lar distribution that no compound states are involved in the low-energy ion-molecule reactions. However, the angular distribution may be an insufficient guide for such a deduction since compound states can have very short lifetimes (~ 10^{-15} sec) and the angular distribution of the heavy particles may not be affected in such a case. Thus, compound states and curve hopping could contribute to the reactions. It is not clear at this time whether the shape of the charge transfer cross section in the range 3–80 eV is a reliable guide for determining electron affinities when both associative detachment and charge transfer are present. Certainly the theoretical basis for such deductions is sparse at the present time.

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On the Application of Faddeev Equations and the Coulomb *t* Matrix to Asymptotic Electron Capture in Hydrogen†

C. P. Carpenter* and T. F. Tuan
Physics Department, University of Cincinnati, Cincinnati, Ohio 45221
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Faddeev equations together with the Coulomb *t* matrix have been used to determine the asymptotic amplitude for electron capture from neutral hydrogen by fast protons. The results show that in the high-energy limit the capture cross section should go down as v^{-11}, where v is the velocity of the incident proton. The capture amplitude is identical to Drisko's second-Born-approximation calculation except for a complex energy-dependent phase factor which ultimately approaches unity with sufficiently high incident energy. The major contribution to the three-body capture amplitude can be shown to come from the on-energy-shell two-body *t* matrix, in agreement with general theorems concerning scattering from complex systems. At high incident energies, the on-energy-shell contribution to the capture amplitude (not the cross section) will decrease as v^{-5}, while the off-energy-shell continuum contribution will decrease as v^{-6}. The contributions from the sum of the infinite number of two-body bound-state poles can be shown to converge, and the sum can be explicitly performed at high enough incident energies in all except the forward direction. The bound-state contributions to the capture amplitude go down as v^{-11}, which is much less than the continuum contributions.

I. INTRODUCTION

Most of the recent investigations in the asymptotic behavior of electron-capture cross section from hydrogen at high energies involve the use of either some kind of Born and distorted-wave approximation[1–3] or the impulse approximation.[4] The approximations usually consist of a Neumann type of iteration of an integral equation whose kernel contains disconnected diagrams. Moreover, the convergence of the Born series for rearrangement three-body scattering has long been questioned.[5]

It is the purpose of the present paper to investigate the asymptotic behavior of electron capture with Faddeev's equations.[6] Other than the obvious advantage that the kernel of this equation does not contain disconnected diagrams and an iteration of such an equation may well converge in the same sense that a Born series converges for sufficiently high incident energies in two-body scattering, there is the additional advantage that the Coulomb two-body *t* matrix[7] is known in closed form. We shall make use of some of the high-energy-approximation techniques developed by Drisko[1] for the Born series which also happen to be applicable to the Faddeev series. To be specific, we shall consider the following reaction at high incident energies:

$$p + \mathrm{H}(1s) \to \mathrm{H}(1s) + p \,. \tag{1}$$

In the following, we will develop the general formulation and introduce the coordinate system as well as the notation in Sec. II. We shall use Lovelace's[8] formulation for the three-body scattering, which is more convenient for our purpose than the original Faddeev[6] equations. In order to facilitate comparison with previous results for the reader, we shall use the same notation as those used by Lovelace,[8] by Drisko,[1] and by Mapleton[3] wherever possible. The actual integral equation used, as well as the series expansion, will also be developed in this section. It will be shown that if we make use of Mott's theorem[9] and neglect the proton-proton interaction, the coupled integral equations reduce to a single integral equation. For the remainder of this paper, we shall be concerned with only this equation. Actually, we can show that there will be two integral equations which are identical on the energy shell but have different analytical continuations off the energy shell. If a Neumann iteration of the two solutions is made, then the first terms correspond to the prior and post first Born matrix elements, which are, of course, equal on the energy shell. The second terms correspond to the second Born approximation with the initial and final-state partial Green's functions. Each of the higher-order terms can be iterated to give a Born-type series, although the convergence of such iterations is open to question.

In Sec. III we shall show that the second term in our iteration in the high-energy limit corresponds to Drisko's[1] and Mapleton's[3] result except for a complex energy-dependent phase factor, which eventually approaches unity as the incident particle velocity increases to sufficiently high values. We will also be able to show explicitly that the principal contribution to the total cross section comes from scattering angles at which the two-body t matrix is on the energy shell.

In Sec. IV, we shall consider the two-body bound-state contributions. Since there are an infinite number of bound states, some speculation[3] has been raised over whether this contribution will be finite. Within the limits of our approximation, we will show that the infinite sum over the bound-state contributions will not only converge, but in the high-energy limit we can actually perform the sum explicitly. Furthermore, the contribution from these bound states will go down with energy much more rapidly than the continuum states and hence cannot be significant at high enough incident energies. In the special case of resonant symmetric capture given by Eq. (1), the bound-state contributions diverge in the forward direction. If, however, the incident particle is a deuteron, or, if the final unperturbed state is not identical with the initial unperturbed state (for example, an excited state), then no such divergence occurs and the entire bound-state contribution remains small in comparison with the continuum-state contributions at high energies.

II. GENERAL FORMULATION

We consider an incident ion 3 (e.g., a proton or a deuteron), which captures an electron 1 originally bound to a nucleus 2. Equation (1) can now be expressed as

$$3+(12)\rightarrow 2+(13)\ . \tag{2}$$

As mentioned in the Introduction, the Faddeev equations for rearrangement scattering consists of two sets of coupled integral equations: One set corresponds to using the initial-state interaction and the other set corresponds to the final-state interaction. Using Lovelace's[8] notation, we can write

$$(U^+_{31}\,U^+_{32}\;U^+_{33}) = (V_1+V_2) - (U^+_{31}\,U^+_{32}\,U^+_{33})\begin{pmatrix} 0 & G_0T_1 & G_0T_1 \\ G_0T_2 & 0 & G_0T_2 \\ G_0T_3 & G_0T_3 & 0\end{pmatrix},$$

$$\begin{pmatrix} U^-_{12} \\ U^-_{22} \\ U^-_{32}\end{pmatrix} = (V_1+V_3) - \begin{pmatrix} 0 & T_2G_0 & T_3G_0 \\ T_1G_0 & 0 & T_3G_0 \\ T_1G_0 & T_2G_0 & 0\end{pmatrix}\begin{pmatrix} U^-_{12} \\ U^-_{22} \\ U^-_{32}\end{pmatrix}\ , \tag{3}$$

where the + superscript denotes initial-state interaction and the − superscript denotes final-state interaction; U_{ij} is the three-body amplitude going from an initial state with particle i free and the other two particles bound together to a final state with particle j free and the two other particles bound together; and T_i is a generalized two-body t matrix in the three-body system and occurs as the product of the usual two-body t matrix and the δ function in momenta for the free particle i. The energy variable of the two-body t matrix is the total energy minus the kinetic energy of particle i. V_i denotes the two-body interaction between the two remaining particles when i is the third particle.

