exact eikonal total cross section with the correct boundary conditions for electron capture from hydrogenlike atoms (Z_T,e) by bare nuclei of charge Z_P can be obtained by retaining only one Coulomb-logarithmic phase factor $\exp[+i(Z_T/v - Z_P/v)\ln(vR - \mathbf{v}\cdot\mathbf{R})]$ in the most general case of the heteronuclear collision $(Z_P \neq Z_T)$. Even this remaining term disappears for homonuclear scatterings $(Z_P = Z_T)$, in which case an easier formalism of the standard collision theory can be employed with merely a slight modification of the total and perturbation potentials.

Next, we replace an exact eikonal reduced transition amplitude $R_{if}^{+(e)}$ by a Schwinger-type variational estimate $\bar{R}_{if}^{+(e)} = R_{if}^{+(\mathrm{CB2})} + S_{if}^{+(e)}$, where label CB2 denotes the corrected second Born approximation and $S_{if}^{+(e)}$ is the stationary part. Each contribution $R_{if}^{+(\mathrm{CB2})}$ and $S_{if}^{+(e)}$ is given in terms of free-particle Green's function G_{0e}^{+} in which the kinetic energy operator for the heavy-particle motions is linearized (eikonal hypothesis). In an analogy with $R_{if}^{+(e)}$, the proper boundary conditions are also preserved in our variational approximation $\bar{R}_{if}^{+(e)}$ whose terms $R_{if}^{+(\mathrm{CB2})}$ and $S_{if}^{+(e)}$ contain only one Coulomb-phase factor $\exp[+i(Z_T/v - Z_P/v)\ln(vR - \mathbf{v}\cdot\mathbf{R})]$ in the most general case of heteronuclear collisions. This is particularly advantageous for homonuclear scattering in which case the full, variational T matrix reduces to, at most, two-dimensional numerical quadratures with smooth integrands. The present general expression for $\bar{R}_{if}^{+(e)}$ is free from the characteristic Coulomb divergencies, which are customarily encountered in the theories with incorrect boundary conditions, such as the strong-potential Born approximation. Two factored constituents $R_{if}^{+(\mathrm{CB2})}$ and $S_{if}^{+(e)}$ of $\bar{R}_{if}^{+(e)}$ are respectively due to the second order of a *perturbation* series and to a contribution from an L^2-*expansion* method. Hence, total estimate $\bar{R}_{if}^{+(e)}$ represents a variational unification of perturbation theories and L^2-close-coupling methods. As such, our variational principle exhibits many advantages over all the existing theories for charge exchange. The present method is valid at all incident energies for which the eikonal hypothesis is applicable (from very high, through intermediate, and down to low energies of the order of 100 eV/amu). In practice, at most the second order can be computed exactly from a perturbation series. The resulting data are inferior to the proposed variational principle containing $T_{if}^{+(\mathrm{CB2})}$ *and* stationary part $S_{if}^{+(e)}$. The latter term could be, therefore, interpreted as a variational approximation to all the otherwise uncalculable higher-order terms beyond the fraction given by $T_{if}^{+(\mathrm{CB2})}$. At the same time, the present theory is superior to the usual close-coupling methods, since the high-energy lead-

ing term $T_{if}^{+(CB2)}$ is accounted for along with the L^2-discretization portion $S_{if}^{+(e)}$, which projects a part of the full transition T operator onto a complete basis set. Stationary function $S_{if}^{+(e)}$ approximately incorporates the same physical effects as do the close-coupling methods through inclusion of virtual transitions in intermediate channels. Rather than solving a system of coupled differential equations, which becomes unwieldy for multielectron targets, multiply charged ions, or even for simple H^+-H charge exchange at sufficiently high energies, we need only to perform numerical quadratures and invert a matrix. At high energies, where the close-coupling techniques necessitate a large number of basis functions, our variational principle requires low-rank matrices since the major contribution is determined by the second Born approximation $T_{if}^{+(CB2)}$.

In addition to being very attractive from the computational point of view, the present method is also quite flexible concerning the choice of the intermediate state propagator G_x^+ and expansion functions. The L^2 basis set and Green's function G_x^+ are not necessarily interrelated, so that, in general, we can choose them independently. We presently select the Sturmians as the expansion functions and free-particle Green's operator G_{0e}^+ for G_x^+. These two choices are completely independent of each other. Setting $G_x^+ = G_{0e}^+$ leads to the simplest second Born approximation $R_{if}^{+(CB2)}$ with the correct high-energy behavior for which powerful algorithms exist.[27] Our choice of intermediate propagator G_x^+ is very simple and this provides an important flexibility in freely augmenting the size of the Sturmian basis sets whenever necessary. Sturmian negative-energy parameters E_P and E_T can, in principle, be varied in a search for the optimal convergence of stationary part $S_{if}^{+(e)}$. Alternatively, these parameters can be fixed in order to account for a significant fraction of the true physical hydrogenic states, e.g., nodeless wave functions $1s, 2p, 3d, 4f, 5g, \ldots$, as illustrated in the present work. Convenient scaling properties of Sturmian wave functions advantageously simplify the full, variational T matrix to evaluation of the first and second Born-type matrix elements. The present computations show that the second Born-type integrals become progressively less important with decreasing impact energy. They are completely negligible at low as well as at the lower edge of intermediate energies. Hence, in this important energy range, L^2-discretization part $S_{if}^{+(e)}$ needs only to compensate for the deficiencies of the first Born approximation $T_{if}^{+(CB1)}$, which already yields an acceptable order of magnitude for the cross sections in the forward direction.

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