We shall only be concerned with the final-state interaction given by the second set of coupled equations in Eqs. (3). The superscript minus sign will henceforth be dropped. We shall, furthermore, make use of Mott's theorem,[9] which essentially states that in an exact atomic-scattering calculation, the contribution of interactions between the protons to the scattering amplitude should vanish in the limit when the electron-proton mass ratio approaches zero. Thus, we may set V_1 and T_1 to zero. The integral equations can then be simply decoupled and we can very easily obtain the following single integral equation for the reactions given by Eq. (2):

$$U_{32} = V_3 - T_2G_0V_3 + T_2G_0T_3G_0U_{32}\ . \tag{4}$$

This is a single inhomogeneous linear integral equation with the kernel given by $T_2G_0T_3G_0$.

A Neumann iteration of this equation would produce a series expansion in the T operators and the free-space Green's functions. The actual scattering amplitude can be obtained from this series by taking the matrix element between the initial and

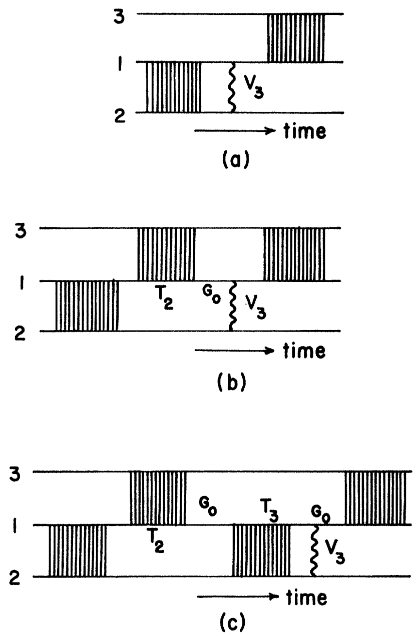

FIG. 1. Diagrams for the first three terms in the expansion for Faddeev's series. (a) Matrix element $\langle f|V_3|i\rangle$, which is identical to the first Born term in final-state interactions; (b) matrix element $\langle f|T_2G_0V_3|i\rangle$, the same as the second Born with final-state partial Green's function; (c) matrix element $\langle f|T_2G_0T_3G_0V_3|i\rangle$, which bears no simple relation to the Born series.

final states. Thus,

$$\langle f|U_{32}|i\rangle = \langle f|V_3|i\rangle - \langle f|T_2G_0V_3|i\rangle + \langle f|T_2G_0T_3G_0V_3|i\rangle - \langle f|T_2G_0T_3G_0T_2G_0V_3|i\rangle + \cdots . \quad (5)$$

Each term in this series represents a connected diagram. The first three terms are given by Figs. 1(a), 1(b), and 1(c), respectively.

It is easy to see that the first term on the right-hand side of Eq. (5) is just the first Born term in the final-state representation. The second term and the higher-order terms can be easily iterated to produce the Drisko[1] Born series.

The Neumann iteration can only provide a means for studying the high-energy behavior and, of course, will not provide any information on three-body bound states, which can only be studied if a proper Fredholm expansion is made of the integral equation given by Eq. (4).

We shall, for the most part, be concerned with the second term on the right-hand side of Eq. (5) and will consider the resonant symmetric reaction given by Eq. (1).

If $\vec{p}_1$, $\vec{p}_2$, and $\vec{p}_3$ are the center-of-mass momentum coordinates of all three particles and $\vec{k}_a$ and $\vec{k}_b$ are the initial and final reduced momenta of the free particle with respect to the center of mass of the initial and final bound systems, then we may write

$$\langle a|T_2G_0V_3|b\rangle = -\int g_a^*\left(\vec{p}_2{}' - \frac{M}{M+m}\,\vec{k}_a\right)\delta(\vec{p}_3{}'+\vec{k}_a)\,\delta(\vec{p}_2{}''-\vec{p}_2{}')\langle \vec{p}_2{}'\,\vec{p}_3{}'|T_2(k)|\vec{p}_2{}''\vec{p}_3{}''\rangle$$
$$\times\frac{V_3(\vec{p}_2{}'-\vec{p}_2)\delta(\vec{p}_3{}''-\vec{p}_3)}{(\vec{p}_2{}''+\vec{p}_3{}'')^2/2m+\vec{p}_2{}''^2/2M+\vec{p}_3{}''^2/2M-s-i\epsilon}$$
$$\times g_b\left(\vec{p}_3+\frac{M}{M+m}\,\vec{k}_b\right)\delta(\vec{p}_2-\vec{k}_b)\;d^3p_2'\,d^3p_3'\,d^3p_2''\,d^3p_3''\,d^3p_2\,d^3p_3\;, \quad (6)$$

where $\vec{p}_1$ has been eliminated by using the center-of-mass system, g_a and g_b are the initial and final ground-state hydrogen wave functions in momentum space, $\delta(\vec{p}_3+\vec{k}_a)$ is the plane wave of the incident particle 3 with respect to (1, 2), $\delta(\vec{p}_2-\vec{k}_b)$ is the plane wave of particle 2 with respect to (1, 3), S is the total energy, and k is the reduced momentum vector of particle 1 relative to 3. Thus,

$$\vec{k}_a = \frac{M(M+m)}{2M+m}\,\vec{v}_a = \mu\vec{v}_a\,,$$
$$\vec{k}_b = \frac{M(M+m)}{2M+m}\,\vec{v}_b = \mu\vec{v}_b\,, \quad (7)$$
$$\vec{k} = \vec{p}_3 + \frac{M}{M+m}\,\vec{p}_2\;\;,$$

where $\vec{v}_a$ and $\vec{v}_b$ are the initial and final relative velocities of the free particle with respect to the center of mass of the initial and final hydrogen atoms.

Conservation of total initial and final energy enables us to write

$$\frac{k_a^2}{2\mu} - \frac{mM}{2(M+m)}\,\alpha^2 = \frac{k_b^2}{2\mu} - \frac{mM}{2(M+m)}\,\alpha\;, \quad (8)$$

where we have set $\hbar = c = 1$ and the fine-structure constant $\alpha = e^2$. From Eq. (8), $|\vec{k}_a| = |\vec{k}_b|$ for the resonant symmetric reaction in Eq. (1). Hence we may set $v_a = v_b = v$.

III. CONTINUUM-STATE CONTRIBUTIONS

The matrix element in Eq. (6) can be evaluated by using the closed-form expression for the two-body t matrix,[10] which is given by

$$\langle \vec{k}_2' | T_2(k_2) | \vec{k}_2'' \rangle = -\frac{\alpha}{2\pi^2} \frac{1+I(x)}{|\vec{k}_2' - \vec{k}_2''|^2}, \tag{9}$$

where

$$I(x) = 2i\zeta(1-e^{-2\pi\zeta})^{-1} \int_\infty^{(1+)} \left(\frac{t+1}{t-1}\right)^{-i\zeta} \frac{dt}{t^2-x^2}, \tag{10}$$

$$x^2 = 1 + \frac{(k_2'^2 - k_2^2)(k_2''^2 - k_2^2)}{k_2^2(\vec{k}_2' - \vec{k}_2'')^2}, \tag{11}$$

$$\zeta = -\frac{mM}{M+m}\frac{\alpha}{k_2} = -\alpha\left(\tfrac{1}{2}m\right)^{1/2} \times \left(S - \frac{2M+m}{2M(M+m)}\vec{p}_2^{\,2}\right)^{-1/2}\left(1+\frac{m}{M}\right)^{-1/2}. \tag{12}$$

The contour for the integral in Eq. (10) is given by Fig. 2(a).

By substituting Eq. (9) in Eq. (6) we obtain a sum of two terms, corresponding to the two terms on the right-hand side of Eq. (9). The first term, which we shall denote by $L_2^{(1)}$, is given by

$$L_2^{(1)} = \frac{1}{2\pi^2}\int g_a^*\left(\vec{p}_2' - \frac{M}{M+m}\vec{k}_a\right)\delta(\vec{p}_3' + \vec{k}_a)\,\delta(\vec{p}_2'' - \vec{p}_2') \times \frac{\alpha(M+m)^2}{[M(\vec{p}_2' - \vec{p}_2'') + (M+m)(\vec{p}_3' - \vec{p}_3'')]^2}\,\frac{V_3(\vec{p}_2'' - \vec{p}_2)}{(p_2'' + p_3'')^2/2m + p_2''^2/2M + p_3''^2/2M - S - i\epsilon}$$
$$\times\,\delta(\vec{p}_3'' - \vec{p}_3)\, g_b\left(\vec{p}_3 + \frac{M}{M+m}\vec{k}_b\right)\delta(\vec{p}_2 - \vec{k}_b)\, d^3p_2'\, d^3p_3'\, d^3p_2''\, d^3p_3''\, d^3p_2\, d^3p_3, \tag{13}$$

where $\vec{k}_2'$, the relative momentum between particles 1 and 3, is expressed in terms of the center-of-mass momenta p_2' and p_3' through the relation $\vec{k}_2' = \vec{p}_3' + (M/M+m)\,\vec{p}_2'$. A corresponding expression holds, of course, for k_3''. Equation (13) is identical with the second Born matrix element $M(V_2, V_3)$ of Drisko[1] and may therefore be evaluated in the high-energy limit in the same way. If no other terms were considered, the total cross section from $L_2^{(1)}$ should show a velocity dependence of v^{-11} at high energies. This term predominates over the first Born (v^{-12}) and the third- or higher-order Born terms.[1]

The second term $L_2^{(2)}$ corresponding to substituting the second term on the right-hand side of Eq. (9) into Eq. (6) is given by

$$L_2^{(2)} = \frac{-im\alpha^2}{\pi^2(1+m/M)}\int g_a^*\left(\vec{p}_2' - \frac{M}{M+m}\vec{k}_a\right)\frac{2m/(1+m/M)A}{1-\exp(\pi\alpha A)}\int_\infty^{(1+)}\left(\frac{t+1}{t-1}\right)^{i\alpha G/2}$$
$$\times\, dt\left\{\frac{2m}{1+m/M}(t^2-1)\left(S - \frac{2M+m}{2M(M+m)}\vec{p}_2'^{\,2}\right)(\vec{p}_3 + \vec{k}_a)^2 - \left[\left(\frac{M}{M+m}\vec{p}_2' - \vec{k}_a\right)^2 + \frac{m(2M+m)}{(M+m)^2}\vec{p}_2'^{\,2} - \frac{2mS}{1+m/M}\right]\right.$$
$$\left.\times\left[\left(\vec{p}_3 + \frac{M}{M+m}\vec{p}_2'\right)^2 + \frac{m(2M+m)}{(M+m)^2}\vec{p}_2'^{\,2} - \frac{2mS}{1+m/M}\right]\right\}^{-1}\frac{V_3(\vec{p}_2' - \vec{k}_b)\, g_b(\vec{p}_3 + [M/(M+m)]\vec{k}_b)}{(\vec{p}_2' + \vec{p}_3)^2/2m + p_2'^2/2M + p_3^2/2M - S - i\epsilon}\, d^3p_2'\, d^3p_3, \tag{14}$$

where

$$G = \left(\frac{2m/(1+m/M)}{S - [(2M+m)/2M(M+m)]\vec{p}_2'^{\,2}}\right)^{1/2}.$$

The integrand in Eq. (14) contains both the bound-state contributions from the two-body t matrix and the continuum contributions. We shall consider only the continuum contributions in this section and will consider the bound states in Sec. IV.

To evaluate the integral in Eq. (14) in the high-energy limit, we note that as $\vec{k}_a$ and $\vec{k}_b$ increase with incident energy, the integrand is always dominated[1] by the two peaks from the initial- and final-state wave function

$$g_a\left(\vec{p}_2 - \frac{M}{M+m}\vec{k}_b\right) \text{ and } g_b\left(\vec{p}_3 + \frac{M}{M+m}\vec{k}_b\right).$$

The peaks occur at $\vec{p}_2' = [M/(M+m)]\vec{k}_a$ and $\vec{p}_3 = -[M/(M+m)]\vec{k}_b$. The only other sharp peaks in the in-

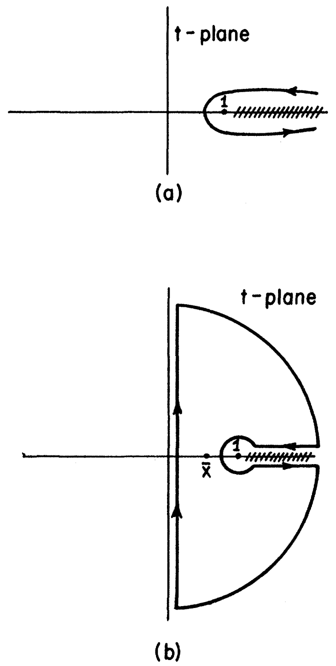

FIG. 2. (a) Contour for the integral representation of the two-body t matrix. (b) Contour for the evaluation of the integral in the complex t plane at high energies for the continuum contribution to the capture amplitude. The diagram shows a pole at $t=\bar{x}$ for a scattering angle $\theta<\sqrt{3}\,m/M$.

tegrand occur at the poles of the two-body t matrix. These poles occur when the variable $\vec{p}_2'$ takes on such values that the expression $[1-\exp(\pi\alpha A)]^{-1}$ diverges. These values for $\vec{p}_2'$ are far from the region where $g_a(\vec{p}_2'-[M/(M+m)]\vec{k}_b)$ peaks. In fact, where the latter peaks, the rest of the integrand including the above expression for the two-body poles are slowly varying functions of $\vec{p}_2'$. We can hence use the integral-mean-value theorem for $\vec{p}_2'$ and factorize out of the integrand[1] all the slowly varying functions, replacing $\vec{p}_2'=[M/(M+M)]\vec{k}_a$. Thus

$$[1-\exp(\pi\alpha G)]^{-1} =\left[1-\exp\left(\frac{2\pi}{[(1+m/M)\,(4n^2-1)]^{1/2}}\right)\right]^{-1} \sim(1-e^{2\pi(4n^2-1)^{-1/2}}), \tag{15}$$

where the incident velocity is expressed in terms of the dimensionless quantity $n=v_a/2\alpha$ and the last step is obtained through neglecting m/M in comparison with unity.

The interaction $V_3(\vec{p}_2'-\vec{k}_b)$ may be taken out of the integrand in the same way. Thus,

$$V_3\left(\frac{M}{M+m}\,\vec{k}_a-\vec{k}_b\right)=-\frac{\alpha}{2\pi^2\{[M/(M+m)]\,\vec{k}_a-\vec{k}_b\}^2}\ . \tag{16}$$

Since the initial direction is fixed and the kinetic energy is conserved, the initial and final reduced momenta $\vec{k}_a$ and $\vec{k}_b$ contain only two variables and may be expressed in terms of the incident velocity and the scattering angle. Furthermore, most of the scattering occurs at such small angles (of the order of m/M) that it is convenient to introduce the parameter λ given by

$$\lambda=\left(\frac{2\sin\frac{1}{2}\theta}{m/M}\right)^2\ , \tag{17}$$

where θ is the scattering angle. Neglecting terms of order m/M, we can write

$$V_3\{[M/(M+m)]\vec{k}_a-\vec{k}_b\}\sim-[2\pi^2m^2\alpha(1+\lambda)n^2]^{-1}\ . \tag{18}$$

Thus $n\gg 1$ implies that the incident velocity is much greater than the orbital electron velocity of the hydrogen atom.

By the same token, since the final-state wave function $g_b(\vec{p}_3+[M/(M+m)]\vec{k}_b)$ has a sharp peak at $\vec{p}_3=-(M/M+m)\,\vec{k}_b$, we may factorize out the denominator involving simultaneously t, $\vec{p}_2'$, and $\vec{p}_3$ from the integration over $\vec{p}_2'$ and $\vec{p}_3$ by replacing $\vec{p}_2'$ with $(M/M+m)\,\vec{k}_a$ and $\vec{p}_3$ with $-(M/M+m)\,\vec{k}_b$. Thus we finally obtain

$$L_2^{(2)}=-\frac{i}{2\pi^4m^4\alpha^2n^4}\ \frac{1}{(4n^2-1)^{1/2}(1+\lambda)^2}\left[\exp\left(\frac{2\pi}{(4n^2-1)^{1/2}}\right)-1\right]^{-1}\int_\infty^{(1^+)}\left(\frac{t+1}{t-1}\right)^{i[(1+m/M)(4n^2-1)]^{-1/2}}$$

$$\times\frac{dt}{t^2-\bar{x}^2}\int\frac{g_a^*(\vec{p}_2'-[M/(M+m)]\vec{k}_a)\,g_b^*(\vec{p}_3+[M/(M+m)]\vec{k}_b)}{(\vec{p}_2'+\vec{p}_3)^2/2m+p_2'^2/2M+p_3^2/2M-S-i\epsilon}\ d^3p_2'\,d^3p_3\ , \tag{19}$$

where

$$\bar{x}^2=1+\frac{1+\frac{21}{2}(m/M)^2n^2}{4(1-m/M)n^2-1}-\frac{1+\frac{21}{2}(m/M)^2n^2}{(1+\lambda)n^2}-(m/M)\frac{1+\frac{21}{2}(m/M)^2n^2}{4(1-m/M)n^2-1}\ \frac{3\lambda-1}{\lambda+1}=x^2\left(\vec{p}_2'=\frac{M}{M+m}\,\vec{k}_a,\ p_3=\frac{-M}{M+m}\,\vec{k}_b\right). \tag{20}$$

The integral over $\vec{p}_2'$ and $\vec{p}_3$ can be transformed into cylindrical coordinates and expressed in terms of n and λ^1. Thus, in the limit when we again neglect terms of order m/M in comparison with unity, and 1 in comparison with $4n^2$,

$$L_2^{(2)} = -\frac{4i}{\pi^2 m^2 \alpha n^7 (1+\lambda)^2 (e^{\pi/n}-1)} \frac{1}{\lambda - 3 - (4i/n)(1+\lambda)^{1/2}} \times \int_\infty^{(1^+)} \left(\frac{t+1}{t-1}\right)^{i/2n} \frac{dt}{t^2 - \bar{x}^2}$$

$$\sim -\frac{4i}{\pi^3 m^2 \alpha n^6 (1+\lambda)^2} \frac{1}{\lambda - 3 - (4i/n)(1+\lambda)^{1/2}} \times \int_\infty^{(1^+)} \left(\frac{t+1}{t-1}\right)^{i/2n} \frac{dt}{t^2 - \bar{x}^2}, \quad (21)$$

where

$$\bar{x} \sim 1 + \frac{1}{8n^2}\left(1 - \frac{4+2(m/M)\lambda}{1+\lambda}\right) \quad (n \gg 1) \quad .$$

Hence, in the high-energy limit $\bar{x} \sim 1$. Actually $\bar{x} < 1$ for $\lambda < 3$ $[\theta < \sqrt{3}m/M]$, where the major contribution to the scattering occurs, and $\bar{x} > 1$ for $\lambda > 3$.

The integral in Eq. (21) may be evaluated by considering the integral over the contour in Fig. 2(b). If we neglect contributions to the integral from $|t| \to \infty$, we may write for the case when $\bar{x} < 1$ and $\lambda < 3$

$$\int_\infty^{(1^+)} \left(\frac{t+1}{t-1}\right)^{i/2n} \frac{dt}{t^2 - \bar{x}^2} = -\int_{-i\infty}^{i\infty} \left(\frac{t+1}{t-1}\right)^{i/2n} \frac{dt}{t^2 - \bar{x}^2} - 2\pi i C, \quad (22)$$

where C is the residue at $t = \bar{x}$ and is given by

$$C \sim \frac{1}{2}\left[\frac{1}{16n^2}\left(1 - \frac{4+2(m/M)\lambda}{1+\lambda}\right)\right]^{-i/2n} \quad . \quad (23)$$

For the case when $\bar{x} > 1$ $(\theta > \sqrt{3}m/M)$, the pole lies on the right-hand cut. In Hostler's[10] paper, a condition is introduced which excludes the pole from the interior of the integration path of the Coulomb Green's function. Such a condition is equivalent in our case to adding a small negative imaginary part to λ and then letting it approach zero at the end of the calculation. The result for both $\lambda < 3$ and $\lambda > 3$ is hence given by

$$\int_\infty^{(1^+)} \left(\frac{t+1}{t-1}\right)^{i/2n} \frac{dt}{t^2 - \bar{x}^2} = -in(1 - e^{\pi/n}) + in(\bar{x} - 1)(1 - e^{\pi/n}) - 2\pi i c$$

$$\sim i\pi\left(1 - \frac{1}{8n^2}\frac{\lambda - 3}{\lambda + 1} - 2C\right). \quad (24)$$

Substituting Eq. (24) into Eq. (21), we obtain

$$L_2^{(2)} \sim \frac{4[1 - 8n^2(\lambda-3)/(\lambda+1) - 2C]}{\pi^2 m^2 \alpha n^6 (1+\lambda)^2 [\lambda - 3 - (4i/n)(1+\lambda)^{1/2}]} \quad . \quad (25)$$

As mentioned above, the term $L_2^{(1)}$ is identical with Drisko's second Born approximation. The first term in the numerator of Eq. (25) is in fact identical with $L_2^{(1)}$ except for a sign. Hence the entire matrix element L_2 is given by

$$L_2 = L_2^{(1)} + L_2^{(2)} = -\frac{2n^{-2}(\lambda-3)/(\lambda+1) + 8C}{\pi^2 m^2 \alpha n^6 (1+\lambda)^2 [\lambda - 3 - (4i/n)(1+\lambda)^{1/2}]} \cdot \quad (26)$$

Hence, in the high-energy limit $n \gg 1$, we have

$$L_2 \sim -\frac{8C}{\pi^2 m^2 \alpha n^6 (1+\lambda)^2 [\lambda - 3 - (4i/n)(1+\lambda)^{1/2}]} \cdot \quad (27)$$

From the expression for C given by Eq. (23), we obtain $|2C| = 1$. Furthermore, as $n \to \infty$, the quantity $2C \to 1$; hence we can write

$$L_2 \sim -\frac{4e^{i\varphi(n)}}{\pi^2 m^2 \alpha n^6 (1+\lambda)^2 [\lambda - 3 - (4i/n)(1+\lambda)^{1/2}]}, \quad (28)$$

where $\varphi(n) \to 0$ as $n \to \infty$.

Equation (28) is identical to the second-Born term except for the complex phase factor, which, in any case, approaches unity for sufficiently high incident velocity. Thus, for large n the matrix element L_2 goes down as n^{-6} power for all values of λ, except at $\lambda = 3$, where it goes down as n^{-5}. Since L_1, which is identical to the first Born approximation, goes down as n^{-6} for all angles, L_2 is obviously the dominant term at sufficiently high incident energies. One can also show that the higher-order terms in the Faddeev expansion of Eq. (4) must necessarily go down more steeply with increasing n. Thus, for sufficiently high incident energy L_2 becomes the only important term, and it is trivial to show that the total cross section is given by

$$\sigma \sim \int_0^\infty |L_2|^2 d\lambda \sim 1/n^{11} \quad . \quad (29)$$

This assumes, of course, that the bound-state contribution to L_2, which we will consider in Sec. IV, is negligible in comparison with the continuum states.

It is interesting to note that the principal contribution to the capture amplitude occurs at $\lambda = 3$ for high incident energy $(n \gg 1)$, where the amplitude decreases with n as n^{-5} instead of n^{-6} for other values of λ. From Eqs. (20) and (21) this means that

$$\bar{x}^2 = x^2\left(\vec{p}_2' = \frac{M}{M+m}\vec{k}_a, \ \vec{p}_3 = -\frac{M}{M+m}\vec{k}_b\right) = 1 ,$$

which from Eqs. (11) and (9) implies, in turn, that the two-body t matrix is on the energy shell. Hence, it would appear that we have here a direct verification of the theorem that at high incident energies the major contribution to scattering from complex systems arises from the on-energy-shell two-body t matrix. The reason why the two-body t matrix should be on the energy shell for $\lambda = 3$ instead of some other value can be understood by considering the classical Thomas[1,11,12] model for high-energy capture and energy-momentum conservation. Actually, from Eq. (21), $x = 1$ for $n \gg 1$ irrespective of λ; hence at sufficiently high energies, the two-body t matrix is always on the energy shell irrespective of the scattering angle.

IV. BOUND-STATE CONTRIBUTIONS

The high-energy-limit result for the matrix element L_2 in Eq. (28) does not contain the two-body bound-state contributions which should, in principle, be less important at high enough incident energies, since the singularities arising from the two-body poles are much farther away than the two-body continuum. We shall evaluate the bound-state contributions in a way similar to what we did for the continuum. Each bound-state pole has an inifinitely sharp peak and we can make the same type of approximation as we did for the peaking of g_a and g_b.

From Eq. (14) we note that the bound states occur when

$$\vec{p}_2'^{\,2} = \vec{k}_a^2 - \frac{mM^2\alpha^2}{2M+m}\left(1 - \frac{1}{N^2} = \vec{J}_N^2\right), \tag{30}$$

where $N = 1, 2, 3, \ldots.$ The direction of $\vec{J}_N$ is arbitrary as given by Eq. (30) and may be taken as along $\vec{k}_a$.

We shall divide the domain of integration for $\vec{p}_2'$ into shells such that each bound state occurs at a value of $\vec{p}_2'$ between two consecutive shells. In this way we have divided our integration domain for $\vec{p}_2'$ into an infinite number of small domains. The expression for $L_2^{(2)}$ given by Eq. (14) then becomes an infinite sum over such domains. We can then first make a Taylor-series expansion of the expression which gives us the bound states [i.e., the left-hand side of Eq. (15)] about each bound state $\vec{p}_2' = \vec{J}_n$. Thus we may write

$$1 - \exp(\pi\alpha H) = -\frac{2\pi i(2 + m/M)N^3}{mM\alpha^2}\,\vec{J}_N \cdot \vec{y}_N\,, \tag{31}$$

where

$$H = \left(\frac{2m/(1+m/M)}{S - [(2M+m)/2M(M+m)]\,(\vec{y}_N + \vec{J}_N)^2}\right)^{1/2},$$

and where $\vec{y}_N = \vec{p}_2' - \vec{J}_N$.

We shall then make the further approximation that the limits of each domain in the integration over $\vec{y}_N$ be replaced by infinite limits. Such an approximation can only overestimate the sum total of the bound-state contributions and hence does not present a special problem to our efforts to show that the bound-state contributions are small.

The matrix element $L_2^{(2)}$ given by Eq. (14) becomes, neglecting terms of order m/M,

$$\begin{aligned} L_2^{(2)} = {} & \frac{(m\alpha^2)^2 M}{4\pi^3} \sum_{n=1}^{\infty} \frac{1}{N^3} \int g_a^*\left(\vec{y}_N + \vec{J}_N - \frac{M}{M+m}\,\vec{k}_a\right) V\,(\vec{y}_N + \vec{J}_N - \vec{k}_b)\,\frac{1}{\vec{J}_N \cdot \vec{y}_N} \int \left(\frac{t+1}{t-1}\right)^{i\alpha H/2} [2m/(1+m/M)H] \\ & \times \left\{ (t^2-1)\,(\vec{p}_3 + \vec{k}_a)^2 \left(\frac{2mMS}{M+m} - \frac{m(2M+m)}{(M+m)^2}\,(\vec{y}_N + \vec{J}_N)^2\right) - \left[\left(\frac{(\vec{J}_N + \vec{y}_N)M}{M+m} - \vec{k}_a\right)^2 \right.\right. \\ & \left.\left. + \frac{m(2M+m)}{(M+m)^2}\,(\vec{y}_N + \vec{J}_N)^2 - \frac{2mMS}{M+m}\right] \left[\left(\vec{p}_3 + \frac{M}{M+m}\,(\vec{y}_N + \vec{J}_N)\right)^2 + m\,\frac{(2M+m)}{(M+m)^2}\,(y_n + J_n)^2 - \frac{2mMS}{M+m}\right]\right\}^{-1} \\ & \times \frac{g_b(\vec{p}_3 + [M/(M+m)]\vec{k}_b)}{(\vec{y}_N + \vec{J}_N + \vec{p}_3)^2/2m + (\vec{y}_N + \vec{J}_N)^2/2M + p_3^2/2M - S - i\epsilon}\, d^3y_N\, d^3p_3\, dt\ . \end{aligned} \tag{32}$$

We shall first consider the integral over p_3. This can be done in the same way that we did for the continuum contribution to L_2. Since in the term L_2 we only have a complete two-body t matrix for particles 3 and 1, the only prominent peak for the integral over $\vec{p}_3$ comes from the final-state wave function $g_b(\vec{p}_3 + [M/(M+m)]\vec{k}_b)$ at $\vec{p}_3 = -(M/M+m)\vec{k}_b$.

In order to facilitate approximation procedures, we introduce $\vec{q} = \vec{p}_3 + (M/M+m)\vec{k}_b$. Thus, we now have an integral over $\vec{y}_N$, $\vec{q}$, and t and $g_b(\vec{q})$ peaks at $\vec{q} = 0$.

By neglecting all terms of order m/M or higher in the denominator for the free-space Green's function, we obtain

$$\frac{(\vec{y}_N+\vec{J}_N+\vec{p}_3)^2}{2m}+\frac{(\vec{y}_N+\vec{J}_N)^2}{2M}+\frac{\vec{p}_3^{\,2}}{2M}-S-i\epsilon$$
$$\sim\frac{(\vec{y}_N+\vec{q})\cdot(\vec{J}_N-\vec{k}_b)}{m}+\frac{m\alpha^2}{2}\left(\lambda n^2+\frac{1}{N^2}\right)-i\epsilon\,. \quad (33)$$

In deriving Eq. (33) we have dropped terms such as $(\vec{y}_N+\vec{q})^2$ which can be neglected in comparison with $(\vec{y}_N+\vec{q})\cdot(\vec{J}_N-\vec{k}_b)$, since $\vec{J}_N-\vec{k}_b$ is of the order of $m\alpha n\sqrt{\lambda}$ in the high-energy limit. We shall assume that the rest of the denominator involving t^2-1, $\vec{y}_N$, and $\vec{q}$ may be taken out of the integral over $\vec{y}_N$ and $\vec{q}$, with the variables $\vec{y}_N$ and $\vec{q}$ set equal to zero where the integrand peaks.

Thus, again neglecting terms of order m/M and using Eqs. (7) and (17), we obtain

$$(t^2-1)\left(\vec{k}_a-\frac{M}{M+m}\vec{k}_b\right)^2\left(\frac{2mMS}{M+m}-\frac{m(2M+m)}{(M+m)^2}(\vec{y}_N+\vec{J}_N)^2\right)-\left[\left(\frac{(\vec{y}_N+\vec{J}_N)M}{M+m}-\vec{k}_a\right)^2+\frac{m(2M+m)}{(M+m)^2}(\vec{y}_N+\vec{J}_N)^2-\frac{2mMS}{M+m}\right]$$
$$\times\left[\left(\vec{q}-\frac{M}{M+m}\vec{k}_b+\frac{M}{M+m}(\vec{y}_N+\vec{J}_N)\right)^2+\frac{m(2M+m)}{(M+m)}(\vec{y}_N+\vec{J}_N)^2-\frac{2mMS}{M+m}\right]-t^2+\frac{1}{1+\lambda}\left[\lambda N^2\left(\frac{v^2}{4\alpha^2}+\frac{\sigma_N}{2}\right)\right.$$
$$\left.+\frac{1}{v^2}\left(2\alpha^2\sigma_N+\frac{4\alpha^2}{N^2}\right)\right]=t^2+\gamma_N^2 \quad \text{as } \vec{y}_N\to 0,\ \vec{q}\to 0, \quad (34)$$

where γ_N^2 is defined by the last equality in Eq. (34) and σ_N is defined by $\sigma_N=1-1/N^2\geq 0$. It is at once clear that $\gamma_N^2>0$ for all N, λ, and v.

Hence, upon taking the entire t integral outside the integral over $\vec{y}_N$ with its dependence on $\vec{y}_N$ set to zero, we obtain

$$L_2^{(2)}=\frac{M\alpha^2}{4\pi^3m^2v^2}\sum_{n=1}^{\infty}\left(-\frac{4}{N(1+\lambda)}\right)\int g_a^*\left(\vec{y}_N+\vec{J}_N-\frac{M}{M+m}\vec{k}_a\right)V(\vec{y}_N+\vec{J}_N-\vec{k}_b)\frac{1}{\vec{J}_N\cdot\vec{y}_N}\int\left(\frac{t+1}{t-1}\right)^N\frac{dt}{t^2+\gamma_N^2}$$
$$\times\int\left\{g_b(\vec{q})\left[\frac{2mM}{M+m}\left(S-\frac{2M+m}{2M(M+m)}(\vec{y}_N+\vec{J}_N)^2\right)\right]^{1/2}\Big/\left[\frac{(\vec{y}_N+\vec{q})\cdot(\vec{J}_N-\vec{k}_b)}{m}+\frac{m\alpha^2}{2}\left(\lambda n^2+\frac{1}{N^2}\right)-i\epsilon\right]\right\}d^3q\,d^3y_N\,. \quad (35)$$

We may evaluate the integral over $\vec{q}$ by introducing cylindrical coordinates, with the z axis along the vector $\vec{k}_b-\vec{J}_N$. Thus, denoting the $\vec{q}$ integral by $\vec{I}_q$, we have

$$I_q=2m\int\frac{g_b(\vec{q})\,d^3q}{2\vec{q}\cdot(\vec{J}_N-\vec{k}_b)+2\vec{y}_N\cdot(\vec{J}_N-\vec{k}_b)+m^2\alpha^2(\lambda n^2+1/N^2)-i\epsilon}$$
$$=\frac{4\sqrt{2}m}{\pi}\int\frac{(m\alpha)^{5/2}\,d^3q}{[(m\alpha)^2+(\vec{q})^2]^2[2\vec{q}\cdot(\vec{J}_N-\vec{k}_b)+2\vec{y}_N\cdot(\vec{J}_N-\vec{k}_b)+m^2\alpha^2(\lambda n^2+1/N^2)-i\epsilon]}$$
$$=4\sqrt{2}m\int_{-\infty}^{\infty}\frac{(m\alpha)^{5/2}\,dq_z}{[(m\alpha)^2+q_z^2][-2q_z|\vec{J}_n-\vec{k}_b|+2\vec{y}_N\cdot(\vec{J}_N-\vec{k}_b)+m^2\alpha^2(\lambda n^2+1/N^2)-i\epsilon]}\,. \quad (36)$$

The integrand of the last term in Eq. (36) contain two poles at $q_z=\pm im\alpha$ and one pole at

$$q_z=\frac{2\vec{y}\cdot(\vec{J}_N-\vec{k}_b)+m^2\alpha^2(\lambda n^2+1/N^2)}{2|\vec{J}_N-\vec{k}_b|}\,.$$

The integrand vanishes for large q_z in the complex q_z plane in both the upper and the lower half-planes. We would obtain the same result as $\epsilon\to 0$ irrespective of whether we chose our contour in the upper or the lower half-plane. Hence, for simplicity, we choose our contour in the upper half-plane and obtain

$$I=\frac{4\sqrt{2}\,\pi\,m(m\alpha)^{3/2}}{[2\vec{y}_N\cdot(\vec{J}_N-\vec{k}_b)-2im\,\alpha|\vec{J}_N-\vec{k}_b|+m^2\alpha^2(\lambda n^2+1/N^2)-i\epsilon]}\,. \quad (37)$$

The integration over $\vec{y}_N$ may be performed by first making the additional assumption that since $y_N=0$ corresponds to the pole for the Nth bound state, we may also remove the function

$$\left[\frac{2mM}{M+m}\left(S-\frac{2M+m}{2M(M+m)}(\vec{y}_N+\vec{J}_N)^2\right)\right]^{1/2},$$

which is slowly varying in the neighborhood of the bound-state pole from the integrand, with $\vec{y}_N$ again set equal to zero. The integration over $\vec{y}_N$ now becomes

$$\int \frac{g_a^*(\vec{y}_N+\vec{J}_N-[M/(M+m)]\vec{k}_a)\,V(\vec{y}_N+\vec{J}_N-\vec{k}_b)}{\vec{J}_N\cdot\vec{y}_N}\,d^3y_N$$

$$=-(\sqrt{2}/\pi^3)\,(m\alpha)^{5/2}\,\alpha I_{\vec{y}_N}\,, \tag{38}$$

where

$$\vec{I}_{\gamma_N}=\int\frac{d^3y_N}{[(m\alpha^2+(\vec{B}+\vec{y}_N)^2]^2[\vec{A}+\vec{y}_N]^2\vec{k}_a\cdot\vec{y}_N}\quad\text{for } n\gg 1,$$

$$\vec{A}=\vec{J}_N-\vec{k}_b,\quad |\vec{A}|\underset{n\gg1}{\longrightarrow} m\,\alpha\, n\sqrt{\lambda}\,,$$

$$\vec{B}=\vec{J}_N-(M/M+m)\vec{k}_a,\ |\vec{B}|\underset{n\gg1}{\longrightarrow}\frac{m}{M+m}\,\vec{k}_a=\frac{mM}{2M+m}\,\vec{v}_a\sim\frac{m\vec{v}}{2}\,.$$

It can be seen that near the bound state ($\vec{y}_N=0$) and in the high-energy limit, the term $(m\alpha)^2$ is small compared with $B^2\sim\frac{1}{4}m^2v^2$. We can introduce the small parameter $x=(m\alpha)^2$ and use differentiation with respect to the parameter x, together with Feynman's parametrization technique and the approximation

$$x=(m\alpha)^2\ll(\vec{B}-\vec{A})^2\sim\tfrac{1}{4}m^2v^2(1+\lambda)\,,$$

to obtain (see the Appendix)

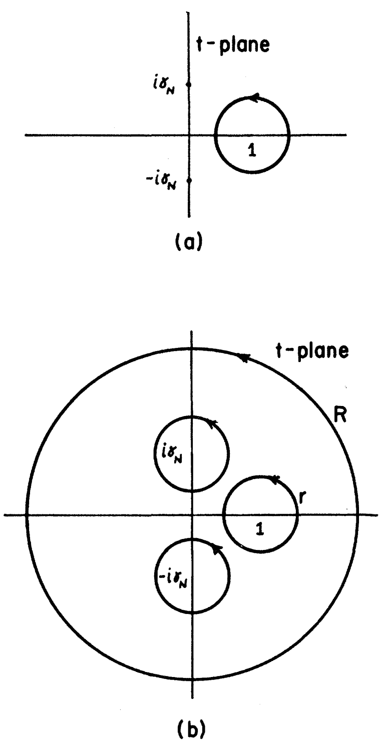

FIG. 3. (a) Contour for the integral is a representation of the two-body t matrix at the bound-state poles. (b) Contour chosen for the evaluation of the integral which avoids evaluating the integral over the Nth-order pole.

$$I_{\vec{y}_N}=\frac{2\pi^2}{m^4M(1+\lambda)^2\alpha^5n^5}$$

$$\times\left(2\tan^{-1}\frac{-i}{\{1+[2\lambda/(1+\lambda)](m/M)\}^{1/2}}-(\pi-i)\right).\tag{39}$$

Combining Eqs. (37)–(39) and (35), we obtain

$$L_2^{(2)}=-\frac{4i}{\pi^3m^2\alpha}\left(\frac{1}{n^7}\right)\sum_N\frac{1}{N^2(1+\lambda)^3}$$

$$\times\frac{1}{(\lambda n^2+1/N^2)-2in\sqrt{\lambda}-i\epsilon}$$

$$\times\left(2\tan^{-1}\frac{-i}{\{1+[2\lambda/(1+\lambda)](m/M)\}^{1/2}}-(\pi-i)\right)$$

$$\times\int\left(\frac{t+1}{t-1}\right)^N\frac{dt}{t^2+\gamma_N^2}\,.\tag{40}$$

Since, from Eq. (34), $\gamma_N^2>0$ and N is a positive integer, the contour for the integration over t is reduced to the one shown in Fig. 3(a). To avoid the troublesome Nth-order pole at $t=1$, we consider the integral over the large circle R [Fig. 3(b)] and write

$$\oint_{R\to\infty}\left(\frac{t+1}{t-1}\right)^N\frac{dt}{t^2+\gamma_N^2}=0=\oint_{+i\gamma_N}\left(\frac{t+1}{t-1}\right)^N\frac{dt}{t^2+\gamma_N^2}$$

$$+\oint_{-i\gamma_N}\left(\frac{t+1}{t-1}\right)^N\frac{dt}{t^2+\gamma_N^2}+\oint_r\left(\frac{t+1}{t-1}\right)^N\frac{dt}{t^2+\gamma_N^2}\,,\tag{41}$$

where r represents the small circle, and the integrals are all taken counterclockwise. In this way the integral over the Nth-order pole (where N can go to infinity) is expressed in terms of integrals over two simple poles. Thus,

$$\int_\infty^{(1^+)}\left(\frac{t+1}{t-1}\right)^N\frac{dt}{t^2+\gamma_N^2}=\oint_r\left(\frac{t+1}{t-1}\right)^N\frac{dt}{t^2+\gamma_N^2}$$

$$=\frac{-2i\pi(-1)^N\sin 2N\theta}{\gamma_N}\,,\tag{42}$$

where $\theta=\tan^{-1}\gamma_N$.

Substituting Eq. (42) into (40), our final result for the bound-state contribution $L_2^{(2)}$ is given by

$$L_2^{(2)}=\frac{-8}{\pi^2m^2\alpha}\left(\frac{1}{n^7}\right)\sum_{N=1}^{\infty}\left(\frac{(-1)^N}{N^2(1+\lambda)^3}\,\frac{\sin 2N\theta}{\gamma_N}\right.$$

$$\left.\times\frac{1}{(\lambda n^2+1/N^2)-2in(\lambda-i\epsilon)^{1/2}}\right)$$

$$\times\left(2\tan^{-1}\frac{-i}{\{1+[2\lambda/(1+\lambda)](m/M)\}^{1/2}}-(\pi-i)\right).\tag{43}$$

Since $\gamma_N \propto N$ for large N, it is easy to see that the infinite sum for the infinite number of bound states converges by trivial application of the Weierstrass M test. The convergence becomes even more obvious if we apply the high-energy-limit approximation. We first consider nonforward scattering. This would include $\lambda = 3$, where we get our maximum capture from continuum intermediate states. From Eq. (34) we have

$$\gamma_N^2 \propto \lambda n^2 N^2/(1+\lambda) \quad (n \gg 1).$$

Hence, in the high-energy limit,

$$\frac{\sin(2N\tan^{-1}\gamma_N)}{\gamma_N} \xrightarrow[n\gg 1]{} -\frac{(-1)^N 2N}{\gamma_N^2} \sim -\frac{(-1)^N 2N(1+\lambda)}{\lambda n^2 N^2} . \tag{44}$$

The matrix element $L_2^{(2)}$ is then given by

$$L_2^{(2)} = \frac{16}{\pi^2 m^2 \alpha}\left(\frac{1}{n^{11}}\right)\left(\sum_{N=1}^{\infty}\frac{1}{N^3}\right)\left(\frac{1}{(1+\lambda)^2}\right)\frac{1}{\lambda[\lambda - 2i(\sqrt{\lambda})/n]}$$

$$\times\left(2\tan^{-1}\frac{-i}{\{1+[2\lambda/(1+\lambda)](m/M)\}^{1/2}} - (\pi - i)\right),$$

where the infinite sum is now given explicitly by

$$\sum_{N=1}^{\infty}\frac{1}{N^3} = 1.202 .$$

In the forward direction $\lambda = 0$, the contribution from the ground bound state diverges logarithmically. A divergence also occurs in Mapleton's paper when he considers the second Born matrix element with the ground intermediate state. However, this divergence was canceled by the inclusion of the proton-proton–interaction term into the second-Born term. In our case, however, the proton-proton interaction cannot be so simply included, since, as we have shown in Sec. II, the Faddeev equations will only decouple into a single integral equation without this interaction. So, with this interaction included, there is no simple connection between the Faddeev equations and the Lippmann-Schwinger equations other than the inhomogenous terms which are just the first Born approximations.

To summarize our results, we have found that if Faddeev equations are used to investigate the electron capture by protons from hydrogen atoms, we obtain identical results as the second Born high-energy-limit result of Drisko[1] except for a complex energy-dependent phase factor which approaches unity for sufficiently high incident energies.

The major contribution to the capture amplitude from the continuum intermediate states comes from the on-energy-shell two-body t matrix. In the ultimate mathematical high-energy limit all the contributions will come from the on-energy-shell t matrix.

The sum over the infinite number of bound-state poles converges. Furthermore, the amplitude goes down as n^{-11} as compared with n^{-6} or n^{-5} at $\lambda = 3$ for the continuum-state contribution.

For symmetrically resonant capture, which is the reaction we have been considering in this paper, the forward capture amplitude from the bound-state contribution diverges. Preliminary results seem to show that the divergence vanishes for nonsymmetrically resonant capture.

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APPENDIX

We consider the integral over $I_{\vec{y}_N}$ as given by Eq. (38). Since $(m\alpha)^2$ is small compared with the rest of the terms in the bracket, we replace it by the small parameter x and differentiate with respect to x. Thus,

$$I_{\vec{y}_N} = \int \frac{d^3 y_N}{[x+(\vec{B}+\vec{y}_N)^2][\vec{A}+\vec{y}_N]^2\,\vec{k}_a\cdot\vec{y}_N} = -\frac{\partial}{\partial x}\int\frac{d^3\vec{y}_N}{[x+(\vec{B}+\vec{y}_N)^2][\vec{A}+\vec{y}_N]^2\,\vec{k}_a\cdot\vec{y}_N} . \tag{A1}$$

Consider the integral I′, where

$$I' = \int\frac{d^3 y_N}{[x+(\vec{B}+\vec{y}_N)^2][\vec{A}+\vec{y}_N]^2\,\vec{k}_a\cdot\vec{y}_N} = \iint_0^1 \frac{d^3 y_N\,du}{\{[x+(\vec{B}+\vec{y}_N)^2]u + (1-u)(\vec{A}+\vec{y}_N)^2\}^2\,\vec{k}_a\cdot\vec{y}_N}$$

$$= \iint_0^1 \frac{d^3 y_N\,du}{\{[xu+(\vec{B}^2-\vec{A}^2)u+\vec{A}^2] - [\vec{A}(1-u)+\vec{B}u]^2 + [\vec{A}(1-u)+\vec{B}u+\vec{y}_N]^2\}^2\,\vec{k}_a\cdot\vec{y}_N} . \tag{A2}$$

Introducing $\vec{W} = \vec{y}_N + \vec{A}(1-u) + \vec{B}u$, $X = xu + (\vec{B}-\vec{A})^2 u(1-u)$, and $Y = \vec{k}_a\cdot[\vec{A}(1-u)+\vec{B}u]$, we obtain

$$I' = \iint_0^1 \frac{du\,d^3W}{(X+W^2)^2(\vec{k}_a\cdot\vec{W} - Y + i\epsilon)} . \tag{A3}$$

Integrating with respect to the $\vec{W}$ variable first, using cylindrical coordinates, with $\vec{k}_a$ as axis, we obtain

$$I' = \frac{1}{2}\iint \frac{du\, d[X+W_z^2+W_R^2]\, dW_\theta\, dW_z}{(X+W_z^2+W_R^2)(|\vec{k}_a|W_z - Y + i\epsilon)} = \pi\int_0^1\int_{-\infty}^{\infty} \frac{dW_z\, du}{(X+W_z^2)(|\vec{k}_a|W_z - Y+i\epsilon)} \quad . \tag{A4}$$

By considering the contour integral over the upper half w_z plane, we obtain

$$I' = -\pi^2\int_0^1 \frac{du}{[(a-bu)u]^{1/2}\{\vec{k}_a\cdot\vec{A} + \vec{k}_a\cdot(\vec{B}-\vec{A})u - ik_a[(a-bu)u]^{1/2}\}} \quad , \tag{A5}$$

where $a = x + (\vec{B}-\vec{A})^2$ and $b = (\vec{B}-\vec{A})^2$. We now make the approximation that since x is small, $b \sim x + (\vec{B}-\vec{A})^2 = a$. This is a fair approximation, since the error we make is the insertion of an additional term xu in the denominator, but x is a small parameter and u only takes on values between 0 and 1.

We may now introduce the variable r given by

$$u = r^2/(1+r^2) \quad .$$

We obtain

$$I' = -\frac{2\pi^2}{\sqrt{a}}\int \frac{dr}{\vec{k}_a\vec{B}r^2 - ik_a(\sqrt{a})r + \vec{k}_a\cdot\vec{A}} \quad . \tag{A6}$$

The rest of the integration and the subsequent differentiation with respect to x follow readily.

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*Present address: Wright Patterson Base, Dayton, Ohio.

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Na-Cs Differential Spin-Exchange Scattering*

C. K. Chang† and R. H. Walker
Physics Department, University of Houston, Houston, Texas 77004
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Unpolarized and spin-exchange differential-scattering cross sections of Na-Cs are calculated using our phenomenological potentials for $r < 14$ a.u. and the difference potential of Dalgarno and Rudge for $r \geq 14$ a.u. The calculated results are in good agreement with the experimental results.

Spin-exchange scattering is known to play an important role in many phenomena such as the spin temperature of interstellar hydrogen,[1] radio-frequency spectroscopy experiments,[2] optical pumping,[3] and orienting free electrons.[4] Various total spin-exchange cross sections of alkali atoms have been measured or calculated.[5,6] More recently Pritchard, Burnham, and Kleppner[7] (PBK) have measured unpolarized and spin-exchange differential cross sections using cross-beam techniques. The work reported here was undertaken as a sensitive test of the validity of the phenomenological method of generating the interatomic potentials of alkali atoms suggested by Chang and Walker.[5]

The method of generating the interatomic potentials of like alkali atoms may be extended to include